



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:33 am BST

PDB ID : 4V7X
Title : Structure of the *Thermus thermophilus* ribosome complexed with erythromycin.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-17
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

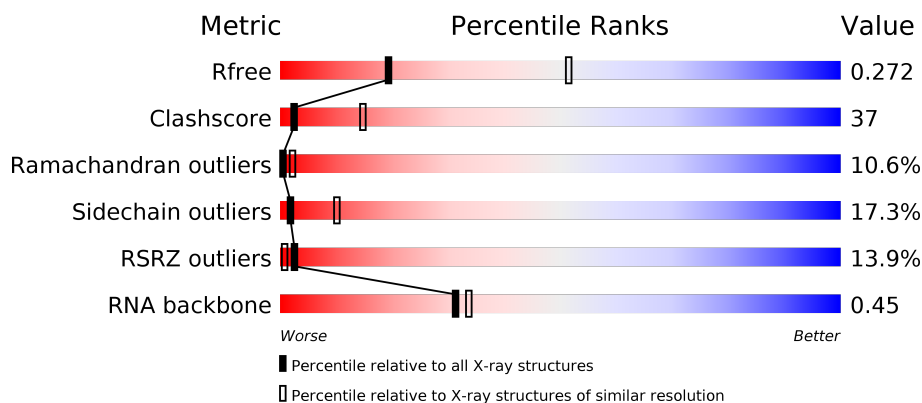
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 2092 (3.00-3.00) |
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |
| RNA backbone | 3102 | 1173 (3.30-2.70) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | AA | 1522 | <div> <div>20%</div> <div>25%</div> <div>59%</div> <div>15%</div> <div>.</div> </div> |
| 1 | CA | 1522 | <div> <div>20%</div> <div>25%</div> <div>58%</div> <div>15%</div> <div>.</div> </div> |
| 2 | AB | 256 | <div> <div>25%</div> <div>34%</div> <div>46%</div> <div>11%</div> <div>8%</div> <div>.</div> </div> |
| 2 | CB | 256 | <div> <div>30%</div> <div>34%</div> <div>46%</div> <div>11%</div> <div>8%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AC | 239 | |
| 3 | CC | 239 | |
| 4 | AD | 209 | |
| 4 | CD | 209 | |
| 5 | AE | 160 | |
| 5 | CE | 160 | |
| 6 | AF | 101 | |
| 6 | CF | 101 | |
| 7 | AG | 156 | |
| 7 | CG | 156 | |
| 8 | AH | 138 | |
| 8 | CH | 138 | |
| 9 | AI | 128 | |
| 9 | CI | 128 | |
| 10 | AJ | 105 | |
| 10 | CJ | 105 | |
| 11 | AK | 129 | |
| 11 | CK | 129 | |
| 12 | AL | 135 | |
| 12 | CL | 135 | |
| 13 | AM | 126 | |
| 13 | CM | 126 | |
| 14 | AN | 61 | |
| 14 | CN | 61 | |
| 15 | AO | 89 | |

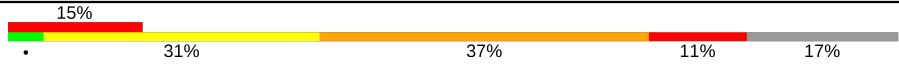


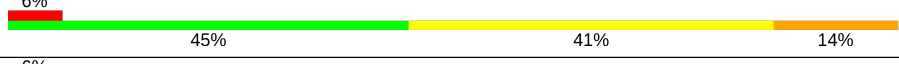
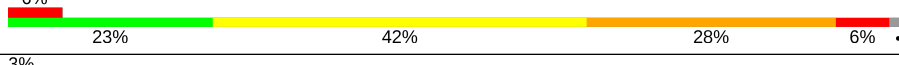
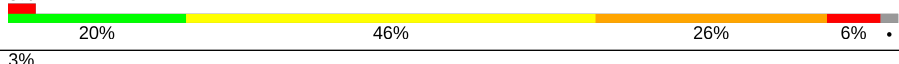
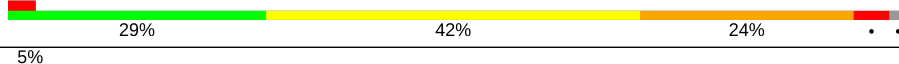
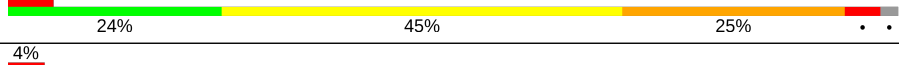
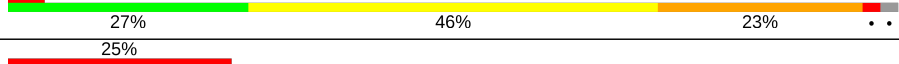
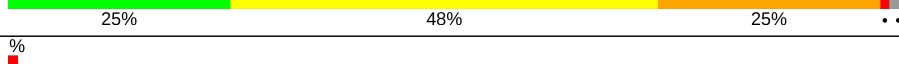

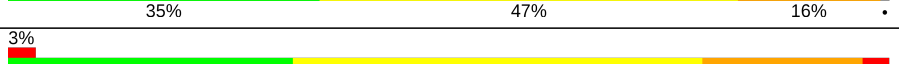
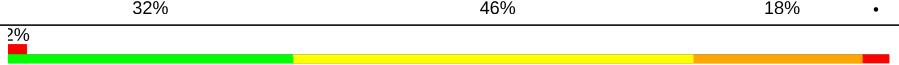
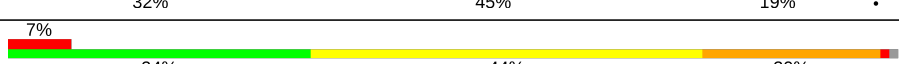
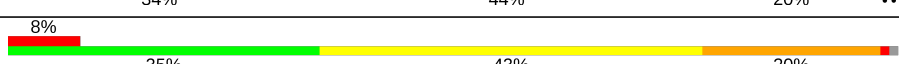

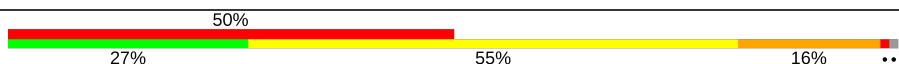
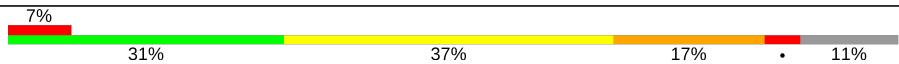
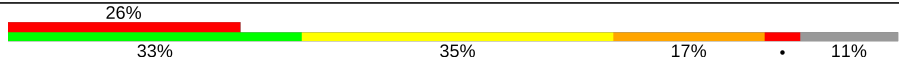

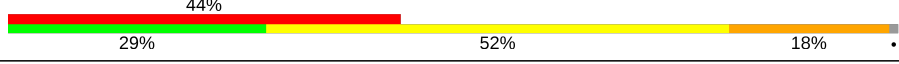
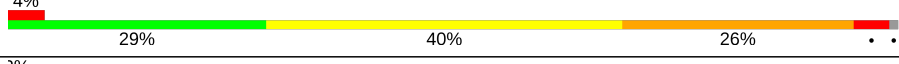
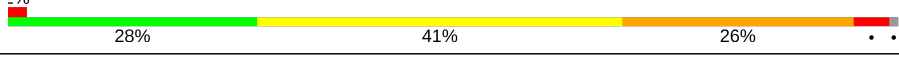


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | CO | 89 | |
| 16 | AP | 88 | |
| 16 | CP | 88 | |
| 17 | AQ | 105 | |
| 17 | CQ | 105 | |
| 18 | AR | 88 | |
| 18 | CR | 88 | |
| 19 | AS | 93 | |
| 19 | CS | 93 | |
| 20 | AT | 106 | |
| 20 | CT | 106 | |
| 21 | AU | 27 | |
| 21 | CU | 27 | |
| 22 | B0 | 85 | |
| 22 | D0 | 85 | |
| 23 | B1 | 98 | |
| 23 | D1 | 98 | |
| 24 | B2 | 72 | |
| 24 | D2 | 72 | |
| 25 | B3 | 60 | |
| 25 | D3 | 60 | |
| 26 | B4 | 71 | |
| 26 | D4 | 71 | |
| 27 | B5 | 60 | |
| 27 | D5 | 60 | |

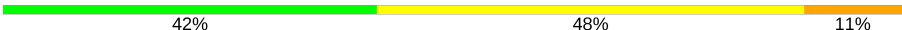

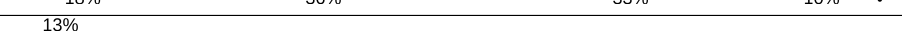

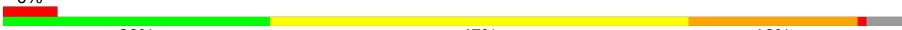
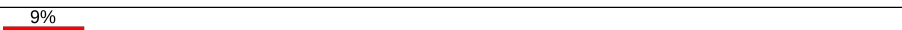
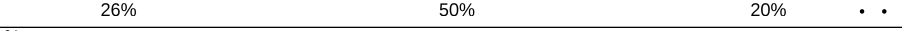
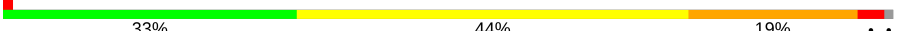

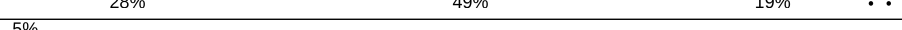
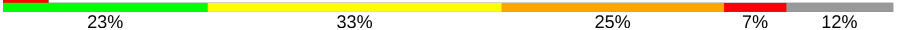



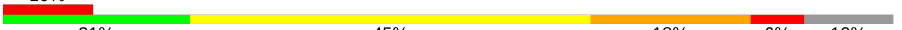


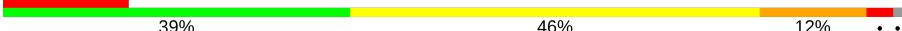



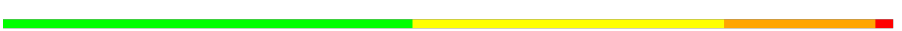

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | B6 | 54 |  |
| 28 | D6 | 54 |  |
| 29 | B7 | 49 |  |
| 29 | D7 | 49 |  |
| 30 | B8 | 65 |  |
| 30 | D8 | 65 |  |
| 31 | BA | 2787 |  |
| 31 | DA | 2787 |  |
| 32 | BB | 122 |  |
| 32 | DB | 122 |  |
| 33 | BD | 276 |  |
| 33 | DD | 276 |  |
| 34 | BE | 206 |  |
| 34 | DE | 206 |  |
| 35 | BF | 210 |  |
| 35 | DF | 210 |  |
| 36 | BG | 182 |  |
| 36 | DG | 182 |  |
| 37 | BH | 180 |  |
| 37 | DH | 180 |  |
| 38 | BI | 148 |  |
| 38 | DI | 148 |  |
| 39 | BN | 140 |  |
| 39 | DN | 140 |  |
| 40 | BO | 122 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 40 | DO | 122 |  |
| 41 | BP | 150 |  |
| 41 | DP | 150 |  |
| 42 | BQ | 141 |  |
| 42 | DQ | 141 |  |
| 43 | BR | 118 |  |
| 43 | DR | 118 |  |
| 44 | BS | 112 |  |
| 44 | DS | 112 |  |
| 45 | BT | 146 |  |
| 45 | DT | 146 |  |
| 46 | BU | 118 |  |
| 46 | DU | 118 |  |
| 47 | BV | 101 |  |
| 47 | DV | 101 |  |
| 48 | BW | 113 |  |
| 48 | DW | 113 |  |
| 49 | BX | 96 |  |
| 49 | DX | 96 |  |
| 50 | BY | 110 |  |
| 50 | DY | 110 |  |
| 51 | BZ | 206 |  |
| 51 | DZ | 206 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 52 | MG | AA | 1634 | - | - | - | X |
| 52 | MG | AA | 1642 | - | - | - | X |
| 52 | MG | AA | 1645 | - | - | - | X |
| 52 | MG | BA | 3074 | - | - | - | X |
| 52 | MG | BA | 3151 | - | - | - | X |
| 52 | MG | BA | 3206 | - | - | - | X |
| 52 | MG | BA | 3245 | - | - | - | X |
| 52 | MG | BA | 3304 | - | - | - | X |
| 52 | MG | BA | 3319 | - | - | - | X |
| 52 | MG | BA | 3327 | - | - | - | X |
| 52 | MG | BA | 3358 | - | - | - | X |
| 52 | MG | CA | 1613 | - | - | - | X |
| 52 | MG | CA | 1628 | - | - | - | X |
| 52 | MG | CA | 1630 | - | - | - | X |
| 52 | MG | CA | 1635 | - | - | - | X |
| 52 | MG | DA | 3191 | - | - | - | X |
| 52 | MG | DA | 3205 | - | - | - | X |
| 52 | MG | DA | 3231 | - | - | - | X |
| 52 | MG | DA | 3247 | - | - | - | X |
| 52 | MG | DA | 3264 | - | - | - | X |
| 52 | MG | DA | 3276 | - | - | - | X |
| 52 | MG | DA | 3278 | - | - | - | X |
| 52 | MG | DA | 3280 | - | - | - | X |
| 52 | MG | DA | 3291 | - | - | - | X |
| 52 | MG | DA | 3309 | - | - | - | X |
| 52 | MG | DA | 3316 | - | - | - | X |
| 52 | MG | DA | 3324 | - | - | - | X |

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 278034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 235 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1901 | 1213 | 342 | 341 | 5 | | | |
| 2 | CB | 235 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1901 | 1213 | 342 | 341 | 5 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AC | 207 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1613 | 1016 | 315 | 281 | 1 | | | |
| 3 | CC | 207 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1613 | 1016 | 315 | 281 | 1 | | | |

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

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 201 | 4 | | | |
| 5 | CE | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 201 | 4 | | | |

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

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

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

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

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

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| AI | 58 | ARG | HIS | CONFLICT | UNP P80374 |
| CI | 58 | ARG | HIS | CONFLICT | UNP P80374 |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AJ | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 795 | 499 | 157 | 138 | 1 | | | |
| 10 | CJ | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 795 | 499 | 157 | 138 | 1 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 971 | 611 | 196 | 163 | 1 | | | |
| 12 | CL | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 971 | 611 | 196 | 163 | 1 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| AL | 2 | VAL | - | INSERTION | UNP Q5SHN3 |
| AL | 3 | ALA | - | INSERTION | UNP Q5SHN3 |
| AL | 4 | LEU | - | INSERTION | UNP Q5SHN3 |
| CL | 2 | VAL | - | INSERTION | UNP Q5SHN3 |
| CL | 3 | ALA | - | INSERTION | UNP Q5SHN3 |
| CL | 4 | LEU | - | INSERTION | UNP Q5SHN3 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 115 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 921 | 569 | 190 | 160 | 2 | | | |
| 13 | CM | 115 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 921 | 569 | 190 | 160 | 2 | | | |

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

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 117 | 1 | | | |
| 16 | CP | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 117 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 100 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 824 | 528 | 152 | 142 | 2 | | | |
| 17 | CQ | 100 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 824 | 528 | 152 | 142 | 2 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 79 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 630 | 403 | 115 | 110 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | CS | 79 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 630 | 403 | 115 | 110 | 2 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AU | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |
| 21 | CU | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | B0 | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 650 | 401 | 137 | 111 | 1 | | | |
| 22 | D0 | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 650 | 401 | 137 | 111 | 1 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 23 | B1 | 89 | Total | C | N | O | 0 | 0 | 1 |
| | | | 693 | 435 | 140 | 118 | | | |
| 23 | D1 | 89 | Total | C | N | O | 0 | 0 | 1 |
| | | | 693 | 435 | 140 | 118 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 24 | B2 | 51 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 421 | 263 | 85 | 72 | 1 | | | |
| 24 | D2 | 51 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 421 | 263 | 85 | 72 | 1 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 25 | B3 | 60 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 468 | 298 | 91 | 78 | 1 | | | |
| 25 | D3 | 60 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 468 | 298 | 91 | 78 | 1 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 26 | B4 | 32 | Total | C | N | O | 0 | 0 | 0 |
| | | | 157 | 93 | 32 | 32 | | | |
| 26 | D4 | 32 | Total | C | N | O | 0 | 0 | 0 |
| | | | 157 | 93 | 32 | 32 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | B5 | 59 | Total | C | N | O | S | 9 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 27 | D5 | 59 | Total | C | N | O | S | 9 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | B6 | 45 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 381 | 235 | 78 | 64 | 4 | | | |
| 28 | D6 | 45 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 381 | 235 | 78 | 64 | 4 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29 | B7 | 49 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 419 | 257 | 105 | 55 | 2 | | | |
| 29 | D7 | 49 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 419 | 257 | 105 | 55 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 508 | 326 | 102 | 78 | 2 | | | |
| 30 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 508 | 326 | 102 | 78 | 2 | | | |

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 31 | BA | 2725 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 58698 | 26124 | 10986 | 18864 | 2724 | | | |
| 31 | DA | 2725 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 58698 | 26124 | 10986 | 18864 | 2724 | | | |

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 32 | BB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |
| 32 | DB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 33 | BD | 272 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2105 | 1329 | 417 | 356 | 3 | | | |
| 33 | DD | 272 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2105 | 1329 | 417 | 356 | 3 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | BE | 205 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1564 | 988 | 300 | 270 | 6 | | | |
| 34 | DE | 205 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1564 | 988 | 300 | 270 | 6 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35 | BF | 208 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1624 | 1035 | 304 | 282 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35 | DF | 208 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1624 | 1035 | 304 | 282 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 36 | DG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BH | 160 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1223 | 773 | 229 | 220 | 1 | | | |
| 37 | DH | 160 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1223 | 773 | 229 | 220 | 1 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BI | 146 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1132 | 723 | 201 | 207 | 1 | | | |
| 38 | DI | 146 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1132 | 723 | 201 | 207 | 1 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | BN | 139 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1105 | 712 | 207 | 182 | 4 | | | |
| 39 | DN | 139 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1105 | 712 | 207 | 182 | 4 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 40 | DO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BP | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |
| 41 | DP | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BQ | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1080 | 688 | 204 | 183 | 5 | | | |
| 42 | DQ | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1080 | 688 | 204 | 183 | 5 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43 | BR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |
| 43 | DR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 44 | BS | 99 | Total | C | N | O | 0 | 0 | 1 |
| | | | 771 | 486 | 155 | 130 | | | |
| 44 | DS | 99 | Total | C | N | O | 0 | 0 | 1 |
| | | | 771 | 486 | 155 | 130 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BT | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1100 | 686 | 227 | 186 | 1 | | | |
| 45 | DT | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1100 | 686 | 227 | 186 | 1 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 604 | 202 | 151 | 1 | | | |
| 46 | DU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 604 | 202 | 151 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | BV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 47 | DV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | BW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 896 | 563 | 176 | 155 | 2 | | | |
| 48 | DW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 896 | 563 | 176 | 155 | 2 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 49 | BX | 93 | Total | C | N | O | | 0 | 0 | 1 |
| | | | 726 | 471 | 132 | 123 | | | | |
| 49 | DX | 93 | Total | C | N | O | | 0 | 0 | 1 |
| | | | 726 | 471 | 132 | 123 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | BY | 101 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 776 | 500 | 149 | 123 | 4 | | | |
| 50 | DY | 101 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 776 | 500 | 149 | 123 | 4 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51 | BZ | 177 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1404 | 897 | 253 | 252 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51 | DZ | 177 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1404 | 897 | 253 | 252 | 2 | | | |

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 52 | BA | 362 | Total | Mg | 0 | 0 |
| | | | 362 | 362 | | |
| 52 | CA | 50 | Total | Mg | 0 | 0 |
| | | | 50 | 50 | | |
| 52 | DQ | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | DF | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | BE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | DU | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | B1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | BP | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 52 | DR | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | B5 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 52 | BB | 7 | Total | Mg | 0 | 0 |
| | | | 7 | 7 | | |
| 52 | D3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | BF | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | BX | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | AA | 54 | Total | Mg | 0 | 0 |
| | | | 54 | 54 | | |
| 52 | BQ | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 52 | D7 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 52 | BU | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 52 | D0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 52 | BR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 52 | DA | 328 | Total 328 | Mg 328 | 0 | 0 |
| 52 | DE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 52 | DX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 52 | DP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 52 | D5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 52 | BD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 52 | B0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 52 | DB | 3 | Total 3 | Mg 3 | 0 | 0 |

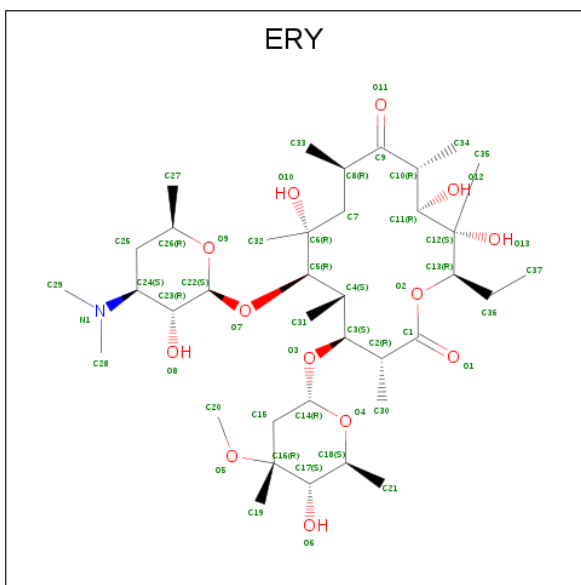
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 53 | CN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 53 | AD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 53 | CD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 53 | AN | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 54 | BA | 1 | Total 1 | K 1 | 0 | 0 |
| 54 | DA | 1 | Total 1 | K 1 | 0 | 0 |

- Molecule 55 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C₃₇H₆₇NO₁₃).

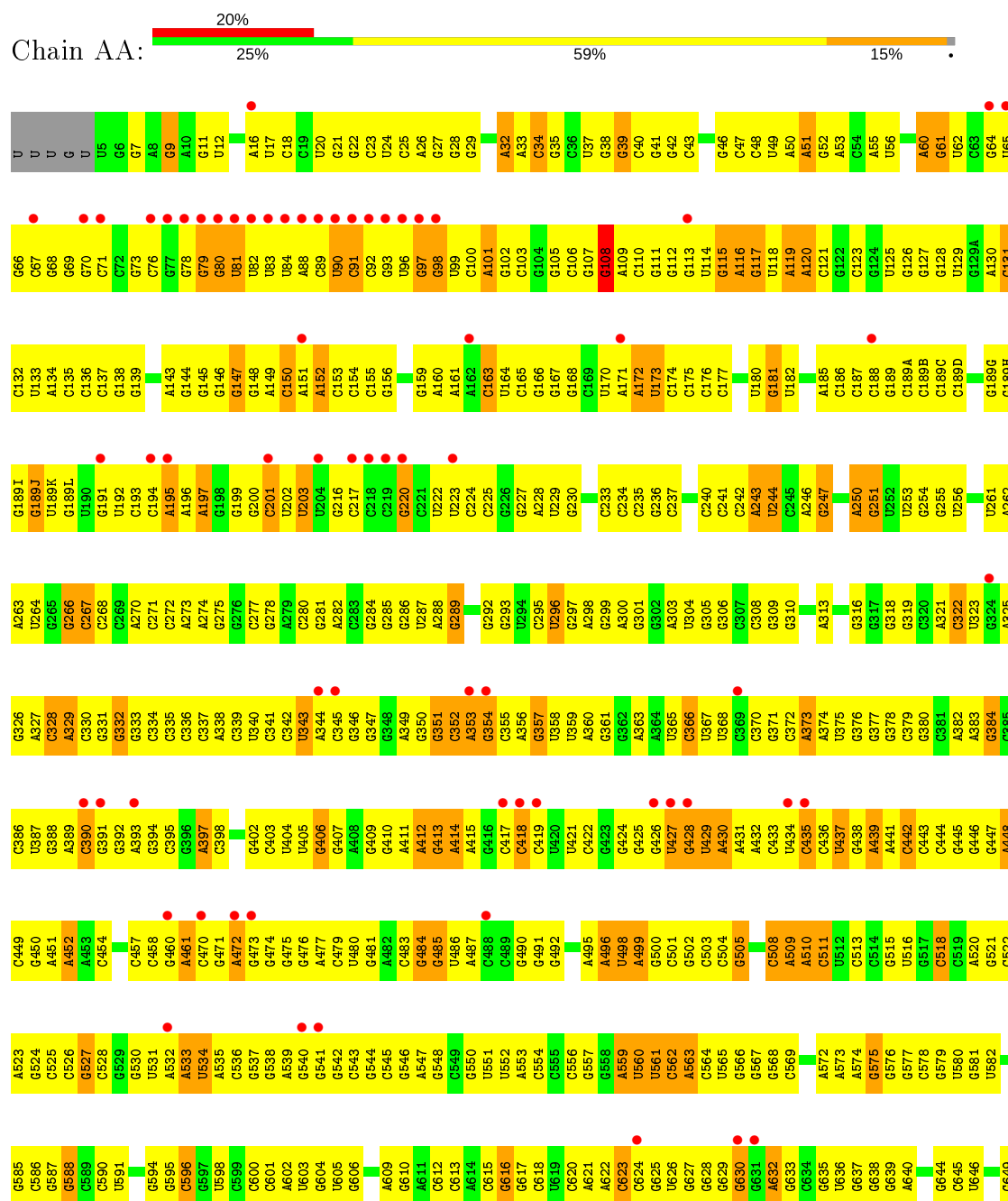


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|
| 55 | BA | 1 | Total 51 | C 37 | N 1 | O 13 | 0 | 0 |
| 55 | DA | 1 | Total 51 | C 37 | N 1 | O 13 | 0 | 0 |

3 Residue-property plots

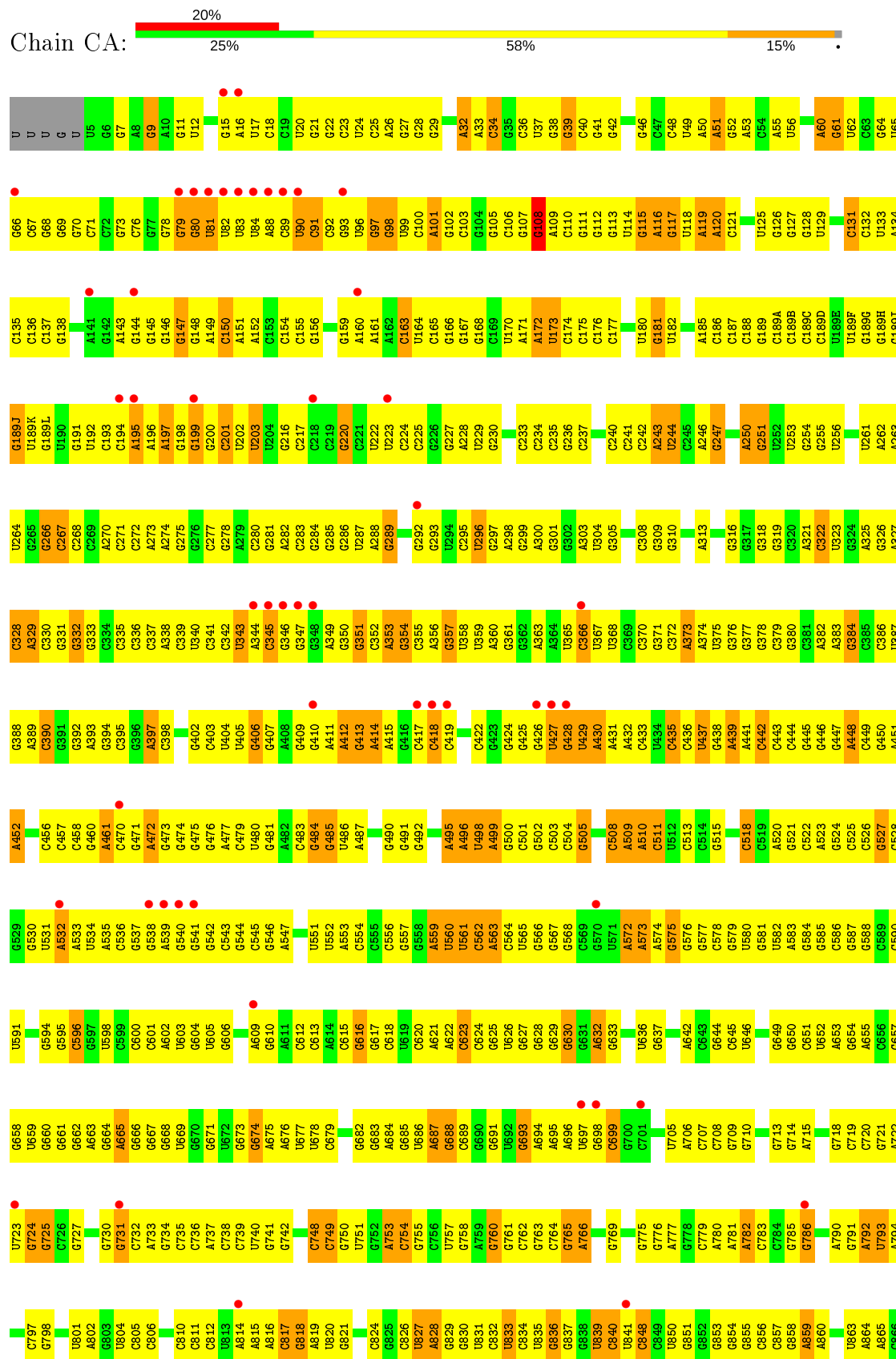
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

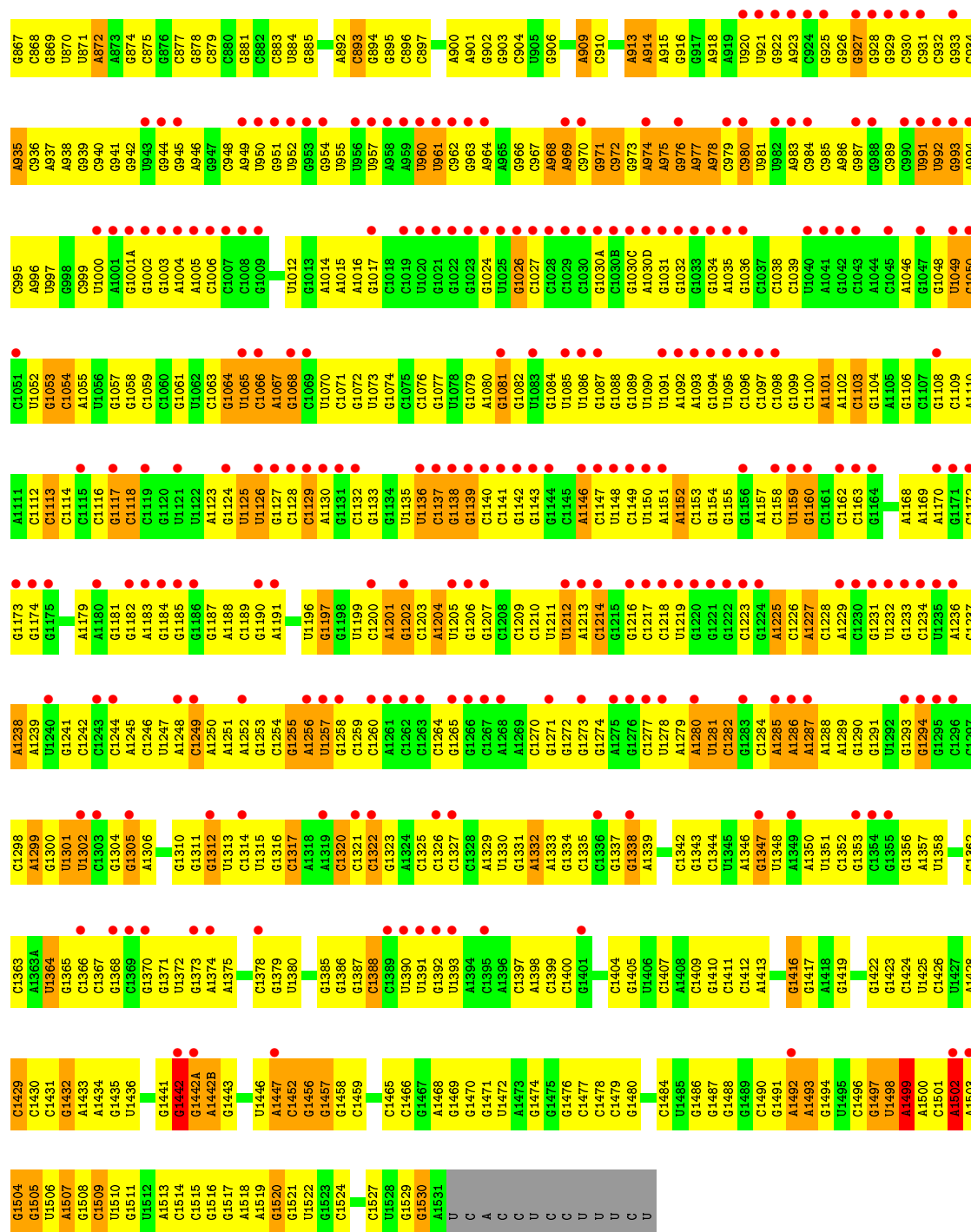
• Molecule 1: 16S rRNA

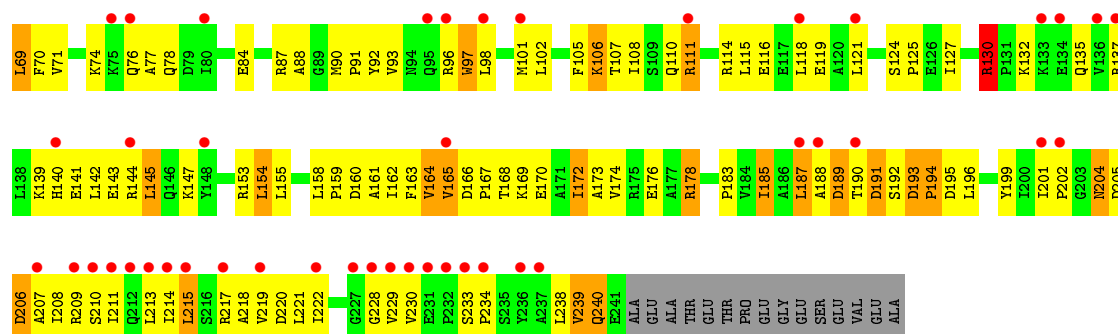


| | | | | | | | | | | | | | |
|--------|-------|--------|-------|-------|-------|-------|-------|--------|------|------|------|------|------|
| A1507 | C1429 | G1361 | G1300 | A1239 | A1179 | G1112 | G1051 | A996 | C936 | U863 | U786 | G713 | G650 |
| G1508 | C1430 | C1362 | U1301 | U1240 | A1180 | G1113 | U1052 | U997 | A937 | A864 | U789 | G714 | C651 |
| G1509 | C1431 | C1363 | U1302 | G1241 | G1181 | C1114 | C1053 | G998 | A938 | A865 | A790 | A715 | U652 |
| U1510 | G1432 | A1363A | C1303 | C1242 | G1182 | C1115 | C1054 | C999 | G939 | C866 | G791 | | A653 |
| G1511 | A1433 | U1364 | G1304 | C1243 | A1183 | G1116 | U1055 | U1000 | C940 | C867 | A792 | G718 | G654 |
| U1512 | A1434 | G1365 | G1305 | C1244 | A1184 | G1117 | U1056 | A1001 | G941 | C868 | U793 | G719 | A655 |
| A1513 | G1435 | C1366 | A1306 | A1245 | G1185 | C1118 | G1057 | G1001A | G942 | C869 | U794 | C720 | C656 |
| G1514 | U1436 | U1367 | U1307 | C1246 | G1186 | C1119 | G1058 | G1002 | U943 | U870 | | G721 | C657 |
| C1515 | G1368 | U1287 | U1308 | U1247 | G1186 | G1120 | C1059 | G1003 | G944 | C875 | G725 | A722 | G658 |
| G1516 | C1369 | C1248 | G1309 | A1249 | A1187 | U1121 | U1060 | A1004 | G945 | A872 | C797 | U723 | U659 |
| G1517 | G1370 | A1250 | G1310 | C1249 | A1188 | U1122 | G1061 | A1005 | A946 | A873 | U798 | U724 | G660 |
| A1518 | G1371 | A1251 | G1311 | A1250 | C1189 | U1123 | U1062 | C1006 | G947 | G874 | G726 | G725 | G661 |
| A1442B | U1372 | A1252 | G1312 | A1251 | G1190 | A1124 | C1063 | G1007 | C948 | A802 | C727 | G726 | G662 |
| G1443 | G1373 | A1253 | U1313 | A1252 | A1191 | U1125 | G1064 | C1008 | A949 | C875 | | | A663 |
| | A1374 | G1253 | C1314 | G1253 | | U1126 | U1065 | G1009 | U950 | G876 | | | G664 |
| U1446 | A1375 | C1254 | U1315 | C1254 | U1194 | G1127 | C1066 | G1010 | G951 | C877 | G730 | | A665 |
| A1447 | | G1255 | G1316 | A1256 | U1195 | U1128 | A1067 | U1011 | U952 | C878 | G731 | | G666 |
| C1452 | G1378 | U1257 | C1317 | U1257 | U1196 | C1129 | C1068 | G1012 | G953 | C879 | G732 | | G667 |
| A1456 | U1379 | G1197 | A1318 | U1197 | G1197 | A1130 | U1070 | U1013 | G954 | C880 | A733 | | G668 |
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| | | C1259 | G1320 | C1259 | U1199 | C1132 | U1072 | A1015 | U956 | C882 | G735 | | G670 |
| C1458 | | G1260 | C1321 | G1260 | C1200 | G1133 | U1073 | A1016 | U957 | C883 | G736 | | G671 |
| U1528 | | A1281 | C1322 | A1281 | A1134 | G1134 | U1074 | G1017 | A958 | C884 | A737 | | U672 |
| G1529 | | G1262 | G1323 | C1262 | A1201 | U1135 | G1074 | C1018 | A959 | C885 | C738 | | G673 |
| G1530 | G1463 | C1263 | C1324 | C1263 | C1203 | U1136 | | C1019 | U960 | G888 | C739 | | G674 |
| A1531 | G1464 | C1264 | A1324 | C1264 | A1204 | C1137 | G1077 | U1020 | U961 | C896 | G740 | | A675 |
| U | | G1265 | C1325 | G1265 | U1205 | G1138 | U1078 | G1021 | C962 | C896 | G741 | | U676 |
| C | A1468 | C1266 | C1326 | C1266 | G1206 | C1139 | U1079 | C1022 | G963 | A901 | G742 | | U677 |
| A | G1469 | G1267 | C1327 | G1267 | U1207 | G1140 | G1080 | G1023 | A964 | G902 | | | U678 |
| C | G1470 | C1268 | C1328 | C1268 | C1208 | C1141 | G1081 | G1024 | A965 | G903 | | | C679 |
| C | U1471 | A1269 | U1330 | A1269 | C1209 | G1142 | G1082 | U1025 | G966 | | | | |
| U | U1472 | C1270 | G1331 | C1270 | C1210 | G1143 | U1083 | G1026 | C967 | | | | |
| C | | G1271 | A1332 | G1271 | U1211 | | U1084 | C1027 | A968 | | | | |
| C | C1477 | A1395 | C1333 | G1272 | U1212 | A1146 | U1085 | C1028 | C969 | | | | G682 |
| U | C1478 | C1397 | A1334 | G1273 | C1213 | U1147 | U1086 | C1029 | C826 | | | | G683 |
| U | G1479 | A1398 | G1335 | G1274 | C1214 | U1148 | G1087 | C1030 | C827 | | | | A684 |
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| | | | A1339 | U1278 | C1218 | A1152 | U1091 | A914 | C831 | | | | G688 |
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| | | | | C1284 | G1224 | U1158 | C1096 | U921 | U839 | | | | A695 |
| | | | | A1285 | A1225 | C1159 | C1097 | G922 | C840 | | | | U696 |
| | | | | C1286 | G1226 | G1160 | U1098 | A923 | U841 | | | | G697 |
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| | | | | A1289 | A1229 | C1163 | A1102 | G926 | | | | | A702 |
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| | | | | U1292 | U1232 | A1169 | A1105 | G929 | | | | | U705 |
| | | | | G1293 | G1233 | G1170 | G1106 | C930 | | | | | G706 |
| | | | | G1294 | C1234 | G1171 | C1045 | C931 | | | | | A707 |
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| | | | | C1296 | A1236 | C1173 | G1047 | U992 | | | | | G708 |
| | | | | A1298 | C1237 | G1174 | U1049 | G993 | | | | | U709 |
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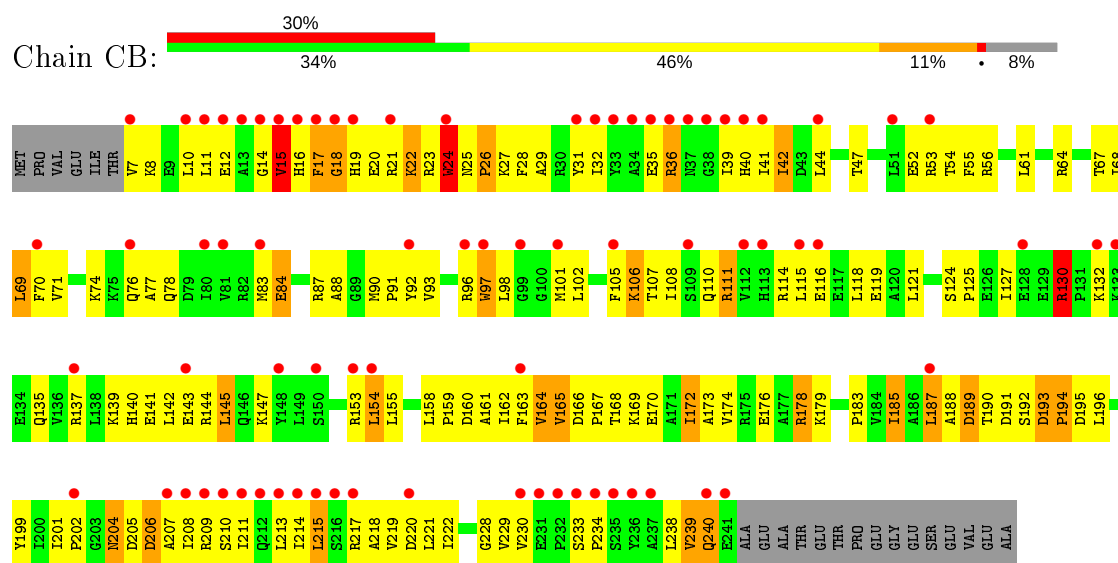
- Molecule 1: 16S rRNA



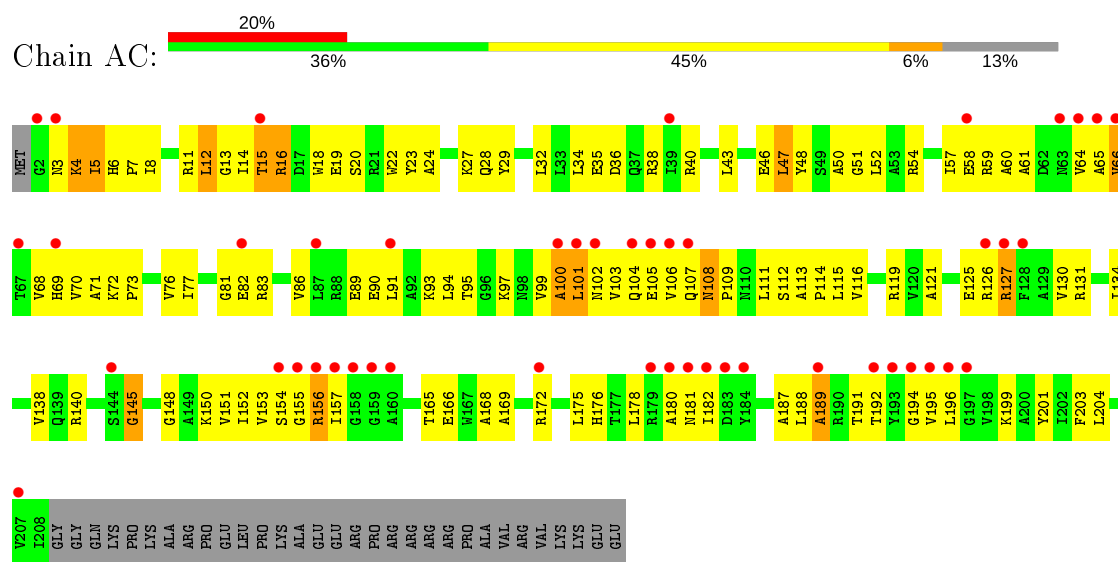




• Molecule 2: 30S ribosomal protein S2

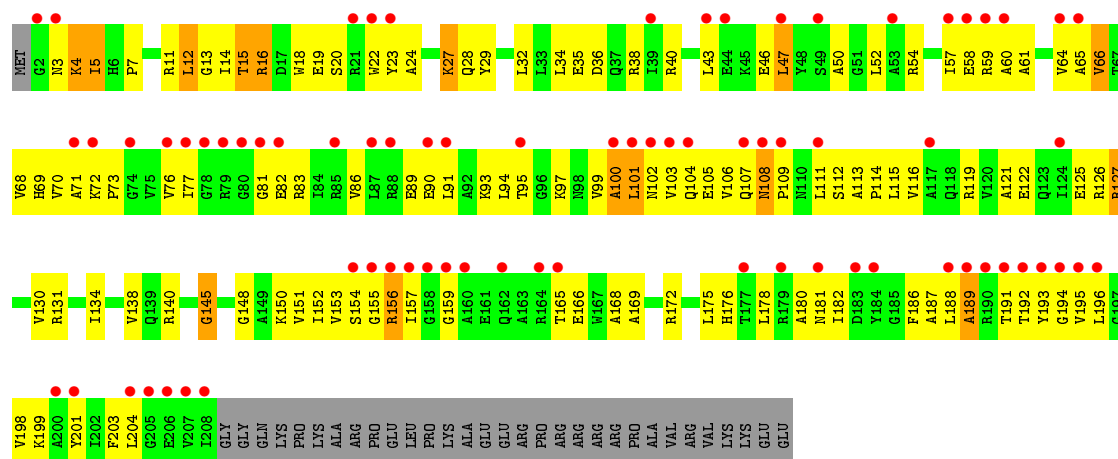


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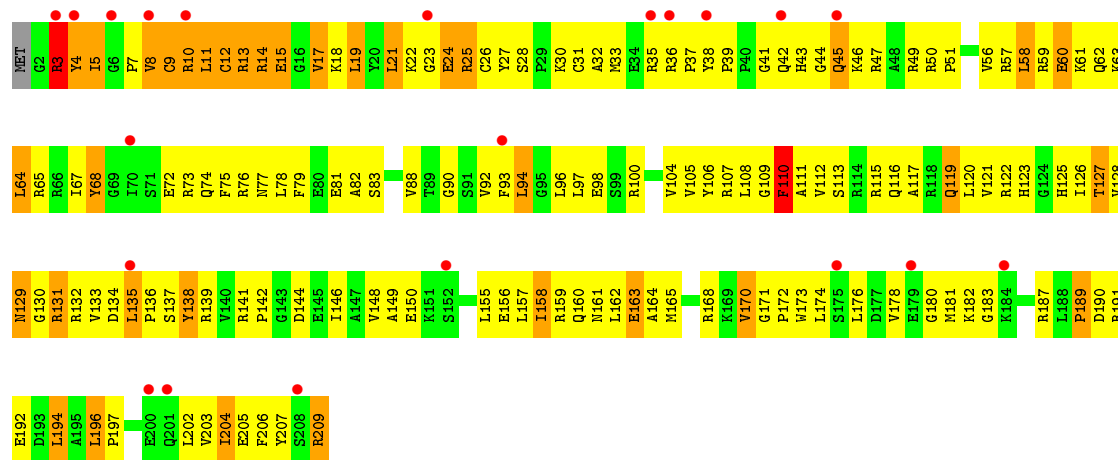


• Molecule 3: 30S ribosomal protein S3

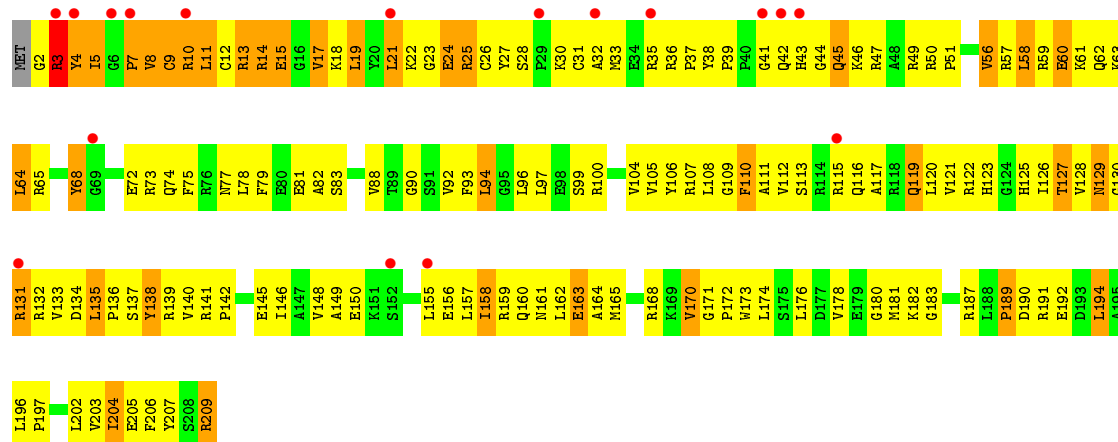




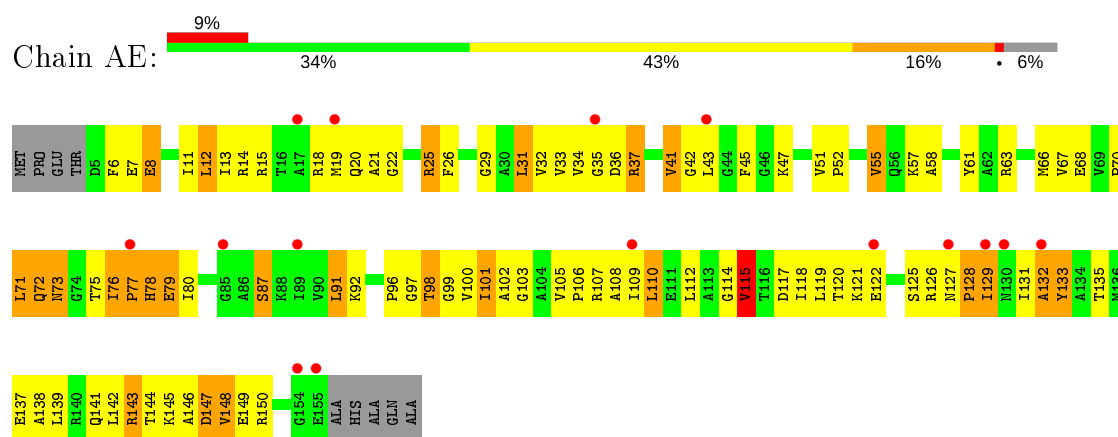
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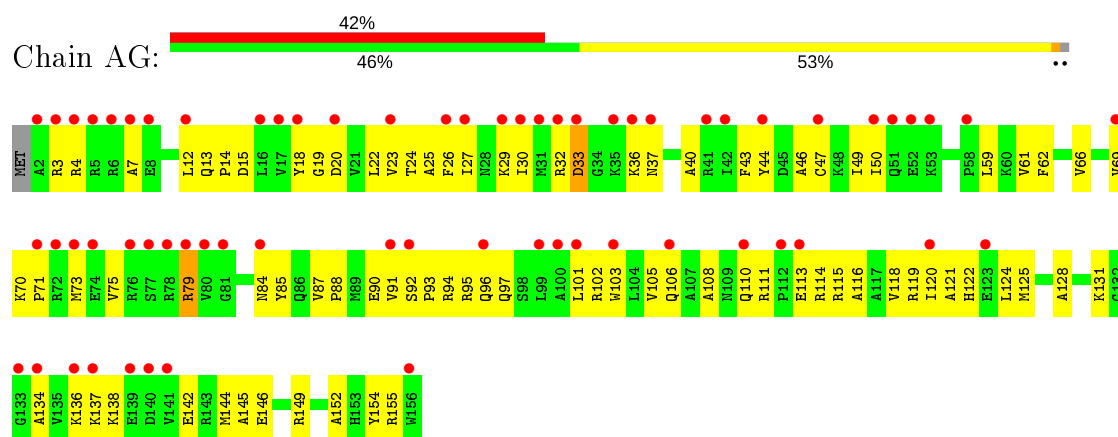


• Molecule 4: 30S ribosomal protein S4

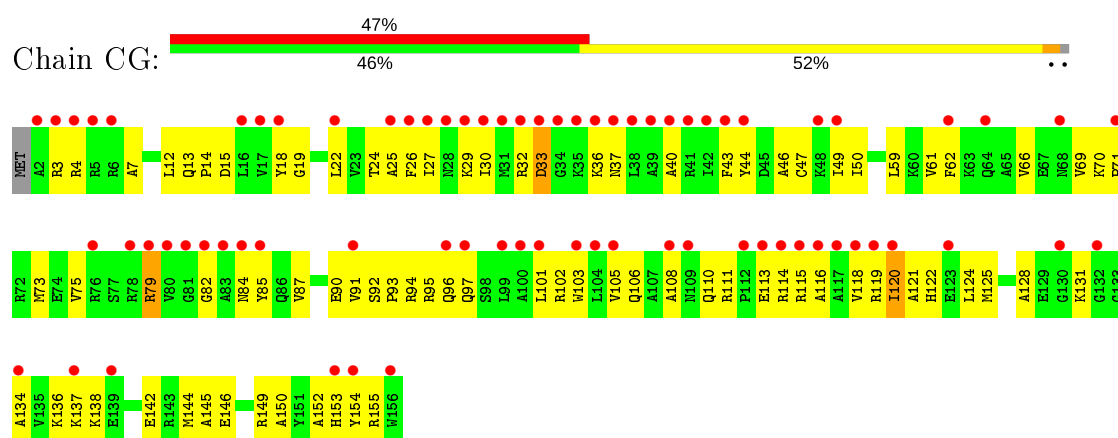


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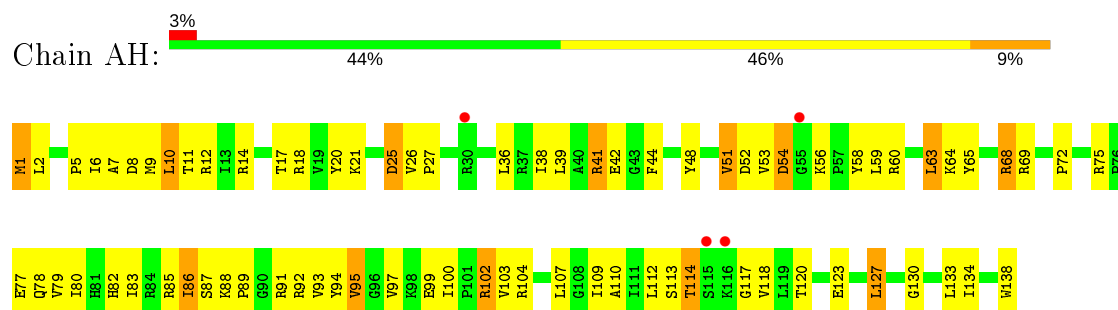




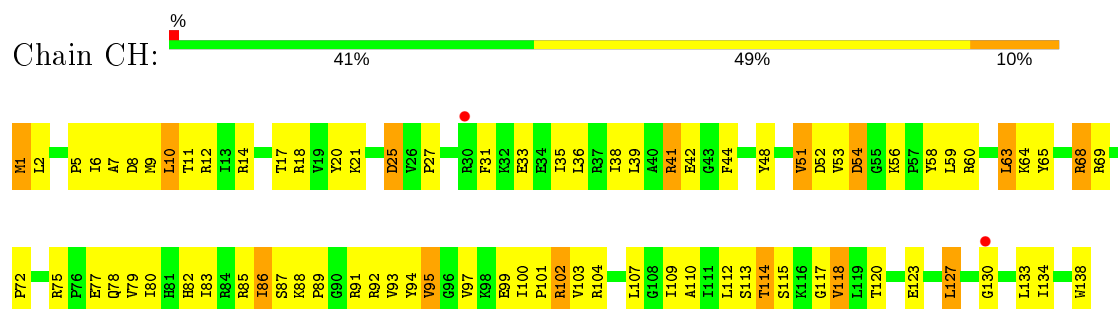
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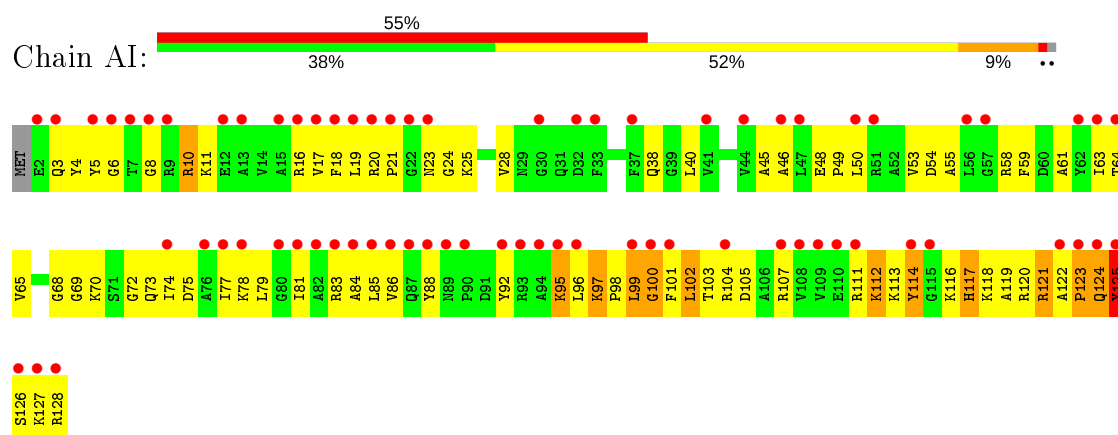
• Molecule 8: 30S ribosomal protein S8



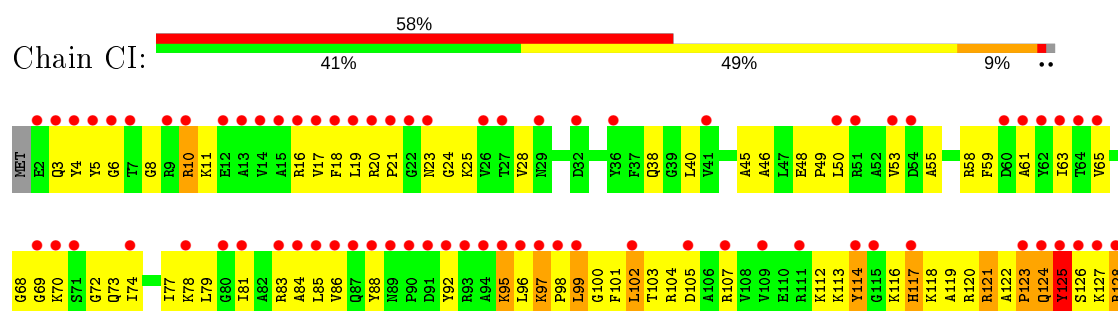
• Molecule 8: 30S ribosomal protein S8



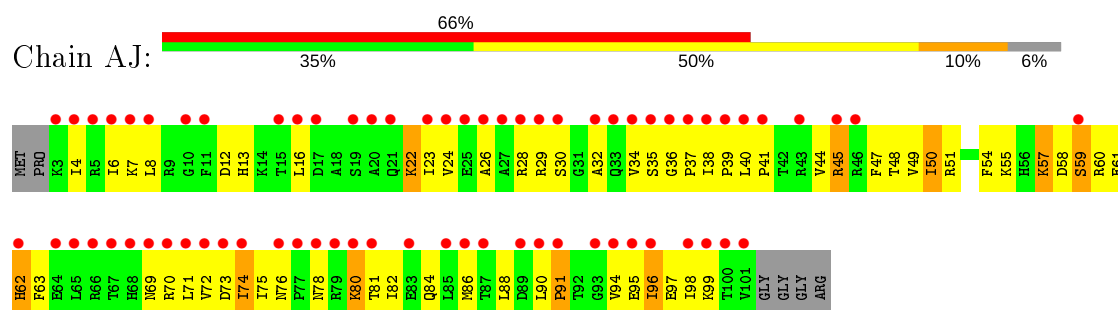
• Molecule 9: 30S ribosomal protein S9



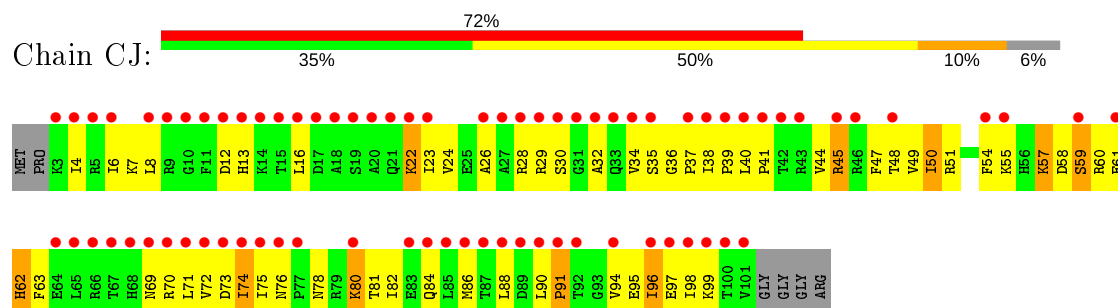
• Molecule 9: 30S ribosomal protein S9



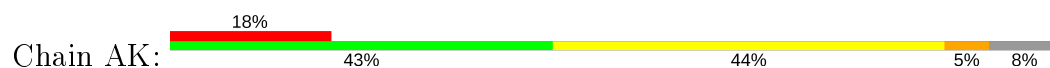
• Molecule 10: 30S ribosomal protein S10

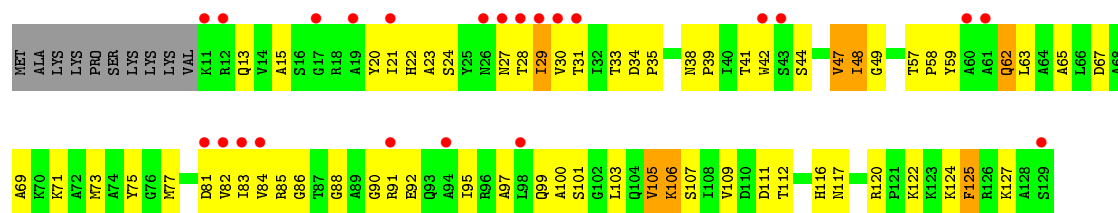


• Molecule 10: 30S ribosomal protein S10

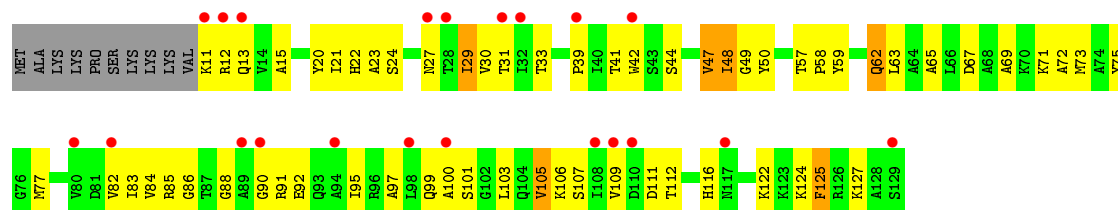


• Molecule 11: 30S ribosomal protein S11

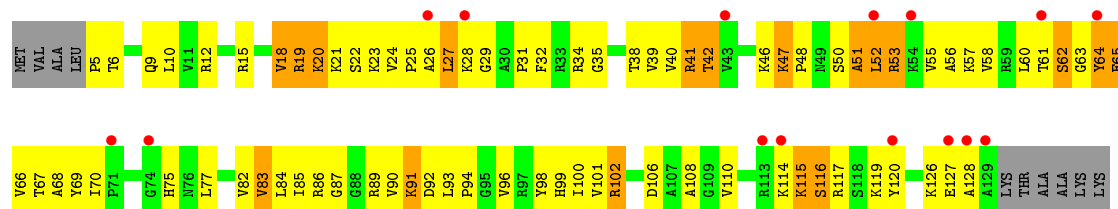




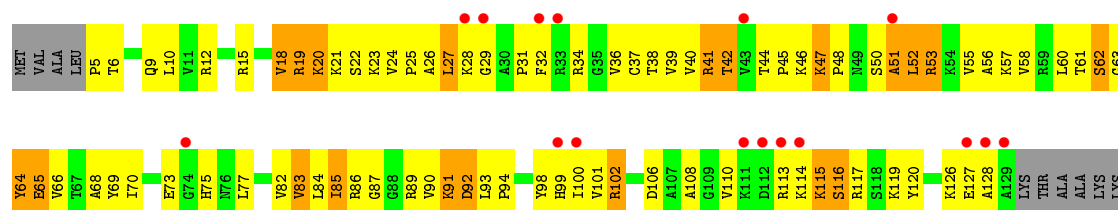
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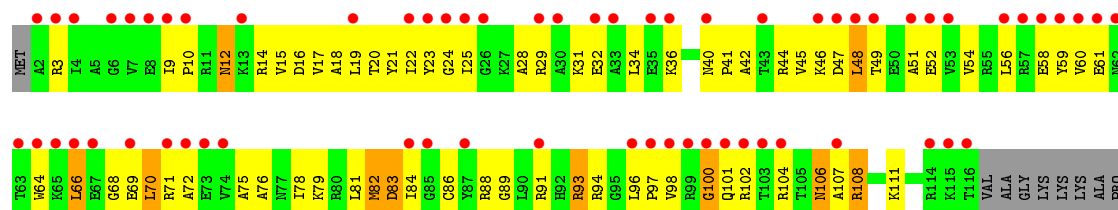
• Molecule 12: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S12

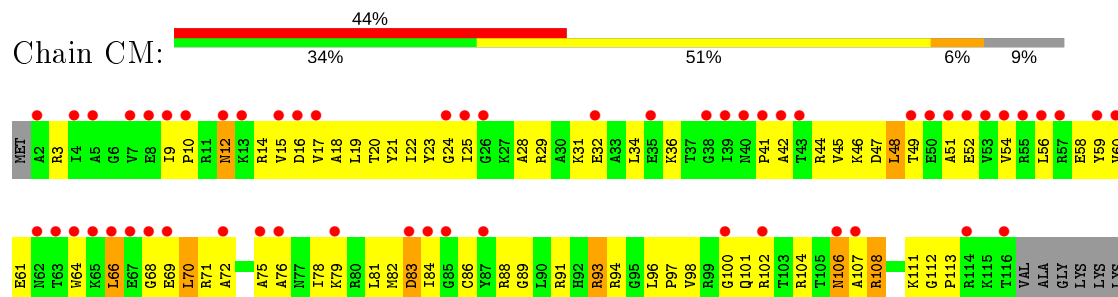


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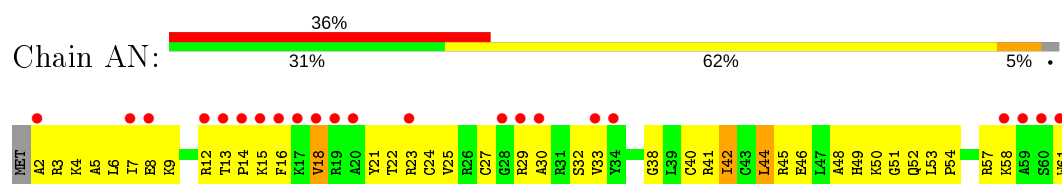
ARG
LYS

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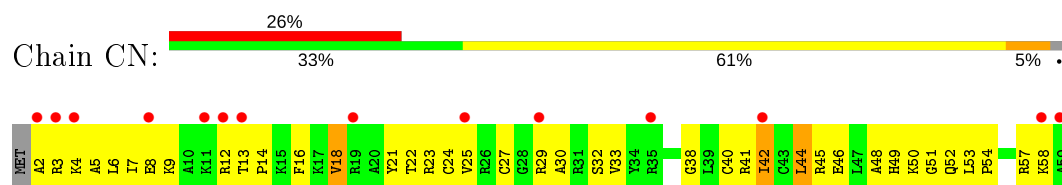


ALA
PRO
ARG
LYS

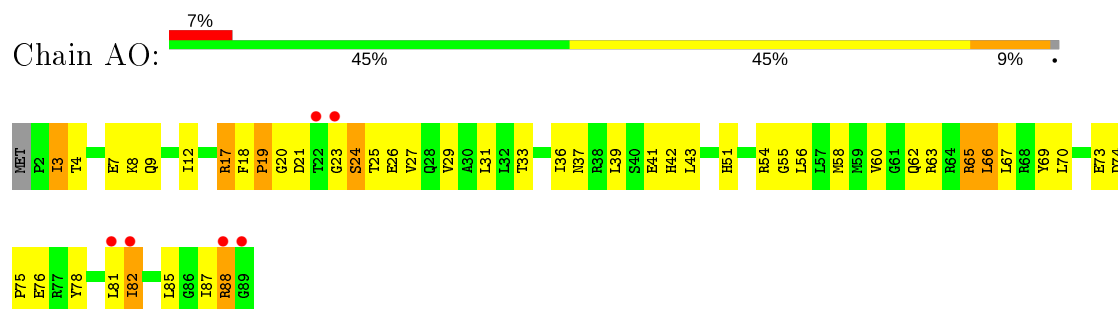
• Molecule 14: 30S ribosomal protein S14



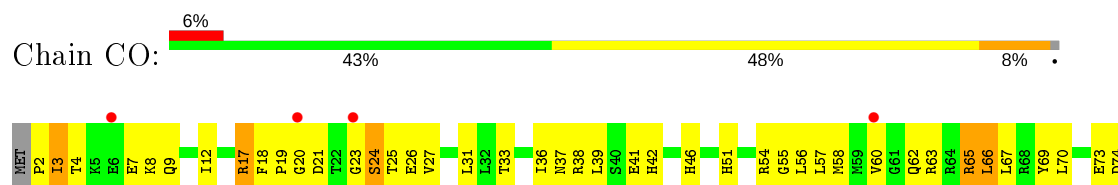
• Molecule 14: 30S ribosomal protein S14

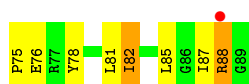


• Molecule 15: 30S ribosomal protein S15

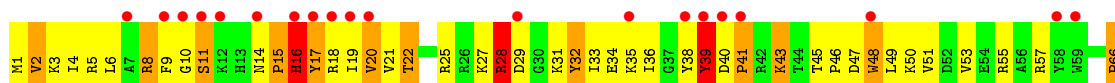


• Molecule 15: 30S ribosomal protein S15

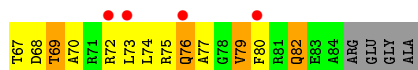
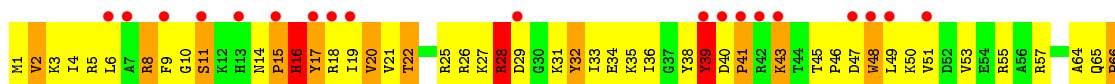




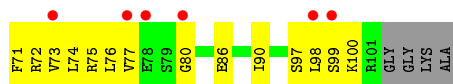
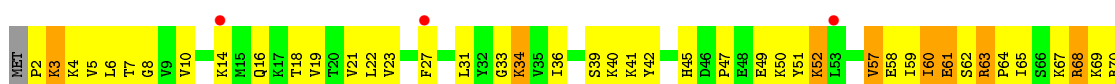
• Molecule 16: 30S ribosomal protein S16



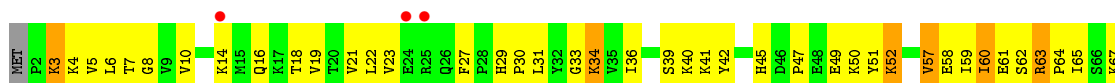
• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17

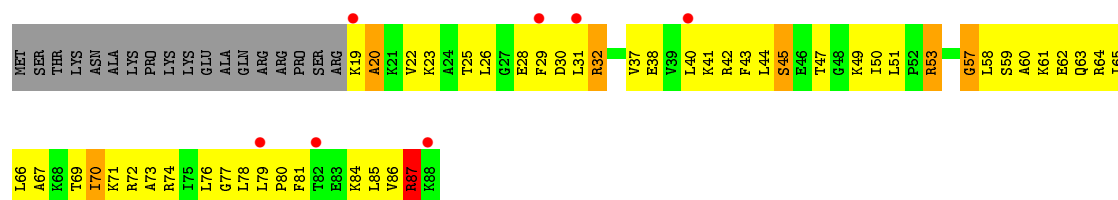


• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

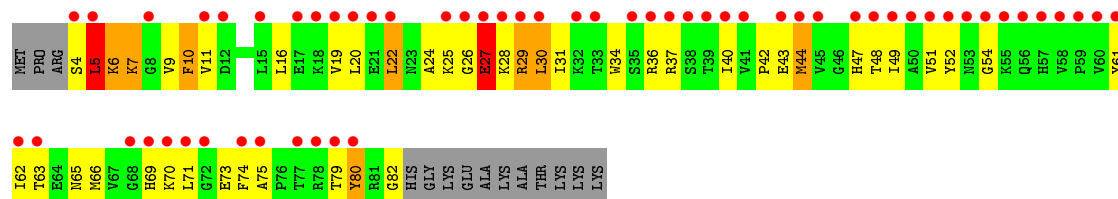




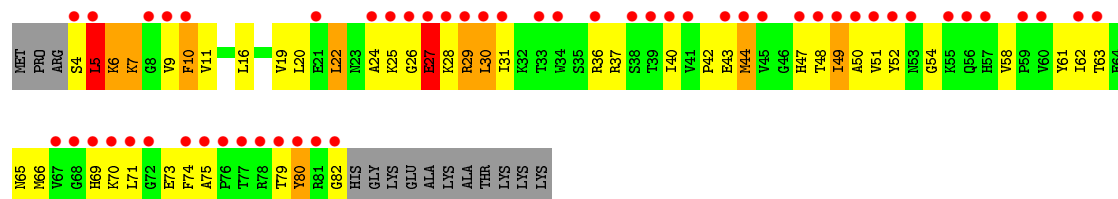
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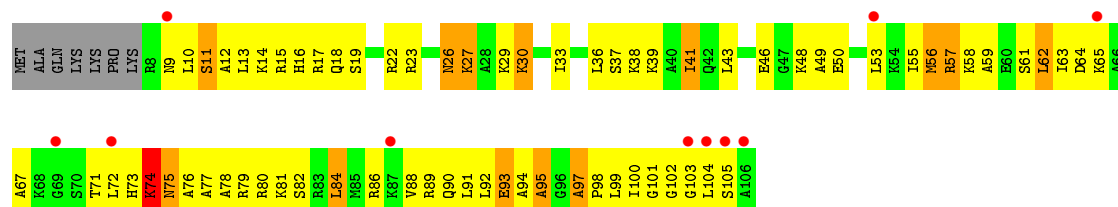
• Molecule 19: 30S ribosomal protein S19



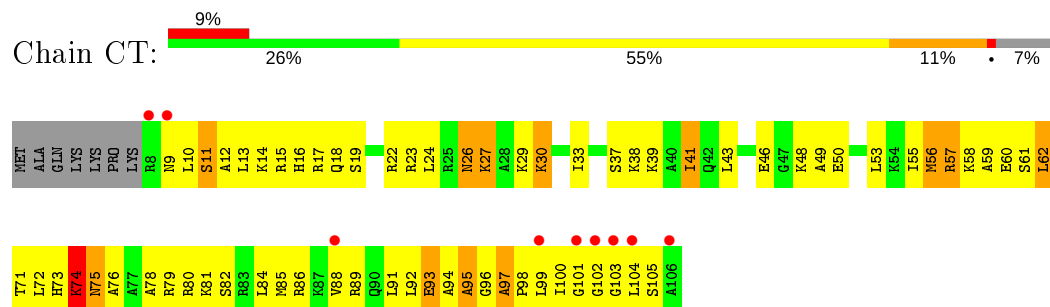
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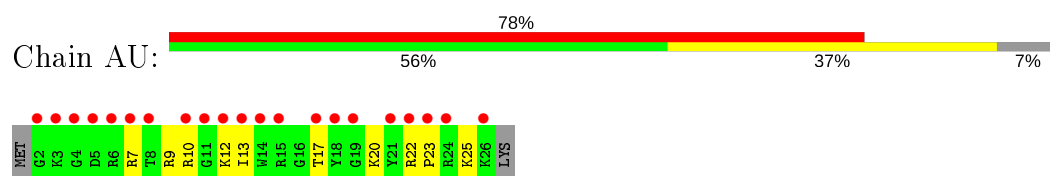
• Molecule 20: 30S ribosomal protein S20



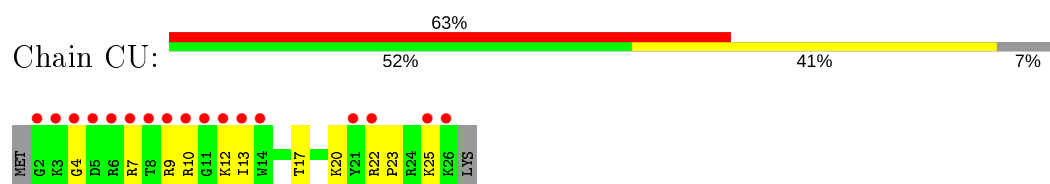
- Molecule 20: 30S ribosomal protein S20



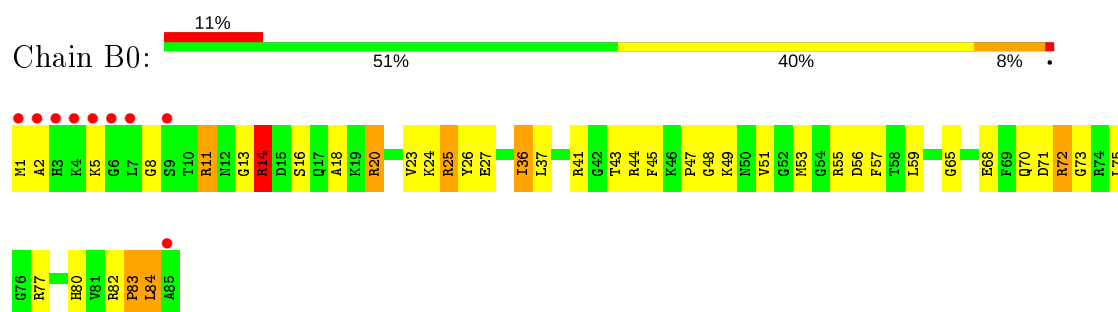
- Molecule 21: 30S ribosomal protein Thx



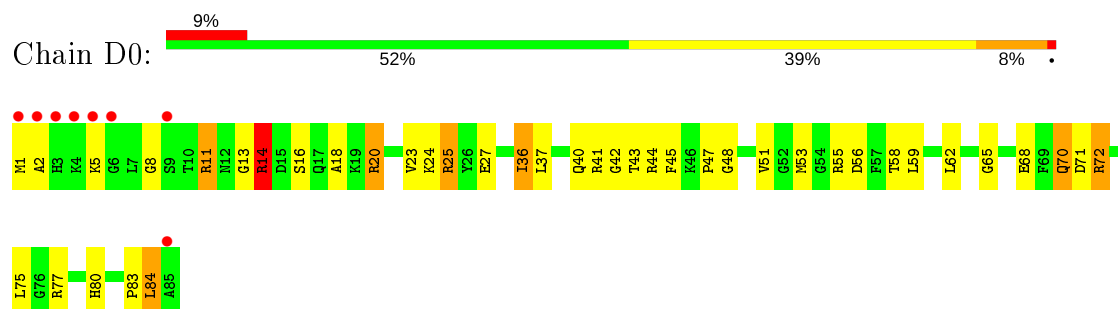
- Molecule 21: 30S ribosomal protein Thx



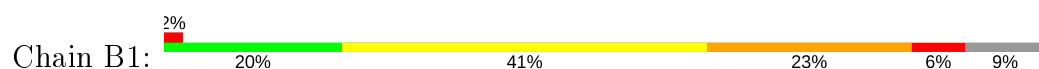
- Molecule 22: 50S ribosomal protein L27

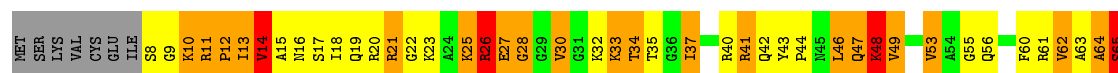


- Molecule 22: 50S ribosomal protein L27

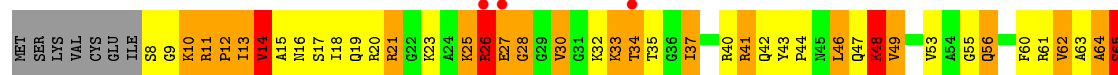
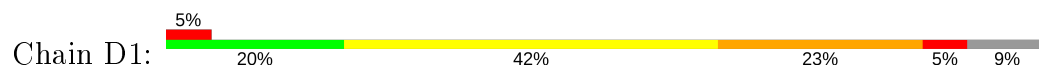


- Molecule 23: 50S ribosomal protein L28





• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



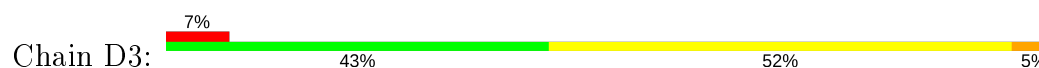
• Molecule 24: 50S ribosomal protein L29



• Molecule 25: 50S ribosomal protein L30

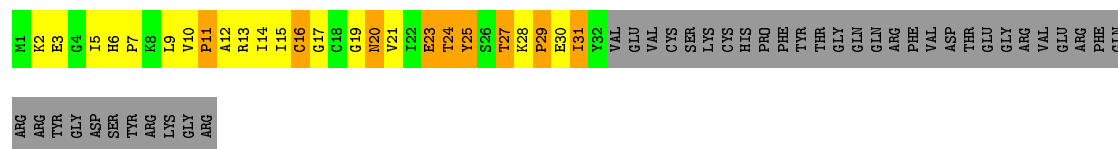
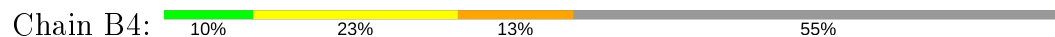


• Molecule 25: 50S ribosomal protein L30

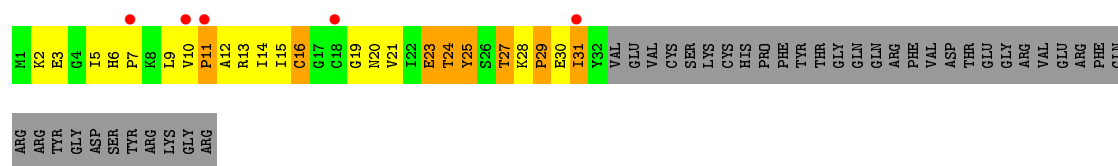
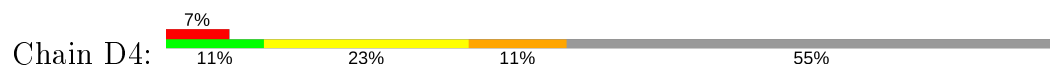




- Molecule 26: 50S ribosomal protein L31



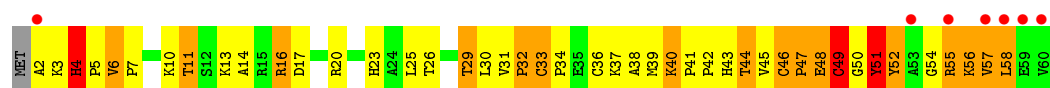
- Molecule 26: 50S ribosomal protein L31



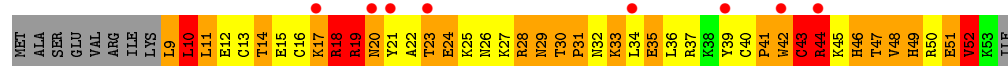
- Molecule 27: 50S ribosomal protein L32



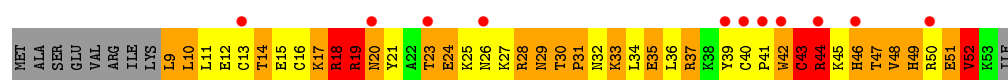
- Molecule 27: 50S ribosomal protein L32



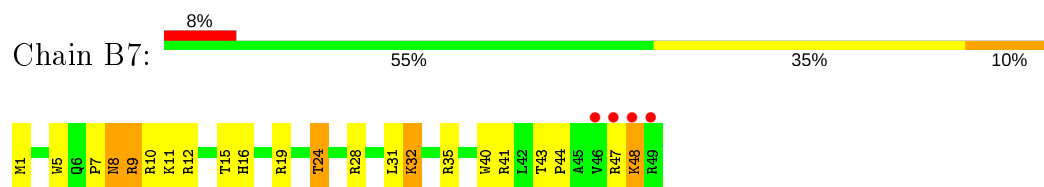
- Molecule 28: 50S ribosomal protein L33



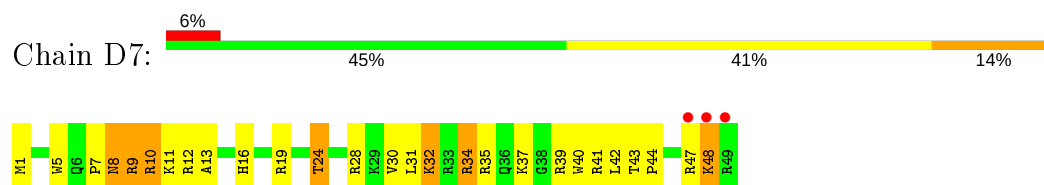
- Molecule 28: 50S ribosomal protein L33



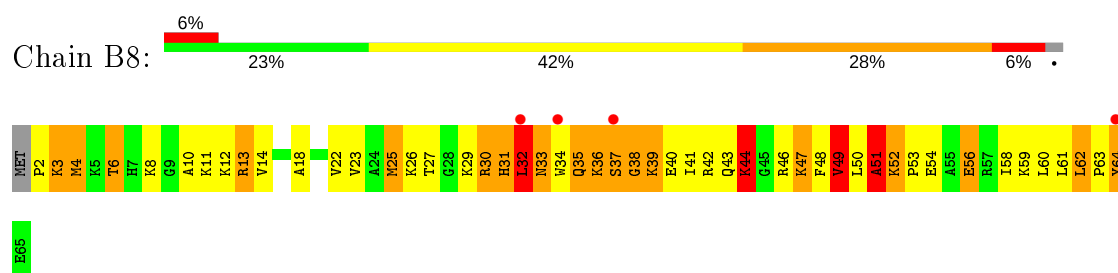
- Molecule 29: 50S ribosomal protein L34



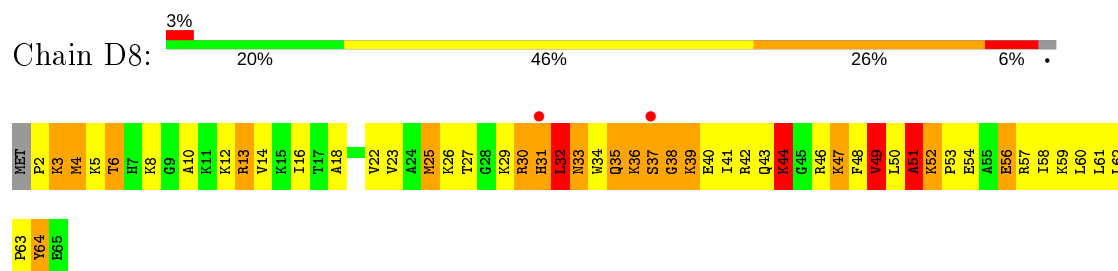
- Molecule 29: 50S ribosomal protein L34



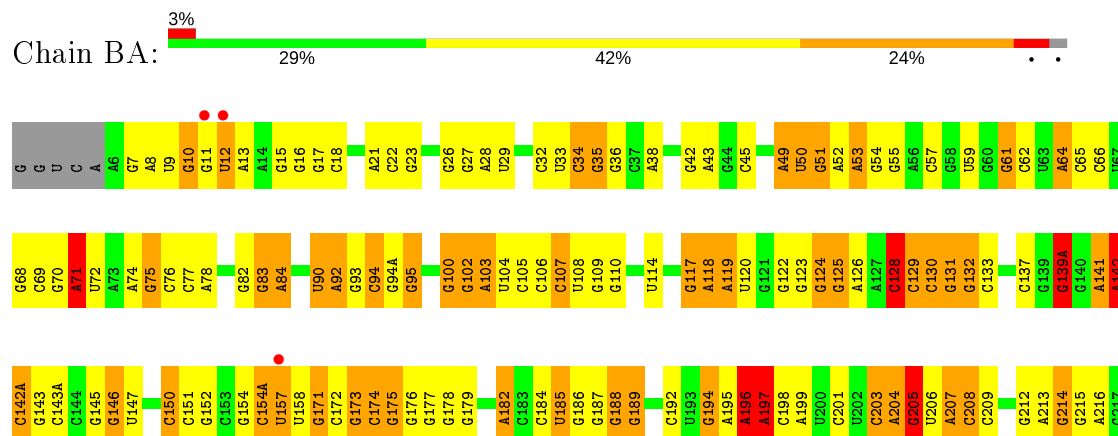
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

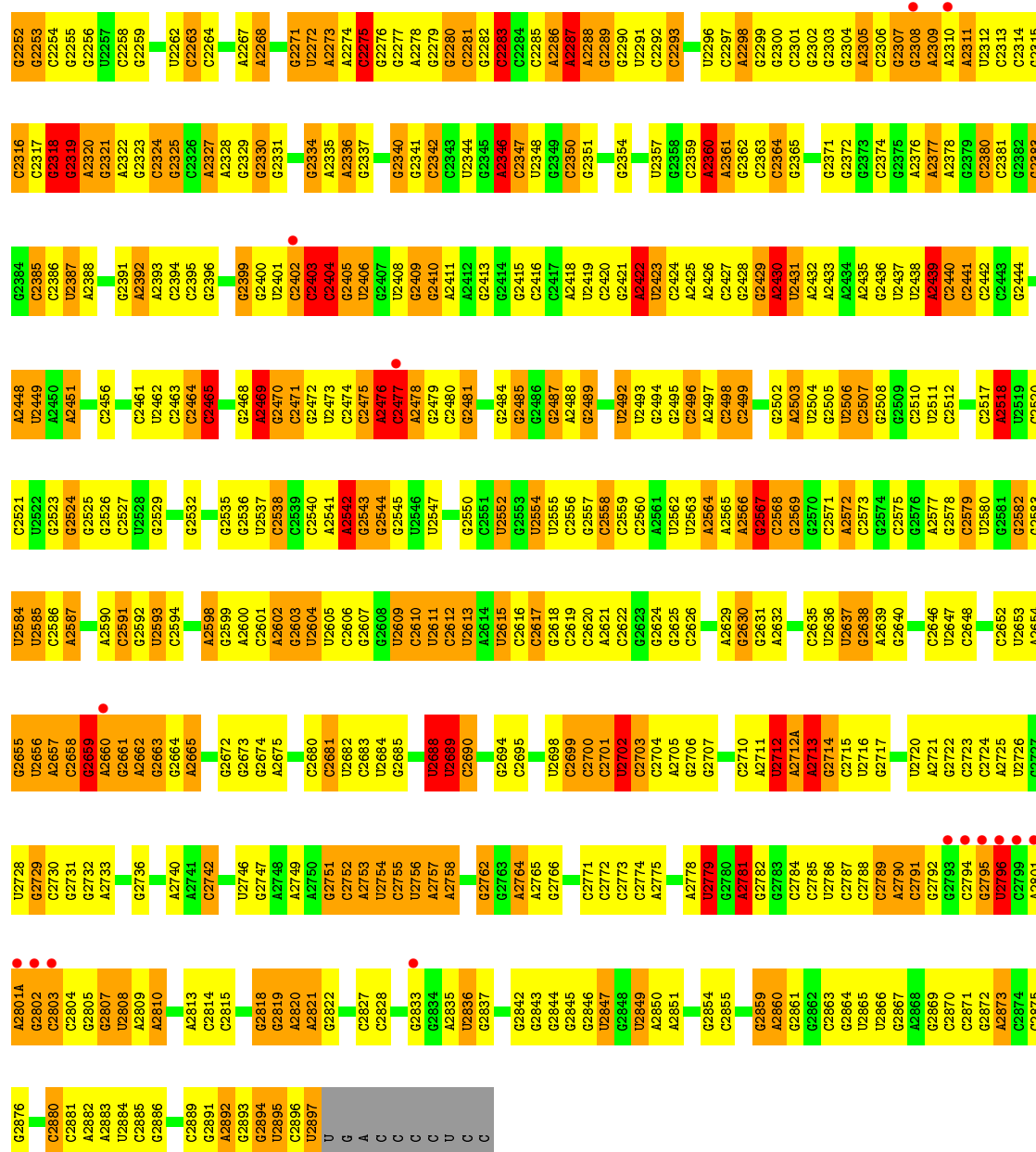


- Molecule 31: 23S ribosomal RNA



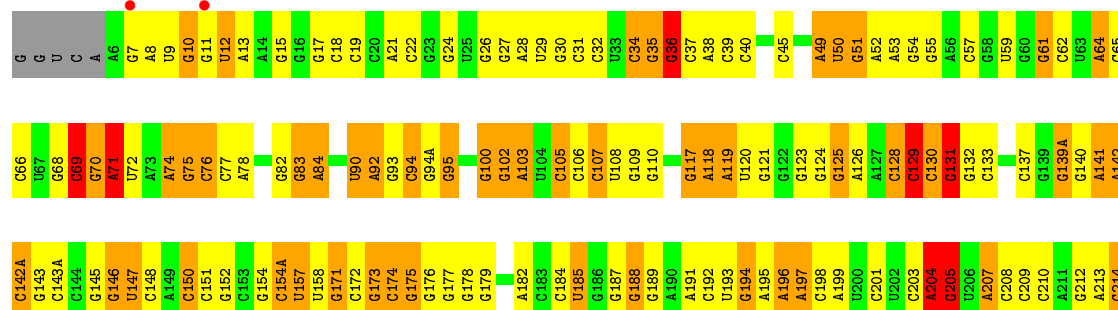
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|
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| U606 | U607 | U608 | U609 | U610 | U611 | U612 | U613 | U614 | U615 | U616 | U617 | U618 | U619 | U620 | U621 | U622 | U623 | U624 | U625 | U626 | U627 | U628 | U629 | U630 | U631 | U632 | U633 | U634 | U635 | U636 | U637 | U638 | U639 | U640 | U641 | U642 | U643 | U644 | U645 | U646 | U647 | U648 | U649 | U650 | U651 | U652 | U653 | U654 | U655 | U656 | U657 | U658 | U659 | U660 | U661 | U662 | U663 | U664 | U665 | U666 | U667 | U668 | U669 | U670 | U671 | U672 | U673 | U674 | U675 | U676 | U677 | U678 | U679 | U680 | U681 | U682 | U683 | U684 | U685 | U686 | U687 | U688 | U689 | U690 | U691 | U692 | U693 | U694 | U695 | U696 | U697 | U698 | U699 | U700 | U701 | U702 | U703 | U704 | U705 | U706 | U707 | U708 | U709 | U710 | U711 | U712 | U713 | U714 | U715 | U716 | U717 | U718 | U719 | U720 | U721 | U722 | U723 | U724 | U725 | U726 | U727 | U728 | U729 | U730 | U731 | U732 | U733 | U734 | U735 | U736 | U737 | U738 | U739 | U740 | U741 | U742 | U743 | U744 | U745 | U746 | U747 | U748 | U749 | U750 | U751 | U752 | U753 | U754 | U755 | U756 | U757 | U758 | U759 | U760 | U761 | U762 | U763 | U764 | U765 | U766 | U767 | U768 | U769 | U770 | U771 | U772 | U773 | U774 | U775 | U776 | U777 | U778 | U779 | U780 | U781 | U782 | U783 | U784 | U785 | U786 | U787 | U788 | U789 | U790 | U791 | U792 | U793 | U794 | U795 | U796 | U797 | U798 | U799 | U800 | U801 | U802 | U803 | U804 | U805 | U806 | U807 | U808 | U809 | U810 | U811 | U812 | U813 | U814 | U815 | U816 | U817 | U818 | U819 | U820 | U821 | U822 | U823 | U824 | U825 | U826 | U827 | U828 | U829 | U830 | U831 | U832 | U833 | U834 | U835 | U836 | U837 | U838 | U839 | U840 | U841 | U842 | U843 | U844 | U845 | U846 | U847 | U848 | U849 | U850 | U851 | U852 | U853 | U854 | U855 | U856 | U857 | U858 | U859 | U860 | U861 | U862 | U863 | U864 | U865 | U866 | U867 | U868 | U869 | U870 | U871 | U872 | U873 | U874 | U875 | U876 | U877 | U878 | U879 | U880 | U881 | U882 | U883 | U884 | U885 | U886 | U887 | U888 | U889 | U890 | U891 | U892 | U893 | U894 | U895 | U896 | U897 | U898 | U899 | U900 | U901 | U902 | U903 | U904 | U905 | U906 | U907 | U908 | U909 | U910 | U911 | U912 | U913 | U914 | U915 | U916 | U917 | U918 | U919 | U920 | U921 | U922 | U923 | U924 | U925 | U926 | U927 | U928 | U929 | U930 | U931 | U932 | U933 | U934 | U935 | U936 | U937 | U938 | U939 | U940 | U941 | U942 | U943 | U944 | U945 | U946 | U947 | U948 | U949 | U950 | U951 | U952 | U953 | U954 | U955 | U956 | U957 | U958 | U959 | U960 | U961 | U962 | U963 | U964 | U965 | U966 | U967 | U968 | U969 | U970 | U971 | U972 | U973 | U974 | U975 | U976 | U977 | U978 | U979 | U980 | U981 | U982 | U983 | U984 | U985 | U986 | U987 | U988 | U989 | U990 | U991 | U992 | U993 | U994 | U995 | U996 | U997 | U998 | U999 | G1000 | G1001 | G1002 | G1003 | G1004 | G1005 |
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|---|-------|-------|-------|-------|-------|-------|--------|--------|-------|-------|--------|
| A | C2085 | U2017 | A1877 | G1696 | G1626 | G1552 | G1482 | G1417 | U1340 | G1271 | G1197 |
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| C | G2087 | A2019 | C1879 | A1698 | G1628 | C1557 | G1485 | A1419 | A1342 | U1273 | C1201 |
| C | A2020 | G1948 | C1880 | G1699 | U1629 | G1558 | G1486 | A1420 | G1343 | A1274 | A1204 |
| U | C2021 | C1881 | A1700 | A1701 | A1632 | G1559 | G1488 | G1421 | G1344 | A1275 | A1205 |
| G | U2091 | G1950 | U1794 | G1702 | G1635 | G1563 | U1489 | G1425 | G1345 | A1276 | U1206 |
| C | G2093 | G1883 | C1795 | G1703 | G1636 | C1564 | A1490 | G1426 | G1348 | A1277 | G1207 |
| G | G2094 | A1884 | U1796 | G1704 | G1637 | C1565 | A1491 | A1427 | A1349 | G1278 | G1208 |
| C | C2095 | A1885 | C1797 | G1705 | A1637 | G1566 | G1492 | G1428 | C1350 | G1279 | C1209 |
| C | U2096 | G1886 | U1798 | G1706 | C1638 | A1567 | G1493 | G1429 | A1353 | U1282 | G1210 |
| C | G2097 | C1887 | U1799 | U1706 | U1639 | G1568 | G1494 | C1430 | A1354 | G1283 | A1210 |
| C | U2098 | G1888 | C1800 | U1709 | C1640 | A1569 | A1495 | U1431 | A1355 | A1284 | G1211 |
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| C | G2100 | A1890 | A1802 | U1709 | G1642 | A1571 | A1497 | U1431 | G1357 | A1286 | A1213 |
| C | U2101 | G1891 | A1803 | U1713 | G1643 | A1572 | U1497 | A1434 | U1358 | A1287 | G1216 |
| C | G2102 | C1892 | G1804 | G1714 | G1644 | A1573 | G1498 | G1435 | G1359 | U1288 | G1217 |
| C | A2031 | C1893 | U1905 | G1717 | C1644 | G1572 | G1499 | G1436 | G1360 | G1289 | G1218 |
| C | A2033 | G1894 | G1718 | G1719 | G1647 | C1574 | G1500 | C1437 | A1361 | U1290 | G1219 |
| C | G2036 | C1895 | G1719 | U1720 | G1648 | C1577 | G1501 | U1438 | U1362 | U1291 | A1220 |
| C | C2039 | G1896 | U1721 | U1720 | G1649 | C1578 | G1502 | A1439 | U1292 | U1292 | C1221A |
| C | G2040 | G1897 | A1812 | G1721 | G1649 | C1579 | U1503 | G1440 | G1364 | U1293 | G1222A |
| C | A2041 | G1898 | G1813 | A1722 | A1652 | A1578 | C1504 | G1441 | A1365 | U1294 | G1223 |
| C | U2042 | A1900 | U1739 | U1739 | G1653 | A1579 | C1505 | G1442 | G1366 | C1298 | G1224 |
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| C | A2054 | A1912 | G1749 | G1749 | C1662 | U1590 | C1513 | C1451 | G1380 | G1311 | A1241 |
| C | C2055 | A1913 | G1750 | G1750 | C1663 | G1591 | U1514 | G1455 | G1381 | U1312 | A1242 |
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| C | C2065 | C1920 | G1756 | G1756 | G1674 | C1598 | G1525 | G1462 | G1388 | C1320 | A1263 |
| C | G2066 | C1925 | A1762 | A1762 | C1675 | U1602 | G1526 | C1463 | A1395 | C1321 | G1254 |
| C | U2067 | U1926 | G1763 | G1763 | A1676 | A1603 | G1527 | C1464 | U1396 | A1322 | A1264 |
| C | G2068 | A1927 | G1764 | G1764 | A1677 | C1604 | A1528 | G1465 | U1397 | U1323 | U1265 |
| C | U2069 | C1928 | G1771 | C1771 | G1678 | C1605 | A1528A | G1466 | C1398 | G1324 | G1266 |
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| C | A2073 | A1932 | C1774 | C1774 | A1685 | A1609 | C1532 | A1471 | U1405 | G1328 | G1261 |
| C | U2074 | G1933 | A1847 | U1777 | C1686 | A1610 | G1533 | A1472 | U1406 | U1329 | A1262 |
| C | G2075 | C1934 | G1856 | U1778 | C1687 | A1614 | C1543 | G1473 | C1407 | C1330 | U1263 |
| C | C2076 | G1935 | G1857 | U1779 | G1688 | C1615 | A1544 | C1474 | C1408 | A1331 | G1264 |
| C | U2077 | A1936 | G1858 | U1779 | A1689 | A1616 | A1545 | G1475 | C1409 | G1332 | A1265 |
| C | G2078 | C1937 | C1780 | A1780 | U1699 | C1617 | C1546 | C1476 | C1410 | C1333 | A1266 |
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| C | G2080 | U1939 | G1783 | G1783 | U1693 | A1619 | C1548 | G1478 | A1412 | A1337 | A1268 |
| C | C2081 | G1865 | A1783 | A1783 | C1694 | G1624 | C1549 | G1479 | G1413 | G1337 | A1269 |
| C | A2082 | C1866 | A1784 | A1784 | U1695 | G1625 | C1550 | U1481 | G1338 | G1339 | C1270 |
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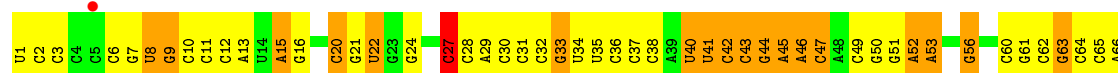
• Molecule 31: 23S ribosomal RNA

Chain DA: 5% 24% 45% 25%

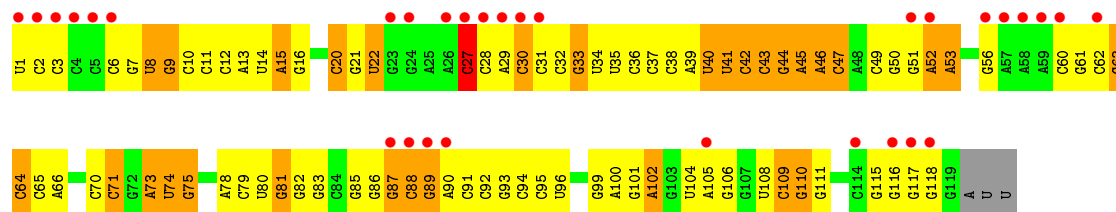




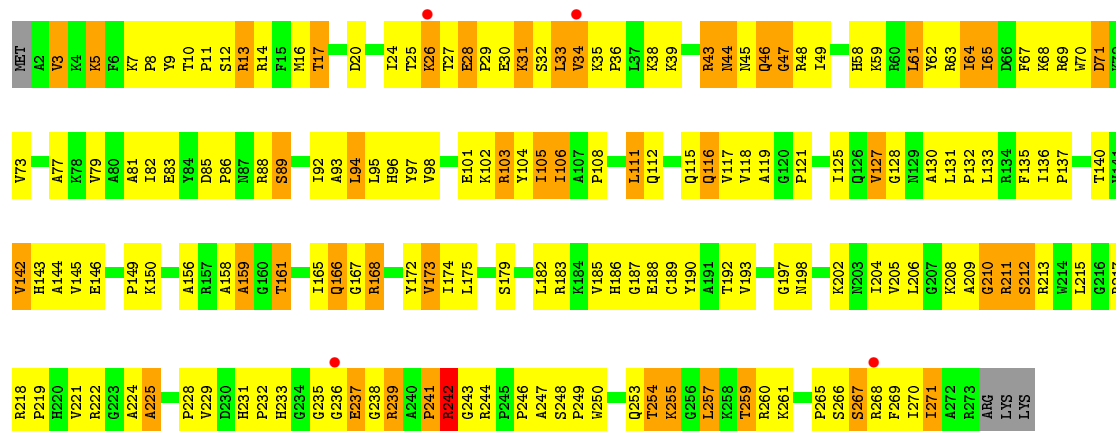
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| G2023 | G2023 | A1953 | C1886 | C1800 | G1717 | A1641 | C1577 | C1505 | G1441 | C1370 | G1243 | U1175 |
| G2024 | G1954 | G1954 | G1887 | G1810 | G1718 | G1642 | U1578 | C1506 | G1442 | G1371 | G1244 | G1176 |
| G2025 | G1955 | G1955 | G1888 | A1802 | G1719 | G1643 | U1579 | A1507 | G1443 | U1372 | G1245 | A1177 |
| G2026 | U1956 | U1956 | A1889 | C1803 | U1720 | A1580 | A1580 | C1508 | G1444 | G1373 | A1246 | C1178 |
| G2027 | G2027 | A1957 | A1890 | C1804 | G1721 | G1648 | G1581 | C1509 | A1445 | A1374 | A1247 | C1179 |
| G2095 | U2028 | C1958 | G1891 | U1805 | A1722 | G1649 | C1582 | A1509A | C1445A | C1375 | G1247 | C1180 |
| G2029 | G1959 | G1959 | C1892 | A1809 | U1739 | A1649 | A1583 | A1509B | C1446 | | G1250 | C1181 |
| G2097 | A2030 | A1960 | C1893 | A1816 | G1740 | A1652 | U1584 | C1510 | G1447 | A1378 | G1251 | A1182 |
| A2031 | G1961 | A1969 | C1894 | A1810 | A1741 | G1653 | A1586 | C1511 | G1448 | A1379 | G1252 | G1183 |
| G2032 | C1962 | C1962 | C1895 | A1811 | G1742 | A1654 | A1587 | C1512 | A1449 | A1380 | A1253 | G1184 |
| U2099 | U1963 | U1963 | G1896 | A1812 | G1743 | A1655 | C1588 | C1513 | G1450 | G1381 | A1254 | C1185 |
| A2033 | G1964 | G1964 | G1897 | A1813 | G1744 | C1656 | C1589 | U1514 | C1450A | G1382 | U1255 | G1186 |
| G2101 | | | U1898 | G1814 | C1745 | C1657 | U1590 | G1515 | C1451 | C1383 | G1256 | G1187 |
| U2102 | G2036 | | G1899 | G1815 | G1746 | C1658 | A1591 | C1516 | | A1321 | C1257 | U1188 |
| C2103 | G2037 | G1968 | A1900 | A1816 | G1746 | U1659 | C1592 | C1517 | G1455 | G1385 | C1258 | A1189 |
| G2104 | G2038 | C1968 | A1901 | A1817 | G1747 | G1660 | G1593 | U1518 | | G1386 | G1259 | G1190 |
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| G2106 | U2041 | A1971 | G1903 | U1820 | G1748 | C1662 | G1595 | U1520 | G1459 | G1388 | C1261 | G1192 |
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| U | G2043 | G1973 | C1905 | G1822 | A1750 | A1665 | C1598 | G1526 | G1461 | A1395 | U1263 | A1934 |
| G | C2044 | C1974 | G1906 | A1829 | C1751 | G1666 | C1599 | G1527 | C1462 | U1396 | G1264 | G1195 |
| C | G2045 | G1974 | G1907 | G1830 | | G1667 | C1599 | G1528 | C1463 | U1397 | A1265 | C1196 |
| G | G1980 | G1980 | G1908 | G1826 | C1754 | G1667 | G1600 | A1528A | G1464 | C1398 | G1266 | G1197 |
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| U | G2049 | G1982 | C1909 | A1829 | G1756 | A1669 | U1602 | G1529 | G1466 | A1268 | A1268 | U1199 |
| A | C2050 | C1983 | G1910 | G1830 | U1757 | C1670 | U1603 | C1530 | G1467 | A1269 | C1270 | G1200 |
| G | A2051 | G1984 | A1913 | | G1758 | C1671 | C1604 | C1531 | | U1270 | C1201 | |
| A | G2052 | G1985 | C1914 | U1833 | A1759 | G1674 | C1605 | C1532 | A1471 | A1336 | G1271 | A1204 |
| U | | | U1915 | U1834 | | C1675 | C1606 | G1533 | A1472 | C1377 | A1272 | |
| A | C2055 | G1989 | A1916 | G1835 | A1762 | A1676 | C1607 | C1543 | G1473 | C1378 | U1273 | U1205 |
| G | G2056 | C1990 | U1917 | C1836 | G1763 | A1677 | A1608 | A1544 | C1474 | C1339 | A1274 | U1206 |
| G | A2057 | U1991 | A1918 | C1837 | G1764 | G1678 | A1609 | A1545 | G1475 | U1340 | A1275 | C1207 |
| U | C2058 | G1992 | G1921 | C1838 | | | C1610 | C1546 | C1476 | C1411 | A1276 | C1208 |
| U | A2059 | U1993 | G1922 | G1840 | C1771 | G1681 | C1612 | C1547 | A1477 | G1343 | G1277 | G1209 |
| G | C1994 | C1994 | | | A1772 | G1682 | G1613 | C1548 | G1478 | A1278 | A1210 | |
| C | U1995 | U1995 | | | G1773 | | C1614 | C1549 | G1479 | G1414 | G1279 | U1211 |
| C | A2060 | G1996 | C1925 | C1844 | C1774 | C1685 | C1615 | C1550 | G1480 | G1280 | G1280 | G1212 |
| A | A2062 | G1997 | U1926 | | U1775 | C1686 | C1616 | C1551 | U1481 | G1281 | G1281 | G1213 |
| G | C2063 | C1998 | A1927 | A1847 | G1776 | G1687 | A1616 | G1552 | G1482 | C1417 | U1282 | A1214 |
| C | C2064 | C1999 | A1928 | | U1777 | U1688 | C1617 | A1553 | G1484 | G1418 | G1283 | G1215 |
| U | C2065 | G2000 | G1929 | G1850 | U1778 | A1689 | A1618 | A1554 | G1485 | A1419 | A1284 | G1216 |
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| C | U2068 | | U1931 | | A1780 | U1692 | | | G1487 | G1421 | A1286 | A1220 |
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| G | G2070 | C2006 | G1933 | G1857 | C1782 | C1694 | G1623 | G1559 | U1489 | | U1288 | C1221A |
| C | A2071 | | C1934 | G1858 | A1783 | G1695 | G1624 | | A1490 | G1425 | U1289 | |
| C | | | G1935 | A1859 | A1784 | G1696 | C1625 | G1563 | G1491 | G1426 | C1290 | C1224 |
| C | | | A1936 | A1785 | A1785 | G1697 | G1626 | C1564 | G1492 | A1427 | G1291 | G1225 |
| G | U2074 | | A1937 | G1865 | A1786 | A1698 | G1627 | C1565 | C1493 | U1292 | A1296 | A1296 |
| U | U2075 | | U1938 | C1866 | | G1699 | G1628 | A1566 | A1494 | G1429 | C1293 | |
| U | | G2012 | U1939 | A1876 | C1790 | A1700 | U1629 | A1567 | A1495 | C1430 | | G1227 |
| G | | A2013 | U1940 | A1877 | A1791 | A1701 | G1630 | G1568 | A1496 | U1431 | C1297 | G1228 |
| A | | A2014 | | G1878 | G1792 | G1702 | | A1569 | U1497 | | C1298 | G1229 |
| A | G2010 | A2015 | G1945 | G1879 | U1793 | G1703 | | A1570 | C1498 | A1434 | G1299 | C1230 |
| U | U2016 | U2017 | U1946 | C1880 | U1794 | | | A1571 | C1499 | G1435 | U1300 | |
| U | A2082 | U2017 | C1947 | C1881 | C1795 | C1708 | C1636 | A1572 | G1500 | G1436 | A1301 | G1235 |
| C | G2083 | G2018 | G1948 | C1882 | C1796 | U1709 | A1637 | G1573 | C1501 | C1437 | A1302 | |
| C | C2084 | A2019 | G1949 | G1883 | C1797 | U1797 | C1638 | C1574 | C1502 | U1438 | G1303 | U1240 |
| A | C2085 | A2020 | | A1884 | U1798 | | U1639 | C1575 | U1503 | A1439 | C1304 | A1241 |
| C | U2086 | C2021 | | | | | | | | | | |



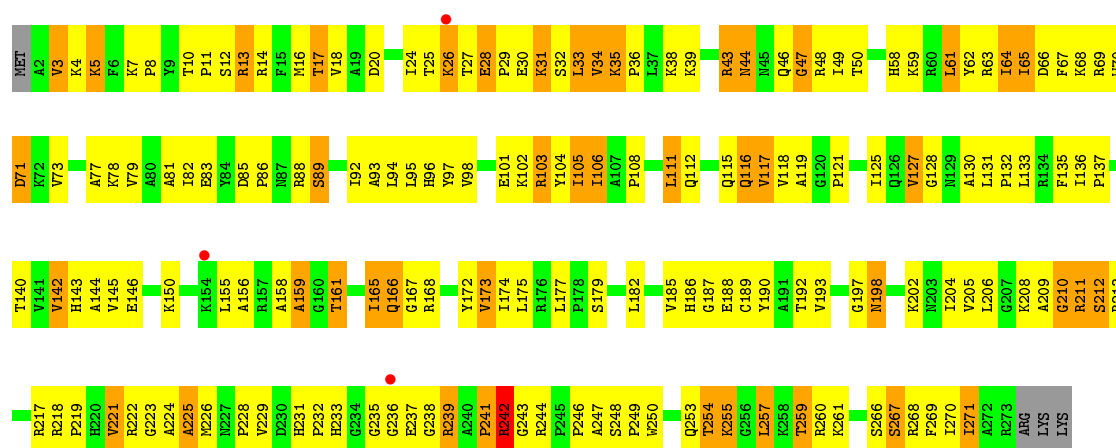
- Molecule 32: 5S ribosomal RNA



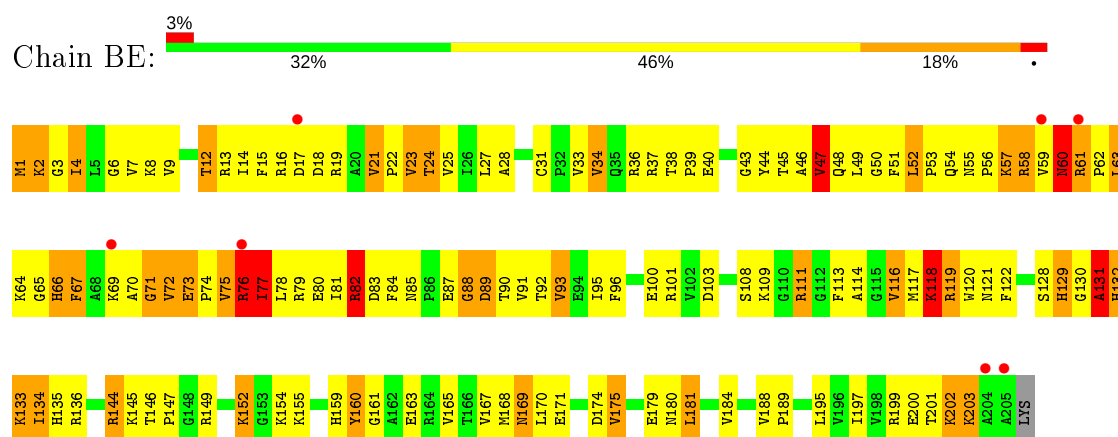
- Molecule 33: 50S ribosomal protein L2



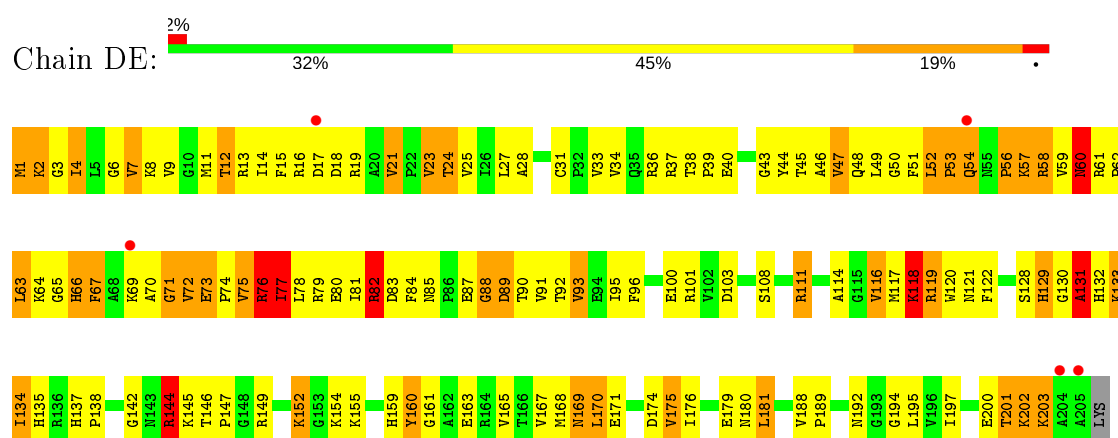
- Molecule 33: 50S ribosomal protein L2



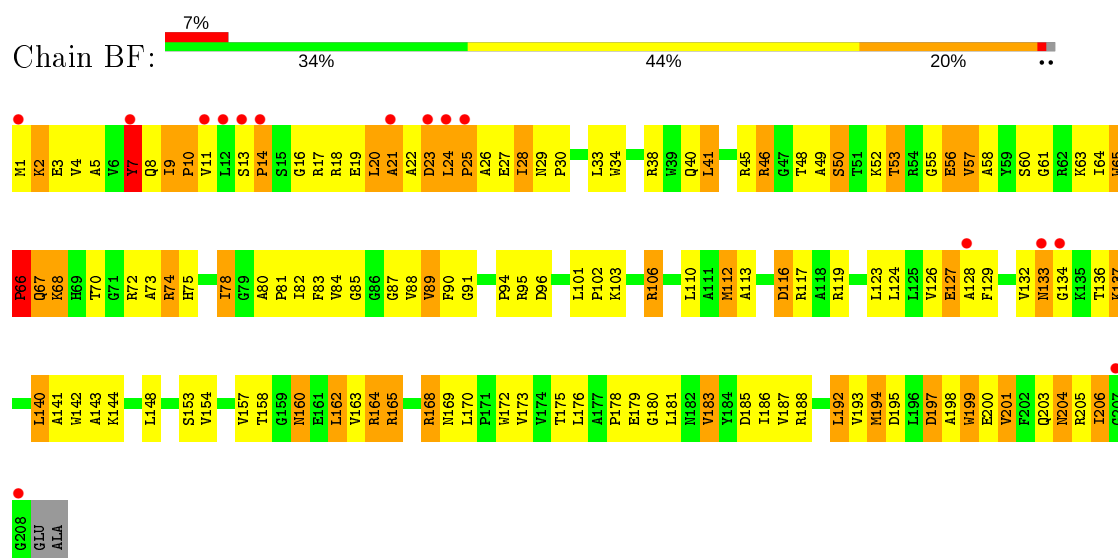
- Molecule 34: 50S ribosomal protein L3



• Molecule 34: 50S ribosomal protein L3

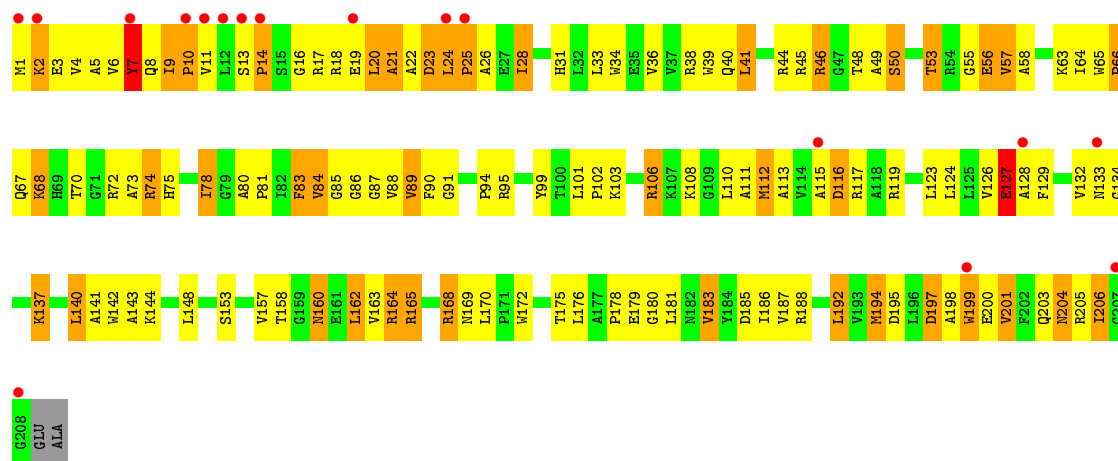


• Molecule 35: 50S ribosomal protein L4

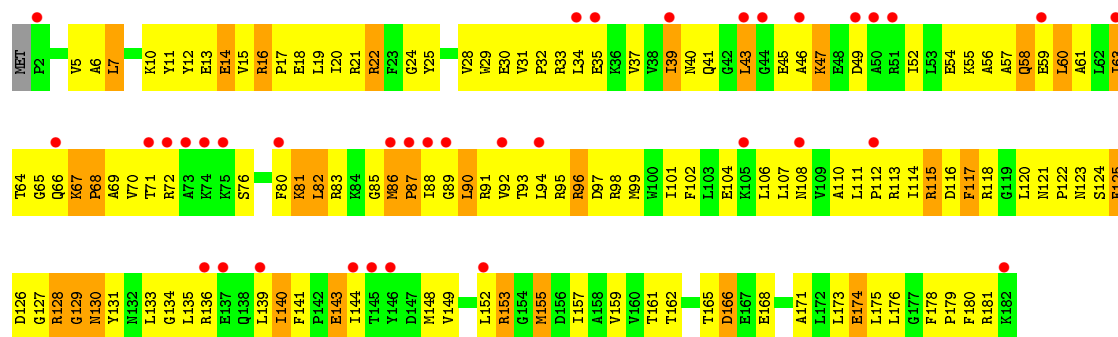


• Molecule 35: 50S ribosomal protein L4

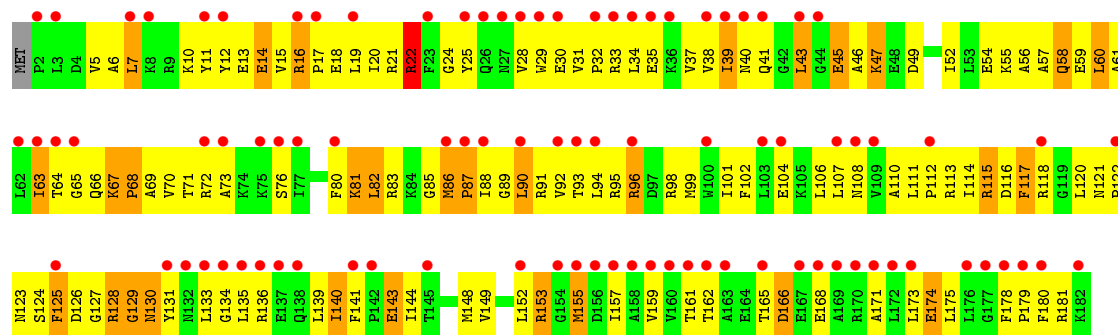




• Molecule 36: 50S ribosomal protein L5

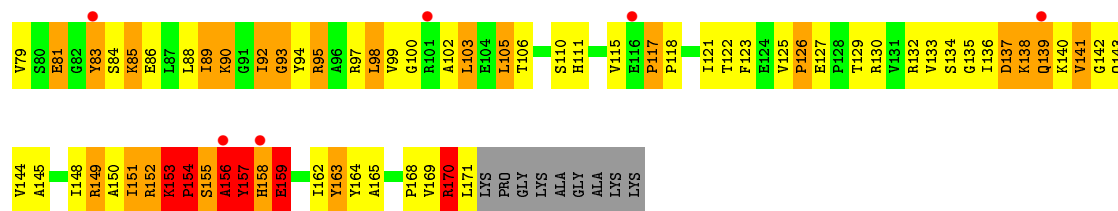


• Molecule 36: 50S ribosomal protein L5

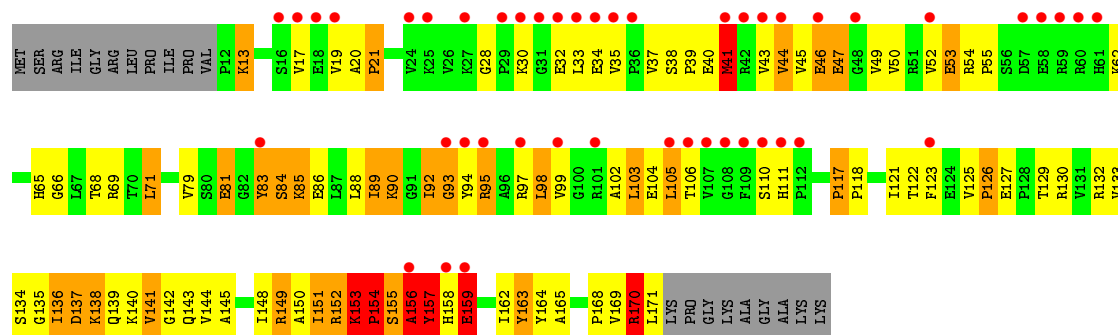


• Molecule 37: 50S ribosomal protein L6

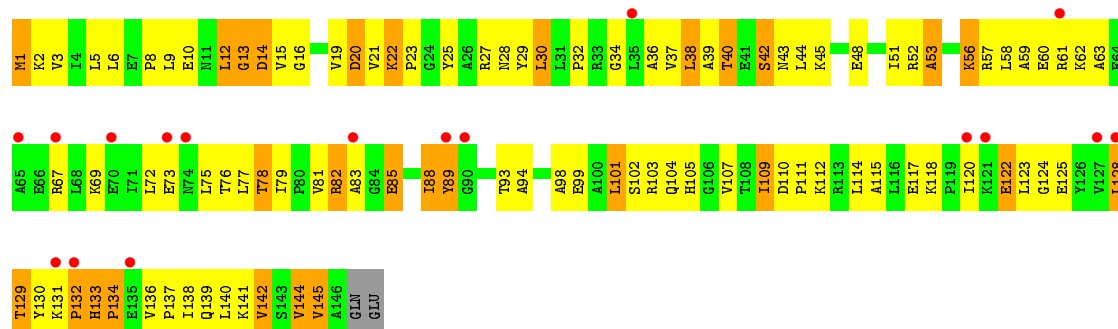




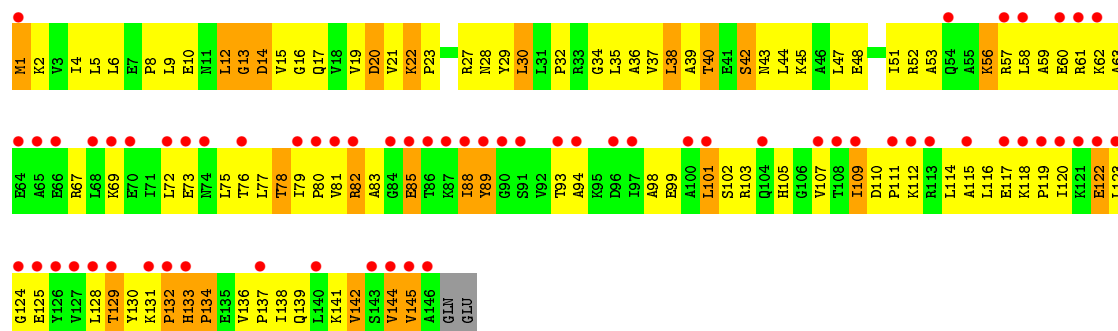
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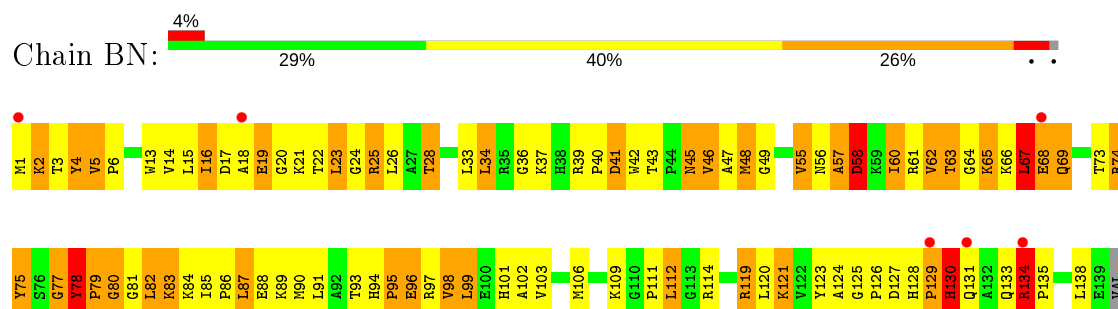
• Molecule 38: 50S ribosomal protein L9



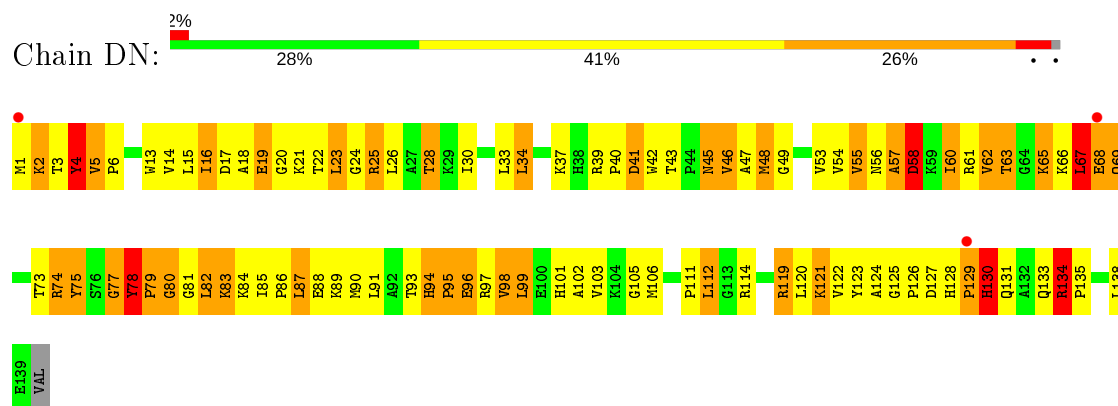
• Molecule 38: 50S ribosomal protein L9



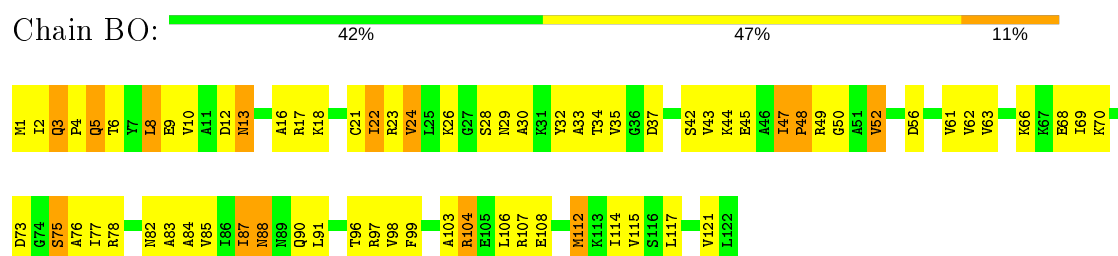
- Molecule 39: 50S ribosomal protein L13



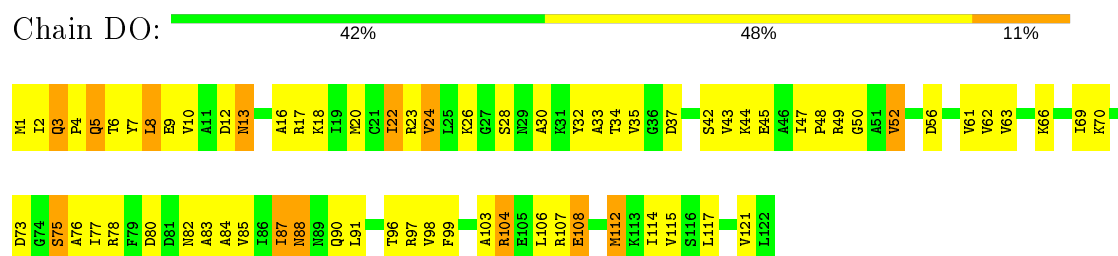
- Molecule 39: 50S ribosomal protein L13



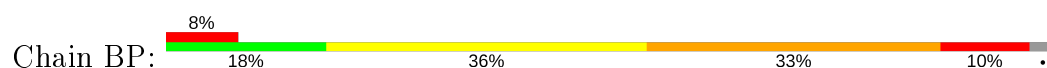
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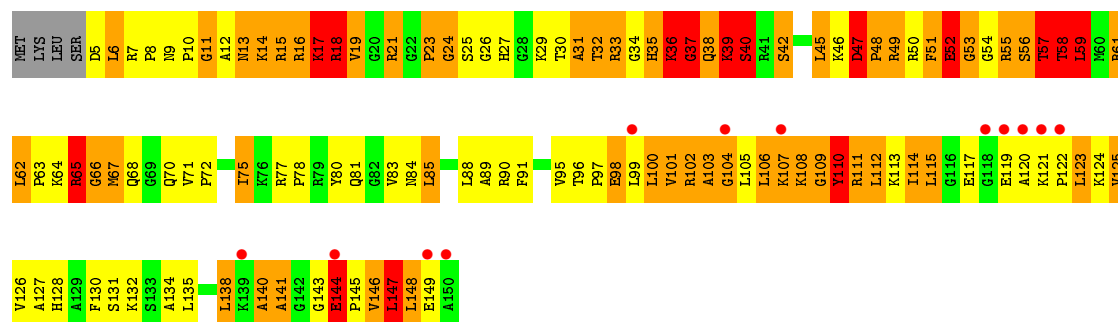


- Molecule 40: 50S ribosomal protein L14

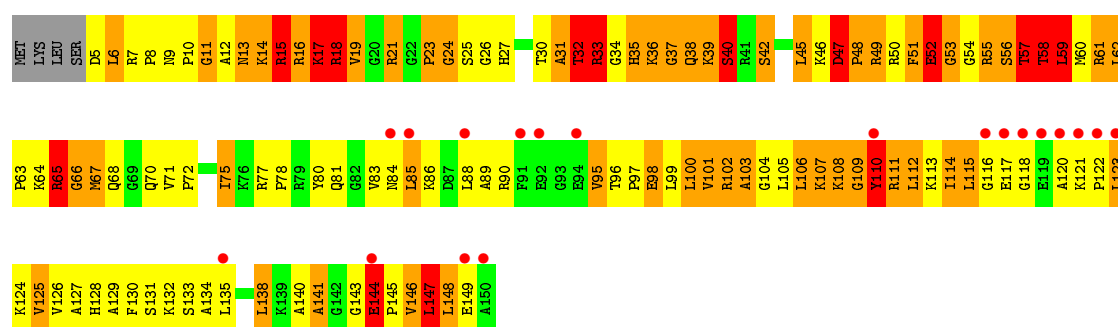
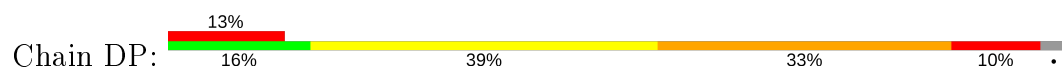


- Molecule 41: 50S ribosomal protein L15

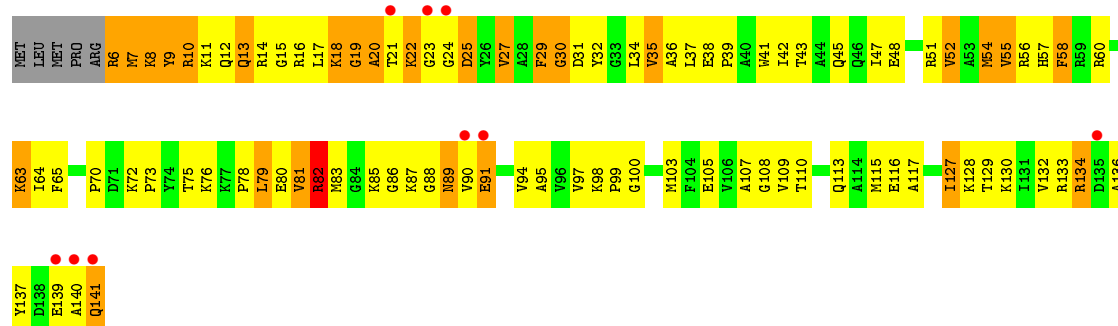
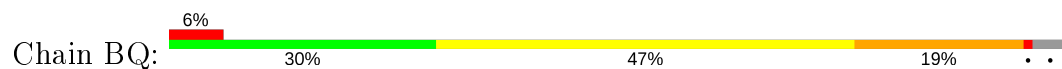




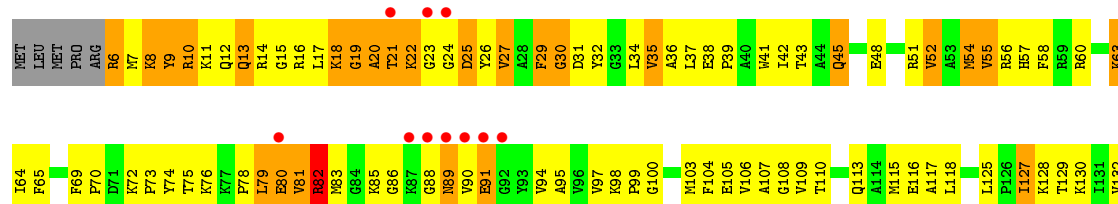
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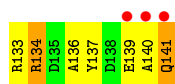


• Molecule 42: 50S ribosomal protein L16



• Molecule 42: 50S ribosomal protein L16

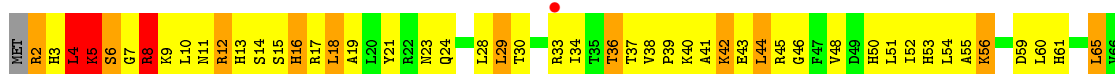




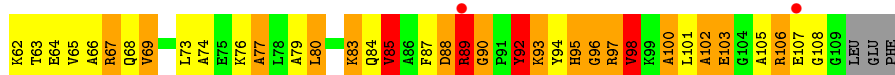
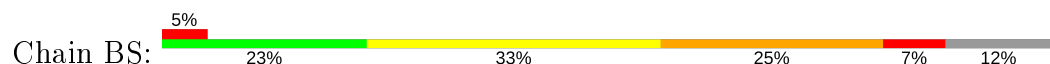
- Molecule 43: 50S ribosomal protein L17



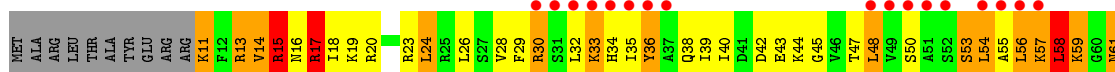
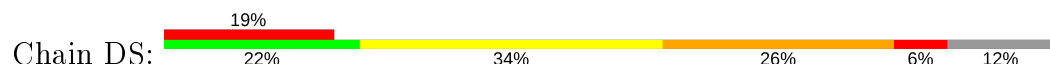
- Molecule 43: 50S ribosomal protein L17



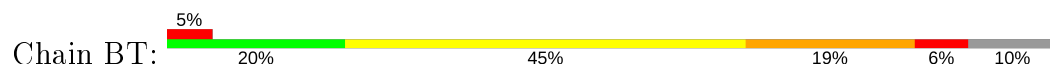
- Molecule 44: 50S ribosomal protein L18

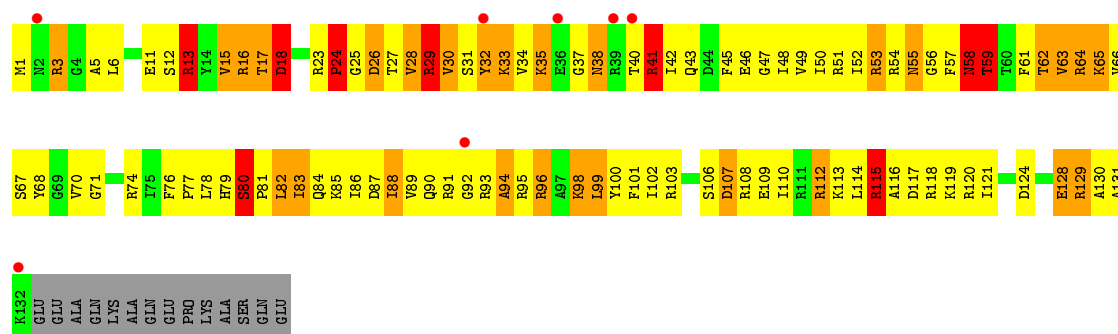


- Molecule 44: 50S ribosomal protein L18

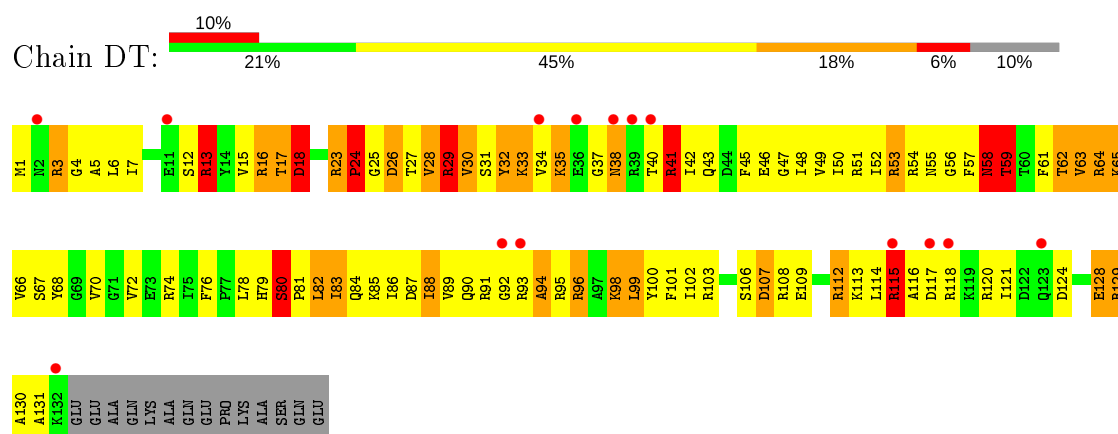


- Molecule 45: 50S ribosomal protein L19

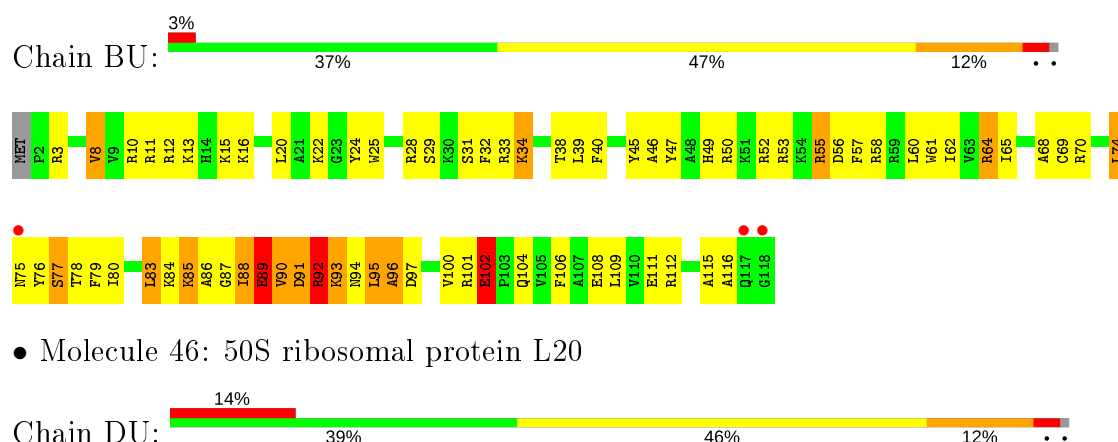




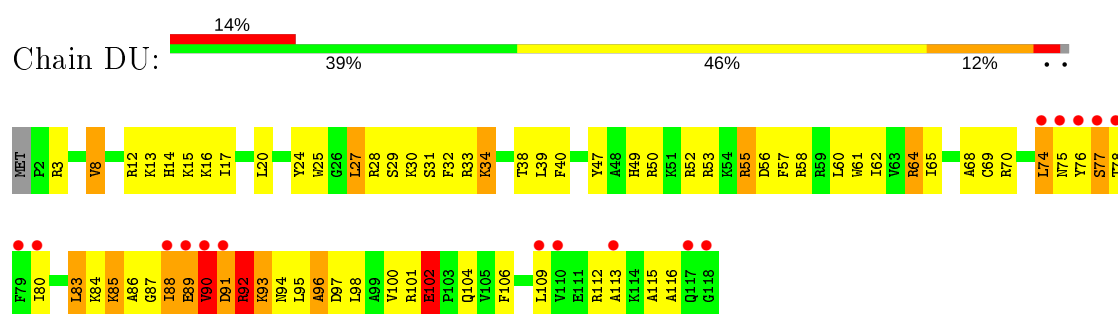
• Molecule 45: 50S ribosomal protein L19



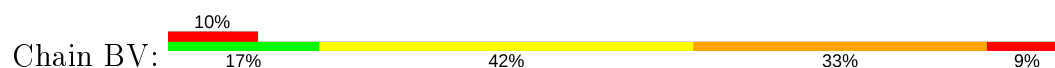
• Molecule 46: 50S ribosomal protein L20

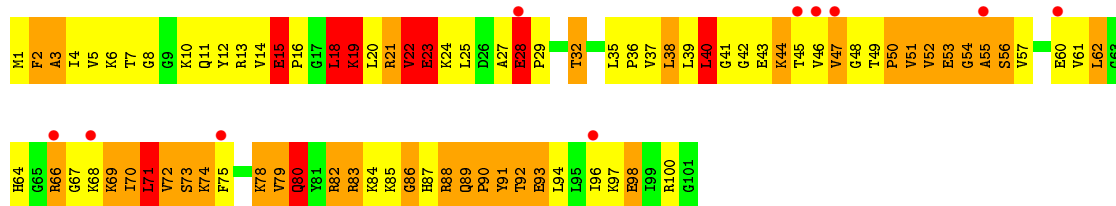


• Molecule 46: 50S ribosomal protein L20

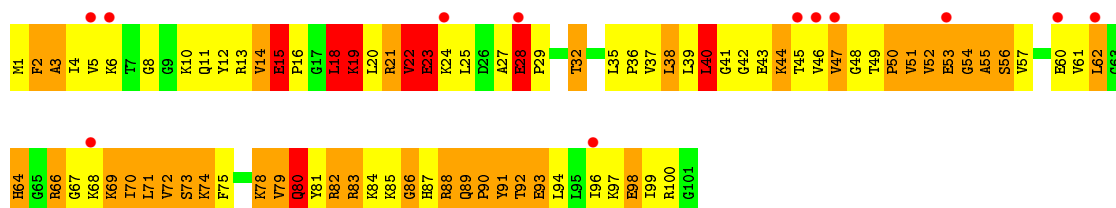
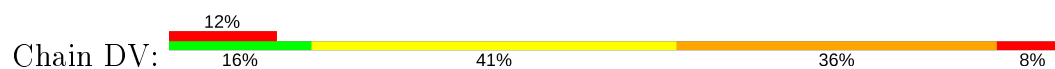


• Molecule 47: 50S ribosomal protein L21

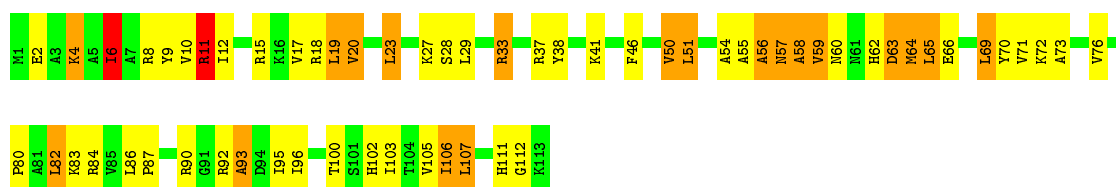




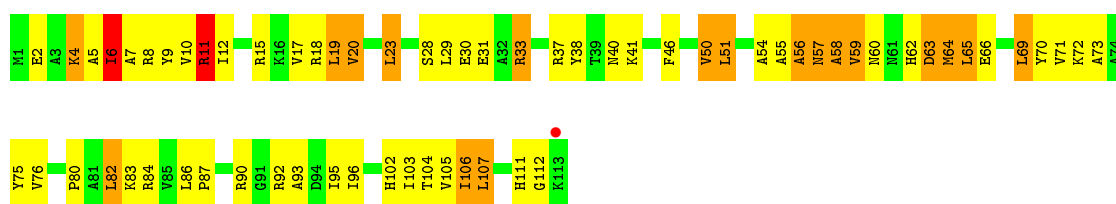
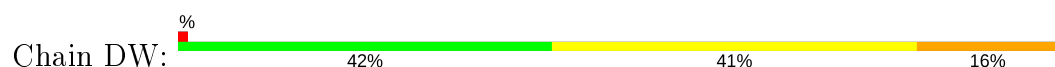
• Molecule 47: 50S ribosomal protein L21



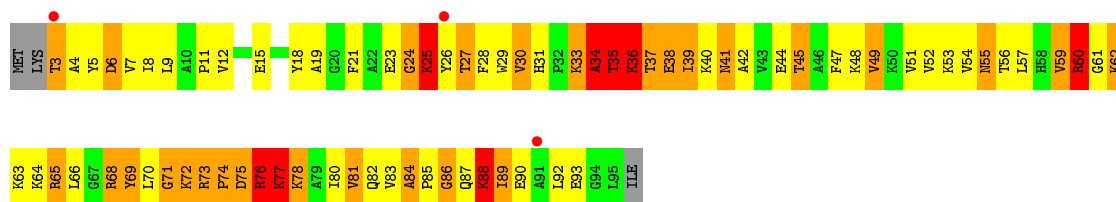
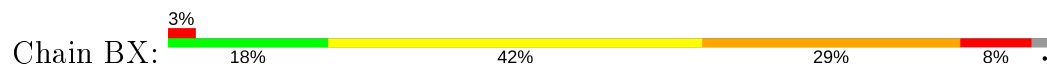
• Molecule 48: 50S ribosomal protein L22



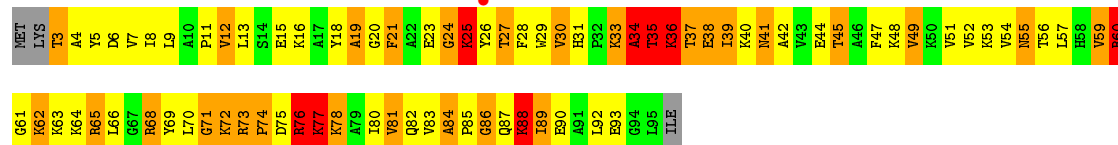
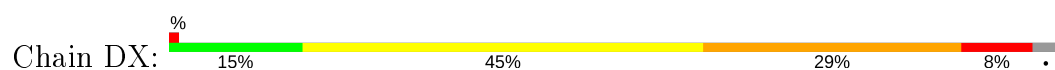
• Molecule 48: 50S ribosomal protein L22



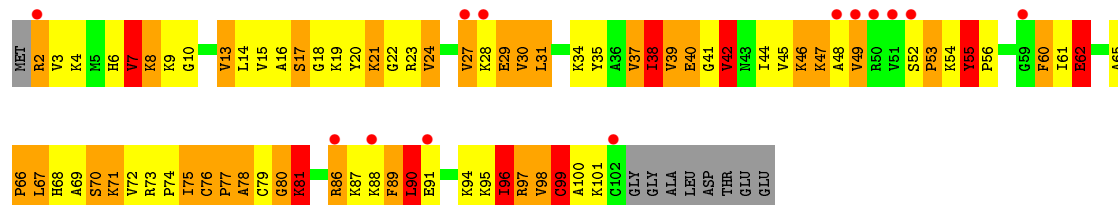
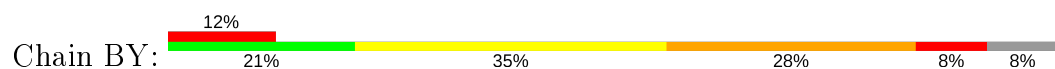
• Molecule 49: 50S ribosomal protein L23



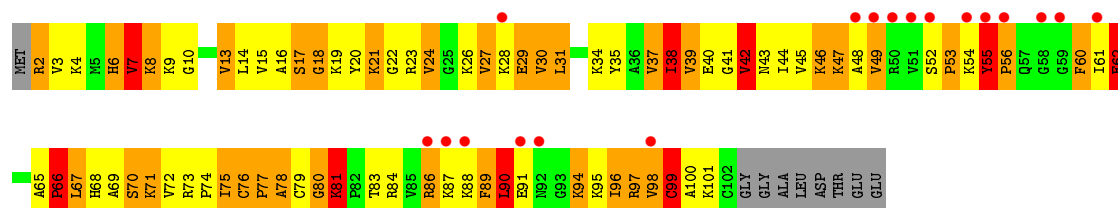
• Molecule 49: 50S ribosomal protein L23



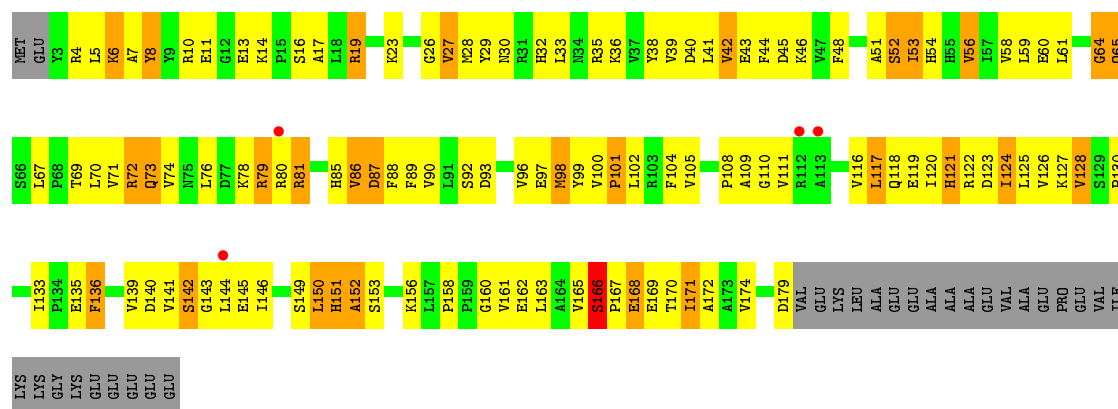
• Molecule 50: 50S ribosomal protein L24



• Molecule 50: 50S ribosomal protein L24

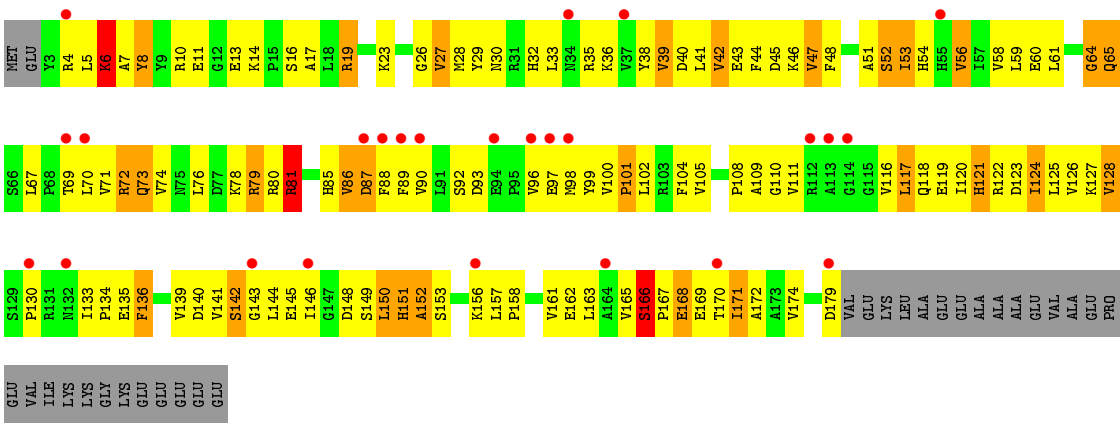


• Molecule 51: 50S ribosomal protein L25



• Molecule 51: 50S ribosomal protein L25





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.47Å 447.96Å 620.17Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.61 – 3.00 49.88 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (49.61-3.00) 99.8 (49.88-3.00) | Depositor EDS |
| R_{merge} | 0.27 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.22 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.243 , 0.278 0.239 , 0.272 | Depositor DCC |
| R_{free} test set | 57768 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 66.5 | Xtriage |
| Anisotropy | 0.273 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 86.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.88 | EDS |
| Total number of atoms | 278034 | wwPDB-VP |
| Average B, all atoms (Å ²) | 93.0 | wwPDB-VP |

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

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: K, MG, ZN, ERY

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 | 0.49 | 0/36190 | 0.86 | 24/56486 (0.0%) |
| 1 | CA | 0.49 | 0/36190 | 0.87 | 35/56486 (0.1%) |
| 2 | AB | 0.28 | 0/1936 | 0.49 | 0/2611 |
| 2 | CB | 0.28 | 0/1936 | 0.49 | 0/2611 |
| 3 | AC | 0.26 | 0/1637 | 0.46 | 0/2207 |
| 3 | CC | 0.26 | 0/1637 | 0.45 | 0/2207 |
| 4 | AD | 0.34 | 0/1733 | 0.52 | 0/2318 |
| 4 | CD | 0.35 | 0/1733 | 0.53 | 0/2318 |
| 5 | AE | 0.32 | 0/1163 | 0.52 | 0/1566 |
| 5 | CE | 0.33 | 0/1163 | 0.54 | 0/1566 |
| 6 | AF | 0.33 | 0/856 | 0.53 | 0/1154 |
| 6 | CF | 0.33 | 0/856 | 0.53 | 0/1154 |
| 7 | AG | 0.24 | 0/1276 | 0.43 | 0/1709 |
| 7 | CG | 0.24 | 0/1276 | 0.43 | 0/1709 |
| 8 | AH | 0.33 | 0/1136 | 0.54 | 0/1527 |
| 8 | CH | 0.31 | 0/1136 | 0.53 | 0/1527 |
| 9 | AI | 0.26 | 0/1028 | 0.42 | 0/1375 |
| 9 | CI | 0.26 | 0/1028 | 0.42 | 0/1375 |
| 10 | AJ | 0.27 | 0/808 | 0.46 | 0/1087 |
| 10 | CJ | 0.27 | 0/808 | 0.47 | 0/1087 |
| 11 | AK | 0.31 | 0/900 | 0.52 | 0/1213 |
| 11 | CK | 0.32 | 0/900 | 0.53 | 0/1213 |
| 12 | AL | 0.39 | 0/987 | 0.61 | 0/1322 |
| 12 | CL | 0.41 | 0/987 | 0.61 | 0/1322 |
| 13 | AM | 0.24 | 0/928 | 0.45 | 0/1238 |
| 13 | CM | 0.25 | 0/928 | 0.45 | 0/1238 |
| 14 | AN | 0.28 | 0/501 | 0.43 | 0/664 |
| 14 | CN | 0.27 | 0/501 | 0.43 | 0/664 |
| 15 | AO | 0.34 | 0/745 | 0.53 | 0/992 |
| 15 | CO | 0.33 | 0/745 | 0.52 | 0/992 |
| 16 | AP | 0.32 | 0/717 | 0.54 | 0/965 |
| 16 | CP | 0.31 | 0/717 | 0.55 | 0/965 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.34 | 0/837 | 0.53 | 0/1119 |
| 17 | CQ | 0.33 | 0/837 | 0.53 | 0/1119 |
| 18 | AR | 0.33 | 0/579 | 0.57 | 0/768 |
| 18 | CR | 0.32 | 0/579 | 0.56 | 0/768 |
| 19 | AS | 0.25 | 0/643 | 0.42 | 0/867 |
| 19 | CS | 0.25 | 0/643 | 0.42 | 0/867 |
| 20 | AT | 0.35 | 0/765 | 0.55 | 0/1007 |
| 20 | CT | 0.34 | 0/765 | 0.55 | 0/1007 |
| 21 | AU | 0.26 | 0/213 | 0.42 | 0/279 |
| 21 | CU | 0.26 | 0/213 | 0.42 | 0/279 |
| 22 | B0 | 0.52 | 0/658 | 0.70 | 0/878 |
| 22 | D0 | 0.52 | 0/658 | 0.70 | 0/878 |
| 23 | B1 | 0.76 | 0/700 | 1.02 | 2/931 (0.2%) |
| 23 | D1 | 0.73 | 0/700 | 0.99 | 2/931 (0.2%) |
| 24 | B2 | 0.65 | 0/423 | 0.99 | 1/560 (0.2%) |
| 24 | D2 | 0.57 | 0/423 | 0.92 | 1/560 (0.2%) |
| 25 | B3 | 0.61 | 0/473 | 0.71 | 0/636 |
| 25 | D3 | 0.48 | 0/473 | 0.68 | 0/636 |
| 26 | B4 | 0.28 | 0/156 | 0.57 | 0/215 |
| 26 | D4 | 0.27 | 0/156 | 0.55 | 0/215 |
| 27 | B5 | 0.85 | 0/473 | 1.06 | 3/639 (0.5%) |
| 27 | D5 | 0.78 | 0/473 | 1.01 | 3/639 (0.5%) |
| 28 | B6 | 0.80 | 0/387 | 1.04 | 2/517 (0.4%) |
| 28 | D6 | 0.67 | 0/387 | 0.94 | 0/517 |
| 29 | B7 | 0.63 | 0/427 | 0.84 | 0/563 |
| 29 | D7 | 0.64 | 0/427 | 0.83 | 1/563 (0.2%) |
| 30 | B8 | 0.73 | 0/516 | 1.07 | 3/681 (0.4%) |
| 30 | D8 | 0.65 | 0/516 | 1.03 | 3/681 (0.4%) |
| 31 | BA | 1.06 | 67/65745 (0.1%) | 1.40 | 967/102639 (0.9%) |
| 31 | DA | 0.87 | 39/65745 (0.1%) | 1.40 | 970/102639 (0.9%) |
| 32 | BB | 0.80 | 0/2853 | 1.13 | 12/4451 (0.3%) |
| 32 | DB | 0.69 | 0/2853 | 1.13 | 20/4451 (0.4%) |
| 33 | BD | 0.63 | 0/2155 | 0.84 | 1/2907 (0.0%) |
| 33 | DD | 0.60 | 0/2155 | 0.83 | 0/2907 |
| 34 | BE | 0.62 | 0/1597 | 0.83 | 2/2155 (0.1%) |
| 34 | DE | 0.55 | 0/1597 | 0.81 | 0/2155 |
| 35 | BF | 0.61 | 1/1659 (0.1%) | 0.76 | 1/2246 (0.0%) |
| 35 | DF | 0.52 | 0/1659 | 0.76 | 2/2246 (0.1%) |
| 36 | BG | 0.31 | 0/1498 | 0.53 | 0/2013 |
| 36 | DG | 0.29 | 0/1498 | 0.52 | 0/2013 |
| 37 | BH | 0.60 | 0/1246 | 0.73 | 0/1684 |
| 37 | DH | 0.42 | 0/1246 | 0.68 | 0/1684 |
| 38 | BI | 0.35 | 0/1147 | 0.59 | 0/1553 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DI | 0.38 | 0/1147 | 0.59 | 0/1553 |
| 39 | BN | 0.72 | 0/1132 | 0.90 | 1/1527 (0.1%) |
| 39 | DN | 0.57 | 0/1132 | 0.86 | 1/1527 (0.1%) |
| 40 | BO | 0.59 | 1/943 (0.1%) | 0.70 | 0/1269 |
| 40 | DO | 0.51 | 0/943 | 0.69 | 0/1269 |
| 41 | BP | 0.73 | 0/1131 | 1.07 | 9/1504 (0.6%) |
| 41 | DP | 0.64 | 0/1131 | 1.00 | 5/1504 (0.3%) |
| 42 | BQ | 0.69 | 0/1100 | 0.85 | 2/1470 (0.1%) |
| 42 | DQ | 0.61 | 0/1100 | 0.85 | 2/1470 (0.1%) |
| 43 | BR | 0.63 | 0/974 | 0.85 | 2/1302 (0.2%) |
| 43 | DR | 0.57 | 0/974 | 0.84 | 2/1302 (0.2%) |
| 44 | BS | 0.51 | 0/779 | 0.79 | 0/1038 |
| 44 | DS | 0.45 | 0/779 | 0.76 | 0/1038 |
| 45 | BT | 0.58 | 0/1114 | 0.86 | 1/1488 (0.1%) |
| 45 | DT | 0.55 | 0/1114 | 0.85 | 2/1488 (0.1%) |
| 46 | BU | 0.69 | 0/975 | 0.79 | 0/1297 |
| 46 | DU | 0.55 | 0/975 | 0.79 | 0/1297 |
| 47 | BV | 0.75 | 0/790 | 0.97 | 1/1057 (0.1%) |
| 47 | DV | 0.60 | 0/790 | 0.92 | 1/1057 (0.1%) |
| 48 | BW | 0.69 | 0/907 | 0.85 | 2/1216 (0.2%) |
| 48 | DW | 0.60 | 0/907 | 0.82 | 2/1216 (0.2%) |
| 49 | BX | 0.74 | 0/740 | 0.97 | 2/995 (0.2%) |
| 49 | DX | 0.65 | 0/740 | 0.96 | 1/995 (0.1%) |
| 50 | BY | 0.67 | 0/789 | 0.86 | 0/1053 |
| 50 | DY | 0.56 | 0/789 | 0.81 | 0/1053 |
| 51 | BZ | 0.45 | 0/1436 | 0.64 | 1/1951 (0.1%) |
| 51 | DZ | 0.40 | 0/1436 | 0.63 | 1/1951 (0.1%) |
| All | All | 0.74 | 108/301002 (0.0%) | 1.11 | 2093/449818 (0.5%) |

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 |
|-----|-------|---------------------|---------------------|
| 23 | B1 | 0 | 1 |
| 23 | D1 | 0 | 1 |
| 27 | B5 | 0 | 1 |
| 27 | D5 | 0 | 1 |
| 30 | B8 | 0 | 1 |
| 30 | D8 | 0 | 1 |
| 31 | BA | 21 | 0 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 31 | DA | 21 | 0 |
| 33 | BD | 0 | 2 |
| 33 | DD | 0 | 2 |
| 34 | BE | 0 | 2 |
| 34 | DE | 0 | 2 |
| 37 | BH | 0 | 2 |
| 37 | DH | 0 | 2 |
| 41 | BP | 0 | 5 |
| 41 | DP | 0 | 3 |
| 42 | BQ | 0 | 1 |
| 42 | DQ | 0 | 1 |
| 43 | BR | 0 | 2 |
| 43 | DR | 0 | 2 |
| 44 | BS | 0 | 1 |
| 44 | DS | 0 | 1 |
| 45 | BT | 0 | 1 |
| 45 | DT | 0 | 1 |
| 46 | BU | 0 | 1 |
| 46 | DU | 0 | 1 |
| 47 | BV | 0 | 1 |
| 47 | DV | 0 | 1 |
| 49 | BX | 0 | 5 |
| 49 | DX | 0 | 5 |
| All | All | 42 | 50 |

All (108) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|--------|-------------|----------|
| 31 | BA | 783 | A | N9-C4 | -14.89 | 1.28 | 1.37 |
| 31 | BA | 783 | A | N3-C4 | -11.41 | 1.28 | 1.34 |
| 31 | BA | 669 | G | C4'-C3' | -11.35 | 1.40 | 1.53 |
| 31 | BA | 1300 | U | C4'-C3' | -10.54 | 1.41 | 1.53 |
| 31 | DA | 783 | A | N9-C4 | -10.54 | 1.31 | 1.37 |
| 31 | BA | 2346 | A | N3-C4 | -10.28 | 1.28 | 1.34 |
| 31 | DA | 669 | G | C4'-C3' | -10.22 | 1.42 | 1.53 |
| 31 | DA | 1300 | U | C4'-C3' | -9.59 | 1.42 | 1.53 |
| 31 | BA | 1142(A) | A | N9-C4 | -9.49 | 1.32 | 1.37 |
| 31 | BA | 1332 | G | N9-C4 | -9.28 | 1.30 | 1.38 |
| 31 | BA | 1694 | C | C4'-C3' | -9.14 | 1.43 | 1.53 |
| 31 | BA | 1021 | A | N9-C4 | -8.87 | 1.32 | 1.37 |
| 31 | DA | 1694 | C | C4'-C3' | -8.81 | 1.43 | 1.53 |
| 31 | BA | 2346 | A | N9-C4 | -8.70 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 31 | DA | 1142(A) | A | N9-C4 | -8.70 | 1.32 | 1.37 |
| 31 | BA | 774 | A | N9-C4 | -8.33 | 1.32 | 1.37 |
| 31 | BA | 330 | A | N9-C4 | -8.19 | 1.32 | 1.37 |
| 31 | DA | 2346 | A | N3-C4 | -7.91 | 1.30 | 1.34 |
| 31 | DA | 2346 | A | N9-C4 | -7.85 | 1.33 | 1.37 |
| 31 | DA | 1332 | G | N9-C4 | -7.82 | 1.31 | 1.38 |
| 31 | BA | 676 | A | N9-C4 | -7.75 | 1.33 | 1.37 |
| 31 | BA | 1786 | A | N9-C4 | -7.68 | 1.33 | 1.37 |
| 31 | BA | 933 | A | N9-C4 | -7.66 | 1.33 | 1.37 |
| 31 | DA | 2430 | A | N9-C4 | -7.58 | 1.33 | 1.37 |
| 31 | DA | 1021 | A | N9-C4 | -7.37 | 1.33 | 1.37 |
| 31 | BA | 2430 | A | N9-C4 | -7.34 | 1.33 | 1.37 |
| 31 | BA | 2713 | A | N9-C4 | -7.31 | 1.33 | 1.37 |
| 31 | BA | 1674 | G | N7-C5 | -7.28 | 1.34 | 1.39 |
| 31 | BA | 783 | A | N7-C5 | -7.26 | 1.34 | 1.39 |
| 31 | BA | 2518 | A | N9-C4 | -7.05 | 1.33 | 1.37 |
| 31 | DA | 528 | A | N9-C4 | -6.91 | 1.33 | 1.37 |
| 31 | DA | 774 | A | N9-C4 | -6.85 | 1.33 | 1.37 |
| 31 | BA | 652 | C | O3'-P | 6.61 | 1.69 | 1.61 |
| 31 | BA | 945 | A | N9-C4 | -6.56 | 1.33 | 1.37 |
| 31 | BA | 1332 | G | N9-C8 | 6.53 | 1.42 | 1.37 |
| 31 | BA | 528 | A | N9-C4 | -6.49 | 1.33 | 1.37 |
| 31 | DA | 652 | C | O3'-P | 6.41 | 1.68 | 1.61 |
| 31 | DA | 2518 | A | N9-C4 | -6.39 | 1.34 | 1.37 |
| 31 | BA | 1829 | A | N9-C4 | -6.39 | 1.34 | 1.37 |
| 31 | DA | 1786 | A | C5-C6 | -6.33 | 1.35 | 1.41 |
| 31 | BA | 945 | A | N3-C4 | -6.30 | 1.31 | 1.34 |
| 31 | DA | 2287 | A | N9-C4 | -6.27 | 1.34 | 1.37 |
| 31 | BA | 2392 | A | N9-C4 | -6.26 | 1.34 | 1.37 |
| 31 | BA | 1204 | A | C5-C6 | -6.26 | 1.35 | 1.41 |
| 31 | BA | 1616 | A | N9-C4 | -6.19 | 1.34 | 1.37 |
| 31 | DA | 2587 | A | N7-C5 | -6.16 | 1.35 | 1.39 |
| 31 | BA | 1762 | A | N9-C4 | 6.09 | 1.41 | 1.37 |
| 31 | DA | 1786 | A | N9-C4 | -6.07 | 1.34 | 1.37 |
| 31 | DA | 783 | A | N3-C4 | -6.07 | 1.31 | 1.34 |
| 31 | BA | 1021 | A | N7-C5 | -6.05 | 1.35 | 1.39 |
| 31 | BA | 2287 | A | N9-C4 | -6.01 | 1.34 | 1.37 |
| 31 | DA | 2821 | A | N9-C4 | -5.93 | 1.34 | 1.37 |
| 31 | DA | 1021 | A | N7-C5 | -5.92 | 1.35 | 1.39 |
| 31 | BA | 652 | C | C3'-O3' | 5.92 | 1.50 | 1.42 |
| 31 | BA | 933 | A | N3-C4 | -5.87 | 1.31 | 1.34 |
| 31 | DA | 1899 | G | N9-C4 | -5.84 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 31 | BA | 2430 | A | C5-C6 | -5.75 | 1.35 | 1.41 |
| 31 | BA | 1332 | G | N3-C4 | -5.74 | 1.31 | 1.35 |
| 31 | BA | 783 | A | C5-C6 | -5.74 | 1.35 | 1.41 |
| 31 | BA | 2346 | A | N7-C5 | -5.73 | 1.35 | 1.39 |
| 31 | DA | 2014 | A | N9-C4 | -5.63 | 1.34 | 1.37 |
| 31 | DA | 652 | C | C3'-O3' | 5.61 | 1.50 | 1.42 |
| 31 | BA | 527 | C | N3-C4 | -5.53 | 1.30 | 1.33 |
| 31 | BA | 585 | G | N7-C5 | -5.52 | 1.35 | 1.39 |
| 31 | DA | 652 | C | P-O5' | 5.50 | 1.65 | 1.59 |
| 31 | BA | 652 | C | P-O5' | 5.49 | 1.65 | 1.59 |
| 31 | BA | 2061 | G | N1-C2 | -5.42 | 1.33 | 1.37 |
| 31 | BA | 330 | A | N3-C4 | -5.41 | 1.31 | 1.34 |
| 31 | BA | 579 | G | C2-N3 | -5.41 | 1.28 | 1.32 |
| 31 | BA | 1802 | A | N7-C5 | -5.39 | 1.36 | 1.39 |
| 31 | BA | 1142(A) | A | N3-C4 | -5.37 | 1.31 | 1.34 |
| 40 | BO | 21 | CYS | CB-SG | -5.36 | 1.73 | 1.81 |
| 31 | DA | 2252 | G | N3-C4 | -5.34 | 1.31 | 1.35 |
| 31 | DA | 1681 | G | N9-C4 | -5.33 | 1.33 | 1.38 |
| 31 | DA | 1786 | A | N7-C5 | -5.30 | 1.36 | 1.39 |
| 31 | DA | 272 | G | N9-C4 | 5.30 | 1.42 | 1.38 |
| 31 | DA | 1829 | A | N9-C4 | -5.30 | 1.34 | 1.37 |
| 31 | BA | 2542 | A | C5-C6 | -5.29 | 1.36 | 1.41 |
| 31 | BA | 71 | A | N9-C4 | -5.28 | 1.34 | 1.37 |
| 31 | BA | 1332 | G | C5-C6 | -5.27 | 1.37 | 1.42 |
| 31 | BA | 788 | A | N7-C5 | -5.26 | 1.36 | 1.39 |
| 31 | BA | 1139 | G | N7-C5 | -5.25 | 1.36 | 1.39 |
| 31 | BA | 2432 | A | C5-C6 | -5.23 | 1.36 | 1.41 |
| 31 | BA | 2711 | A | N9-C4 | -5.22 | 1.34 | 1.37 |
| 31 | DA | 1269 | A | N9-C4 | -5.20 | 1.34 | 1.37 |
| 31 | BA | 2430 | A | N7-C5 | -5.20 | 1.36 | 1.39 |
| 31 | DA | 656 | G | P-O5' | 5.19 | 1.65 | 1.59 |
| 31 | DA | 2476 | A | N9-C4 | 5.18 | 1.41 | 1.37 |
| 31 | DA | 783 | A | C5-C6 | -5.17 | 1.36 | 1.41 |
| 31 | BA | 470 | A | N9-C4 | -5.16 | 1.34 | 1.37 |
| 35 | BF | 65 | TRP | CB-CG | -5.16 | 1.41 | 1.50 |
| 31 | BA | 197 | A | N9-C4 | -5.14 | 1.34 | 1.37 |
| 31 | BA | 950 | G | C6-N1 | -5.13 | 1.35 | 1.39 |
| 31 | BA | 2014 | A | C5-C6 | -5.13 | 1.36 | 1.41 |
| 31 | BA | 1899 | G | N9-C4 | -5.11 | 1.33 | 1.38 |
| 31 | BA | 774 | A | N3-C4 | -5.11 | 1.31 | 1.34 |
| 31 | DA | 1762 | A | N9-C4 | 5.11 | 1.41 | 1.37 |
| 31 | BA | 971 | C | N1-C6 | -5.07 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 31 | BA | 651 | G | N9-C4 | 5.07 | 1.42 | 1.38 |
| 31 | DA | 330 | A | N9-C4 | -5.06 | 1.34 | 1.37 |
| 31 | BA | 71 | A | C5-C6 | -5.06 | 1.36 | 1.41 |
| 31 | BA | 2436 | G | N3-C4 | -5.06 | 1.31 | 1.35 |
| 31 | BA | 1624 | G | C5-C4 | -5.04 | 1.34 | 1.38 |
| 31 | BA | 1162 | G | N9-C8 | -5.04 | 1.34 | 1.37 |
| 31 | DA | 528 | A | N3-C4 | -5.03 | 1.31 | 1.34 |
| 31 | DA | 945 | A | C5-C6 | -5.03 | 1.36 | 1.41 |
| 31 | BA | 1786 | A | N3-C4 | -5.01 | 1.31 | 1.34 |
| 31 | DA | 945 | A | N7-C5 | -5.01 | 1.36 | 1.39 |

All (2093) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|--------|-------------|----------|
| 31 | BA | 1332 | G | N3-C4-C5 | 21.05 | 139.12 | 128.60 |
| 31 | BA | 1332 | G | N3-C4-N9 | -19.19 | 114.49 | 126.00 |
| 31 | DA | 1779 | U | C5-C6-N1 | -16.63 | 114.39 | 122.70 |
| 31 | BA | 1332 | G | C2-N3-C4 | -16.06 | 103.87 | 111.90 |
| 31 | BA | 1779 | U | C5-C6-N1 | -15.89 | 114.75 | 122.70 |
| 31 | DA | 1332 | G | N3-C4-C5 | 15.36 | 136.28 | 128.60 |
| 31 | DA | 1332 | G | N3-C4-N9 | -15.10 | 116.94 | 126.00 |
| 31 | DA | 1899 | G | N3-C4-N9 | -14.36 | 117.38 | 126.00 |
| 31 | BA | 2346 | A | C2-N3-C4 | -14.16 | 103.52 | 110.60 |
| 31 | BA | 1142(A) | A | C2-N3-C4 | -13.17 | 104.02 | 110.60 |
| 31 | BA | 1678 | G | C4-C5-N7 | 13.17 | 116.07 | 110.80 |
| 31 | BA | 1899 | G | N3-C4-N9 | -13.15 | 118.11 | 126.00 |
| 31 | BA | 945 | A | N1-C6-N6 | 13.15 | 126.49 | 118.60 |
| 31 | BA | 2518 | A | C5-N7-C8 | -12.98 | 97.41 | 103.90 |
| 31 | BA | 1204 | A | C2-N3-C4 | -12.66 | 104.27 | 110.60 |
| 31 | BA | 783 | A | C2-N3-C4 | -12.47 | 104.36 | 110.60 |
| 31 | BA | 1616 | A | C5-N7-C8 | -12.43 | 97.69 | 103.90 |
| 32 | BB | 81 | G | C4-C5-N7 | 12.31 | 115.72 | 110.80 |
| 31 | BA | 676 | A | C2-N3-C4 | -12.21 | 104.49 | 110.60 |
| 31 | BA | 1678 | G | C5-N7-C8 | -12.19 | 98.20 | 104.30 |
| 31 | DA | 1786 | A | C5-N7-C8 | -12.15 | 97.82 | 103.90 |
| 31 | DA | 2430 | A | C2-N3-C4 | -12.11 | 104.54 | 110.60 |
| 31 | DA | 2346 | A | C2-N3-C4 | -12.10 | 104.55 | 110.60 |
| 31 | BA | 1022 | G | C8-N9-C4 | -12.03 | 101.59 | 106.40 |
| 31 | DA | 2828 | C | C6-N1-C2 | 11.88 | 125.05 | 120.30 |
| 31 | DA | 1899 | G | C8-N9-C1' | 11.61 | 142.09 | 127.00 |
| 31 | BA | 1899 | G | C8-N9-C1' | 11.59 | 142.07 | 127.00 |
| 31 | BA | 1616 | A | N7-C8-N9 | 11.53 | 119.57 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 31 | DA | 783 | A | C5-N7-C8 | -11.53 | 98.14 | 103.90 |
| 31 | BA | 1678 | G | C6-C5-N7 | -11.48 | 123.51 | 130.40 |
| 32 | BB | 81 | G | C6-C5-N7 | -11.46 | 123.52 | 130.40 |
| 31 | DA | 1678 | G | C6-C5-N7 | -11.46 | 123.52 | 130.40 |
| 31 | BA | 2346 | A | N1-C2-N3 | 11.39 | 135.00 | 129.30 |
| 31 | DA | 1786 | A | N1-C6-N6 | 11.35 | 125.41 | 118.60 |
| 31 | DA | 1207 | C | C6-N1-C2 | 11.28 | 124.81 | 120.30 |
| 31 | BA | 141 | A | N1-C6-N6 | 11.26 | 125.36 | 118.60 |
| 31 | DA | 945 | A | N1-C6-N6 | 11.15 | 125.29 | 118.60 |
| 31 | BA | 2713 | A | C5-N7-C8 | -11.12 | 98.34 | 103.90 |
| 31 | BA | 2287 | A | C2-N3-C4 | -11.11 | 105.04 | 110.60 |
| 31 | DA | 783 | A | C2-N3-C4 | -11.11 | 105.04 | 110.60 |
| 31 | BA | 330 | A | C2-N3-C4 | -11.10 | 105.05 | 110.60 |
| 31 | BA | 1332 | G | C5-N7-C8 | -11.09 | 98.76 | 104.30 |
| 31 | BA | 1022 | G | N9-C4-C5 | 11.06 | 109.83 | 105.40 |
| 32 | DB | 81 | G | C4-N9-C1' | 10.96 | 140.75 | 126.50 |
| 31 | DA | 1678 | G | C5-N7-C8 | -10.94 | 98.83 | 104.30 |
| 31 | BA | 409 | C | C6-N1-C2 | 10.93 | 124.67 | 120.30 |
| 31 | BA | 1899 | G | C4-N9-C1' | -10.92 | 112.30 | 126.50 |
| 31 | BA | 1786 | A | C2-N3-C4 | -10.88 | 105.16 | 110.60 |
| 32 | DB | 81 | G | C6-C5-N7 | -10.87 | 123.88 | 130.40 |
| 31 | DA | 1899 | G | C4-N9-C1' | -10.79 | 112.48 | 126.50 |
| 32 | BB | 81 | G | C4-N9-C1' | 10.78 | 140.51 | 126.50 |
| 31 | DA | 1779 | U | C2-N1-C1' | -10.74 | 104.81 | 117.70 |
| 31 | DA | 1021 | A | C2-N3-C4 | -10.69 | 105.25 | 110.60 |
| 31 | BA | 1779 | U | C2-N1-C1' | -10.69 | 104.88 | 117.70 |
| 31 | DA | 1786 | A | C4-C5-N7 | 10.68 | 116.04 | 110.70 |
| 31 | DA | 1678 | G | C4-C5-N7 | 10.64 | 115.06 | 110.80 |
| 31 | BA | 1204 | A | C6-C5-N7 | -10.56 | 124.91 | 132.30 |
| 31 | BA | 530 | G | N3-C4-N9 | -10.54 | 119.68 | 126.00 |
| 31 | DA | 1022 | G | C8-N9-C4 | -10.51 | 102.20 | 106.40 |
| 31 | BA | 2346 | A | C5-C6-N1 | -10.48 | 112.46 | 117.70 |
| 31 | BA | 783 | A | N1-C6-N6 | 10.44 | 124.87 | 118.60 |
| 31 | BA | 2430 | A | N1-C6-N6 | 10.44 | 124.86 | 118.60 |
| 31 | BA | 1021 | A | C2-N3-C4 | -10.40 | 105.40 | 110.60 |
| 31 | BA | 945 | A | C2-N3-C4 | -10.35 | 105.43 | 110.60 |
| 31 | BA | 1786 | A | C5-N7-C8 | -10.32 | 98.74 | 103.90 |
| 31 | BA | 2518 | A | C4-C5-N7 | 10.27 | 115.83 | 110.70 |
| 31 | DA | 2542 | A | N1-C6-N6 | 10.22 | 124.73 | 118.60 |
| 31 | DA | 130 | C | C6-N1-C2 | 10.21 | 124.39 | 120.30 |
| 31 | BA | 2544 | G | N1-C6-O6 | 10.19 | 126.01 | 119.90 |
| 32 | DB | 81 | G | C4-C5-N7 | 10.18 | 114.87 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|--------|-------------|----------|
| 31 | BA | 528 | A | C2-N3-C4 | -10.17 | 105.51 | 110.60 |
| 31 | DA | 1142(A) | A | C2-N3-C4 | -10.14 | 105.53 | 110.60 |
| 31 | BA | 783 | A | C5-N7-C8 | -10.09 | 98.86 | 103.90 |
| 31 | BA | 1678 | G | C2-N3-C4 | -10.08 | 106.86 | 111.90 |
| 31 | BA | 1241 | A | C2-N3-C4 | -10.07 | 105.57 | 110.60 |
| 31 | BA | 2430 | A | C2-N3-C4 | -10.06 | 105.57 | 110.60 |
| 31 | DA | 676 | A | C5-N7-C8 | -10.05 | 98.87 | 103.90 |
| 31 | DA | 2742 | C | C6-N1-C2 | 10.01 | 124.31 | 120.30 |
| 31 | BA | 1678 | G | N7-C8-N9 | 10.01 | 118.10 | 113.10 |
| 31 | DA | 1899 | G | N3-C4-C5 | 10.00 | 133.60 | 128.60 |
| 31 | DA | 783 | A | N1-C6-N6 | 9.99 | 124.59 | 118.60 |
| 32 | DB | 81 | G | C8-N9-C1' | -9.96 | 114.05 | 127.00 |
| 31 | DA | 566 | U | C5-C6-N1 | -9.89 | 117.75 | 122.70 |
| 31 | BA | 272 | G | N3-C4-C5 | -9.88 | 123.66 | 128.60 |
| 31 | DA | 2231 | C | C5-C6-N1 | -9.81 | 116.10 | 121.00 |
| 31 | BA | 1397 | U | N3-C2-O2 | -9.79 | 115.35 | 122.20 |
| 31 | BA | 1779 | U | C5-C4-O4 | 9.78 | 131.77 | 125.90 |
| 31 | BA | 2392 | A | C2-N3-C4 | -9.75 | 105.73 | 110.60 |
| 31 | DA | 1332 | G | C2-N3-C4 | -9.73 | 107.03 | 111.90 |
| 31 | BA | 1543 | C | C5-C6-N1 | 9.72 | 125.86 | 121.00 |
| 31 | BA | 676 | A | C5-N7-C8 | -9.69 | 99.06 | 103.90 |
| 31 | DA | 1698 | A | N1-C6-N6 | 9.68 | 124.41 | 118.60 |
| 31 | BA | 933 | A | C5-N7-C8 | -9.66 | 99.07 | 103.90 |
| 32 | BB | 81 | G | C8-N9-C1' | -9.65 | 114.45 | 127.00 |
| 31 | DA | 678 | C | C6-N1-C2 | 9.65 | 124.16 | 120.30 |
| 31 | DA | 1678 | G | N7-C8-N9 | 9.64 | 117.92 | 113.10 |
| 31 | DA | 1698 | A | C2-N3-C4 | -9.63 | 105.79 | 110.60 |
| 31 | BA | 130 | C | C6-N1-C2 | 9.62 | 124.15 | 120.30 |
| 31 | DA | 2346 | A | C5-C6-N1 | -9.58 | 112.91 | 117.70 |
| 31 | DA | 1962 | C | O4'-C1'-N1 | 9.56 | 115.85 | 108.20 |
| 31 | BA | 621 | A | C5-N7-C8 | -9.50 | 99.15 | 103.90 |
| 31 | DA | 783 | A | C4-C5-N7 | 9.47 | 115.44 | 110.70 |
| 31 | DA | 1204 | A | C2-N3-C4 | -9.47 | 105.87 | 110.60 |
| 31 | BA | 2713 | A | C2-N3-C4 | -9.45 | 105.87 | 110.60 |
| 31 | DA | 2518 | A | N1-C6-N6 | 9.44 | 124.27 | 118.60 |
| 31 | DA | 1204 | A | C6-C5-N7 | -9.40 | 125.72 | 132.30 |
| 31 | DA | 774 | A | C5-N7-C8 | -9.39 | 99.21 | 103.90 |
| 31 | DA | 2287 | A | C2-N3-C4 | -9.37 | 105.92 | 110.60 |
| 31 | BA | 446 | G | C5-C6-O6 | -9.36 | 122.98 | 128.60 |
| 31 | BA | 201 | C | N3-C4-C5 | 9.36 | 125.64 | 121.90 |
| 31 | DA | 1786 | A | C6-C5-N7 | -9.35 | 125.75 | 132.30 |
| 31 | BA | 1698 | A | C2-N3-C4 | -9.30 | 105.95 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 31 | BA | 71 | A | C5-N7-C8 | -9.29 | 99.25 | 103.90 |
| 31 | BA | 1616 | A | C8-N9-C4 | -9.26 | 102.10 | 105.80 |
| 31 | DA | 2231 | C | C6-N1-C2 | 9.24 | 124.00 | 120.30 |
| 31 | BA | 1899 | G | N3-C4-C5 | 9.19 | 133.20 | 128.60 |
| 31 | BA | 678 | C | C6-N1-C2 | 9.16 | 123.97 | 120.30 |
| 31 | DA | 2518 | A | C5-N7-C8 | -9.15 | 99.32 | 103.90 |
| 31 | BA | 2346 | A | C6-C5-N7 | -9.15 | 125.89 | 132.30 |
| 31 | DA | 141 | A | N1-C6-N6 | 9.15 | 124.09 | 118.60 |
| 31 | BA | 2713 | A | N1-C6-N6 | 9.13 | 124.08 | 118.60 |
| 31 | BA | 1142(A) | A | C5-C6-N1 | -9.12 | 113.14 | 117.70 |
| 31 | DA | 1786 | A | N7-C8-N9 | 9.11 | 118.36 | 113.80 |
| 32 | BB | 81 | G | C5-N7-C8 | -9.11 | 99.75 | 104.30 |
| 31 | DA | 1204 | A | N1-C6-N6 | 9.11 | 124.06 | 118.60 |
| 31 | DA | 1332 | G | C5-N7-C8 | -9.11 | 99.75 | 104.30 |
| 31 | BA | 945 | A | N1-C2-N3 | 9.10 | 133.85 | 129.30 |
| 31 | BA | 774 | A | C5-N7-C8 | -9.07 | 99.36 | 103.90 |
| 31 | DA | 2512 | C | C6-N1-C2 | 9.06 | 123.92 | 120.30 |
| 31 | DA | 1698 | A | C4-C5-N7 | 9.05 | 115.22 | 110.70 |
| 31 | DA | 1899 | G | N9-C4-C5 | 9.04 | 109.01 | 105.40 |
| 31 | BA | 1204 | A | N1-C6-N6 | 9.02 | 124.01 | 118.60 |
| 31 | DA | 330 | A | N9-C4-C5 | -9.00 | 102.20 | 105.80 |
| 31 | BA | 528 | A | C5-N7-C8 | -8.97 | 99.42 | 103.90 |
| 31 | DA | 179 | G | C8-N9-C4 | 8.95 | 109.98 | 106.40 |
| 31 | DA | 1829 | A | C8-N9-C4 | 8.92 | 109.37 | 105.80 |
| 31 | DA | 451 | C | C6-N1-C2 | 8.89 | 123.86 | 120.30 |
| 31 | BA | 1207 | C | C6-N1-C2 | 8.89 | 123.86 | 120.30 |
| 1 | CA | 117 | G | N1-C6-O6 | 8.87 | 125.22 | 119.90 |
| 31 | BA | 2392 | A | C5-N7-C8 | -8.85 | 99.47 | 103.90 |
| 31 | DA | 409 | C | C6-N1-C2 | 8.84 | 123.83 | 120.30 |
| 31 | DA | 2544 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |
| 31 | BA | 1021 | A | C5-N7-C8 | -8.81 | 99.50 | 103.90 |
| 31 | DA | 1241 | A | C2-N3-C4 | -8.79 | 106.21 | 110.60 |
| 31 | DA | 1022 | G | N9-C4-C5 | 8.78 | 108.91 | 105.40 |
| 31 | BA | 856 | C | C6-N1-C2 | -8.76 | 116.80 | 120.30 |
| 31 | BA | 1962 | C | O4'-C1'-N1 | 8.75 | 115.20 | 108.20 |
| 31 | DA | 133 | C | C5-C6-N1 | -8.75 | 116.62 | 121.00 |
| 31 | DA | 330 | A | C4-C5-N7 | 8.75 | 115.08 | 110.70 |
| 31 | DA | 530 | G | N3-C4-N9 | -8.73 | 120.76 | 126.00 |
| 31 | BA | 446 | G | N1-C6-O6 | 8.73 | 125.14 | 119.90 |
| 31 | BA | 2346 | A | C5-N7-C8 | -8.70 | 99.55 | 103.90 |
| 31 | BA | 2422 | A | C8-N9-C4 | -8.68 | 102.33 | 105.80 |
| 31 | DA | 1786 | A | C2-N3-C4 | -8.68 | 106.26 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 31 | DA | 1204 | A | C5-N7-C8 | -8.66 | 99.57 | 103.90 |
| 31 | BA | 141 | A | C6-C5-N7 | -8.66 | 126.24 | 132.30 |
| 31 | BA | 856 | C | C2-N1-C1' | 8.65 | 128.31 | 118.80 |
| 31 | DA | 1373 | A | C8-N9-C4 | 8.64 | 109.26 | 105.80 |
| 31 | BA | 786 | C | C5-C6-N1 | -8.64 | 116.68 | 121.00 |
| 31 | DA | 71 | A | C5-N7-C8 | -8.63 | 99.59 | 103.90 |
| 31 | BA | 1786 | A | C6-C5-N7 | -8.60 | 126.28 | 132.30 |
| 31 | DA | 1698 | A | C5-N7-C8 | -8.60 | 99.60 | 103.90 |
| 31 | DA | 1663 | C | C2-N3-C4 | -8.58 | 115.61 | 119.90 |
| 31 | BA | 1332 | G | C4-C5-N7 | 8.58 | 114.23 | 110.80 |
| 31 | DA | 676 | A | N1-C6-N6 | 8.57 | 123.74 | 118.60 |
| 31 | DA | 1123 | C | C6-N1-C2 | 8.57 | 123.73 | 120.30 |
| 31 | BA | 845 | G | N7-C8-N9 | 8.56 | 117.38 | 113.10 |
| 31 | DA | 1698 | A | C6-C5-N7 | -8.54 | 126.32 | 132.30 |
| 31 | BA | 1332 | G | C5-C6-N1 | -8.54 | 107.23 | 111.50 |
| 31 | DA | 928 | G | N1-C6-O6 | 8.54 | 125.02 | 119.90 |
| 31 | BA | 2230 | G | N1-C6-O6 | 8.52 | 125.01 | 119.90 |
| 31 | DA | 2346 | A | N1-C2-N3 | 8.51 | 133.56 | 129.30 |
| 31 | BA | 1204 | A | C5-N7-C8 | -8.51 | 99.65 | 103.90 |
| 31 | DA | 376 | C | C6-N1-C2 | 8.51 | 123.70 | 120.30 |
| 31 | DA | 2463 | C | C6-N1-C2 | 8.50 | 123.70 | 120.30 |
| 31 | BA | 1022 | G | N3-C4-C5 | -8.50 | 124.35 | 128.60 |
| 31 | DA | 566 | U | C6-N1-C2 | 8.50 | 126.10 | 121.00 |
| 31 | DA | 1779 | U | C2-N3-C4 | -8.48 | 121.91 | 127.00 |
| 31 | DA | 2330 | G | C8-N9-C4 | 8.47 | 109.79 | 106.40 |
| 31 | BA | 2518 | A | N7-C8-N9 | 8.46 | 118.03 | 113.80 |
| 31 | BA | 2287 | A | N1-C2-N3 | 8.46 | 133.53 | 129.30 |
| 31 | BA | 828 | U | C5-C4-O4 | 8.46 | 130.98 | 125.90 |
| 31 | DA | 933 | A | C5-N7-C8 | -8.43 | 99.69 | 103.90 |
| 31 | BA | 2542 | A | N1-C6-N6 | 8.42 | 123.65 | 118.60 |
| 31 | BA | 142 | A | N1-C6-N6 | 8.42 | 123.65 | 118.60 |
| 31 | BA | 1779 | U | N3-C4-O4 | -8.42 | 113.51 | 119.40 |
| 31 | DA | 528 | A | C2-N3-C4 | -8.41 | 106.39 | 110.60 |
| 31 | DA | 2742 | C | C5-C6-N1 | -8.41 | 116.80 | 121.00 |
| 31 | BA | 1332 | G | C6-N1-C2 | 8.39 | 130.14 | 125.10 |
| 31 | BA | 100 | G | O4'-C1'-N9 | 8.38 | 114.91 | 108.20 |
| 31 | BA | 1694 | C | C2-N1-C1' | 8.38 | 128.02 | 118.80 |
| 31 | DA | 1616 | A | C5-N7-C8 | -8.38 | 99.71 | 103.90 |
| 31 | DA | 676 | A | C2-N3-C4 | -8.37 | 106.42 | 110.60 |
| 31 | DA | 933 | A | C2-N3-C4 | -8.37 | 106.41 | 110.60 |
| 31 | BA | 945 | A | C6-C5-N7 | -8.37 | 126.44 | 132.30 |
| 31 | BA | 1786 | A | N1-C6-N6 | 8.37 | 123.62 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 31 | BA | 621 | A | N7-C8-N9 | 8.36 | 117.98 | 113.80 |
| 31 | BA | 2392 | A | N1-C6-N6 | 8.35 | 123.61 | 118.60 |
| 31 | DA | 1543 | C | C5-C6-N1 | 8.34 | 125.17 | 121.00 |
| 31 | DA | 577 | G | C8-N9-C4 | 8.32 | 109.73 | 106.40 |
| 31 | DA | 100 | G | O4'-C1'-N9 | 8.31 | 114.85 | 108.20 |
| 31 | DA | 2346 | A | N7-C8-N9 | 8.30 | 117.95 | 113.80 |
| 31 | BA | 2518 | A | N1-C6-N6 | 8.30 | 123.58 | 118.60 |
| 32 | DB | 115 | G | C8-N9-C4 | 8.27 | 109.71 | 106.40 |
| 31 | BA | 1616 | A | C4-C5-N7 | 8.27 | 114.83 | 110.70 |
| 31 | DA | 71 | A | N1-C6-N6 | 8.27 | 123.56 | 118.60 |
| 31 | DA | 1261 | C | N3-C4-C5 | 8.27 | 125.21 | 121.90 |
| 31 | DA | 2544 | G | C5-C6-O6 | -8.27 | 123.64 | 128.60 |
| 31 | BA | 62 | C | C6-N1-C2 | 8.26 | 123.61 | 120.30 |
| 31 | BA | 564 | C | N1-C2-O2 | -8.26 | 113.94 | 118.90 |
| 31 | DA | 1333 | C | N3-C4-C5 | 8.25 | 125.20 | 121.90 |
| 31 | BA | 1899 | G | N9-C4-C5 | 8.24 | 108.70 | 105.40 |
| 31 | BA | 774 | A | N7-C8-N9 | 8.23 | 117.92 | 113.80 |
| 31 | DA | 133 | C | C2-N3-C4 | -8.23 | 115.78 | 119.90 |
| 31 | DA | 945 | A | C2-N3-C4 | -8.23 | 106.49 | 110.60 |
| 31 | DA | 272 | G | N3-C4-C5 | -8.22 | 124.49 | 128.60 |
| 31 | BA | 1204 | A | N1-C2-N3 | 8.21 | 133.41 | 129.30 |
| 31 | DA | 1694 | C | C2-N1-C1' | 8.21 | 127.83 | 118.80 |
| 31 | BA | 1786 | A | N7-C8-N9 | 8.21 | 117.90 | 113.80 |
| 31 | DA | 1123 | C | C2-N3-C4 | -8.19 | 115.80 | 119.90 |
| 31 | DA | 1204 | A | N7-C8-N9 | 8.18 | 117.89 | 113.80 |
| 31 | DA | 272(B) | G | N1-C6-O6 | -8.17 | 115.00 | 119.90 |
| 31 | BA | 2084 | C | C5-C6-N1 | -8.16 | 116.92 | 121.00 |
| 31 | DA | 1678 | G | C4-N9-C1' | 8.16 | 137.11 | 126.50 |
| 32 | BB | 81 | G | N7-C8-N9 | 8.16 | 117.18 | 113.10 |
| 31 | BA | 1694 | C | C5-C6-N1 | 8.15 | 125.08 | 121.00 |
| 31 | BA | 945 | A | C4-C5-C6 | 8.15 | 121.07 | 117.00 |
| 31 | DA | 2522 | U | C5-C6-N1 | -8.14 | 118.63 | 122.70 |
| 31 | BA | 1142(A) | A | N3-C4-C5 | 8.13 | 132.49 | 126.80 |
| 31 | BA | 330 | A | C5-N7-C8 | -8.12 | 99.84 | 103.90 |
| 31 | DA | 465 | G | C8-N9-C4 | -8.11 | 103.16 | 106.40 |
| 31 | DA | 2713 | A | C5-N7-C8 | -8.11 | 99.85 | 103.90 |
| 31 | DA | 133 | C | C6-N1-C2 | 8.10 | 123.54 | 120.30 |
| 31 | BA | 1495 | A | N7-C8-N9 | 8.10 | 117.85 | 113.80 |
| 31 | BA | 2404 | C | C6-N1-C2 | 8.09 | 123.54 | 120.30 |
| 31 | BA | 1653 | G | N3-C4-C5 | -8.08 | 124.56 | 128.60 |
| 31 | BA | 2542 | A | C2-N3-C4 | -8.08 | 106.56 | 110.60 |
| 31 | BA | 814 | C | C6-N1-C2 | 8.07 | 123.53 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 41 | BP | 37 | GLY | N-CA-C | 8.07 | 133.28 | 113.10 |
| 31 | DA | 2512 | C | C5-C6-N1 | -8.07 | 116.97 | 121.00 |
| 31 | DA | 330 | A | N1-C6-N6 | 8.06 | 123.44 | 118.60 |
| 31 | BA | 845 | G | C5-N7-C8 | -8.06 | 100.27 | 104.30 |
| 31 | BA | 1495 | A | C8-N9-C4 | -8.05 | 102.58 | 105.80 |
| 31 | DA | 330 | A | C2-N3-C4 | -8.05 | 106.58 | 110.60 |
| 31 | BA | 226 | G | N1-C6-O6 | 8.04 | 124.72 | 119.90 |
| 31 | BA | 2346 | A | N7-C8-N9 | 8.02 | 117.81 | 113.80 |
| 31 | DA | 933 | A | N1-C6-N6 | 8.01 | 123.41 | 118.60 |
| 31 | BA | 676 | A | C4-C5-N7 | 8.01 | 114.70 | 110.70 |
| 31 | BA | 933 | A | C2-N3-C4 | -8.00 | 106.60 | 110.60 |
| 31 | BA | 141 | A | C5-N7-C8 | -7.99 | 99.90 | 103.90 |
| 31 | DA | 2346 | A | C5-N7-C8 | -7.98 | 99.91 | 103.90 |
| 31 | DA | 1616 | A | N7-C8-N9 | 7.98 | 117.79 | 113.80 |
| 31 | DA | 783 | A | N3-C4-C5 | 7.96 | 132.38 | 126.80 |
| 31 | DA | 2713 | A | N1-C6-N6 | 7.96 | 123.38 | 118.60 |
| 31 | BA | 676 | A | N3-C4-C5 | 7.96 | 132.37 | 126.80 |
| 31 | DA | 2622 | C | C6-N1-C2 | 7.95 | 123.48 | 120.30 |
| 31 | DA | 529 | A | N1-C6-N6 | 7.95 | 123.37 | 118.60 |
| 31 | DA | 2364 | C | C6-N1-C2 | 7.93 | 123.47 | 120.30 |
| 31 | BA | 1698 | A | N1-C6-N6 | 7.93 | 123.36 | 118.60 |
| 31 | BA | 1698 | A | C6-C5-N7 | -7.92 | 126.75 | 132.30 |
| 31 | BA | 2346 | A | C4-C5-C6 | 7.92 | 120.96 | 117.00 |
| 31 | DA | 201 | C | C6-N1-C2 | 7.91 | 123.46 | 120.30 |
| 31 | BA | 1762 | A | C8-N9-C4 | -7.90 | 102.64 | 105.80 |
| 31 | BA | 208 | C | C6-N1-C2 | 7.90 | 123.46 | 120.30 |
| 31 | DA | 856 | C | C2-N1-C1' | 7.89 | 127.48 | 118.80 |
| 31 | BA | 2476 | A | C2-N3-C4 | 7.89 | 114.55 | 110.60 |
| 31 | BA | 71 | A | C2-N3-C4 | -7.86 | 106.67 | 110.60 |
| 32 | DB | 81 | G | N3-C4-N9 | 7.86 | 130.71 | 126.00 |
| 31 | DA | 2542 | A | C5-N7-C8 | -7.84 | 99.98 | 103.90 |
| 31 | BA | 1204 | A | C4-C5-N7 | 7.84 | 114.62 | 110.70 |
| 31 | BA | 201 | C | C2-N3-C4 | -7.84 | 115.98 | 119.90 |
| 31 | DA | 945 | A | C6-C5-N7 | -7.83 | 126.82 | 132.30 |
| 31 | DA | 1653 | G | N3-C4-C5 | -7.83 | 124.69 | 128.60 |
| 31 | DA | 2518 | A | C4-C5-N7 | 7.82 | 114.61 | 110.70 |
| 31 | BA | 1829 | A | C8-N9-C4 | 7.81 | 108.92 | 105.80 |
| 31 | DA | 2392 | A | C2-N3-C4 | -7.81 | 106.69 | 110.60 |
| 31 | DA | 774 | A | C2-N3-C4 | -7.81 | 106.70 | 110.60 |
| 31 | BA | 2430 | A | C5-N7-C8 | -7.80 | 100.00 | 103.90 |
| 31 | BA | 71 | A | N1-C6-N6 | 7.80 | 123.28 | 118.60 |
| 31 | BA | 774 | A | C8-N9-C4 | -7.79 | 102.68 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 31 | BA | 71 | A | C4-C5-N7 | 7.79 | 114.59 | 110.70 |
| 1 | AA | 322 | C | C6-N1-C2 | 7.78 | 123.41 | 120.30 |
| 31 | BA | 2713 | A | C4-C5-N7 | 7.78 | 114.59 | 110.70 |
| 31 | BA | 1409 | C | C6-N1-C2 | 7.77 | 123.41 | 120.30 |
| 31 | DA | 1614 | A | N7-C8-N9 | 7.77 | 117.68 | 113.80 |
| 31 | BA | 2713 | A | N7-C8-N9 | 7.75 | 117.68 | 113.80 |
| 31 | BA | 783 | A | N3-C4-C5 | 7.72 | 132.21 | 126.80 |
| 31 | DA | 2741 | A | C8-N9-C4 | 7.72 | 108.89 | 105.80 |
| 31 | BA | 2711 | A | C8-N9-C4 | 7.71 | 108.89 | 105.80 |
| 31 | BA | 1774 | C | N1-C2-O2 | -7.71 | 114.27 | 118.90 |
| 31 | BA | 2552 | U | N1-C2-O2 | -7.71 | 117.41 | 122.80 |
| 31 | DA | 2042 | A | C8-N9-C4 | 7.68 | 108.87 | 105.80 |
| 31 | DA | 1558 | A | C2-N3-C4 | -7.67 | 106.77 | 110.60 |
| 31 | DA | 837 | C | C6-N1-C2 | -7.66 | 117.23 | 120.30 |
| 31 | BA | 1784 | A | C8-N9-C4 | 7.66 | 108.86 | 105.80 |
| 31 | DA | 676 | A | N7-C8-N9 | 7.66 | 117.63 | 113.80 |
| 31 | BA | 130 | C | C5-C6-N1 | -7.65 | 117.18 | 121.00 |
| 31 | BA | 2512 | C | C6-N1-C2 | 7.62 | 123.35 | 120.30 |
| 31 | DA | 2827 | C | C6-N1-C2 | 7.62 | 123.35 | 120.30 |
| 31 | BA | 528 | A | N3-C4-C5 | 7.62 | 132.13 | 126.80 |
| 31 | BA | 451 | C | C6-N1-C2 | 7.60 | 123.34 | 120.30 |
| 31 | BA | 1786 | A | C4-C5-N7 | 7.59 | 114.50 | 110.70 |
| 31 | BA | 847 | U | C2-N1-C1' | -7.58 | 108.61 | 117.70 |
| 31 | DA | 330 | A | C5-N7-C8 | -7.57 | 100.12 | 103.90 |
| 31 | DA | 1123 | C | C5-C6-N1 | -7.56 | 117.22 | 121.00 |
| 31 | DA | 2346 | A | C6-C5-N7 | -7.56 | 127.01 | 132.30 |
| 31 | DA | 1820 | U | C6-N1-C2 | 7.55 | 125.53 | 121.00 |
| 31 | DA | 1261 | C | C6-N1-C2 | 7.55 | 123.32 | 120.30 |
| 31 | DA | 207 | A | C8-N9-C4 | 7.55 | 108.82 | 105.80 |
| 31 | BA | 265 | A | C5-N7-C8 | -7.55 | 100.13 | 103.90 |
| 31 | DA | 1962 | C | N1-C1'-C2' | 7.55 | 123.81 | 114.00 |
| 31 | BA | 330 | A | N3-C4-C5 | 7.54 | 132.08 | 126.80 |
| 31 | BA | 1543 | C | N3-C2-O2 | 7.54 | 127.18 | 121.90 |
| 31 | BA | 1614 | A | C5-N7-C8 | -7.54 | 100.13 | 103.90 |
| 31 | DA | 1820 | U | C5-C6-N1 | -7.54 | 118.93 | 122.70 |
| 31 | BA | 1698 | A | C4-C5-N7 | 7.53 | 114.47 | 110.70 |
| 31 | DA | 2253 | G | C5-C6-O6 | -7.53 | 124.08 | 128.60 |
| 31 | DA | 2258 | C | C5-C4-N4 | -7.52 | 114.93 | 120.20 |
| 31 | DA | 2016 | U | C5-C6-N1 | -7.52 | 118.94 | 122.70 |
| 31 | DA | 141 | A | C6-C5-N7 | -7.51 | 127.04 | 132.30 |
| 31 | DA | 2006 | C | C6-N1-C2 | 7.50 | 123.30 | 120.30 |
| 32 | BB | 81 | G | N9-C4-C5 | -7.49 | 102.40 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 31 | DA | 1359 | A | C8-N9-C4 | 7.49 | 108.80 | 105.80 |
| 31 | BA | 1543 | C | C2-N3-C4 | 7.49 | 123.64 | 119.90 |
| 31 | DA | 2463 | C | C2-N3-C4 | -7.49 | 116.16 | 119.90 |
| 31 | BA | 659 | C | C6-N1-C2 | 7.48 | 123.29 | 120.30 |
| 31 | DA | 330 | A | N3-C4-C5 | 7.47 | 132.03 | 126.80 |
| 31 | DA | 2441 | C | C2-N3-C4 | -7.47 | 116.16 | 119.90 |
| 32 | DB | 64 | C | C6-N1-C2 | 7.47 | 123.29 | 120.30 |
| 31 | BA | 1543 | C | N3-C4-C5 | -7.46 | 118.92 | 121.90 |
| 31 | BA | 1204 | A | C5-C6-N1 | -7.45 | 113.97 | 117.70 |
| 31 | DA | 193 | U | N3-C4-O4 | 7.45 | 124.61 | 119.40 |
| 31 | DA | 1126 | A | C8-N9-C4 | 7.45 | 108.78 | 105.80 |
| 31 | BA | 141 | A | C5-C6-N6 | -7.44 | 117.75 | 123.70 |
| 31 | DA | 1258 | C | C6-N1-C2 | 7.44 | 123.28 | 120.30 |
| 31 | DA | 1678 | G | C2-N3-C4 | -7.44 | 108.18 | 111.90 |
| 31 | BA | 2432 | A | N1-C6-N6 | 7.43 | 123.06 | 118.60 |
| 31 | DA | 2828 | C | C5-C6-N1 | -7.42 | 117.29 | 121.00 |
| 31 | DA | 2463 | C | C5-C6-N1 | -7.42 | 117.29 | 121.00 |
| 31 | BA | 272 | G | N3-C4-N9 | 7.42 | 130.45 | 126.00 |
| 31 | DA | 1762 | A | C8-N9-C4 | -7.42 | 102.83 | 105.80 |
| 31 | BA | 1616 | A | C6-C5-N7 | -7.41 | 127.11 | 132.30 |
| 31 | DA | 774 | A | N7-C8-N9 | 7.41 | 117.50 | 113.80 |
| 42 | DQ | 82 | ARG | NE-CZ-NH2 | -7.40 | 116.60 | 120.30 |
| 31 | DA | 484 | C | C2-N3-C4 | -7.40 | 116.20 | 119.90 |
| 31 | DA | 621 | A | C2-N3-C4 | -7.39 | 106.90 | 110.60 |
| 31 | DA | 1269 | A | C8-N9-C4 | 7.39 | 108.76 | 105.80 |
| 31 | BA | 2688 | U | C5-C4-O4 | 7.39 | 130.33 | 125.90 |
| 31 | DA | 2287 | A | N1-C2-N3 | 7.38 | 132.99 | 129.30 |
| 31 | BA | 62 | C | C5-C6-N1 | -7.38 | 117.31 | 121.00 |
| 31 | BA | 1658 | C | N1-C2-O2 | -7.37 | 114.48 | 118.90 |
| 31 | DA | 621 | A | C5-N7-C8 | -7.37 | 100.22 | 103.90 |
| 31 | DA | 1350 | C | N1-C2-O2 | -7.37 | 114.48 | 118.90 |
| 31 | BA | 1698 | A | C5-N7-C8 | -7.37 | 100.22 | 103.90 |
| 31 | DA | 2293 | C | C6-N1-C2 | 7.36 | 123.24 | 120.30 |
| 31 | DA | 2346 | A | C8-N9-C4 | -7.36 | 102.86 | 105.80 |
| 31 | DA | 560 | C | C6-N1-C2 | 7.35 | 123.24 | 120.30 |
| 31 | BA | 265 | A | N7-C8-N9 | 7.34 | 117.47 | 113.80 |
| 31 | BA | 272(D) | G | C8-N9-C4 | 7.34 | 109.34 | 106.40 |
| 31 | BA | 774 | A | C2-N3-C4 | -7.34 | 106.93 | 110.60 |
| 31 | BA | 1779 | U | C4-C5-C6 | 7.34 | 124.10 | 119.70 |
| 32 | BB | 81 | G | N3-C4-N9 | 7.33 | 130.40 | 126.00 |
| 31 | DA | 847 | U | C5-C4-O4 | 7.33 | 130.30 | 125.90 |
| 31 | BA | 2616 | C | N1-C2-O2 | -7.31 | 114.51 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 31 | BA | 2392 | A | C5-C6-N1 | -7.31 | 114.04 | 117.70 |
| 31 | DA | 1826 | G | N1-C6-O6 | -7.31 | 115.51 | 119.90 |
| 31 | BA | 676 | A | N1-C6-N6 | 7.30 | 122.98 | 118.60 |
| 31 | BA | 950 | G | C5-C6-O6 | 7.30 | 132.98 | 128.60 |
| 31 | BA | 139(A) | G | N7-C8-N9 | 7.30 | 116.75 | 113.10 |
| 31 | BA | 2779 | U | N3-C4-O4 | -7.30 | 114.29 | 119.40 |
| 31 | BA | 1326 | U | C6-N1-C2 | 7.30 | 125.38 | 121.00 |
| 31 | BA | 205 | G | C8-N9-C4 | 7.29 | 109.32 | 106.40 |
| 1 | CA | 117 | G | C5-C6-O6 | -7.29 | 124.22 | 128.60 |
| 31 | BA | 530 | G | N3-C4-C5 | 7.29 | 132.24 | 128.60 |
| 31 | DA | 1349 | A | C5-N7-C8 | -7.29 | 100.25 | 103.90 |
| 39 | BN | 67 | LEU | CA-CB-CG | 7.28 | 132.04 | 115.30 |
| 31 | DA | 528 | A | C5-N7-C8 | -7.28 | 100.26 | 103.90 |
| 31 | BA | 949 | C | C6-N1-C2 | 7.27 | 123.21 | 120.30 |
| 31 | BA | 1021 | A | C5-C6-N1 | -7.27 | 114.07 | 117.70 |
| 31 | DA | 2084 | C | C5-C6-N1 | -7.26 | 117.37 | 121.00 |
| 31 | BA | 845 | G | C8-N9-C4 | -7.25 | 103.50 | 106.40 |
| 31 | BA | 1962 | C | C5-C6-N1 | 7.25 | 124.63 | 121.00 |
| 31 | DA | 1544 | A | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |
| 31 | DA | 1204 | A | C4-C5-N7 | 7.24 | 114.32 | 110.70 |
| 31 | BA | 2073 | C | N1-C2-O2 | -7.24 | 114.56 | 118.90 |
| 31 | BA | 1332 | G | C8-N9-C1' | 7.23 | 136.40 | 127.00 |
| 31 | DA | 584 | C | C6-N1-C2 | 7.21 | 123.19 | 120.30 |
| 31 | DA | 1204 | A | N1-C2-N3 | 7.21 | 132.91 | 129.30 |
| 31 | DA | 2253 | G | N1-C6-O6 | 7.21 | 124.23 | 119.90 |
| 31 | BA | 1962 | C | N1-C1'-C2' | 7.20 | 123.36 | 114.00 |
| 1 | CA | 1524 | C | C6-N1-C2 | 7.20 | 123.18 | 120.30 |
| 31 | BA | 783 | A | C6-C5-N7 | -7.20 | 127.26 | 132.30 |
| 31 | DA | 796 | C | C6-N1-C2 | 7.18 | 123.17 | 120.30 |
| 31 | BA | 2518 | A | C2-N3-C4 | -7.18 | 107.01 | 110.60 |
| 31 | DA | 1313 | U | C5-C4-O4 | -7.18 | 121.59 | 125.90 |
| 31 | DA | 1779 | U | N3-C4-O4 | -7.18 | 114.38 | 119.40 |
| 31 | BA | 1558 | A | C2-N3-C4 | -7.17 | 107.01 | 110.60 |
| 31 | BA | 1544 | A | O4'-C1'-N9 | 7.16 | 113.93 | 108.20 |
| 31 | BA | 1617 | C | C5-C6-N1 | -7.16 | 117.42 | 121.00 |
| 31 | DA | 678 | C | N3-C4-C5 | 7.15 | 124.76 | 121.90 |
| 31 | DA | 2579 | C | C6-N1-C2 | 7.15 | 123.16 | 120.30 |
| 31 | DA | 1899 | G | C6-C5-N7 | 7.13 | 134.68 | 130.40 |
| 31 | BA | 845 | G | C4-C5-N7 | 7.13 | 113.65 | 110.80 |
| 31 | BA | 1349 | A | C5-N7-C8 | -7.12 | 100.34 | 103.90 |
| 31 | BA | 828 | U | N3-C4-O4 | -7.12 | 114.42 | 119.40 |
| 31 | DA | 1126 | A | N7-C8-N9 | -7.12 | 110.24 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 31 | BA | 1493 | C | C2-N1-C1' | 7.11 | 126.62 | 118.80 |
| 31 | DA | 1328 | G | N3-C4-N9 | 7.11 | 130.27 | 126.00 |
| 31 | DA | 1207 | C | C5-C6-N1 | -7.11 | 117.44 | 121.00 |
| 31 | DA | 1313 | U | N3-C4-O4 | 7.11 | 124.38 | 119.40 |
| 32 | DB | 81 | G | N7-C8-N9 | 7.10 | 116.65 | 113.10 |
| 31 | BA | 1021 | A | N7-C8-N9 | 7.10 | 117.35 | 113.80 |
| 31 | BA | 142 | A | C5-N7-C8 | -7.10 | 100.35 | 103.90 |
| 31 | DA | 1829 | A | N7-C8-N9 | -7.10 | 110.25 | 113.80 |
| 31 | DA | 1021 | A | C5-C6-N1 | -7.10 | 114.15 | 117.70 |
| 31 | BA | 1300 | U | O4'-C1'-N1 | 7.09 | 113.88 | 108.20 |
| 31 | DA | 1397 | U | C5-C4-O4 | 7.09 | 130.16 | 125.90 |
| 31 | BA | 2430 | A | C4-C5-N7 | 7.09 | 114.25 | 110.70 |
| 31 | BA | 686 | G | C5-C6-O6 | -7.09 | 124.34 | 128.60 |
| 31 | BA | 783 | A | N3-C4-N9 | -7.09 | 121.73 | 127.40 |
| 31 | BA | 1373 | A | C8-N9-C4 | 7.09 | 108.64 | 105.80 |
| 31 | DA | 1830 | C | C6-N1-C2 | 7.08 | 123.13 | 120.30 |
| 31 | BA | 759 | G | C8-N9-C4 | 7.08 | 109.23 | 106.40 |
| 31 | DA | 2346 | A | C4-C5-C6 | 7.07 | 120.54 | 117.00 |
| 31 | BA | 1820 | U | C5-C6-N1 | -7.07 | 119.16 | 122.70 |
| 31 | DA | 1779 | U | C4-C5-C6 | 7.07 | 123.94 | 119.70 |
| 31 | DA | 2891 | G | C8-N9-C4 | 7.07 | 109.23 | 106.40 |
| 31 | DA | 652 | C | C6-N1-C2 | -7.06 | 117.47 | 120.30 |
| 31 | BA | 139(A) | G | C8-N9-C4 | -7.06 | 103.58 | 106.40 |
| 31 | BA | 679 | C | C6-N1-C2 | 7.05 | 123.12 | 120.30 |
| 31 | DA | 1959 | G | N1-C6-O6 | -7.05 | 115.67 | 119.90 |
| 31 | BA | 1241 | A | N1-C2-N3 | 7.04 | 132.82 | 129.30 |
| 31 | DA | 1315 | C | N1-C2-O2 | -7.04 | 114.67 | 118.90 |
| 43 | DR | 4 | LEU | CB-CG-CD1 | 7.04 | 122.97 | 111.00 |
| 31 | BA | 2230 | G | C5-C6-O6 | -7.04 | 124.38 | 128.60 |
| 31 | BA | 1678 | G | N1-C2-N2 | -7.03 | 109.87 | 116.20 |
| 31 | DA | 484 | C | C5-C6-N1 | -7.03 | 117.48 | 121.00 |
| 32 | DB | 81 | G | C5-N7-C8 | -7.03 | 100.78 | 104.30 |
| 31 | DA | 272 | G | N3-C4-N9 | 7.03 | 130.22 | 126.00 |
| 31 | DA | 585 | G | C5-C6-O6 | -7.02 | 124.39 | 128.60 |
| 31 | DA | 2542 | A | C2-N3-C4 | -7.02 | 107.09 | 110.60 |
| 31 | BA | 652 | C | C6-N1-C2 | -7.01 | 117.50 | 120.30 |
| 31 | DA | 1328 | G | C5-C6-N1 | 7.01 | 115.01 | 111.50 |
| 31 | BA | 2392 | A | C4-C5-N7 | 7.01 | 114.21 | 110.70 |
| 31 | BA | 528 | A | N3-C4-N9 | -7.00 | 121.80 | 127.40 |
| 31 | BA | 856 | C | C5-C6-N1 | 7.00 | 124.50 | 121.00 |
| 31 | BA | 2346 | A | C8-N9-C4 | -6.99 | 103.00 | 105.80 |
| 31 | DA | 1332 | G | C8-N9-C1' | 6.99 | 136.09 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 31 | BA | 2508 | G | N3-C2-N2 | -6.99 | 115.01 | 119.90 |
| 31 | DA | 2258 | C | N3-C4-N4 | 6.99 | 122.89 | 118.00 |
| 31 | BA | 2318 | G | N7-C8-N9 | 6.97 | 116.58 | 113.10 |
| 31 | BA | 1158 | C | C6-N1-C1' | -6.97 | 112.44 | 120.80 |
| 31 | DA | 1930 | G | C8-N9-C4 | 6.97 | 109.19 | 106.40 |
| 31 | BA | 2319 | G | N3-C4-C5 | -6.96 | 125.12 | 128.60 |
| 31 | DA | 244 | A | N1-C6-N6 | 6.96 | 122.77 | 118.60 |
| 31 | BA | 2014 | A | N1-C6-N6 | 6.95 | 122.77 | 118.60 |
| 31 | DA | 847 | U | C2-N1-C1' | -6.95 | 109.36 | 117.70 |
| 31 | DA | 2430 | A | N1-C2-N3 | 6.95 | 132.78 | 129.30 |
| 39 | DN | 67 | LEU | CA-CB-CG | 6.95 | 131.29 | 115.30 |
| 31 | BA | 2512 | C | C2-N3-C4 | -6.95 | 116.43 | 119.90 |
| 31 | BA | 1204 | A | C4-C5-C6 | 6.95 | 120.47 | 117.00 |
| 31 | DA | 1698 | A | N9-C4-C5 | -6.94 | 103.02 | 105.80 |
| 31 | DA | 2828 | C | N3-C4-C5 | 6.94 | 124.67 | 121.90 |
| 31 | BA | 1830 | C | N1-C2-O2 | -6.93 | 114.74 | 118.90 |
| 31 | BA | 2433 | A | N1-C6-N6 | 6.93 | 122.76 | 118.60 |
| 31 | BA | 1899 | G | C2-N3-C4 | -6.93 | 108.44 | 111.90 |
| 31 | DA | 1158 | C | C6-N1-C1' | -6.93 | 112.49 | 120.80 |
| 31 | DA | 2575 | C | C6-N1-C2 | 6.92 | 123.07 | 120.30 |
| 31 | DA | 2435 | A | C8-N9-C4 | -6.91 | 103.03 | 105.80 |
| 31 | BA | 2713 | A | C6-C5-N7 | -6.91 | 127.46 | 132.30 |
| 1 | CA | 893 | C | C6-N1-C2 | 6.90 | 123.06 | 120.30 |
| 31 | BA | 1204 | A | N7-C8-N9 | 6.90 | 117.25 | 113.80 |
| 31 | BA | 141 | A | N7-C8-N9 | 6.89 | 117.25 | 113.80 |
| 31 | BA | 1899 | G | C6-C5-N7 | 6.89 | 134.53 | 130.40 |
| 31 | BA | 57 | C | C6-N1-C2 | 6.88 | 123.05 | 120.30 |
| 31 | BA | 201 | C | C6-N1-C2 | 6.88 | 123.05 | 120.30 |
| 31 | BA | 330 | A | C4-C5-N7 | 6.88 | 114.14 | 110.70 |
| 31 | BA | 1142(A) | A | N3-C4-N9 | -6.87 | 121.90 | 127.40 |
| 31 | DA | 1529 | G | C4-N9-C1' | 6.87 | 135.43 | 126.50 |
| 31 | DA | 1326 | U | C5-C6-N1 | -6.87 | 119.27 | 122.70 |
| 1 | AA | 896 | C | C6-N1-C2 | 6.86 | 123.05 | 120.30 |
| 31 | BA | 2430 | A | N3-C4-C5 | 6.86 | 131.60 | 126.80 |
| 31 | BA | 1497 | U | N1-C2-N3 | -6.86 | 110.78 | 114.90 |
| 31 | DA | 2232 | U | C5-C6-N1 | -6.86 | 119.27 | 122.70 |
| 32 | DB | 81 | G | N9-C4-C5 | -6.86 | 102.66 | 105.40 |
| 31 | BA | 1142(A) | A | C5-N7-C8 | -6.85 | 100.47 | 103.90 |
| 31 | DA | 69 | C | C6-N1-C2 | 6.85 | 123.04 | 120.30 |
| 31 | DA | 621 | A | N7-C8-N9 | 6.85 | 117.23 | 113.80 |
| 31 | BA | 847 | U | C5-C6-N1 | -6.85 | 119.28 | 122.70 |
| 31 | DA | 584 | C | C5-C6-N1 | -6.84 | 117.58 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | DA | 2681 | C | N3-C4-N4 | -6.84 | 113.21 | 118.00 |
| 31 | BA | 2689 | U | N3-C4-O4 | -6.84 | 114.61 | 119.40 |
| 31 | DA | 141 | A | C4-C5-N7 | 6.84 | 114.12 | 110.70 |
| 31 | DA | 528 | A | N3-C4-N9 | -6.84 | 121.93 | 127.40 |
| 31 | DA | 265 | A | N7-C8-N9 | 6.84 | 117.22 | 113.80 |
| 31 | DA | 2504 | U | C6-N1-C2 | 6.83 | 125.10 | 121.00 |
| 31 | DA | 837 | C | N3-C2-O2 | -6.83 | 117.12 | 121.90 |
| 31 | BA | 847 | U | C5-C4-O4 | 6.83 | 130.00 | 125.90 |
| 31 | DA | 1614 | A | C5-N7-C8 | -6.83 | 100.49 | 103.90 |
| 31 | BA | 621 | A | C8-N9-C4 | -6.83 | 103.07 | 105.80 |
| 31 | BA | 788 | A | N1-C6-N6 | 6.82 | 122.69 | 118.60 |
| 31 | DA | 1962 | C | C5-C6-N1 | 6.82 | 124.41 | 121.00 |
| 31 | DA | 2651 | C | C6-N1-C2 | 6.81 | 123.03 | 120.30 |
| 31 | DA | 586 | A | N1-C2-N3 | -6.81 | 125.89 | 129.30 |
| 31 | DA | 185 | U | C5-C6-N1 | -6.81 | 119.30 | 122.70 |
| 31 | DA | 484 | C | N3-C4-C5 | 6.81 | 124.62 | 121.90 |
| 31 | DA | 1397 | U | N3-C2-O2 | -6.81 | 117.43 | 122.20 |
| 31 | BA | 945 | A | C5-C6-N6 | -6.81 | 118.25 | 123.70 |
| 31 | DA | 2606 | C | C6-N1-C2 | 6.81 | 123.02 | 120.30 |
| 31 | DA | 1493 | C | C2-N1-C1' | 6.80 | 126.28 | 118.80 |
| 31 | BA | 933 | A | C4-C5-N7 | 6.79 | 114.10 | 110.70 |
| 31 | BA | 2201 | C | C6-N1-C2 | 6.79 | 123.02 | 120.30 |
| 31 | DA | 2017 | U | N1-C2-N3 | 6.79 | 118.97 | 114.90 |
| 31 | BA | 1373 | A | N7-C8-N9 | -6.79 | 110.41 | 113.80 |
| 31 | DA | 62 | C | C5-C6-N1 | -6.79 | 117.61 | 121.00 |
| 31 | DA | 1657 | C | C5-C6-N1 | -6.79 | 117.61 | 121.00 |
| 24 | B2 | 53 | LEU | CA-CB-CG | 6.78 | 130.90 | 115.30 |
| 31 | BA | 2061 | G | N3-C2-N2 | 6.78 | 124.65 | 119.90 |
| 31 | BA | 2318 | G | C8-N9-C4 | -6.78 | 103.69 | 106.40 |
| 31 | BA | 735 | A | C8-N9-C4 | 6.78 | 108.51 | 105.80 |
| 31 | BA | 2024 | G | C8-N9-C4 | 6.78 | 109.11 | 106.40 |
| 31 | DA | 1497 | U | N1-C2-N3 | -6.78 | 110.83 | 114.90 |
| 41 | DP | 37 | GLY | N-CA-C | 6.78 | 130.05 | 113.10 |
| 31 | DA | 71 | A | C4-C5-N7 | 6.78 | 114.09 | 110.70 |
| 31 | BA | 1049 | C | C6-N1-C2 | -6.78 | 117.59 | 120.30 |
| 31 | DA | 207 | A | N7-C8-N9 | -6.78 | 110.41 | 113.80 |
| 31 | DA | 1617 | C | N1-C2-O2 | -6.78 | 114.83 | 118.90 |
| 31 | BA | 2451 | A | N9-C4-C5 | 6.77 | 108.51 | 105.80 |
| 31 | DA | 679 | C | C6-N1-C2 | 6.77 | 123.01 | 120.30 |
| 31 | BA | 995 | C | N1-C2-O2 | -6.77 | 114.84 | 118.90 |
| 31 | BA | 1495 | A | C5-N7-C8 | -6.77 | 100.51 | 103.90 |
| 31 | DA | 676 | A | C4-C5-N7 | 6.77 | 114.08 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 1 | AA | 1459 | C | C6-N1-C2 | 6.77 | 123.01 | 120.30 |
| 31 | BA | 2689 | U | C5-C4-O4 | 6.76 | 129.96 | 125.90 |
| 31 | DA | 577 | G | N7-C8-N9 | -6.76 | 109.72 | 113.10 |
| 31 | BA | 1779 | U | C6-N1-C2 | 6.76 | 125.06 | 121.00 |
| 31 | DA | 1962 | C | C2-N1-C1' | 6.76 | 126.23 | 118.80 |
| 1 | CA | 810 | C | C6-N1-C2 | 6.75 | 123.00 | 120.30 |
| 31 | DA | 1573 | G | C8-N9-C4 | 6.75 | 109.10 | 106.40 |
| 31 | DA | 2681 | C | C5-C4-N4 | 6.75 | 124.93 | 120.20 |
| 31 | BA | 2053 | G | N1-C6-O6 | 6.75 | 123.95 | 119.90 |
| 31 | DA | 1349 | A | N7-C8-N9 | 6.74 | 117.17 | 113.80 |
| 31 | DA | 1142(A) | A | C5-C6-N1 | -6.74 | 114.33 | 117.70 |
| 31 | DA | 1653 | G | C4-N9-C1' | 6.74 | 135.26 | 126.50 |
| 31 | BA | 1158 | C | C2-N1-C1' | 6.74 | 126.21 | 118.80 |
| 31 | DA | 591 | C | C5-C6-N1 | -6.74 | 117.63 | 121.00 |
| 31 | DA | 828 | U | C5-C4-O4 | 6.74 | 129.94 | 125.90 |
| 31 | DA | 1799 | G | C8-N9-C4 | 6.73 | 109.09 | 106.40 |
| 31 | BA | 2796 | U | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 31 | BA | 446 | G | N9-C4-C5 | -6.72 | 102.71 | 105.40 |
| 31 | DA | 2044 | C | C6-N1-C2 | 6.72 | 122.99 | 120.30 |
| 31 | DA | 2364 | C | C5-C6-N1 | -6.72 | 117.64 | 121.00 |
| 31 | DA | 2014 | A | N1-C6-N6 | 6.72 | 122.63 | 118.60 |
| 31 | DA | 783 | A | C6-C5-N7 | -6.72 | 127.59 | 132.30 |
| 31 | DA | 1300 | U | O4'-C1'-N1 | 6.72 | 113.57 | 108.20 |
| 31 | BA | 1382 | G | N3-C4-C5 | 6.71 | 131.96 | 128.60 |
| 31 | DA | 1304 | C | N3-C4-C5 | 6.71 | 124.58 | 121.90 |
| 31 | BA | 194 | G | N1-C6-O6 | 6.71 | 123.92 | 119.90 |
| 31 | BA | 2688 | U | C5-C6-N1 | -6.71 | 119.35 | 122.70 |
| 31 | DA | 2594 | C | N1-C2-O2 | -6.71 | 114.88 | 118.90 |
| 31 | DA | 567 | A | C5-N7-C8 | -6.70 | 100.55 | 103.90 |
| 31 | DA | 2432 | A | N1-C6-N6 | 6.70 | 122.62 | 118.60 |
| 31 | BA | 1674 | G | C6-C5-N7 | -6.70 | 126.38 | 130.40 |
| 31 | BA | 786 | C | C6-N1-C2 | 6.69 | 122.98 | 120.30 |
| 31 | BA | 1617 | C | N1-C2-O2 | -6.69 | 114.89 | 118.90 |
| 31 | BA | 141 | A | C4-C5-N7 | 6.69 | 114.05 | 110.70 |
| 31 | BA | 676 | A | N7-C8-N9 | 6.69 | 117.14 | 113.80 |
| 31 | DA | 1021 | A | N1-C6-N6 | 6.69 | 122.61 | 118.60 |
| 31 | DA | 1609 | A | C3'-C2'-C1' | 6.68 | 106.85 | 101.50 |
| 31 | BA | 530 | G | N9-C4-C5 | 6.68 | 108.07 | 105.40 |
| 31 | BA | 2043 | C | N1-C2-O2 | -6.68 | 114.89 | 118.90 |
| 31 | DA | 2017 | U | C5-C6-N1 | -6.68 | 119.36 | 122.70 |
| 31 | BA | 2084 | C | C4-C5-C6 | 6.68 | 120.74 | 117.40 |
| 31 | BA | 1326 | U | C5-C6-N1 | -6.67 | 119.36 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 31 | DA | 2427 | C | N1-C2-O2 | -6.67 | 114.89 | 118.90 |
| 31 | BA | 1653 | G | C4-N9-C1' | 6.67 | 135.17 | 126.50 |
| 31 | BA | 2591 | C | C2-N3-C4 | -6.67 | 116.57 | 119.90 |
| 31 | BA | 2512 | C | C5-C6-N1 | -6.67 | 117.67 | 121.00 |
| 31 | BA | 2363 | C | C5-C6-N1 | -6.66 | 117.67 | 121.00 |
| 31 | DA | 1999 | C | C6-N1-C2 | 6.66 | 122.97 | 120.30 |
| 31 | DA | 2796 | U | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 31 | BA | 837 | C | C6-N1-C2 | -6.66 | 117.64 | 120.30 |
| 31 | DA | 2433 | A | N1-C6-N6 | 6.66 | 122.59 | 118.60 |
| 31 | DA | 265 | A | C5-N7-C8 | -6.65 | 100.57 | 103.90 |
| 31 | DA | 659 | C | C6-N1-C2 | 6.65 | 122.96 | 120.30 |
| 31 | DA | 486 | C | N1-C2-O2 | -6.65 | 114.91 | 118.90 |
| 1 | AA | 1524 | C | N1-C2-O2 | -6.65 | 114.91 | 118.90 |
| 31 | DA | 2464 | C | C6-N1-C2 | 6.65 | 122.96 | 120.30 |
| 31 | BA | 142 | A | C6-C5-N7 | -6.65 | 127.65 | 132.30 |
| 31 | BA | 2498 | C | C6-N1-C2 | 6.64 | 122.96 | 120.30 |
| 31 | BA | 1198 | U | C5-C6-N1 | -6.64 | 119.38 | 122.70 |
| 31 | BA | 142 | A | N7-C8-N9 | 6.64 | 117.12 | 113.80 |
| 31 | DA | 1930 | G | N7-C8-N9 | -6.64 | 109.78 | 113.10 |
| 32 | BB | 81 | G | C5-C6-O6 | -6.63 | 124.62 | 128.60 |
| 31 | BA | 736 | C | N1-C2-O2 | -6.63 | 114.92 | 118.90 |
| 31 | BA | 768 | G | N1-C6-O6 | 6.63 | 123.88 | 119.90 |
| 31 | DA | 945 | A | C5-C6-N6 | -6.63 | 118.40 | 123.70 |
| 31 | DA | 2475 | C | C6-N1-C1' | -6.63 | 112.84 | 120.80 |
| 31 | DA | 2774 | C | C6-N1-C2 | 6.63 | 122.95 | 120.30 |
| 31 | DA | 968 | G | C8-N9-C4 | 6.62 | 109.05 | 106.40 |
| 31 | DA | 1678 | G | N1-C2-N2 | -6.62 | 110.24 | 116.20 |
| 42 | DQ | 82 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 31 | BA | 206 | U | C5-C6-N1 | -6.61 | 119.39 | 122.70 |
| 31 | BA | 1614 | A | N7-C8-N9 | 6.61 | 117.11 | 113.80 |
| 31 | BA | 2672 | G | C5-C6-O6 | -6.61 | 124.63 | 128.60 |
| 31 | DA | 201 | C | C5-C6-N1 | -6.61 | 117.70 | 121.00 |
| 31 | BA | 107 | C | N1-C2-O2 | -6.61 | 114.94 | 118.90 |
| 31 | BA | 933 | A | N7-C8-N9 | 6.61 | 117.10 | 113.80 |
| 31 | DA | 2253 | G | N9-C4-C5 | -6.61 | 102.76 | 105.40 |
| 31 | DA | 2680 | C | C6-N1-C2 | 6.61 | 122.94 | 120.30 |
| 31 | DA | 2475 | C | C2-N1-C1' | 6.60 | 126.06 | 118.80 |
| 31 | DA | 1021 | A | C5-N7-C8 | -6.60 | 100.60 | 103.90 |
| 31 | BA | 737 | C | C5-C6-N1 | -6.60 | 117.70 | 121.00 |
| 31 | BA | 2701 | C | C6-N1-C2 | -6.60 | 117.66 | 120.30 |
| 31 | DA | 179 | G | N3-C4-C5 | 6.60 | 131.90 | 128.60 |
| 31 | DA | 1779 | U | N1-C2-N3 | 6.60 | 118.86 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | DA | 2084 | C | C6-N1-C2 | 6.59 | 122.94 | 120.30 |
| 1 | AA | 117 | G | N1-C6-O6 | 6.59 | 123.85 | 119.90 |
| 31 | DA | 2441 | C | N3-C4-C5 | 6.58 | 124.53 | 121.90 |
| 31 | BA | 1653 | G | C4-C5-C6 | 6.58 | 122.75 | 118.80 |
| 31 | BA | 2363 | C | C2-N3-C4 | -6.58 | 116.61 | 119.90 |
| 31 | BA | 1543 | C | N1-C2-O2 | -6.58 | 114.95 | 118.90 |
| 31 | DA | 444 | C | N1-C2-O2 | -6.57 | 114.96 | 118.90 |
| 31 | BA | 604 | G | C8-N9-C4 | 6.57 | 109.03 | 106.40 |
| 31 | DA | 2361 | A | N1-C6-N6 | 6.57 | 122.54 | 118.60 |
| 31 | BA | 735 | A | N7-C8-N9 | -6.57 | 110.52 | 113.80 |
| 31 | DA | 774 | A | C4-C5-N7 | 6.57 | 113.98 | 110.70 |
| 31 | BA | 1021 | A | N1-C6-N6 | 6.57 | 122.54 | 118.60 |
| 42 | BQ | 82 | ARG | NE-CZ-NH1 | 6.57 | 123.58 | 120.30 |
| 31 | BA | 124 | G | C5-C6-O6 | -6.56 | 124.66 | 128.60 |
| 31 | BA | 584 | C | N1-C2-O2 | -6.56 | 114.96 | 118.90 |
| 31 | DA | 2598 | A | C8-N9-C4 | 6.56 | 108.42 | 105.80 |
| 31 | BA | 1663 | C | C2-N3-C4 | -6.56 | 116.62 | 119.90 |
| 31 | BA | 2392 | A | N3-C4-C5 | 6.56 | 131.39 | 126.80 |
| 31 | BA | 2781 | A | N1-C6-N6 | -6.55 | 114.67 | 118.60 |
| 31 | DA | 205 | G | C8-N9-C4 | 6.55 | 109.02 | 106.40 |
| 31 | DA | 226 | G | N1-C6-O6 | 6.54 | 123.83 | 119.90 |
| 31 | BA | 1529 | G | C4-N9-C1' | 6.54 | 135.00 | 126.50 |
| 31 | BA | 1962 | C | C2-N1-C1' | 6.54 | 125.99 | 118.80 |
| 31 | DA | 1022 | G | N7-C8-N9 | 6.54 | 116.37 | 113.10 |
| 31 | DA | 1543 | C | N3-C4-C5 | -6.53 | 119.29 | 121.90 |
| 31 | DA | 210 | C | C5-C6-N1 | -6.53 | 117.73 | 121.00 |
| 31 | DA | 2030 | A | C5-C6-N6 | -6.53 | 118.47 | 123.70 |
| 31 | BA | 2648 | C | C6-N1-C2 | 6.53 | 122.91 | 120.30 |
| 31 | BA | 179 | G | C8-N9-C4 | 6.52 | 109.01 | 106.40 |
| 31 | DA | 1659 | U | C5-C6-N1 | -6.52 | 119.44 | 122.70 |
| 31 | BA | 1799 | G | C8-N9-C4 | 6.51 | 109.01 | 106.40 |
| 31 | BA | 2481 | G | N9-C4-C5 | -6.51 | 102.80 | 105.40 |
| 31 | DA | 1779 | U | C6-N1-C2 | 6.51 | 124.91 | 121.00 |
| 31 | BA | 201 | C | C5-C6-N1 | -6.51 | 117.75 | 121.00 |
| 31 | DA | 2711 | A | C8-N9-C4 | 6.50 | 108.40 | 105.80 |
| 31 | DA | 945 | A | C4-C5-N7 | 6.50 | 113.95 | 110.70 |
| 31 | DA | 2346 | A | C4-N9-C1' | 6.50 | 137.99 | 126.30 |
| 31 | DA | 2715 | C | C5-C6-N1 | -6.50 | 117.75 | 121.00 |
| 31 | BA | 16 | G | C2-N3-C4 | -6.49 | 108.65 | 111.90 |
| 31 | BA | 1158 | C | C5-C6-N1 | 6.49 | 124.25 | 121.00 |
| 31 | BA | 975 | C | C5-C4-N4 | 6.49 | 124.74 | 120.20 |
| 51 | BZ | 110 | GLY | N-CA-C | -6.49 | 96.88 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | BA | 1261 | C | N3-C2-O2 | 6.49 | 126.44 | 121.90 |
| 31 | BA | 2571 | C | N3-C2-O2 | -6.48 | 117.36 | 121.90 |
| 31 | DA | 774 | A | N3-C4-C5 | 6.48 | 131.34 | 126.80 |
| 31 | DA | 847 | U | N3-C4-O4 | -6.48 | 114.87 | 119.40 |
| 31 | DA | 560 | C | C5-C6-N1 | -6.47 | 117.76 | 121.00 |
| 31 | DA | 621 | A | C8-N9-C4 | -6.47 | 103.21 | 105.80 |
| 31 | BA | 2779 | U | C5-C4-O4 | 6.46 | 129.78 | 125.90 |
| 31 | DA | 2498 | C | N1-C2-O2 | -6.46 | 115.02 | 118.90 |
| 31 | BA | 207 | A | C2-N3-C4 | -6.46 | 107.37 | 110.60 |
| 31 | BA | 1811 | G | N3-C2-N2 | -6.46 | 115.38 | 119.90 |
| 31 | DA | 1496 | A | N7-C8-N9 | 6.46 | 117.03 | 113.80 |
| 31 | BA | 2346 | A | C4-N9-C1' | 6.45 | 137.91 | 126.30 |
| 43 | BR | 8 | ARG | N-CA-C | 6.45 | 128.42 | 111.00 |
| 31 | DA | 573 | G | N1-C6-O6 | -6.45 | 116.03 | 119.90 |
| 31 | BA | 1350 | C | N1-C2-O2 | -6.45 | 115.03 | 118.90 |
| 31 | BA | 1241 | A | C5-C6-N1 | -6.45 | 114.48 | 117.70 |
| 31 | BA | 2622 | C | C6-N1-C2 | 6.45 | 122.88 | 120.30 |
| 31 | BA | 2081 | C | N1-C2-O2 | -6.44 | 115.03 | 118.90 |
| 31 | DA | 2014 | A | C5-C6-N6 | -6.44 | 118.55 | 123.70 |
| 31 | DA | 2422 | A | C8-N9-C4 | -6.44 | 103.22 | 105.80 |
| 31 | BA | 1786 | A | C5-C6-N1 | -6.44 | 114.48 | 117.70 |
| 31 | BA | 2518 | A | C5-C6-N6 | -6.44 | 118.55 | 123.70 |
| 31 | DA | 569 | U | C5-C6-N1 | -6.44 | 119.48 | 122.70 |
| 31 | DA | 2363 | C | C2-N1-C1' | -6.44 | 111.72 | 118.80 |
| 31 | BA | 527 | C | N3-C4-N4 | -6.44 | 113.49 | 118.00 |
| 31 | DA | 1678 | G | C8-N9-C4 | -6.44 | 103.82 | 106.40 |
| 31 | BA | 1210 | A | C6-C5-N7 | -6.44 | 127.79 | 132.30 |
| 31 | BA | 1678 | G | C4-N9-C1' | 6.44 | 134.87 | 126.50 |
| 31 | BA | 2681 | C | C5-C4-N4 | 6.43 | 124.70 | 120.20 |
| 32 | DB | 81 | G | C5-C6-O6 | -6.43 | 124.74 | 128.60 |
| 31 | BA | 783 | A | C4-C5-N7 | 6.42 | 113.91 | 110.70 |
| 31 | BA | 71 | A | C6-C5-N7 | -6.42 | 127.81 | 132.30 |
| 31 | DA | 2542 | A | C6-C5-N7 | -6.42 | 127.81 | 132.30 |
| 31 | BA | 1258 | C | C6-N1-C2 | 6.42 | 122.87 | 120.30 |
| 31 | DA | 1614 | A | C6-C5-N7 | -6.42 | 127.81 | 132.30 |
| 31 | DA | 2050 | C | C2-N3-C4 | -6.42 | 116.69 | 119.90 |
| 31 | BA | 1543 | C | C6-N1-C2 | -6.41 | 117.73 | 120.30 |
| 31 | BA | 465 | G | C8-N9-C4 | -6.41 | 103.84 | 106.40 |
| 31 | BA | 1609 | A | C3'-C2'-C1' | 6.41 | 106.62 | 101.50 |
| 31 | DA | 287 | C | C6-N1-C2 | 6.41 | 122.86 | 120.30 |
| 31 | BA | 1543 | C | N3-C4-N4 | 6.40 | 122.48 | 118.00 |
| 31 | BA | 621 | A | C4-C5-N7 | 6.40 | 113.90 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|----------|-------|-------------|----------|
| 31 | DA | 1779 | U | C5-C4-O4 | 6.40 | 129.74 | 125.90 |
| 31 | BA | 797 | C | C2-N3-C4 | -6.39 | 116.70 | 119.90 |
| 31 | DA | 2814 | C | C6-N1-C2 | 6.39 | 122.86 | 120.30 |
| 31 | BA | 265 | A | C8-N9-C4 | -6.39 | 103.24 | 105.80 |
| 31 | DA | 798 | G | N1-C6-O6 | -6.39 | 116.06 | 119.90 |
| 31 | BA | 1328 | G | N3-C4-N9 | 6.39 | 129.83 | 126.00 |
| 31 | DA | 580 | C | N1-C2-O2 | -6.39 | 115.07 | 118.90 |
| 31 | DA | 130 | C | C5-C6-N1 | -6.38 | 117.81 | 121.00 |
| 31 | DA | 791 | C | C5-C6-N1 | -6.38 | 117.81 | 121.00 |
| 31 | BA | 2648 | C | N3-C4-C5 | 6.38 | 124.45 | 121.90 |
| 31 | BA | 446 | G | C4-C5-N7 | 6.38 | 113.35 | 110.80 |
| 31 | DA | 397 | G | N1-C6-O6 | 6.38 | 123.72 | 119.90 |
| 31 | BA | 2587 | A | N1-C2-N3 | 6.37 | 132.49 | 129.30 |
| 31 | DA | 62 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 31 | DA | 1142(A) | A | N3-C4-N9 | -6.36 | 122.31 | 127.40 |
| 31 | BA | 1624 | G | C8-N9-C4 | 6.36 | 108.94 | 106.40 |
| 31 | BA | 2413 | G | C8-N9-C4 | 6.36 | 108.94 | 106.40 |
| 31 | BA | 2477 | C | N3-C4-C5 | -6.36 | 119.36 | 121.90 |
| 31 | DA | 530 | G | N9-C4-C5 | 6.36 | 107.94 | 105.40 |
| 31 | DA | 796 | C | C5-C6-N1 | -6.36 | 117.82 | 121.00 |
| 31 | DA | 1528 | A | N1-C6-N6 | 6.36 | 122.41 | 118.60 |
| 31 | DA | 1367 | A | N1-C6-N6 | -6.35 | 114.79 | 118.60 |
| 31 | DA | 529 | A | C4-C5-N7 | 6.35 | 113.87 | 110.70 |
| 1 | CA | 34 | C | C6-N1-C2 | 6.34 | 122.84 | 120.30 |
| 31 | DA | 2362 | G | C8-N9-C4 | 6.34 | 108.94 | 106.40 |
| 31 | BA | 1991 | U | N1-C2-O2 | -6.34 | 118.36 | 122.80 |
| 31 | DA | 516 | C | C6-N1-C2 | 6.34 | 122.84 | 120.30 |
| 31 | BA | 1021 | A | C6-C5-N7 | -6.34 | 127.86 | 132.30 |
| 31 | DA | 409 | C | N3-C4-C5 | 6.34 | 124.43 | 121.90 |
| 31 | DA | 528 | A | N3-C4-C5 | 6.34 | 131.24 | 126.80 |
| 31 | BA | 1784 | A | N7-C8-N9 | -6.33 | 110.63 | 113.80 |
| 31 | BA | 2552 | U | N3-C2-O2 | 6.33 | 126.63 | 122.20 |
| 31 | BA | 529 | A | C5-N7-C8 | -6.33 | 100.73 | 103.90 |
| 31 | BA | 1977 | A | C8-N9-C4 | 6.33 | 108.33 | 105.80 |
| 24 | D2 | 53 | LEU | CA-CB-CG | 6.33 | 129.86 | 115.30 |
| 31 | DA | 2079 | U | C4-C5-C6 | 6.32 | 123.49 | 119.70 |
| 31 | DA | 933 | A | C4-C5-N7 | 6.32 | 113.86 | 110.70 |
| 31 | DA | 1543 | C | C2-N3-C4 | 6.32 | 123.06 | 119.90 |
| 31 | BA | 130 | C | N3-C4-C5 | 6.32 | 124.43 | 121.90 |
| 31 | DA | 1899 | G | C2-N3-C4 | -6.32 | 108.74 | 111.90 |
| 31 | DA | 2392 | A | N1-C6-N6 | 6.32 | 122.39 | 118.60 |
| 31 | DA | 2420 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | BA | 1397 | U | C6-N1-C2 | -6.31 | 117.21 | 121.00 |
| 31 | DA | 934 | G | C8-N9-C4 | 6.31 | 108.92 | 106.40 |
| 31 | DA | 2241 | A | C8-N9-C4 | 6.31 | 108.33 | 105.80 |
| 31 | BA | 2485 | G | C6-C5-N7 | -6.31 | 126.61 | 130.40 |
| 31 | DA | 1496 | A | N1-C6-N6 | 6.31 | 122.39 | 118.60 |
| 31 | DA | 2361 | A | C2-N3-C4 | -6.31 | 107.45 | 110.60 |
| 31 | BA | 1349 | A | N1-C6-N6 | 6.30 | 122.38 | 118.60 |
| 31 | DA | 1006 | C | C6-N1-C2 | 6.30 | 122.82 | 120.30 |
| 31 | DA | 2680 | C | N3-C4-C5 | 6.30 | 124.42 | 121.90 |
| 32 | DB | 104 | U | C6-N1-C2 | 6.30 | 124.78 | 121.00 |
| 31 | BA | 205 | G | N3-C2-N2 | 6.30 | 124.31 | 119.90 |
| 31 | DA | 1614 | A | C8-N9-C4 | -6.30 | 103.28 | 105.80 |
| 31 | BA | 669 | G | N1-C6-O6 | -6.30 | 116.12 | 119.90 |
| 31 | DA | 2481 | G | N9-C4-C5 | -6.30 | 102.88 | 105.40 |
| 31 | BA | 1207 | C | C5-C6-N1 | -6.30 | 117.85 | 121.00 |
| 31 | BA | 1343 | G | C4-N9-C1' | 6.30 | 134.69 | 126.50 |
| 31 | DA | 1694 | C | C6-N1-C1' | -6.30 | 113.25 | 120.80 |
| 31 | DA | 2713 | A | C2-N3-C4 | -6.30 | 107.45 | 110.60 |
| 31 | BA | 2258 | C | C5-C4-N4 | -6.29 | 115.79 | 120.20 |
| 31 | DA | 2017 | U | C4-C5-C6 | 6.29 | 123.48 | 119.70 |
| 31 | BA | 133 | C | C6-N1-C2 | 6.29 | 122.81 | 120.30 |
| 31 | BA | 783 | A | N1-C2-N3 | 6.28 | 132.44 | 129.30 |
| 31 | BA | 2593 | U | N3-C4-C5 | -6.28 | 110.83 | 114.60 |
| 1 | CA | 1509 | C | C6-N1-C2 | 6.28 | 122.81 | 120.30 |
| 31 | BA | 179 | G | N1-C6-O6 | 6.28 | 123.67 | 119.90 |
| 31 | BA | 1049 | C | C2-N1-C1' | 6.28 | 125.71 | 118.80 |
| 31 | DA | 2476 | A | C2-N3-C4 | 6.28 | 113.74 | 110.60 |
| 31 | DA | 856 | C | C5-C6-N1 | 6.28 | 124.14 | 121.00 |
| 31 | DA | 1328 | G | N3-C4-C5 | -6.27 | 125.47 | 128.60 |
| 31 | BA | 847 | U | N3-C4-O4 | -6.26 | 115.02 | 119.40 |
| 31 | BA | 2498 | C | N1-C2-O2 | -6.26 | 115.14 | 118.90 |
| 31 | BA | 2547 | U | C5-C6-N1 | -6.26 | 119.57 | 122.70 |
| 31 | DA | 1049 | C | C2-N1-C1' | 6.26 | 125.69 | 118.80 |
| 31 | DA | 2542 | A | N7-C8-N9 | 6.25 | 116.93 | 113.80 |
| 31 | DA | 986 | C | C2-N3-C4 | -6.25 | 116.78 | 119.90 |
| 31 | DA | 805 | G | N3-C4-N9 | 6.25 | 129.75 | 126.00 |
| 31 | BA | 463 | G | N1-C6-O6 | -6.25 | 116.15 | 119.90 |
| 31 | BA | 956 | G | C5-C6-N1 | -6.25 | 108.38 | 111.50 |
| 31 | DA | 2438 | U | C5-C6-N1 | -6.25 | 119.58 | 122.70 |
| 31 | DA | 141 | A | C5-N7-C8 | -6.25 | 100.78 | 103.90 |
| 31 | DA | 2624 | G | C5-C6-O6 | -6.24 | 124.85 | 128.60 |
| 31 | BA | 1675 | C | C2-N1-C1' | -6.24 | 111.94 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 31 | BA | 731 | C | N1-C2-O2 | -6.24 | 115.16 | 118.90 |
| 31 | BA | 1279 | G | N1-C6-O6 | -6.24 | 116.16 | 119.90 |
| 31 | BA | 1328 | G | C6-N1-C2 | -6.24 | 121.36 | 125.10 |
| 31 | BA | 2073 | C | N3-C2-O2 | 6.24 | 126.26 | 121.90 |
| 31 | BA | 71 | A | N7-C8-N9 | 6.23 | 116.92 | 113.80 |
| 31 | BA | 189 | G | C2-N3-C4 | -6.23 | 108.78 | 111.90 |
| 31 | DA | 1496 | A | C4-N9-C1' | 6.23 | 137.51 | 126.30 |
| 31 | BA | 205 | G | N9-C4-C5 | -6.22 | 102.91 | 105.40 |
| 31 | DA | 1622 | G | N1-C6-O6 | -6.22 | 116.17 | 119.90 |
| 31 | DA | 2542 | A | C5-C6-N1 | -6.22 | 114.59 | 117.70 |
| 31 | BA | 1261 | C | N1-C2-O2 | -6.22 | 115.17 | 118.90 |
| 43 | DR | 8 | ARG | N-CA-C | 6.22 | 127.78 | 111.00 |
| 31 | BA | 2084 | C | C6-N1-C2 | 6.21 | 122.78 | 120.30 |
| 31 | DA | 2441 | C | N3-C4-N4 | -6.21 | 113.65 | 118.00 |
| 31 | DA | 1123 | C | N3-C4-C5 | 6.21 | 124.38 | 121.90 |
| 31 | DA | 2362 | G | C2-N3-C4 | -6.21 | 108.79 | 111.90 |
| 31 | DA | 71 | A | N7-C8-N9 | 6.21 | 116.91 | 113.80 |
| 31 | DA | 847 | U | C5-C6-N1 | -6.21 | 119.59 | 122.70 |
| 31 | DA | 1543 | C | N3-C2-O2 | 6.21 | 126.25 | 121.90 |
| 31 | BA | 2579 | C | C6-N1-C2 | 6.21 | 122.78 | 120.30 |
| 31 | BA | 647 | G | C4-N9-C1' | 6.20 | 134.56 | 126.50 |
| 31 | DA | 2079 | U | C5-C6-N1 | -6.20 | 119.60 | 122.70 |
| 31 | BA | 847 | U | C6-N1-C1' | 6.20 | 129.88 | 121.20 |
| 31 | BA | 1279 | G | C5-C6-O6 | 6.20 | 132.32 | 128.60 |
| 31 | DA | 1021 | A | C6-C5-N7 | -6.20 | 127.96 | 132.30 |
| 31 | DA | 2659 | G | C4-N9-C1' | 6.20 | 134.56 | 126.50 |
| 31 | BA | 2659 | G | C4-N9-C1' | 6.20 | 134.55 | 126.50 |
| 31 | DA | 1142(A) | A | N3-C4-C5 | 6.20 | 131.14 | 126.80 |
| 31 | BA | 528 | A | C4-C5-N7 | 6.19 | 113.80 | 110.70 |
| 31 | DA | 481 | G | C8-N9-C4 | -6.19 | 103.92 | 106.40 |
| 31 | BA | 1349 | A | C4-C5-N7 | 6.19 | 113.79 | 110.70 |
| 31 | BA | 805 | G | C5-C6-O6 | -6.18 | 124.89 | 128.60 |
| 31 | DA | 2363 | C | N1-C2-O2 | -6.18 | 115.19 | 118.90 |
| 31 | BA | 774 | A | N3-C4-N9 | -6.18 | 122.45 | 127.40 |
| 31 | DA | 1634 | A | N9-C4-C5 | 6.18 | 108.27 | 105.80 |
| 31 | BA | 2475 | C | C2-N1-C1' | 6.18 | 125.59 | 118.80 |
| 31 | DA | 1681 | G | N3-C4-C5 | 6.18 | 131.69 | 128.60 |
| 31 | DA | 1694 | C | C5-C6-N1 | 6.17 | 124.09 | 121.00 |
| 31 | BA | 1678 | G | N9-C4-C5 | -6.17 | 102.93 | 105.40 |
| 31 | BA | 1990 | C | N3-C2-O2 | -6.17 | 117.58 | 121.90 |
| 31 | DA | 1349 | A | N1-C6-N6 | 6.17 | 122.30 | 118.60 |
| 31 | DA | 2421 | G | N1-C6-O6 | 6.16 | 123.60 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | DA | 669 | G | N7-C8-N9 | -6.16 | 110.02 | 113.10 |
| 31 | BA | 1609 | A | C6-N1-C2 | -6.16 | 114.91 | 118.60 |
| 31 | DA | 105 | C | C6-N1-C2 | 6.16 | 122.76 | 120.30 |
| 31 | DA | 378 | C | N3-C4-C5 | 6.16 | 124.36 | 121.90 |
| 31 | BA | 2544 | G | C5-C6-O6 | -6.15 | 124.91 | 128.60 |
| 31 | DA | 1326 | U | C6-N1-C2 | 6.15 | 124.69 | 121.00 |
| 31 | DA | 1902 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 31 | DA | 2253 | G | C4-C5-N7 | 6.15 | 113.26 | 110.80 |
| 31 | DA | 2593 | U | N3-C4-C5 | -6.15 | 110.91 | 114.60 |
| 31 | DA | 141 | A | C5-C6-N6 | -6.15 | 118.78 | 123.70 |
| 31 | DA | 1784 | A | C2-N3-C4 | -6.14 | 107.53 | 110.60 |
| 31 | BA | 1624 | G | N7-C8-N9 | -6.14 | 110.03 | 113.10 |
| 31 | BA | 1397 | U | N1-C2-N3 | 6.14 | 118.58 | 114.90 |
| 31 | DA | 1204 | A | C4-N9-C1' | 6.14 | 137.35 | 126.30 |
| 31 | DA | 1678 | G | C8-N9-C1' | -6.14 | 119.02 | 127.00 |
| 31 | BA | 2362 | G | C8-N9-C4 | 6.14 | 108.86 | 106.40 |
| 31 | DA | 933 | A | N7-C8-N9 | 6.14 | 116.87 | 113.80 |
| 31 | BA | 1332 | G | C4-N9-C1' | -6.14 | 118.52 | 126.50 |
| 31 | DA | 941 | A | C8-N9-C4 | -6.14 | 103.34 | 105.80 |
| 31 | DA | 378 | C | C6-N1-C2 | 6.14 | 122.75 | 120.30 |
| 31 | DA | 529 | A | C5-C6-N6 | -6.14 | 118.79 | 123.70 |
| 1 | CA | 1519 | A | N1-C6-N6 | -6.13 | 114.92 | 118.60 |
| 31 | DA | 24 | G | N1-C6-O6 | 6.13 | 123.58 | 119.90 |
| 31 | DA | 192 | C | C6-N1-C2 | 6.13 | 122.75 | 120.30 |
| 31 | BA | 2711 | A | C2-N3-C4 | -6.13 | 107.53 | 110.60 |
| 31 | DA | 207 | A | C2-N3-C4 | -6.13 | 107.53 | 110.60 |
| 31 | DA | 2011 | U | N3-C2-O2 | 6.13 | 126.49 | 122.20 |
| 31 | DA | 2033 | A | N1-C6-N6 | -6.12 | 114.92 | 118.60 |
| 31 | BA | 2027 | G | C8-N9-C4 | -6.12 | 103.95 | 106.40 |
| 31 | DA | 2626 | C | C4-C5-C6 | 6.12 | 120.46 | 117.40 |
| 31 | BA | 1204 | A | C4-N9-C1' | 6.12 | 137.31 | 126.30 |
| 31 | DA | 1829 | A | C2-N3-C4 | -6.12 | 107.54 | 110.60 |
| 31 | BA | 1210 | A | C5-N7-C8 | -6.12 | 100.84 | 103.90 |
| 31 | BA | 2827 | C | C5-C4-N4 | -6.12 | 115.92 | 120.20 |
| 31 | DA | 664 | C | C6-N1-C2 | 6.11 | 122.75 | 120.30 |
| 27 | B5 | 51 | TYR | CA-CB-CG | 6.11 | 125.01 | 113.40 |
| 31 | BA | 150 | C | C6-N1-C2 | 6.11 | 122.74 | 120.30 |
| 31 | BA | 2014 | A | C5-C6-N6 | -6.11 | 118.81 | 123.70 |
| 31 | DA | 1269 | A | C2-N3-C4 | -6.11 | 107.55 | 110.60 |
| 31 | DA | 1496 | A | C6-C5-N7 | -6.11 | 128.02 | 132.30 |
| 31 | DA | 558 | G | N7-C8-N9 | -6.11 | 110.05 | 113.10 |
| 31 | DA | 612 | C | C6-N1-C2 | 6.11 | 122.74 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 31 | BA | 1279 | G | C8-N9-C4 | -6.11 | 103.96 | 106.40 |
| 31 | BA | 2499 | C | C2-N1-C1' | 6.11 | 125.52 | 118.80 |
| 31 | DA | 2648 | C | C6-N1-C2 | 6.11 | 122.74 | 120.30 |
| 31 | BA | 2385 | C | N1-C2-O2 | -6.10 | 115.24 | 118.90 |
| 31 | DA | 827 | U | N3-C2-O2 | 6.10 | 126.47 | 122.20 |
| 41 | BP | 59 | LEU | N-CA-C | -6.10 | 94.53 | 111.00 |
| 31 | DA | 1382 | G | N3-C4-C5 | 6.10 | 131.65 | 128.60 |
| 31 | DA | 2010 | G | C8-N9-C4 | -6.10 | 103.96 | 106.40 |
| 31 | BA | 2477 | C | C6-N1-C2 | -6.10 | 117.86 | 120.30 |
| 31 | DA | 850 | C | C6-N1-C2 | 6.09 | 122.74 | 120.30 |
| 31 | DA | 2441 | C | C5-C6-N1 | -6.09 | 117.95 | 121.00 |
| 31 | BA | 2544 | G | C6-C5-N7 | -6.09 | 126.75 | 130.40 |
| 41 | DP | 59 | LEU | N-CA-C | -6.09 | 94.56 | 111.00 |
| 48 | BW | 12 | ILE | N-CA-C | -6.09 | 94.57 | 111.00 |
| 31 | BA | 805 | G | N3-C4-N9 | 6.08 | 129.65 | 126.00 |
| 31 | DA | 2432 | A | C5-C6-N6 | -6.08 | 118.84 | 123.70 |
| 31 | BA | 2080 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 31 | DA | 934 | G | N7-C8-N9 | -6.08 | 110.06 | 113.10 |
| 31 | DA | 2531 | A | C8-N9-C4 | 6.08 | 108.23 | 105.80 |
| 31 | BA | 2258 | C | N1-C2-O2 | -6.07 | 115.26 | 118.90 |
| 31 | BA | 529 | A | N1-C6-N6 | 6.07 | 122.24 | 118.60 |
| 31 | DA | 690 | G | C8-N9-C4 | 6.07 | 108.83 | 106.40 |
| 31 | BA | 1022 | G | C6-N1-C2 | -6.07 | 121.46 | 125.10 |
| 31 | BA | 2485 | G | N1-C6-O6 | 6.07 | 123.54 | 119.90 |
| 31 | BA | 995 | C | C6-N1-C1' | 6.07 | 128.08 | 120.80 |
| 31 | DA | 928 | G | C6-C5-N7 | -6.07 | 126.76 | 130.40 |
| 31 | BA | 139(A) | G | C5-N7-C8 | -6.06 | 101.27 | 104.30 |
| 31 | DA | 2013 | A | C8-N9-C4 | 6.06 | 108.22 | 105.80 |
| 31 | BA | 463 | G | C5-C6-O6 | 6.06 | 132.23 | 128.60 |
| 1 | AA | 123 | C | C6-N1-C2 | 6.05 | 122.72 | 120.30 |
| 31 | BA | 1670 | C | N1-C2-O2 | -6.05 | 115.27 | 118.90 |
| 1 | AA | 917 | G | C8-N9-C4 | -6.05 | 103.98 | 106.40 |
| 31 | DA | 148 | C | C6-N1-C2 | 6.05 | 122.72 | 120.30 |
| 31 | DA | 389 | G | C8-N9-C4 | 6.05 | 108.82 | 106.40 |
| 31 | BA | 2002 | G | C5-C6-O6 | -6.05 | 124.97 | 128.60 |
| 31 | BA | 2568 | C | C6-N1-C2 | 6.05 | 122.72 | 120.30 |
| 31 | DA | 672 | C | C5-C6-N1 | -6.05 | 117.97 | 121.00 |
| 31 | DA | 2421 | G | C5-C6-O6 | -6.05 | 124.97 | 128.60 |
| 1 | CA | 699 | C | N1-C2-O2 | -6.05 | 115.27 | 118.90 |
| 31 | DA | 2681 | C | C5-C6-N1 | -6.05 | 117.98 | 121.00 |
| 31 | DA | 2742 | C | C2-N1-C1' | -6.05 | 112.15 | 118.80 |
| 31 | DA | 450 | G | C8-N9-C4 | -6.04 | 103.98 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 31 | BA | 265 | A | C6-C5-N7 | -6.04 | 128.07 | 132.30 |
| 31 | BA | 1049 | C | C5-C6-N1 | 6.04 | 124.02 | 121.00 |
| 31 | BA | 139(A) | G | C5-C6-O6 | -6.04 | 124.98 | 128.60 |
| 31 | DA | 205 | G | N9-C4-C5 | -6.04 | 102.98 | 105.40 |
| 31 | DA | 1997 | G | C6-N1-C2 | -6.04 | 121.48 | 125.10 |
| 31 | DA | 1779 | U | C6-N1-C1' | 6.04 | 129.65 | 121.20 |
| 31 | DA | 1343 | G | N3-C4-C5 | -6.04 | 125.58 | 128.60 |
| 31 | DA | 2399 | G | C4-N9-C1' | 6.04 | 134.35 | 126.50 |
| 31 | DA | 995 | C | C6-N1-C1' | 6.03 | 128.04 | 120.80 |
| 31 | BA | 1559 | G | C4-C5-N7 | 6.03 | 113.21 | 110.80 |
| 31 | DA | 2542 | A | C4-C5-N7 | 6.03 | 113.72 | 110.70 |
| 31 | DA | 728 | G | C8-N9-C4 | 6.03 | 108.81 | 106.40 |
| 31 | DA | 671 | C | N1-C2-O2 | -6.03 | 115.28 | 118.90 |
| 31 | DA | 2571 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 31 | DA | 2698 | U | N1-C2-O2 | -6.03 | 118.58 | 122.80 |
| 31 | DA | 445 | C | C5-C6-N1 | -6.02 | 117.99 | 121.00 |
| 31 | BA | 2399 | G | C4-N9-C1' | 6.02 | 134.33 | 126.50 |
| 31 | BA | 827 | U | C6-N1-C2 | 6.02 | 124.61 | 121.00 |
| 31 | BA | 656 | G | N3-C4-C5 | -6.02 | 125.59 | 128.60 |
| 31 | BA | 2439 | A | N7-C8-N9 | 6.02 | 116.81 | 113.80 |
| 31 | DA | 586 | A | C8-N9-C4 | 6.02 | 108.21 | 105.80 |
| 31 | DA | 2263 | C | N1-C2-O2 | -6.02 | 115.29 | 118.90 |
| 31 | DA | 647 | G | C4-N9-C1' | 6.02 | 134.32 | 126.50 |
| 31 | BA | 1977 | A | C2-N3-C4 | -6.01 | 107.59 | 110.60 |
| 31 | DA | 71 | A | C6-C5-N7 | -6.01 | 128.09 | 132.30 |
| 31 | DA | 530 | G | C8-N9-C1' | 6.01 | 134.82 | 127.00 |
| 31 | DA | 794 | G | C4-C5-N7 | -6.01 | 108.39 | 110.80 |
| 31 | BA | 928 | G | C6-C5-N7 | -6.01 | 126.79 | 130.40 |
| 31 | DA | 1332 | G | C4-N9-C1' | -6.01 | 118.69 | 126.50 |
| 31 | BA | 139(A) | G | C5-C6-N1 | 6.00 | 114.50 | 111.50 |
| 31 | DA | 669 | G | C4-C5-N7 | -6.00 | 108.40 | 110.80 |
| 31 | DA | 2713 | A | C4-C5-N7 | 6.00 | 113.70 | 110.70 |
| 31 | BA | 2275 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 31 | DA | 1351 | C | C6-N1-C2 | 5.99 | 122.70 | 120.30 |
| 31 | BA | 1830 | C | N3-C2-O2 | 5.99 | 126.09 | 121.90 |
| 31 | BA | 2465 | C | C2-N3-C4 | -5.99 | 116.91 | 119.90 |
| 31 | DA | 1948 | G | C8-N9-C4 | -5.99 | 104.01 | 106.40 |
| 31 | DA | 2680 | C | C2-N3-C4 | -5.99 | 116.91 | 119.90 |
| 31 | BA | 128 | C | C6-N1-C2 | -5.98 | 117.91 | 120.30 |
| 31 | BA | 2033 | A | N1-C6-N6 | -5.98 | 115.01 | 118.60 |
| 31 | BA | 673 | C | C5-C4-N4 | -5.98 | 116.01 | 120.20 |
| 31 | BA | 928 | G | N1-C6-O6 | 5.98 | 123.49 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 43 | BR | 4 | LEU | CB-CG-CD1 | 5.98 | 121.16 | 111.00 |
| 31 | BA | 474 | G | C8-N9-C4 | -5.97 | 104.01 | 106.40 |
| 31 | DA | 2503 | A | C5-C6-N1 | 5.97 | 120.69 | 117.70 |
| 31 | DA | 2070 | G | C6-N1-C2 | -5.97 | 121.52 | 125.10 |
| 31 | DA | 774 | A | C8-N9-C4 | -5.96 | 103.41 | 105.80 |
| 31 | DA | 1268 | A | C2-N3-C4 | -5.96 | 107.62 | 110.60 |
| 31 | DA | 2604 | U | C5-C6-N1 | -5.96 | 119.72 | 122.70 |
| 31 | DA | 1617 | C | C6-N1-C2 | 5.96 | 122.69 | 120.30 |
| 31 | DA | 2283 | C | N1-C2-O2 | -5.96 | 115.32 | 118.90 |
| 31 | DA | 59 | U | C5-C4-O4 | 5.96 | 129.48 | 125.90 |
| 31 | BA | 2422 | A | N7-C8-N9 | 5.96 | 116.78 | 113.80 |
| 31 | BA | 2017 | U | N1-C2-N3 | 5.96 | 118.47 | 114.90 |
| 31 | BA | 2293 | C | N1-C2-O2 | -5.96 | 115.33 | 118.90 |
| 31 | DA | 2435 | A | N7-C8-N9 | 5.96 | 116.78 | 113.80 |
| 31 | BA | 768 | G | C5-C6-O6 | -5.95 | 125.03 | 128.60 |
| 31 | DA | 2713 | A | N7-C8-N9 | 5.95 | 116.78 | 113.80 |
| 31 | BA | 1573 | G | C8-N9-C4 | 5.95 | 108.78 | 106.40 |
| 27 | D5 | 4 | HIS | C-N-CD | 5.95 | 140.90 | 128.40 |
| 31 | DA | 1558 | A | N1-C2-N3 | 5.95 | 132.28 | 129.30 |
| 31 | DA | 272(B) | G | C4-C5-N7 | -5.95 | 108.42 | 110.80 |
| 31 | DA | 1252 | G | C8-N9-C4 | 5.95 | 108.78 | 106.40 |
| 31 | BA | 1694 | C | C4-C5-C6 | -5.95 | 114.43 | 117.40 |
| 31 | BA | 800 | A | N1-C6-N6 | -5.95 | 115.03 | 118.60 |
| 31 | BA | 530 | G | C8-N9-C1' | 5.94 | 134.73 | 127.00 |
| 31 | BA | 1162 | G | C4-C5-N7 | -5.94 | 108.42 | 110.80 |
| 31 | BA | 686 | G | C4-C5-N7 | 5.94 | 113.18 | 110.80 |
| 31 | DA | 995 | C | C2-N1-C1' | -5.94 | 112.27 | 118.80 |
| 31 | DA | 1373 | A | N7-C8-N9 | -5.94 | 110.83 | 113.80 |
| 31 | BA | 2518 | A | N3-C4-C5 | 5.94 | 130.96 | 126.80 |
| 31 | BA | 2518 | A | C6-C5-N7 | -5.94 | 128.14 | 132.30 |
| 1 | CA | 904 | C | C6-N1-C2 | 5.94 | 122.67 | 120.30 |
| 1 | CA | 117 | G | N9-C4-C5 | -5.93 | 103.03 | 105.40 |
| 31 | BA | 614 | U | C5-C4-O4 | 5.93 | 129.46 | 125.90 |
| 31 | BA | 676 | A | C6-C5-N7 | -5.93 | 128.15 | 132.30 |
| 31 | BA | 1261 | C | C6-N1-C2 | 5.93 | 122.67 | 120.30 |
| 31 | BA | 2053 | G | C5-C6-O6 | -5.93 | 125.04 | 128.60 |
| 31 | BA | 2681 | C | N3-C4-N4 | -5.93 | 113.85 | 118.00 |
| 28 | B6 | 11 | LEU | CA-CB-CG | 5.93 | 128.94 | 115.30 |
| 31 | BA | 1607 | C | N3-C4-N4 | 5.93 | 122.15 | 118.00 |
| 31 | DA | 2079 | U | N1-C2-N3 | 5.92 | 118.45 | 114.90 |
| 31 | DA | 2043 | C | C2-N3-C4 | -5.92 | 116.94 | 119.90 |
| 31 | BA | 178 | G | N1-C6-O6 | -5.92 | 116.35 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 31 | DA | 1821 | A | N7-C8-N9 | -5.92 | 110.84 | 113.80 |
| 31 | BA | 139(A) | G | C4-N9-C1' | 5.92 | 134.20 | 126.50 |
| 31 | DA | 754 | C | C5-C6-N1 | -5.92 | 118.04 | 121.00 |
| 31 | BA | 1324 | G | N1-C6-O6 | 5.91 | 123.45 | 119.90 |
| 31 | BA | 1992 | G | N3-C4-C5 | -5.91 | 125.64 | 128.60 |
| 31 | DA | 1204 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 31 | BA | 2041 | U | N1-C2-O2 | -5.91 | 118.66 | 122.80 |
| 41 | BP | 53 | GLY | N-CA-C | -5.91 | 98.33 | 113.10 |
| 31 | DA | 1558 | A | C5-C6-N1 | -5.91 | 114.74 | 117.70 |
| 31 | DA | 1616 | A | C4-C5-N7 | 5.91 | 113.66 | 110.70 |
| 31 | BA | 1310 | G | N3-C4-C5 | -5.91 | 125.65 | 128.60 |
| 1 | CA | 1429 | C | C5-C6-N1 | -5.91 | 118.05 | 121.00 |
| 31 | DA | 847 | U | C6-N1-C1' | 5.91 | 129.47 | 121.20 |
| 31 | BA | 1653 | G | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 31 | BA | 686 | G | N1-C6-O6 | 5.91 | 123.44 | 119.90 |
| 31 | DA | 1049 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 31 | DA | 2648 | C | C5-C6-N1 | -5.90 | 118.05 | 121.00 |
| 31 | BA | 142 | A | C4-C5-N7 | 5.90 | 113.65 | 110.70 |
| 31 | DA | 131 | G | C8-N9-C4 | 5.90 | 108.76 | 106.40 |
| 31 | DA | 1708 | C | C6-N1-C2 | 5.90 | 122.66 | 120.30 |
| 31 | BA | 412 | A | C2-N3-C4 | -5.90 | 107.65 | 110.60 |
| 31 | BA | 1496 | A | C4-N9-C1' | 5.90 | 136.91 | 126.30 |
| 31 | DA | 272(B) | G | C5-C6-O6 | 5.90 | 132.14 | 128.60 |
| 31 | DA | 2866 | U | C4-C5-C6 | 5.89 | 123.24 | 119.70 |
| 31 | BA | 1782 | C | C4-C5-C6 | 5.89 | 120.35 | 117.40 |
| 31 | BA | 1994 | C | C5-C6-N1 | -5.89 | 118.05 | 121.00 |
| 1 | CA | 322 | C | C6-N1-C2 | 5.89 | 122.66 | 120.30 |
| 31 | BA | 976 | C | N1-C2-O2 | 5.89 | 122.43 | 118.90 |
| 31 | BA | 2779 | U | C5-C6-N1 | -5.89 | 119.76 | 122.70 |
| 31 | DA | 1771 | C | N1-C2-O2 | -5.89 | 115.37 | 118.90 |
| 31 | DA | 121 | G | C8-N9-C4 | 5.89 | 108.75 | 106.40 |
| 31 | DA | 253 | C | N1-C2-O2 | -5.89 | 115.37 | 118.90 |
| 31 | DA | 1800 | C | C2-N1-C1' | -5.89 | 112.32 | 118.80 |
| 31 | BA | 1332 | G | N1-C6-O6 | 5.88 | 123.43 | 119.90 |
| 31 | BA | 1333 | C | N3-C4-C5 | 5.88 | 124.25 | 121.90 |
| 31 | DA | 584 | C | C2-N1-C1' | -5.88 | 112.33 | 118.80 |
| 31 | DA | 2493 | U | C5-C6-N1 | -5.88 | 119.76 | 122.70 |
| 31 | BA | 579 | G | N1-C6-O6 | 5.88 | 123.43 | 119.90 |
| 31 | DA | 178 | G | N1-C6-O6 | -5.88 | 116.37 | 119.90 |
| 1 | CA | 108 | G | C4-C5-N7 | 5.88 | 113.15 | 110.80 |
| 31 | BA | 194 | G | C5-C6-O6 | -5.87 | 125.08 | 128.60 |
| 31 | BA | 209 | C | C6-N1-C2 | 5.87 | 122.65 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | BA | 594 | U | C5-C6-N1 | -5.87 | 119.76 | 122.70 |
| 31 | BA | 762 | U | C2-N1-C1' | 5.87 | 124.74 | 117.70 |
| 31 | BA | 1256 | G | C8-N9-C1' | -5.87 | 119.37 | 127.00 |
| 31 | BA | 2681 | C | C5-C6-N1 | -5.87 | 118.07 | 121.00 |
| 31 | DA | 2779 | U | N3-C2-O2 | -5.87 | 118.09 | 122.20 |
| 31 | BA | 2475 | C | C6-N1-C1' | -5.86 | 113.77 | 120.80 |
| 31 | BA | 2598 | A | C8-N9-C4 | 5.86 | 108.14 | 105.80 |
| 31 | DA | 1031 | G | C6-N1-C2 | -5.86 | 121.58 | 125.10 |
| 31 | DA | 2778 | A | C2-N3-C4 | -5.86 | 107.67 | 110.60 |
| 31 | BA | 982 | C | C6-N1-C2 | -5.86 | 117.96 | 120.30 |
| 31 | BA | 1268 | A | C5-C6-N1 | -5.86 | 114.77 | 117.70 |
| 31 | BA | 2032 | G | C5-C6-O6 | -5.86 | 125.09 | 128.60 |
| 31 | DA | 1207 | C | N3-C2-O2 | 5.86 | 126.00 | 121.90 |
| 31 | DA | 814 | C | C5-C6-N1 | -5.85 | 118.07 | 121.00 |
| 31 | DA | 2651 | C | C5-C6-N1 | -5.85 | 118.07 | 121.00 |
| 31 | DA | 194 | G | N1-C6-O6 | 5.85 | 123.41 | 119.90 |
| 31 | BA | 1802 | A | N1-C6-N6 | 5.85 | 122.11 | 118.60 |
| 31 | BA | 2626 | C | C2-N3-C4 | -5.85 | 116.98 | 119.90 |
| 31 | DA | 1678 | G | N3-C2-N2 | 5.85 | 123.99 | 119.90 |
| 31 | DA | 2496 | C | C6-N1-C2 | 5.85 | 122.64 | 120.30 |
| 31 | DA | 2011 | U | N1-C2-O2 | -5.84 | 118.71 | 122.80 |
| 31 | BA | 208 | C | C5-C4-N4 | -5.84 | 116.11 | 120.20 |
| 31 | BA | 2363 | C | N1-C2-O2 | -5.84 | 115.39 | 118.90 |
| 31 | DA | 1012 | U | N3-C4-O4 | -5.84 | 115.31 | 119.40 |
| 31 | BA | 2430 | A | C5-C6-N1 | -5.84 | 114.78 | 117.70 |
| 31 | DA | 737 | C | C6-N1-C2 | 5.84 | 122.64 | 120.30 |
| 31 | BA | 1800 | C | C2-N1-C1' | -5.84 | 112.38 | 118.80 |
| 32 | DB | 115 | G | N7-C8-N9 | -5.84 | 110.18 | 113.10 |
| 31 | BA | 1559 | G | N1-C6-O6 | 5.83 | 123.40 | 119.90 |
| 31 | BA | 1779 | U | C6-N1-C1' | 5.83 | 129.37 | 121.20 |
| 31 | DA | 803 | U | C5-C6-N1 | -5.83 | 119.78 | 122.70 |
| 31 | BA | 1959 | G | N1-C6-O6 | -5.83 | 116.40 | 119.90 |
| 31 | BA | 1972 | A | N1-C6-N6 | 5.83 | 122.10 | 118.60 |
| 31 | DA | 2610 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 31 | BA | 122 | G | C8-N9-C4 | 5.83 | 108.73 | 106.40 |
| 31 | DA | 185 | U | C2-N3-C4 | -5.83 | 123.50 | 127.00 |
| 31 | BA | 2403 | C | N1-C2-O2 | -5.83 | 115.40 | 118.90 |
| 31 | DA | 2044 | C | N3-C2-O2 | 5.83 | 125.98 | 121.90 |
| 31 | BA | 774 | A | C5-C6-N1 | -5.83 | 114.79 | 117.70 |
| 31 | DA | 933 | A | C6-C5-N7 | -5.83 | 128.22 | 132.30 |
| 23 | D1 | 43 | TYR | N-CA-C | -5.82 | 95.28 | 111.00 |
| 32 | DB | 104 | U | C5-C6-N1 | -5.82 | 119.79 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 31 | BA | 1256 | G | C4-N9-C1' | 5.82 | 134.07 | 126.50 |
| 31 | BA | 1029 | A | N1-C6-N6 | 5.82 | 122.09 | 118.60 |
| 31 | DA | 74 | A | N1-C6-N6 | -5.82 | 115.11 | 118.60 |
| 31 | DA | 1648 | C | N3-C4-C5 | 5.82 | 124.23 | 121.90 |
| 31 | DA | 2712(A) | A | C8-N9-C4 | -5.82 | 103.47 | 105.80 |
| 31 | BA | 472 | A | C4'-C3'-C2' | 5.82 | 108.42 | 102.60 |
| 31 | BA | 739 | G | C8-N9-C4 | 5.82 | 108.73 | 106.40 |
| 31 | BA | 1694 | C | C6-N1-C1' | -5.82 | 113.82 | 120.80 |
| 31 | DA | 733 | G | C4-C5-N7 | 5.81 | 113.12 | 110.80 |
| 31 | DA | 2689 | U | C5-C6-N1 | -5.81 | 119.79 | 122.70 |
| 31 | BA | 805 | G | C4-C5-N7 | 5.81 | 113.12 | 110.80 |
| 31 | BA | 936 | C | N1-C2-O2 | -5.81 | 115.41 | 118.90 |
| 31 | BA | 481 | G | C8-N9-C4 | -5.81 | 104.08 | 106.40 |
| 31 | BA | 2190 | G | C4-N9-C1' | 5.81 | 134.05 | 126.50 |
| 1 | CA | 906 | G | N9-C4-C5 | -5.81 | 103.08 | 105.40 |
| 31 | BA | 528 | A | N7-C8-N9 | 5.81 | 116.70 | 113.80 |
| 31 | BA | 760 | G | N1-C6-O6 | 5.80 | 123.38 | 119.90 |
| 31 | DA | 444 | C | C5-C6-N1 | -5.80 | 118.10 | 121.00 |
| 31 | DA | 2430 | A | N1-C6-N6 | 5.80 | 122.08 | 118.60 |
| 31 | BA | 783 | A | N7-C8-N9 | 5.80 | 116.70 | 113.80 |
| 31 | BA | 2430 | A | C6-C5-N7 | -5.80 | 128.24 | 132.30 |
| 31 | BA | 2485 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 31 | DA | 558 | G | C8-N9-C4 | 5.80 | 108.72 | 106.40 |
| 31 | DA | 1790 | C | C2-N3-C4 | -5.80 | 117.00 | 119.90 |
| 31 | DA | 591 | C | C2-N3-C4 | -5.79 | 117.00 | 119.90 |
| 31 | DA | 2827 | C | C2-N3-C4 | -5.79 | 117.00 | 119.90 |
| 31 | BA | 950 | G | N1-C6-O6 | -5.79 | 116.42 | 119.90 |
| 31 | DA | 1544 | A | N9-C1'-C2' | 5.79 | 121.53 | 114.00 |
| 31 | DA | 1641 | A | N1-C2-N3 | 5.79 | 132.19 | 129.30 |
| 31 | DA | 2588 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 31 | DA | 584 | C | C4-C5-C6 | 5.79 | 120.30 | 117.40 |
| 31 | DA | 2190 | G | C4-N9-C1' | 5.79 | 134.03 | 126.50 |
| 31 | DA | 2837 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 48 | BW | 6 | ILE | CB-CA-C | -5.79 | 100.03 | 111.60 |
| 31 | BA | 59 | U | N3-C2-O2 | -5.79 | 118.15 | 122.20 |
| 31 | BA | 2584 | U | C5-C4-O4 | 5.78 | 129.37 | 125.90 |
| 31 | DA | 566 | U | C2-N1-C1' | -5.78 | 110.76 | 117.70 |
| 31 | DA | 774 | A | N3-C4-N9 | -5.78 | 122.77 | 127.40 |
| 31 | DA | 1012 | U | C5-C4-O4 | 5.78 | 129.37 | 125.90 |
| 31 | DA | 2626 | C | C5-C6-N1 | -5.78 | 118.11 | 121.00 |
| 31 | BA | 621 | A | N1-C6-N6 | 5.78 | 122.07 | 118.60 |
| 31 | BA | 1291 | C | C5-C6-N1 | -5.78 | 118.11 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | BA | 600 | G | C2-N3-C4 | -5.78 | 109.01 | 111.90 |
| 31 | DA | 669 | G | C5-N7-C8 | 5.78 | 107.19 | 104.30 |
| 31 | DA | 150 | C | C6-N1-C2 | 5.78 | 122.61 | 120.30 |
| 31 | DA | 541 | C | N3-C4-C5 | 5.78 | 124.21 | 121.90 |
| 31 | DA | 671 | C | N3-C4-C5 | -5.78 | 119.59 | 121.90 |
| 32 | BB | 101 | G | C8-N9-C4 | 5.77 | 108.71 | 106.40 |
| 31 | BA | 419 | C | C6-N1-C2 | 5.77 | 122.61 | 120.30 |
| 31 | DA | 1502 | C | C2-N1-C1' | 5.77 | 125.15 | 118.80 |
| 31 | BA | 2243 | U | N1-C2-O2 | -5.77 | 118.76 | 122.80 |
| 27 | D5 | 51 | TYR | CA-CB-CG | 5.77 | 124.36 | 113.40 |
| 31 | BA | 1022 | G | C4-C5-N7 | -5.77 | 108.49 | 110.80 |
| 31 | BA | 265 | A | C2-N3-C4 | -5.77 | 107.72 | 110.60 |
| 31 | BA | 2771 | C | N3-C4-C5 | 5.77 | 124.21 | 121.90 |
| 31 | DA | 141 | A | C2-N3-C4 | -5.77 | 107.72 | 110.60 |
| 31 | BA | 207 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 31 | BA | 826 | U | N3-C2-O2 | 5.77 | 126.24 | 122.20 |
| 31 | DA | 1665 | A | N1-C6-N6 | -5.76 | 115.14 | 118.60 |
| 30 | B8 | 33 | ASN | N-CA-C | -5.76 | 95.44 | 111.00 |
| 31 | BA | 1157 | G | C4-N9-C1' | 5.76 | 133.99 | 126.50 |
| 31 | DA | 1409 | C | C5-C6-N1 | -5.76 | 118.12 | 121.00 |
| 31 | DA | 2555 | U | N1-C2-O2 | -5.76 | 118.77 | 122.80 |
| 31 | BA | 672 | C | C5-C6-N1 | -5.76 | 118.12 | 121.00 |
| 31 | DA | 1312 | U | C5-C6-N1 | -5.76 | 119.82 | 122.70 |
| 31 | DA | 472 | A | C4'-C3'-C2' | 5.76 | 108.36 | 102.60 |
| 31 | DA | 2518 | A | C6-C5-N7 | -5.76 | 128.27 | 132.30 |
| 31 | BA | 730 | C | N3-C4-C5 | 5.76 | 124.20 | 121.90 |
| 31 | BA | 1496 | A | C6-C5-N7 | -5.76 | 128.27 | 132.30 |
| 49 | DX | 62 | LYS | N-CA-C | 5.75 | 126.54 | 111.00 |
| 31 | BA | 2689 | U | C5-C6-N1 | -5.75 | 119.82 | 122.70 |
| 31 | DA | 2231 | C | C2-N3-C4 | -5.75 | 117.02 | 119.90 |
| 31 | DA | 2318 | G | N7-C8-N9 | 5.75 | 115.97 | 113.10 |
| 31 | DA | 2814 | C | N1-C2-O2 | -5.75 | 115.45 | 118.90 |
| 31 | BA | 2613 | U | N3-C4-C5 | 5.75 | 118.05 | 114.60 |
| 31 | BA | 130 | C | C2-N3-C4 | -5.75 | 117.03 | 119.90 |
| 31 | BA | 397 | G | C8-N9-C4 | 5.75 | 108.70 | 106.40 |
| 1 | CA | 572 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 31 | BA | 1370 | C | C2-N1-C1' | -5.75 | 112.48 | 118.80 |
| 31 | DA | 187 | G | C4-C5-N7 | 5.75 | 113.10 | 110.80 |
| 31 | DA | 794 | G | C5-N7-C8 | 5.75 | 107.17 | 104.30 |
| 31 | DA | 1210 | A | N1-C6-N6 | 5.75 | 122.05 | 118.60 |
| 31 | DA | 1758 | G | N3-C4-N9 | -5.75 | 122.55 | 126.00 |
| 31 | DA | 1948 | G | N9-C4-C5 | 5.75 | 107.70 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31 | DA | 2022 | U | C5-C4-O4 | -5.74 | 122.45 | 125.90 |
| 31 | BA | 2318 | G | C6-C5-N7 | -5.74 | 126.96 | 130.40 |
| 31 | BA | 1565 | C | C6-N1-C2 | 5.74 | 122.59 | 120.30 |
| 31 | DA | 2477 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 31 | BA | 139(A) | G | C2-N3-C4 | 5.73 | 114.77 | 111.90 |
| 31 | BA | 647 | G | N3-C4-C5 | -5.73 | 125.73 | 128.60 |
| 31 | DA | 179 | G | C2-N3-C4 | -5.73 | 109.03 | 111.90 |
| 31 | DA | 1210 | A | C5-N7-C8 | -5.73 | 101.03 | 103.90 |
| 31 | BA | 2364 | C | C6-N1-C2 | 5.73 | 122.59 | 120.30 |
| 31 | DA | 928 | G | C5-C6-O6 | -5.73 | 125.16 | 128.60 |
| 1 | CA | 1524 | C | N3-C2-O2 | 5.73 | 125.91 | 121.90 |
| 31 | DA | 1652 | A | C4'-C3'-C2' | 5.73 | 108.33 | 102.60 |
| 31 | BA | 1021 | A | N3-C4-C5 | 5.73 | 130.81 | 126.80 |
| 31 | DA | 2247 | A | C2-N3-C4 | -5.73 | 107.74 | 110.60 |
| 31 | BA | 1698 | A | N1-C2-N3 | 5.72 | 132.16 | 129.30 |
| 31 | BA | 1800 | C | N1-C2-O2 | -5.72 | 115.47 | 118.90 |
| 31 | DA | 594 | U | C5-C6-N1 | -5.72 | 119.84 | 122.70 |
| 31 | BA | 530 | G | C5-C6-O6 | 5.72 | 132.03 | 128.60 |
| 31 | DA | 660 | G | C5-C6-N1 | -5.72 | 108.64 | 111.50 |
| 31 | DA | 2464 | C | N3-C4-C5 | 5.72 | 124.19 | 121.90 |
| 31 | DA | 2711 | A | C2-N3-C4 | -5.72 | 107.74 | 110.60 |
| 31 | DA | 2688 | U | C5-C6-N1 | -5.72 | 119.84 | 122.70 |
| 31 | DA | 1278 | A | N1-C2-N3 | 5.71 | 132.16 | 129.30 |
| 31 | BA | 2243 | U | N3-C2-O2 | 5.71 | 126.20 | 122.20 |
| 31 | BA | 2441 | C | N3-C4-C5 | 5.71 | 124.18 | 121.90 |
| 31 | DA | 57 | C | C6-N1-C2 | 5.71 | 122.58 | 120.30 |
| 31 | BA | 2828 | C | N3-C4-C5 | 5.71 | 124.18 | 121.90 |
| 31 | DA | 2430 | A | C5-C6-N1 | -5.71 | 114.84 | 117.70 |
| 31 | BA | 107 | C | N3-C2-O2 | 5.71 | 125.89 | 121.90 |
| 31 | BA | 683 | C | N3-C4-C5 | 5.71 | 124.18 | 121.90 |
| 31 | DA | 1343 | G | N3-C4-N9 | 5.71 | 129.42 | 126.00 |
| 31 | BA | 1742 | G | C5-C6-O6 | -5.71 | 125.18 | 128.60 |
| 31 | DA | 1972 | A | N1-C6-N6 | 5.71 | 122.02 | 118.60 |
| 31 | BA | 272 | G | N3-C2-N2 | 5.70 | 123.89 | 119.90 |
| 31 | BA | 1033 | U | C2-N1-C1' | 5.70 | 124.55 | 117.70 |
| 1 | CA | 1484 | C | C6-N1-C2 | 5.70 | 122.58 | 120.30 |
| 31 | DA | 2569 | G | C5-C6-O6 | -5.70 | 125.18 | 128.60 |
| 31 | BA | 1359 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |
| 31 | BA | 1381 | G | C8-N9-C4 | -5.70 | 104.12 | 106.40 |
| 31 | DA | 805 | G | C5-C6-O6 | -5.70 | 125.18 | 128.60 |
| 31 | BA | 265 | A | C4-C5-N7 | 5.70 | 113.55 | 110.70 |
| 31 | DA | 2524 | G | C5-C6-O6 | -5.70 | 125.18 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 31 | DA | 2723 | C | C6-N1-C2 | 5.70 | 122.58 | 120.30 |
| 1 | AA | 1524 | C | C6-N1-C2 | 5.69 | 122.58 | 120.30 |
| 23 | B1 | 43 | TYR | N-CA-C | -5.69 | 95.63 | 111.00 |
| 31 | BA | 2538 | C | C6-N1-C2 | 5.69 | 122.58 | 120.30 |
| 41 | BP | 36 | LYS | CD-CE-NZ | 5.69 | 124.79 | 111.70 |
| 31 | DA | 1287 | A | N1-C6-N6 | -5.69 | 115.19 | 118.60 |
| 31 | DA | 2427 | C | N3-C2-O2 | 5.69 | 125.88 | 121.90 |
| 31 | DA | 2522 | U | C4-C5-C6 | 5.69 | 123.11 | 119.70 |
| 31 | DA | 2702 | U | C5-C4-O4 | 5.69 | 129.31 | 125.90 |
| 31 | DA | 2702 | U | N3-C2-O2 | -5.69 | 118.22 | 122.20 |
| 31 | BA | 1336 | A | C5-C6-N1 | 5.69 | 120.54 | 117.70 |
| 31 | DA | 129 | C | C5-C6-N1 | -5.69 | 118.16 | 121.00 |
| 31 | DA | 1142(A) | A | C5-N7-C8 | -5.69 | 101.06 | 103.90 |
| 32 | DB | 101 | G | C8-N9-C4 | 5.69 | 108.67 | 106.40 |
| 31 | BA | 272 | G | N1-C2-N2 | -5.68 | 111.08 | 116.20 |
| 31 | DA | 1948 | G | N3-C2-N2 | -5.68 | 115.92 | 119.90 |
| 31 | BA | 849 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 31 | BA | 2672 | G | C6-C5-N7 | -5.68 | 126.99 | 130.40 |
| 31 | DA | 656 | G | N3-C4-C5 | -5.68 | 125.76 | 128.60 |
| 31 | DA | 2778 | A | N1-C2-N3 | 5.68 | 132.14 | 129.30 |
| 31 | BA | 796 | C | C6-N1-C2 | 5.68 | 122.57 | 120.30 |
| 31 | BA | 53 | A | N1-C2-N3 | 5.68 | 132.14 | 129.30 |
| 31 | BA | 1652 | A | C4'-C3'-C2' | 5.68 | 108.28 | 102.60 |
| 31 | DA | 129 | C | C6-N1-C2 | 5.68 | 122.57 | 120.30 |
| 31 | DA | 1332 | G | C4-C5-N7 | 5.68 | 113.07 | 110.80 |
| 31 | DA | 2822 | G | C8-N9-C4 | 5.67 | 108.67 | 106.40 |
| 1 | AA | 810 | C | C6-N1-C2 | 5.67 | 122.57 | 120.30 |
| 31 | BA | 2256 | G | C4-C5-N7 | 5.67 | 113.07 | 110.80 |
| 31 | DA | 242 | G | C4-N9-C1' | -5.67 | 119.13 | 126.50 |
| 31 | DA | 494 | G | C2-N3-C4 | -5.67 | 109.07 | 111.90 |
| 31 | DA | 690 | G | N7-C8-N9 | -5.67 | 110.27 | 113.10 |
| 31 | DA | 1256 | G | C4-N9-C1' | 5.67 | 133.87 | 126.50 |
| 31 | DA | 1991 | U | C5-C6-N1 | -5.67 | 119.87 | 122.70 |
| 31 | DA | 463 | G | C5-C6-O6 | 5.67 | 132.00 | 128.60 |
| 31 | DA | 2253 | G | C6-C5-N7 | -5.66 | 127.00 | 130.40 |
| 32 | DB | 30 | C | C6-N1-C2 | -5.66 | 118.03 | 120.30 |
| 31 | DA | 1299 | G | N1-C6-O6 | 5.66 | 123.30 | 119.90 |
| 27 | B5 | 4 | HIS | C-N-CD | 5.66 | 140.29 | 128.40 |
| 31 | BA | 2247 | A | C2-N3-C4 | -5.66 | 107.77 | 110.60 |
| 31 | DA | 193 | U | C5-C4-O4 | -5.66 | 122.50 | 125.90 |
| 31 | DA | 2485 | G | N9-C4-C5 | -5.66 | 103.14 | 105.40 |
| 31 | BA | 945 | A | C5-N7-C8 | -5.66 | 101.07 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | DA | 1241 | A | N1-C2-N3 | 5.66 | 132.13 | 129.30 |
| 31 | DA | 2712 | U | N1-C2-N3 | 5.66 | 118.30 | 114.90 |
| 31 | BA | 1213 | A | C8-N9-C4 | -5.66 | 103.54 | 105.80 |
| 31 | DA | 353 | G | N3-C4-N9 | 5.66 | 129.39 | 126.00 |
| 31 | BA | 803 | U | C5-C6-N1 | -5.65 | 119.87 | 122.70 |
| 31 | DA | 739 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 31 | DA | 912 | C | C6-N1-C2 | -5.65 | 118.04 | 120.30 |
| 31 | BA | 132 | G | C5-C6-N1 | -5.65 | 108.67 | 111.50 |
| 31 | BA | 265 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 31 | DA | 2823 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 31 | BA | 1314 | C | C6-N1-C1' | -5.64 | 114.03 | 120.80 |
| 31 | DA | 2230 | G | N1-C6-O6 | 5.64 | 123.29 | 119.90 |
| 31 | DA | 465 | G | N7-C8-N9 | 5.64 | 115.92 | 113.10 |
| 31 | BA | 378 | C | N3-C4-C5 | 5.64 | 124.16 | 121.90 |
| 31 | DA | 2441 | C | C2-N1-C1' | -5.64 | 112.60 | 118.80 |
| 31 | BA | 1544 | A | N9-C1'-C2' | 5.63 | 121.32 | 114.00 |
| 31 | DA | 71 | A | C2-N3-C4 | -5.63 | 107.78 | 110.60 |
| 31 | DA | 1409 | C | C6-N1-C2 | 5.63 | 122.55 | 120.30 |
| 31 | BA | 2230 | G | N3-C2-N2 | -5.63 | 115.96 | 119.90 |
| 31 | BA | 2346 | A | C1'-O4'-C4' | -5.63 | 105.40 | 109.90 |
| 31 | BA | 673 | C | N3-C4-N4 | 5.63 | 121.94 | 118.00 |
| 41 | BP | 58 | THR | N-CA-C | -5.63 | 95.81 | 111.00 |
| 31 | DA | 1327 | C | N1-C2-O2 | -5.63 | 115.52 | 118.90 |
| 31 | DA | 2620 | C | N3-C4-C5 | 5.63 | 124.15 | 121.90 |
| 31 | DA | 762 | U | N3-C4-O4 | 5.62 | 123.34 | 119.40 |
| 31 | DA | 2009 | G | N9-C4-C5 | 5.62 | 107.65 | 105.40 |
| 31 | DA | 2009 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 31 | DA | 1775 | U | C5-C6-N1 | -5.62 | 119.89 | 122.70 |
| 31 | DA | 2430 | A | N3-C4-C5 | 5.62 | 130.73 | 126.80 |
| 31 | BA | 1574 | C | C6-N1-C2 | 5.62 | 122.55 | 120.30 |
| 31 | DA | 1653 | G | C8-N9-C1' | -5.62 | 119.70 | 127.00 |
| 31 | DA | 2414 | G | N1-C6-O6 | 5.62 | 123.27 | 119.90 |
| 31 | DA | 945 | A | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 31 | DA | 784 | A | C2-N3-C4 | -5.61 | 107.79 | 110.60 |
| 31 | BA | 783 | A | C5-C6-N1 | -5.61 | 114.89 | 117.70 |
| 31 | BA | 1605 | C | N3-C2-O2 | -5.61 | 117.97 | 121.90 |
| 31 | DA | 1247 | A | N1-C6-N6 | 5.61 | 121.97 | 118.60 |
| 31 | DA | 2497 | A | C8-N9-C4 | 5.61 | 108.04 | 105.80 |
| 31 | DA | 2678 | C | C5-C6-N1 | -5.61 | 118.19 | 121.00 |
| 31 | BA | 330 | A | N1-C6-N6 | 5.61 | 121.96 | 118.60 |
| 31 | DA | 1201 | C | C6-N1-C2 | 5.61 | 122.54 | 120.30 |
| 30 | B8 | 44 | LYS | CD-CE-NZ | 5.61 | 124.59 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31 | BA | 1204 | A | C3'-C2'-C1' | -5.61 | 97.02 | 101.50 |
| 31 | BA | 1675 | C | N1-C2-O2 | -5.60 | 115.54 | 118.90 |
| 31 | DA | 2814 | C | C2-N3-C4 | -5.60 | 117.10 | 119.90 |
| 31 | DA | 669 | G | C4-N9-C1' | -5.60 | 119.22 | 126.50 |
| 31 | BA | 2579 | C | C5-C6-N1 | -5.60 | 118.20 | 121.00 |
| 31 | DA | 83 | G | N3-C2-N2 | -5.60 | 115.98 | 119.90 |
| 47 | DV | 40 | LEU | CA-CB-CG | 5.60 | 128.18 | 115.30 |
| 48 | DW | 12 | ILE | N-CA-C | -5.60 | 95.88 | 111.00 |
| 31 | BA | 1314 | C | C2-N1-C1' | 5.60 | 124.96 | 118.80 |
| 31 | BA | 1607 | C | N3-C4-C5 | -5.60 | 119.66 | 121.90 |
| 31 | BA | 139(A) | G | C4-C5-N7 | 5.60 | 113.04 | 110.80 |
| 31 | BA | 1333 | C | C2-N3-C4 | -5.59 | 117.10 | 119.90 |
| 31 | DA | 209 | C | C6-N1-C2 | 5.59 | 122.54 | 120.30 |
| 31 | BA | 794 | G | C5-C6-O6 | 5.59 | 131.96 | 128.60 |
| 31 | BA | 1991 | U | N3-C2-O2 | 5.59 | 126.11 | 122.20 |
| 31 | DA | 1158 | C | C2-N1-C1' | 5.59 | 124.95 | 118.80 |
| 31 | DA | 509 | C | C2-N3-C4 | -5.59 | 117.11 | 119.90 |
| 31 | DA | 1614 | A | C5-C6-N1 | -5.59 | 114.91 | 117.70 |
| 31 | BA | 2702 | U | C5-C4-O4 | 5.59 | 129.25 | 125.90 |
| 31 | BA | 1782 | C | C5-C6-N1 | -5.58 | 118.21 | 121.00 |
| 31 | BA | 2699 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 31 | BA | 2073 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 31 | DA | 2468 | G | C8-N9-C1' | 5.58 | 134.26 | 127.00 |
| 31 | DA | 2599 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 31 | BA | 1742 | G | N1-C6-O6 | 5.58 | 123.25 | 119.90 |
| 31 | DA | 2518 | A | C2-N3-C4 | -5.58 | 107.81 | 110.60 |
| 31 | BA | 378 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 31 | BA | 2036 | C | N1-C2-O2 | -5.58 | 115.56 | 118.90 |
| 31 | BA | 2607 | G | N3-C4-N9 | 5.58 | 129.35 | 126.00 |
| 31 | BA | 353 | G | N3-C4-N9 | 5.57 | 129.34 | 126.00 |
| 31 | BA | 2702 | U | N3-C4-O4 | -5.57 | 115.50 | 119.40 |
| 31 | DA | 870 | A | C8-N9-C4 | 5.57 | 108.03 | 105.80 |
| 31 | DA | 945 | A | C5-N7-C8 | -5.57 | 101.11 | 103.90 |
| 31 | DA | 1304 | C | N3-C4-N4 | -5.57 | 114.10 | 118.00 |
| 31 | DA | 1784 | A | N1-C2-N3 | 5.57 | 132.09 | 129.30 |
| 31 | DA | 2502 | G | N3-C2-N2 | 5.57 | 123.80 | 119.90 |
| 31 | DA | 2413 | G | C2-N3-C4 | -5.57 | 109.11 | 111.90 |
| 31 | BA | 133 | C | C5-C6-N1 | -5.57 | 118.22 | 121.00 |
| 31 | BA | 1502 | C | C2-N1-C1' | 5.57 | 124.93 | 118.80 |
| 31 | DA | 2036 | C | N1-C2-O2 | -5.57 | 115.56 | 118.90 |
| 31 | BA | 196 | A | N9-C4-C5 | -5.57 | 103.57 | 105.80 |
| 31 | BA | 812 | C | N1-C2-O2 | -5.57 | 115.56 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | DA | 1997 | G | N1-C2-N2 | -5.57 | 111.19 | 116.20 |
| 31 | BA | 2542 | A | C4-C5-N7 | 5.57 | 113.48 | 110.70 |
| 31 | BA | 2590 | A | C2-N3-C4 | -5.57 | 107.82 | 110.60 |
| 31 | DA | 756 | C | C5-C6-N1 | -5.57 | 118.22 | 121.00 |
| 31 | DA | 2499 | C | C6-N1-C1' | -5.56 | 114.12 | 120.80 |
| 1 | AA | 108 | G | N9-C4-C5 | -5.56 | 103.18 | 105.40 |
| 1 | AA | 117 | G | C5-C6-O6 | -5.56 | 125.26 | 128.60 |
| 31 | DA | 1314 | C | C5-C4-N4 | -5.56 | 116.31 | 120.20 |
| 31 | DA | 2084 | C | C4-C5-C6 | 5.56 | 120.18 | 117.40 |
| 31 | DA | 1675 | C | C2-N1-C1' | -5.56 | 112.69 | 118.80 |
| 31 | BA | 1021 | A | C4-C5-N7 | 5.56 | 113.48 | 110.70 |
| 31 | BA | 2711 | A | N3-C4-C5 | 5.55 | 130.69 | 126.80 |
| 31 | BA | 1333 | C | C6-N1-C2 | 5.55 | 122.52 | 120.30 |
| 31 | DA | 1529 | G | C8-N9-C1' | -5.55 | 119.79 | 127.00 |
| 31 | BA | 2014 | A | N9-C4-C5 | -5.54 | 103.58 | 105.80 |
| 31 | DA | 1674 | G | N3-C4-C5 | -5.54 | 125.83 | 128.60 |
| 31 | BA | 124 | G | N1-C6-O6 | 5.54 | 123.22 | 119.90 |
| 47 | BV | 40 | LEU | CA-CB-CG | 5.54 | 128.05 | 115.30 |
| 31 | DA | 535 | C | C5-C6-N1 | -5.54 | 118.23 | 121.00 |
| 31 | DA | 2447 | G | N7-C8-N9 | -5.54 | 110.33 | 113.10 |
| 31 | DA | 389 | G | N9-C4-C5 | -5.54 | 103.18 | 105.40 |
| 31 | BA | 2024 | G | N7-C8-N9 | -5.53 | 110.33 | 113.10 |
| 31 | BA | 2283 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 31 | DA | 2607 | G | N1-C2-N2 | -5.53 | 111.22 | 116.20 |
| 31 | BA | 179 | G | C2-N3-C4 | -5.53 | 109.14 | 111.90 |
| 31 | BA | 1790 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 31 | DA | 2231 | C | C2-N1-C1' | -5.53 | 112.72 | 118.80 |
| 31 | DA | 2318 | G | C8-N9-C4 | -5.53 | 104.19 | 106.40 |
| 31 | BA | 1496 | A | C4-C5-N7 | 5.53 | 113.47 | 110.70 |
| 31 | DA | 1918 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 31 | BA | 2779 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 31 | DA | 1281 | G | N1-C6-O6 | 5.53 | 123.22 | 119.90 |
| 31 | DA | 2239 | G | N1-C2-N2 | -5.52 | 111.23 | 116.20 |
| 31 | BA | 676 | A | C5-C6-N1 | -5.52 | 114.94 | 117.70 |
| 31 | DA | 1565 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 31 | DA | 2481 | G | N1-C6-O6 | 5.52 | 123.21 | 119.90 |
| 31 | BA | 296 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 31 | BA | 566 | U | C2-N1-C1' | -5.52 | 111.08 | 117.70 |
| 31 | BA | 1397 | U | P-O3'-C3' | 5.52 | 126.32 | 119.70 |
| 31 | BA | 1496 | A | N1-C6-N6 | 5.52 | 121.91 | 118.60 |
| 31 | BA | 150 | C | C5-C6-N1 | -5.51 | 118.24 | 121.00 |
| 31 | DA | 1614 | A | N1-C6-N6 | 5.51 | 121.91 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | DA | 2468 | G | C4-N9-C1' | -5.51 | 119.33 | 126.50 |
| 31 | BA | 1267 | U | N1-C2-O2 | 5.51 | 126.66 | 122.80 |
| 31 | BA | 2392 | A | N7-C8-N9 | 5.51 | 116.56 | 113.80 |
| 31 | DA | 1336 | A | C5-C6-N1 | 5.51 | 120.46 | 117.70 |
| 31 | BA | 1162 | G | N1-C6-O6 | -5.51 | 116.59 | 119.90 |
| 31 | BA | 2432 | A | C5-C6-N6 | -5.51 | 119.29 | 123.70 |
| 31 | DA | 1786 | A | C5-C6-N1 | -5.51 | 114.94 | 117.70 |
| 31 | BA | 234 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 31 | DA | 930 | U | C5-C6-N1 | -5.51 | 119.95 | 122.70 |
| 31 | DA | 1012 | U | N3-C2-O2 | -5.51 | 118.35 | 122.20 |
| 31 | BA | 788 | A | N9-C4-C5 | -5.50 | 103.60 | 105.80 |
| 31 | DA | 2741 | A | N7-C8-N9 | -5.50 | 111.05 | 113.80 |
| 31 | BA | 621 | A | C2-N3-C4 | -5.50 | 107.85 | 110.60 |
| 31 | BA | 1343 | G | C8-N9-C1' | -5.50 | 119.85 | 127.00 |
| 31 | BA | 2426 | A | N1-C6-N6 | 5.50 | 121.90 | 118.60 |
| 31 | BA | 2429 | G | C8-N9-C4 | -5.50 | 104.20 | 106.40 |
| 31 | BA | 2572 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 31 | DA | 2040 | C | C6-N1-C2 | 5.50 | 122.50 | 120.30 |
| 31 | BA | 287 | C | C6-N1-C2 | 5.50 | 122.50 | 120.30 |
| 31 | BA | 2432 | A | C4-C5-N7 | 5.50 | 113.45 | 110.70 |
| 31 | BA | 1934 | C | C4'-C3'-C2' | 5.49 | 108.09 | 102.60 |
| 31 | DA | 2385 | C | N1-C2-O2 | -5.49 | 115.60 | 118.90 |
| 31 | DA | 2563 | U | C5-C6-N1 | -5.49 | 119.95 | 122.70 |
| 31 | BA | 189 | G | N1-C6-O6 | 5.49 | 123.19 | 119.90 |
| 31 | BA | 455 | C | N3-C4-C5 | 5.49 | 124.10 | 121.90 |
| 31 | BA | 527 | C | C2-N3-C4 | -5.49 | 117.16 | 119.90 |
| 42 | BQ | 82 | ARG | NE-CZ-NH2 | -5.49 | 117.55 | 120.30 |
| 31 | DA | 2027 | G | C8-N9-C4 | -5.49 | 104.20 | 106.40 |
| 31 | BA | 1201 | C | C5-C4-N4 | -5.49 | 116.36 | 120.20 |
| 31 | BA | 1340 | U | C2-N3-C4 | -5.49 | 123.71 | 127.00 |
| 31 | BA | 2080 | G | C5-C6-O6 | -5.49 | 125.31 | 128.60 |
| 35 | BF | 68 | LYS | N-CA-C | 5.49 | 125.82 | 111.00 |
| 31 | BA | 2392 | A | C6-C5-N7 | -5.49 | 128.46 | 132.30 |
| 31 | BA | 467 | G | C8-N9-C4 | 5.49 | 108.59 | 106.40 |
| 31 | BA | 1609 | A | N1-C2-N3 | 5.49 | 132.04 | 129.30 |
| 31 | BA | 2281 | C | N1-C2-O2 | -5.49 | 115.61 | 118.90 |
| 31 | BA | 2665 | A | C6-C5-N7 | -5.49 | 128.46 | 132.30 |
| 31 | DA | 783 | A | N7-C8-N9 | 5.49 | 116.54 | 113.80 |
| 31 | BA | 226 | G | C5-C6-O6 | -5.48 | 125.31 | 128.60 |
| 31 | DA | 933 | A | C5-C6-N1 | -5.48 | 114.96 | 117.70 |
| 31 | BA | 395 | U | N3-C2-O2 | -5.48 | 118.36 | 122.20 |
| 31 | BA | 748 | G | N7-C8-N9 | -5.48 | 110.36 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | DA | 2433 | A | C2-N3-C4 | -5.48 | 107.86 | 110.60 |
| 31 | DA | 651 | G | C4-N9-C1' | 5.48 | 133.62 | 126.50 |
| 31 | BA | 1774 | C | N3-C2-O2 | 5.48 | 125.73 | 121.90 |
| 31 | DA | 774 | A | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 31 | DA | 2587 | A | C4-C5-C6 | 5.47 | 119.74 | 117.00 |
| 1 | AA | 1442 | G | C4-N9-C1' | 5.47 | 133.62 | 126.50 |
| 31 | DA | 1833 | U | N1-C2-O2 | -5.47 | 118.97 | 122.80 |
| 31 | DA | 2820 | A | C2-N3-C4 | -5.47 | 107.86 | 110.60 |
| 41 | DP | 53 | GLY | N-CA-C | -5.47 | 99.42 | 113.10 |
| 31 | BA | 1846 | G | N1-C6-O6 | 5.47 | 123.18 | 119.90 |
| 31 | DA | 2522 | U | C6-N1-C2 | 5.47 | 124.28 | 121.00 |
| 31 | BA | 16 | G | N1-C6-O6 | 5.47 | 123.18 | 119.90 |
| 31 | BA | 1291 | C | C6-N1-C2 | 5.47 | 122.49 | 120.30 |
| 31 | BA | 1904 | G | C8-N9-C4 | 5.47 | 108.59 | 106.40 |
| 31 | BA | 2061 | G | N1-C6-O6 | -5.47 | 116.62 | 119.90 |
| 31 | BA | 2715 | C | C5-C6-N1 | -5.47 | 118.27 | 121.00 |
| 31 | BA | 2441 | C | C2-N3-C4 | -5.46 | 117.17 | 119.90 |
| 31 | BA | 451 | C | N3-C2-O2 | 5.46 | 125.72 | 121.90 |
| 31 | DA | 801 | G | C5-C6-O6 | 5.46 | 131.88 | 128.60 |
| 31 | BA | 128 | C | C5-C4-N4 | -5.46 | 116.38 | 120.20 |
| 31 | BA | 1189 | A | N1-C6-N6 | 5.46 | 121.88 | 118.60 |
| 31 | BA | 1653 | G | C8-N9-C1' | -5.46 | 119.90 | 127.00 |
| 31 | DA | 1616 | A | C8-N9-C4 | -5.46 | 103.62 | 105.80 |
| 31 | DA | 2678 | C | C6-N1-C2 | 5.46 | 122.48 | 120.30 |
| 31 | BA | 114 | U | C2-N1-C1' | 5.45 | 124.24 | 117.70 |
| 31 | BA | 805 | G | C6-C5-N7 | -5.45 | 127.13 | 130.40 |
| 31 | BA | 976 | C | N3-C2-O2 | -5.45 | 118.08 | 121.90 |
| 31 | DA | 594 | U | C2-N3-C4 | -5.45 | 123.73 | 127.00 |
| 31 | DA | 2318 | G | C4-N9-C1' | 5.45 | 133.59 | 126.50 |
| 31 | DA | 2544 | G | C6-C5-N7 | -5.45 | 127.13 | 130.40 |
| 31 | DA | 2030 | A | N1-C6-N6 | 5.45 | 121.87 | 118.60 |
| 31 | BA | 2422 | A | N9-C4-C5 | 5.45 | 107.98 | 105.80 |
| 31 | DA | 600 | G | C2-N3-C4 | -5.45 | 109.18 | 111.90 |
| 51 | DZ | 110 | GLY | N-CA-C | -5.45 | 99.48 | 113.10 |
| 31 | BA | 1020 | A | C8-N9-C4 | -5.45 | 103.62 | 105.80 |
| 31 | DA | 2619 | C | C5-C6-N1 | -5.45 | 118.28 | 121.00 |
| 31 | DA | 2244 | U | C5-C6-N1 | -5.44 | 119.98 | 122.70 |
| 31 | DA | 2595 | G | C8-N9-C4 | 5.44 | 108.58 | 106.40 |
| 31 | BA | 512 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 31 | BA | 669 | G | C6-C5-N7 | 5.44 | 133.66 | 130.40 |
| 31 | BA | 1204 | A | C1'-O4'-C4' | -5.44 | 105.55 | 109.90 |
| 31 | BA | 1970 | A | N1-C6-N6 | 5.44 | 121.86 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | DA | 330 | A | C8-N9-C4 | 5.44 | 107.98 | 105.80 |
| 31 | DA | 1371 | G | N1-C6-O6 | 5.44 | 123.16 | 119.90 |
| 31 | DA | 1682 | G | C8-N9-C4 | 5.44 | 108.58 | 106.40 |
| 31 | DA | 2352 | A | C2-N3-C4 | -5.44 | 107.88 | 110.60 |
| 31 | DA | 2607 | G | C6-C5-N7 | -5.44 | 127.14 | 130.40 |
| 32 | DB | 81 | G | N1-C6-O6 | 5.44 | 123.16 | 119.90 |
| 31 | BA | 789 | A | N1-C6-N6 | -5.44 | 115.34 | 118.60 |
| 31 | BA | 1207 | C | N3-C2-O2 | 5.44 | 125.70 | 121.90 |
| 31 | DA | 133 | C | N3-C4-C5 | 5.44 | 124.07 | 121.90 |
| 31 | DA | 762 | U | C2-N1-C1' | 5.43 | 124.22 | 117.70 |
| 31 | BA | 141 | A | C4-C5-C6 | 5.43 | 119.72 | 117.00 |
| 31 | DA | 461 | C | N1-C2-O2 | -5.43 | 115.64 | 118.90 |
| 31 | DA | 2346 | A | C1'-O4'-C4' | -5.43 | 105.55 | 109.90 |
| 31 | BA | 1336 | A | C6-N1-C2 | -5.43 | 115.34 | 118.60 |
| 31 | BA | 1755 | A | N1-C6-N6 | -5.43 | 115.34 | 118.60 |
| 31 | DA | 2463 | C | N3-C4-C5 | 5.43 | 124.07 | 121.90 |
| 31 | BA | 2085 | C | C5-C6-N1 | -5.43 | 118.29 | 121.00 |
| 31 | BA | 2715 | C | C2-N3-C4 | -5.43 | 117.19 | 119.90 |
| 31 | DA | 1797 | C | C5-C6-N1 | -5.42 | 118.29 | 121.00 |
| 31 | DA | 2814 | C | C5-C6-N1 | -5.42 | 118.29 | 121.00 |
| 31 | BA | 2201 | C | C5-C6-N1 | -5.42 | 118.29 | 121.00 |
| 31 | BA | 2374 | C | C5-C6-N1 | -5.42 | 118.29 | 121.00 |
| 31 | BA | 2736 | G | C4-N9-C1' | -5.42 | 119.45 | 126.50 |
| 31 | BA | 531 | C | C5-C6-N1 | -5.42 | 118.29 | 121.00 |
| 31 | BA | 2232 | U | C5-C6-N1 | -5.42 | 119.99 | 122.70 |
| 31 | DA | 856 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 31 | DA | 1833 | U | N3-C2-O2 | 5.42 | 125.99 | 122.20 |
| 31 | DA | 1270 | C | N1-C2-O2 | -5.41 | 115.65 | 118.90 |
| 31 | BA | 527 | C | N1-C2-N3 | 5.41 | 122.99 | 119.20 |
| 32 | BB | 27 | C | C2-N1-C1' | 5.41 | 124.75 | 118.80 |
| 31 | DA | 445 | C | C2-N3-C4 | -5.41 | 117.19 | 119.90 |
| 31 | DA | 2774 | C | N3-C4-C5 | 5.41 | 124.06 | 121.90 |
| 31 | BA | 1614 | A | C4-C5-N7 | 5.41 | 113.41 | 110.70 |
| 31 | BA | 2518 | A | C8-N9-C4 | -5.41 | 103.64 | 105.80 |
| 31 | BA | 542 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 31 | DA | 2579 | C | N3-C2-O2 | 5.41 | 125.69 | 121.90 |
| 31 | BA | 2346 | A | N1-C6-N6 | 5.41 | 121.84 | 118.60 |
| 31 | DA | 1674 | G | C4-N9-C1' | 5.41 | 133.53 | 126.50 |
| 31 | BA | 1674 | G | N3-C4-N9 | 5.40 | 129.24 | 126.00 |
| 31 | BA | 2319 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 31 | BA | 2399 | G | C6-C5-N7 | -5.40 | 127.16 | 130.40 |
| 31 | DA | 2399 | G | N3-C4-C5 | -5.40 | 125.90 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | BA | 192 | C | N1-C2-O2 | -5.40 | 115.66 | 118.90 |
| 31 | BA | 386 | G | C5-C6-O6 | -5.40 | 125.36 | 128.60 |
| 34 | BE | 136 | ARG | NE-CZ-NH1 | -5.40 | 117.60 | 120.30 |
| 1 | CA | 1519 | A | C5-C6-N6 | 5.40 | 128.02 | 123.70 |
| 30 | B8 | 49 | VAL | N-CA-C | -5.40 | 96.42 | 111.00 |
| 31 | BA | 475 | U | C2-N1-C1' | 5.40 | 124.18 | 117.70 |
| 31 | BA | 1349 | A | N7-C8-N9 | 5.40 | 116.50 | 113.80 |
| 31 | BA | 2253 | G | N9-C4-C5 | -5.40 | 103.24 | 105.40 |
| 31 | BA | 529 | A | C4-C5-N7 | 5.40 | 113.40 | 110.70 |
| 1 | AA | 108 | G | C4-C5-N7 | 5.39 | 112.96 | 110.80 |
| 31 | BA | 577 | G | C8-N9-C4 | 5.39 | 108.56 | 106.40 |
| 31 | BA | 1681 | G | N3-C4-C5 | 5.39 | 131.30 | 128.60 |
| 31 | DA | 2055 | C | N3-C4-C5 | 5.39 | 124.06 | 121.90 |
| 31 | DA | 2293 | C | N3-C4-C5 | 5.39 | 124.06 | 121.90 |
| 31 | BA | 640 | C | N3-C4-C5 | -5.39 | 119.74 | 121.90 |
| 31 | BA | 2399 | G | N3-C4-C5 | -5.39 | 125.90 | 128.60 |
| 31 | DA | 1786 | A | C8-N9-C4 | -5.39 | 103.64 | 105.80 |
| 32 | DB | 27 | C | N1-C2-O2 | 5.39 | 122.14 | 118.90 |
| 31 | BA | 2196 | C | C6-N1-C2 | 5.39 | 122.46 | 120.30 |
| 31 | DA | 530 | G | N3-C4-C5 | 5.39 | 131.29 | 128.60 |
| 31 | BA | 1694 | C | C5-C4-N4 | -5.39 | 116.43 | 120.20 |
| 31 | BA | 2240 | C | C5-C4-N4 | -5.39 | 116.43 | 120.20 |
| 31 | DA | 1210 | A | N7-C8-N9 | 5.39 | 116.50 | 113.80 |
| 31 | BA | 1674 | G | C8-N9-C4 | -5.39 | 104.25 | 106.40 |
| 31 | BA | 2600 | A | C5-N7-C8 | 5.39 | 106.59 | 103.90 |
| 49 | BX | 62 | LYS | N-CA-C | 5.39 | 125.55 | 111.00 |
| 31 | DA | 446 | G | C8-N9-C4 | 5.38 | 108.55 | 106.40 |
| 31 | DA | 1340 | U | C2-N3-C4 | -5.38 | 123.77 | 127.00 |
| 31 | BA | 682 | G | N3-C2-N2 | 5.38 | 123.67 | 119.90 |
| 31 | BA | 930 | U | C5-C4-O4 | 5.38 | 129.13 | 125.90 |
| 31 | DA | 265 | A | C6-C5-N7 | -5.38 | 128.53 | 132.30 |
| 31 | BA | 1918 | A | C8-N9-C4 | 5.38 | 107.95 | 105.80 |
| 31 | DA | 859 | G | C4-N9-C1' | -5.38 | 119.51 | 126.50 |
| 31 | DA | 948 | G | N3-C4-C5 | 5.38 | 131.29 | 128.60 |
| 31 | DA | 2455 | G | N1-C6-O6 | 5.38 | 123.12 | 119.90 |
| 31 | BA | 527 | C | C5-C4-N4 | 5.37 | 123.96 | 120.20 |
| 31 | DA | 584 | C | N1-C2-O2 | -5.37 | 115.67 | 118.90 |
| 31 | DA | 2485 | G | N3-C4-N9 | 5.37 | 129.22 | 126.00 |
| 1 | AA | 1502 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |
| 31 | BA | 1617 | C | C4-C5-C6 | 5.37 | 120.09 | 117.40 |
| 31 | BA | 2363 | C | C2-N1-C1' | -5.37 | 112.89 | 118.80 |
| 31 | DA | 2330 | G | N7-C8-N9 | -5.37 | 110.42 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31 | DA | 783 | A | N3-C4-N9 | -5.37 | 123.10 | 127.40 |
| 31 | BA | 791 | C | C6-N1-C2 | 5.37 | 122.45 | 120.30 |
| 31 | BA | 1694 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 35 | DF | 68 | LYS | N-CA-C | 5.37 | 125.49 | 111.00 |
| 31 | DA | 1559 | G | N1-C6-O6 | 5.37 | 123.12 | 119.90 |
| 31 | DA | 2495 | G | C8-N9-C4 | 5.37 | 108.55 | 106.40 |
| 31 | BA | 481 | G | N3-C4-C5 | -5.37 | 125.92 | 128.60 |
| 31 | BA | 1558 | A | N1-C2-N3 | 5.37 | 131.98 | 129.30 |
| 31 | BA | 1653 | G | C5-N7-C8 | 5.37 | 106.98 | 104.30 |
| 31 | DA | 444 | C | C2-N3-C4 | -5.37 | 117.22 | 119.90 |
| 45 | DT | 23 | ARG | NE-CZ-NH2 | -5.37 | 117.62 | 120.30 |
| 31 | BA | 2433 | A | N1-C2-N3 | 5.36 | 131.98 | 129.30 |
| 31 | BA | 2538 | C | C5-C6-N1 | -5.36 | 118.32 | 121.00 |
| 31 | DA | 773 | U | C5-C6-N1 | -5.36 | 120.02 | 122.70 |
| 31 | DA | 1256 | G | N3-C4-C5 | -5.36 | 125.92 | 128.60 |
| 31 | DA | 1349 | A | C6-C5-N7 | -5.36 | 128.55 | 132.30 |
| 31 | DA | 1340 | U | C5-C6-N1 | -5.36 | 120.02 | 122.70 |
| 31 | BA | 1529 | G | C8-N9-C1' | -5.36 | 120.03 | 127.00 |
| 48 | DW | 6 | ILE | CB-CA-C | -5.36 | 100.88 | 111.60 |
| 31 | BA | 2014 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 31 | BA | 2724 | C | N1-C2-O2 | -5.36 | 115.68 | 118.90 |
| 31 | DA | 1934 | C | C4'-C3'-C2' | 5.36 | 107.96 | 102.60 |
| 31 | DA | 2037 | G | C6-N1-C2 | -5.36 | 121.89 | 125.10 |
| 31 | BA | 1674 | G | C4-N9-C1' | 5.36 | 133.47 | 126.50 |
| 31 | BA | 843 | G | C8-N9-C4 | 5.36 | 108.54 | 106.40 |
| 31 | BA | 2688 | U | C4-C5-C6 | 5.36 | 122.91 | 119.70 |
| 31 | DA | 2686 | G | C8-N9-C4 | -5.36 | 104.26 | 106.40 |
| 23 | D1 | 55 | GLY | N-CA-C | -5.35 | 99.72 | 113.10 |
| 31 | DA | 1397 | U | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 31 | DA | 1771 | C | C2-N3-C4 | -5.35 | 117.22 | 119.90 |
| 31 | BA | 272(C) | G | C8-N9-C4 | 5.35 | 108.54 | 106.40 |
| 31 | BA | 729 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 31 | BA | 2439 | A | C5-N7-C8 | -5.35 | 101.22 | 103.90 |
| 31 | DA | 791 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 1 | AA | 43 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 31 | BA | 104 | U | N1-C2-O2 | -5.35 | 119.06 | 122.80 |
| 31 | BA | 2751 | G | C4-N9-C1' | 5.35 | 133.46 | 126.50 |
| 29 | D7 | 34 | ARG | NE-CZ-NH1 | -5.35 | 117.63 | 120.30 |
| 31 | DA | 856 | C | C6-N1-C1' | -5.35 | 114.38 | 120.80 |
| 31 | DA | 1328 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 23 | B1 | 55 | GLY | N-CA-C | -5.35 | 99.73 | 113.10 |
| 31 | BA | 612 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 31 | BA | 1616 | A | C4-N9-C1' | 5.35 | 135.92 | 126.30 |
| 31 | BA | 2318 | G | C5-N7-C8 | -5.35 | 101.63 | 104.30 |
| 31 | DA | 1962 | C | C6-N1-C1' | -5.35 | 114.38 | 120.80 |
| 31 | DA | 2383 | G | N1-C6-O6 | -5.35 | 116.69 | 119.90 |
| 31 | BA | 686 | G | C6-C5-N7 | -5.35 | 127.19 | 130.40 |
| 31 | DA | 676 | A | N3-C4-C5 | 5.35 | 130.54 | 126.80 |
| 31 | DA | 755 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 31 | BA | 1310 | G | C4-C5-N7 | -5.34 | 108.66 | 110.80 |
| 31 | BA | 1349 | A | C6-C5-N7 | -5.34 | 128.56 | 132.30 |
| 31 | BA | 2059 | A | C8-N9-C4 | 5.34 | 107.94 | 105.80 |
| 31 | DA | 2225 | A | C8-N9-C4 | -5.34 | 103.66 | 105.80 |
| 31 | BA | 2618 | G | C8-N9-C4 | -5.34 | 104.26 | 106.40 |
| 31 | DA | 452 | G | C5-C6-O6 | -5.34 | 125.39 | 128.60 |
| 31 | DA | 2736 | G | C4-N9-C1' | -5.34 | 119.56 | 126.50 |
| 31 | DA | 1397 | U | N1-C2-N3 | 5.34 | 118.10 | 114.90 |
| 30 | D8 | 49 | VAL | N-CA-C | -5.34 | 96.59 | 111.00 |
| 31 | BA | 128 | C | C2-N3-C4 | -5.34 | 117.23 | 119.90 |
| 32 | DB | 99 | G | C8-N9-C4 | 5.34 | 108.53 | 106.40 |
| 1 | CA | 1442 | G | C4-N9-C1' | 5.33 | 133.44 | 126.50 |
| 31 | DA | 591 | C | C4-C5-C6 | 5.33 | 120.07 | 117.40 |
| 31 | BA | 2431 | U | C5-C6-N1 | -5.33 | 120.03 | 122.70 |
| 31 | DA | 1244 | G | N3-C4-C5 | 5.33 | 131.27 | 128.60 |
| 31 | DA | 2779 | U | C5-C6-N1 | -5.33 | 120.03 | 122.70 |
| 31 | BA | 2542 | A | C6-C5-N7 | -5.33 | 128.57 | 132.30 |
| 31 | DA | 2827 | C | C5-C6-N1 | -5.33 | 118.33 | 121.00 |
| 31 | BA | 1279 | G | N9-C4-C5 | 5.33 | 107.53 | 105.40 |
| 31 | BA | 2031 | A | C8-N9-C4 | -5.33 | 103.67 | 105.80 |
| 31 | DA | 2607 | G | C8-N9-C1' | -5.33 | 120.08 | 127.00 |
| 31 | DA | 580 | C | N3-C2-O2 | 5.32 | 125.63 | 121.90 |
| 31 | DA | 1985 | G | N1-C2-N3 | 5.32 | 127.09 | 123.90 |
| 31 | DA | 2447 | G | C6-N1-C2 | -5.32 | 121.91 | 125.10 |
| 31 | BA | 585 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 31 | BA | 2048 | G | N9-C4-C5 | 5.32 | 107.53 | 105.40 |
| 27 | B5 | 46 | CYS | N-CA-C | 5.32 | 125.37 | 111.00 |
| 31 | BA | 272(B) | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 31 | BA | 676 | A | N3-C4-N9 | -5.32 | 123.14 | 127.40 |
| 45 | BT | 80 | SER | N-CA-C | 5.32 | 125.37 | 111.00 |
| 31 | DA | 1611 | C | C5-C4-N4 | -5.32 | 116.48 | 120.20 |
| 31 | DA | 1653 | G | N3-C4-N9 | 5.32 | 129.19 | 126.00 |
| 31 | BA | 83 | G | N3-C2-N2 | -5.32 | 116.18 | 119.90 |
| 27 | D5 | 46 | CYS | N-CA-C | 5.32 | 125.36 | 111.00 |
| 31 | DA | 523 | C | N1-C2-O2 | -5.32 | 115.71 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 31 | DA | 587 | C | N3-C2-O2 | -5.31 | 118.18 | 121.90 |
| 31 | BA | 1602 | U | C4-C5-C6 | 5.31 | 122.89 | 119.70 |
| 31 | DA | 1332 | G | C4-C5-C6 | -5.31 | 115.61 | 118.80 |
| 31 | DA | 1485 | G | N3-C4-N9 | 5.31 | 129.19 | 126.00 |
| 31 | DA | 1762 | A | N7-C8-N9 | 5.31 | 116.46 | 113.80 |
| 31 | BA | 1328 | G | C5-C6-O6 | -5.31 | 125.41 | 128.60 |
| 31 | DA | 2050 | C | C5-C6-N1 | -5.31 | 118.34 | 121.00 |
| 31 | BA | 669 | G | C4-N9-C1' | -5.31 | 119.60 | 126.50 |
| 31 | BA | 945 | A | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |
| 31 | BA | 2436 | G | N9-C4-C5 | 5.31 | 107.52 | 105.40 |
| 31 | BA | 2571 | C | C2-N1-C1' | 5.31 | 124.64 | 118.80 |
| 31 | DA | 24 | G | C5-C6-N1 | -5.31 | 108.84 | 111.50 |
| 31 | BA | 389 | G | C8-N9-C4 | 5.31 | 108.52 | 106.40 |
| 31 | BA | 2713 | A | N3-C4-C5 | 5.31 | 130.51 | 126.80 |
| 41 | BP | 47 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 31 | DA | 1681 | G | N1-C6-O6 | 5.31 | 123.08 | 119.90 |
| 31 | DA | 2424 | C | C5-C6-N1 | -5.31 | 118.35 | 121.00 |
| 31 | DA | 2547 | U | C5-C6-N1 | -5.31 | 120.05 | 122.70 |
| 31 | BA | 495 | G | C4-C5-N7 | -5.30 | 108.68 | 110.80 |
| 31 | BA | 1213 | A | N7-C8-N9 | 5.30 | 116.45 | 113.80 |
| 31 | BA | 2700 | C | C6-N1-C2 | 5.30 | 122.42 | 120.30 |
| 31 | DA | 1328 | G | C6-N1-C2 | -5.30 | 121.92 | 125.10 |
| 31 | DA | 2043 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 31 | BA | 1939 | U | N3-C4-C5 | 5.30 | 117.78 | 114.60 |
| 31 | BA | 2729 | G | N1-C6-O6 | 5.30 | 123.08 | 119.90 |
| 31 | DA | 2841 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 41 | DP | 52 | GLU | N-CA-C | 5.30 | 125.31 | 111.00 |
| 31 | BA | 949 | C | C5-C6-N1 | -5.30 | 118.35 | 121.00 |
| 31 | BA | 860 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 31 | DA | 1378 | A | N1-C6-N6 | -5.29 | 115.42 | 118.60 |
| 31 | BA | 962 | G | N1-C6-O6 | 5.29 | 123.08 | 119.90 |
| 1 | CA | 495 | A | N1-C6-N6 | -5.29 | 115.42 | 118.60 |
| 31 | BA | 1674 | G | C5-C6-O6 | -5.29 | 125.42 | 128.60 |
| 31 | BA | 2383 | G | C4-N9-C1' | 5.29 | 133.38 | 126.50 |
| 31 | DA | 736 | C | N1-C2-O2 | -5.29 | 115.73 | 118.90 |
| 31 | DA | 272 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |
| 31 | DA | 1033 | U | C2-N1-C1' | 5.29 | 124.05 | 117.70 |
| 31 | DA | 2363 | C | C6-N1-C2 | 5.29 | 122.42 | 120.30 |
| 31 | BA | 1495 | A | C4-C5-N7 | 5.29 | 113.34 | 110.70 |
| 31 | DA | 673 | C | C6-N1-C2 | 5.29 | 122.41 | 120.30 |
| 31 | DA | 1962 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 31 | DA | 2452 | C | C5-C4-N4 | -5.29 | 116.50 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 31 | DA | 2429 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 31 | DA | 2607 | G | N3-C4-N9 | 5.28 | 129.17 | 126.00 |
| 1 | AA | 139 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 31 | BA | 330 | A | N3-C4-N9 | -5.28 | 123.17 | 127.40 |
| 31 | DA | 791 | C | C2-N3-C4 | -5.28 | 117.26 | 119.90 |
| 31 | BA | 864 | G | C2-N3-C4 | 5.28 | 114.54 | 111.90 |
| 31 | BA | 2688 | U | N1-C2-N3 | 5.28 | 118.07 | 114.90 |
| 31 | DA | 864 | G | C2-N3-C4 | 5.28 | 114.54 | 111.90 |
| 31 | DA | 1301 | A | N1-C6-N6 | 5.28 | 121.77 | 118.60 |
| 1 | CA | 1429 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 31 | BA | 2059 | A | C2-N3-C4 | -5.28 | 107.96 | 110.60 |
| 31 | DA | 2440 | C | C2-N1-C1' | -5.28 | 112.99 | 118.80 |
| 31 | DA | 2518 | A | C5-C6-N6 | -5.28 | 119.48 | 123.70 |
| 41 | DP | 58 | THR | N-CA-C | -5.28 | 96.75 | 111.00 |
| 31 | BA | 2475 | C | C5-C6-N1 | 5.28 | 123.64 | 121.00 |
| 31 | BA | 1559 | G | N3-C4-C5 | 5.27 | 131.24 | 128.60 |
| 31 | DA | 985 | C | C5-C6-N1 | -5.27 | 118.36 | 121.00 |
| 31 | DA | 1363 | C | C2-N1-C1' | -5.27 | 113.00 | 118.80 |
| 31 | DA | 1653 | G | C4-C5-C6 | 5.27 | 121.97 | 118.80 |
| 31 | BA | 1989 | G | N1-C6-O6 | 5.27 | 123.06 | 119.90 |
| 31 | BA | 673 | C | C6-N1-C2 | 5.27 | 122.41 | 120.30 |
| 31 | BA | 2433 | A | C2-N3-C4 | -5.27 | 107.97 | 110.60 |
| 31 | BA | 2819 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 31 | DA | 1674 | G | C8-N9-C1' | -5.27 | 120.15 | 127.00 |
| 31 | BA | 827 | U | N3-C2-O2 | 5.26 | 125.89 | 122.20 |
| 31 | DA | 1543 | C | N3-C4-N4 | 5.26 | 121.69 | 118.00 |
| 31 | DA | 2477 | C | N3-C4-C5 | -5.26 | 119.79 | 121.90 |
| 31 | DA | 814 | C | C6-N1-C2 | 5.26 | 122.41 | 120.30 |
| 31 | BA | 1829 | A | C2-N3-C4 | -5.26 | 107.97 | 110.60 |
| 31 | BA | 1833 | U | N1-C2-O2 | -5.26 | 119.12 | 122.80 |
| 31 | DA | 843 | G | C8-N9-C4 | 5.26 | 108.50 | 106.40 |
| 31 | BA | 678 | C | C2-N3-C4 | -5.26 | 117.27 | 119.90 |
| 31 | BA | 1142(A) | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 31 | BA | 2231 | C | C6-N1-C2 | 5.26 | 122.40 | 120.30 |
| 31 | BA | 2612 | C | C6-N1-C2 | 5.26 | 122.40 | 120.30 |
| 31 | BA | 2278 | A | N9-C4-C5 | 5.26 | 107.90 | 105.80 |
| 31 | DA | 1827 | C | C2-N3-C4 | -5.25 | 117.27 | 119.90 |
| 31 | DA | 2779 | U | N1-C2-N3 | 5.25 | 118.05 | 114.90 |
| 31 | BA | 587 | C | N3-C2-O2 | -5.25 | 118.22 | 121.90 |
| 31 | BA | 1496 | A | C8-N9-C1' | -5.25 | 118.25 | 127.70 |
| 31 | BA | 2346 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 31 | DA | 1286 | A | N9-C4-C5 | 5.25 | 107.90 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | DA | 1698 | A | N7-C8-N9 | 5.25 | 116.43 | 113.80 |
| 31 | DA | 2329 | G | C8-N9-C4 | 5.25 | 108.50 | 106.40 |
| 31 | DA | 2443 | C | N3-C4-N4 | 5.25 | 121.68 | 118.00 |
| 31 | BA | 1942 | C | N1-C2-O2 | -5.25 | 115.75 | 118.90 |
| 31 | BA | 933 | A | N1-C6-N6 | 5.25 | 121.75 | 118.60 |
| 31 | DA | 1797 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 31 | DA | 2037 | G | N1-C2-N3 | 5.25 | 127.05 | 123.90 |
| 31 | DA | 2711 | A | N3-C4-C5 | 5.25 | 130.47 | 126.80 |
| 31 | BA | 518 | G | N3-C4-C5 | -5.25 | 125.98 | 128.60 |
| 31 | BA | 1678 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 31 | DA | 1332 | G | C6-N1-C2 | 5.25 | 128.25 | 125.10 |
| 31 | DA | 2395 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 31 | BA | 1238 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |
| 31 | DA | 843 | G | N7-C8-N9 | -5.24 | 110.48 | 113.10 |
| 31 | DA | 1343 | G | C4-N9-C1' | 5.24 | 133.31 | 126.50 |
| 31 | DA | 1662 | C | N3-C4-C5 | 5.24 | 124.00 | 121.90 |
| 31 | DA | 1193 | G | N1-C6-O6 | 5.24 | 123.05 | 119.90 |
| 31 | DA | 1349 | A | C2-N3-C4 | -5.24 | 107.98 | 110.60 |
| 1 | AA | 34 | C | C6-N1-C2 | 5.24 | 122.39 | 120.30 |
| 31 | BA | 1698 | A | C3'-C2'-C1' | -5.24 | 97.31 | 101.50 |
| 1 | CA | 909 | A | C8-N9-C4 | 5.24 | 107.89 | 105.80 |
| 31 | DA | 192 | C | N1-C2-O2 | -5.24 | 115.76 | 118.90 |
| 31 | BA | 2085 | C | C4-C5-C6 | 5.24 | 120.02 | 117.40 |
| 31 | BA | 565 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 31 | BA | 2070 | G | C5-C6-O6 | -5.23 | 125.46 | 128.60 |
| 31 | BA | 2201 | C | N3-C4-N4 | -5.23 | 114.34 | 118.00 |
| 31 | DA | 1674 | G | N3-C4-N9 | 5.23 | 129.14 | 126.00 |
| 31 | DA | 1682 | G | N9-C4-C5 | -5.23 | 103.31 | 105.40 |
| 31 | BA | 1338 | G | C5-C6-O6 | -5.23 | 125.46 | 128.60 |
| 31 | BA | 774 | A | C3'-C2'-C1' | 5.23 | 105.68 | 101.50 |
| 31 | BA | 2685 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 31 | BA | 2258 | C | N3-C2-O2 | 5.23 | 125.56 | 121.90 |
| 31 | DA | 1163 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 31 | BA | 209 | C | C5-C6-N1 | -5.23 | 118.39 | 121.00 |
| 31 | BA | 2512 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 31 | DA | 2065 | C | C6-N1-C2 | 5.23 | 122.39 | 120.30 |
| 31 | DA | 2599 | G | C5-C6-O6 | 5.23 | 131.74 | 128.60 |
| 31 | BA | 643 | A | C4-C5-C6 | 5.23 | 119.61 | 117.00 |
| 31 | BA | 661 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 31 | BA | 1658 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 31 | DA | 1281 | G | C5-C6-O6 | -5.23 | 125.46 | 128.60 |
| 31 | BA | 990 | A | C2-N3-C4 | -5.22 | 107.99 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | BA | 2558 | C | N3-C4-C5 | 5.22 | 123.99 | 121.90 |
| 1 | CA | 117 | G | C6-C5-N7 | -5.22 | 127.27 | 130.40 |
| 31 | BA | 933 | A | C6-C5-N7 | -5.22 | 128.64 | 132.30 |
| 31 | DA | 2383 | G | N3-C4-C5 | -5.22 | 125.99 | 128.60 |
| 31 | BA | 196 | A | C4-C5-N7 | 5.22 | 113.31 | 110.70 |
| 31 | BA | 2318 | G | C4-N9-C1' | 5.22 | 133.29 | 126.50 |
| 31 | BA | 2607 | G | C6-C5-N7 | -5.22 | 127.27 | 130.40 |
| 31 | DA | 527 | C | N3-C4-N4 | -5.22 | 114.34 | 118.00 |
| 1 | AA | 906 | G | N9-C4-C5 | -5.22 | 103.31 | 105.40 |
| 31 | BA | 748 | G | C4-C5-N7 | -5.22 | 108.71 | 110.80 |
| 31 | BA | 1251 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 34 | BE | 47 | VAL | CB-CA-C | -5.22 | 101.48 | 111.40 |
| 31 | DA | 2469 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 31 | BA | 2252 | G | C2-N3-C4 | -5.22 | 109.29 | 111.90 |
| 31 | DA | 376 | C | C2-N1-C1' | -5.22 | 113.06 | 118.80 |
| 31 | DA | 948 | G | N3-C4-N9 | -5.21 | 122.87 | 126.00 |
| 31 | DA | 797 | C | C4-C5-C6 | 5.21 | 120.01 | 117.40 |
| 31 | DA | 2430 | A | C5-N7-C8 | -5.21 | 101.29 | 103.90 |
| 31 | BA | 1201 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90 |
| 31 | BA | 272 | G | C8-N9-C4 | -5.21 | 104.32 | 106.40 |
| 31 | DA | 1698 | A | C3'-C2'-C1' | -5.21 | 97.33 | 101.50 |
| 31 | DA | 1819 | A | N1-C2-N3 | 5.21 | 131.90 | 129.30 |
| 31 | DA | 2676 | C | C5-C6-N1 | -5.21 | 118.40 | 121.00 |
| 31 | DA | 397 | G | C2-N3-C4 | -5.21 | 109.30 | 111.90 |
| 31 | DA | 529 | A | N9-C4-C5 | -5.21 | 103.72 | 105.80 |
| 31 | DA | 2572 | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |
| 31 | BA | 530 | G | C2-N3-C4 | -5.20 | 109.30 | 111.90 |
| 31 | DA | 2383 | G | C4-N9-C1' | 5.20 | 133.26 | 126.50 |
| 31 | BA | 2024 | G | C5-N7-C8 | 5.20 | 106.90 | 104.30 |
| 31 | BA | 2070 | G | N9-C4-C5 | -5.20 | 103.32 | 105.40 |
| 31 | BA | 2254 | C | N1-C2-O2 | -5.20 | 115.78 | 118.90 |
| 31 | DA | 205 | G | N3-C2-N2 | 5.20 | 123.54 | 119.90 |
| 31 | DA | 2399 | G | C8-N9-C1' | -5.20 | 120.24 | 127.00 |
| 31 | BA | 2712 | U | N3-C4-O4 | -5.20 | 115.76 | 119.40 |
| 31 | BA | 2828 | C | C6-N1-C2 | 5.20 | 122.38 | 120.30 |
| 41 | BP | 29 | LYS | CD-CE-NZ | 5.20 | 123.66 | 111.70 |
| 31 | BA | 185 | U | C2-N3-C4 | -5.20 | 123.88 | 127.00 |
| 31 | BA | 1660 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 31 | BA | 2258 | C | N3-C4-N4 | 5.20 | 121.64 | 118.00 |
| 31 | DA | 1349 | A | C4-C5-N7 | 5.20 | 113.30 | 110.70 |
| 31 | BA | 678 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 49 | BX | 75 | ASP | N-CA-C | -5.20 | 96.97 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 31 | DA | 786 | C | C5-C6-N1 | -5.20 | 118.40 | 121.00 |
| 35 | DF | 83 | PHE | N-CA-C | 5.19 | 125.02 | 111.00 |
| 31 | BA | 23 | G | C8-N9-C4 | 5.19 | 108.48 | 106.40 |
| 31 | BA | 651 | G | C4-N9-C1' | 5.19 | 133.25 | 126.50 |
| 1 | CA | 1524 | C | N1-C2-O2 | -5.19 | 115.78 | 118.90 |
| 31 | DA | 179 | G | N7-C8-N9 | -5.19 | 110.50 | 113.10 |
| 31 | DA | 2612 | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 31 | BA | 1762 | A | N7-C8-N9 | 5.19 | 116.39 | 113.80 |
| 31 | DA | 292 | C | N3-C4-C5 | 5.19 | 123.97 | 121.90 |
| 31 | DA | 1317 | A | C6-N1-C2 | -5.19 | 115.49 | 118.60 |
| 31 | DA | 1960 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 31 | BA | 1131 | G | N3-C2-N2 | 5.19 | 123.53 | 119.90 |
| 31 | BA | 2672 | G | N1-C6-O6 | 5.19 | 123.01 | 119.90 |
| 31 | BA | 650 | C | C6-N1-C2 | -5.18 | 118.23 | 120.30 |
| 31 | BA | 1204 | A | O4'-C1'-N9 | 5.18 | 112.35 | 108.20 |
| 31 | BA | 1614 | A | C6-C5-N7 | -5.18 | 128.67 | 132.30 |
| 41 | BP | 39 | LYS | CD-CE-NZ | -5.18 | 99.78 | 111.70 |
| 31 | DA | 621 | A | C5-C6-N1 | -5.18 | 115.11 | 117.70 |
| 31 | DA | 2512 | C | C2-N3-C4 | -5.18 | 117.31 | 119.90 |
| 31 | DA | 1573 | G | N7-C8-N9 | -5.18 | 110.51 | 113.10 |
| 31 | DA | 1983 | C | N1-C2-O2 | -5.18 | 115.79 | 118.90 |
| 1 | CA | 1432 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 31 | DA | 564 | C | N1-C2-O2 | -5.18 | 115.79 | 118.90 |
| 31 | DA | 730 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 31 | DA | 1794 | U | N1-C2-O2 | 5.18 | 126.42 | 122.80 |
| 31 | DA | 754 | C | C2-N3-C4 | -5.18 | 117.31 | 119.90 |
| 31 | DA | 1574 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 31 | DA | 2469 | A | N1-C2-N3 | 5.18 | 131.89 | 129.30 |
| 31 | BA | 1678 | G | C8-N9-C1' | -5.17 | 120.27 | 127.00 |
| 31 | BA | 2607 | G | C4-N9-C1' | 5.17 | 133.23 | 126.50 |
| 31 | DA | 1658 | C | N1-C2-O2 | -5.17 | 115.80 | 118.90 |
| 1 | CA | 894 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 31 | DA | 192 | C | N3-C2-O2 | 5.17 | 125.52 | 121.90 |
| 31 | DA | 2045 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 31 | DA | 2087 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 31 | BA | 38 | A | C8-N9-C4 | -5.17 | 103.73 | 105.80 |
| 31 | BA | 2771 | C | N3-C4-N4 | -5.17 | 114.38 | 118.00 |
| 31 | DA | 1790 | C | C2-N1-C1' | -5.17 | 113.11 | 118.80 |
| 31 | BA | 774 | A | N3-C4-C5 | 5.17 | 130.42 | 126.80 |
| 31 | BA | 669 | G | C5-C6-O6 | 5.17 | 131.70 | 128.60 |
| 31 | DA | 2685 | G | C5-C6-N1 | -5.17 | 108.92 | 111.50 |
| 31 | BA | 316 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31 | BA | 2469 | A | C8-N9-C4 | -5.16 | 103.73 | 105.80 |
| 31 | DA | 1617 | C | N3-C2-O2 | 5.16 | 125.51 | 121.90 |
| 31 | DA | 2443 | C | C5-C4-N4 | -5.16 | 116.59 | 120.20 |
| 31 | BA | 1204 | A | C8-N9-C1' | -5.16 | 118.41 | 127.70 |
| 31 | BA | 1210 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |
| 31 | DA | 2475 | C | C5-C4-N4 | -5.16 | 116.59 | 120.20 |
| 31 | BA | 814 | C | C5-C6-N1 | -5.16 | 118.42 | 121.00 |
| 31 | BA | 2503 | A | C2-N3-C4 | 5.16 | 113.18 | 110.60 |
| 31 | BA | 1782 | C | C2-N3-C4 | -5.16 | 117.32 | 119.90 |
| 31 | BA | 2027 | G | N7-C8-N9 | 5.16 | 115.68 | 113.10 |
| 31 | DA | 555 | U | C2-N1-C1' | -5.16 | 111.51 | 117.70 |
| 31 | DA | 1204 | A | C8-N9-C1' | -5.16 | 118.42 | 127.70 |
| 1 | AA | 569 | C | N3-C2-O2 | -5.15 | 118.29 | 121.90 |
| 31 | DA | 569 | U | C6-N1-C2 | 5.15 | 124.09 | 121.00 |
| 31 | DA | 671 | C | C4-C5-C6 | 5.15 | 119.98 | 117.40 |
| 31 | BA | 2409 | G | N3-C4-N9 | 5.15 | 129.09 | 126.00 |
| 31 | DA | 1821 | A | C8-N9-C4 | 5.15 | 107.86 | 105.80 |
| 31 | DA | 2713 | A | C6-C5-N7 | -5.15 | 128.69 | 132.30 |
| 1 | AA | 123 | C | C5-C6-N1 | -5.15 | 118.42 | 121.00 |
| 31 | DA | 486 | C | N3-C2-O2 | 5.15 | 125.50 | 121.90 |
| 31 | BA | 1238 | G | N9-C4-C5 | 5.15 | 107.46 | 105.40 |
| 31 | DA | 1333 | C | C6-N1-C2 | 5.15 | 122.36 | 120.30 |
| 1 | AA | 1432 | G | C5-C6-N1 | -5.15 | 108.93 | 111.50 |
| 31 | BA | 737 | C | C2-N3-C4 | -5.14 | 117.33 | 119.90 |
| 31 | BA | 1241 | A | C6-C5-N7 | -5.14 | 128.70 | 132.30 |
| 31 | BA | 1659 | U | N1-C2-O2 | -5.14 | 119.20 | 122.80 |
| 31 | BA | 266 | G | N1-C6-O6 | 5.14 | 122.99 | 119.90 |
| 1 | CA | 897 | C | C5-C6-N1 | -5.14 | 118.43 | 121.00 |
| 31 | DA | 484 | C | C6-N1-C2 | 5.14 | 122.36 | 120.30 |
| 31 | BA | 2499 | C | N3-C4-N4 | 5.14 | 121.60 | 118.00 |
| 31 | BA | 683 | C | C2-N3-C4 | -5.14 | 117.33 | 119.90 |
| 31 | DA | 107 | C | C5-C6-N1 | -5.14 | 118.43 | 121.00 |
| 31 | DA | 1780 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 31 | BA | 1253 | A | C2-N3-C4 | 5.14 | 113.17 | 110.60 |
| 31 | DA | 1992 | G | N1-C6-O6 | -5.14 | 116.82 | 119.90 |
| 31 | BA | 2672 | G | N3-C4-N9 | 5.14 | 129.08 | 126.00 |
| 31 | DA | 847 | U | N1-C2-N3 | 5.13 | 117.98 | 114.90 |
| 31 | BA | 272(B) | G | C4-C5-N7 | -5.13 | 108.75 | 110.80 |
| 31 | BA | 587 | C | C3'-C2'-C1' | 5.13 | 105.61 | 101.50 |
| 31 | DA | 1792 | G | C8-N9-C4 | 5.13 | 108.45 | 106.40 |
| 31 | DA | 2503 | A | C2-N3-C4 | 5.13 | 113.17 | 110.60 |
| 30 | D8 | 44 | LYS | CD-CE-NZ | 5.13 | 123.50 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | DA | 474 | G | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 31 | DA | 1543 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 1 | AA | 1524 | C | N3-C2-O2 | 5.13 | 125.49 | 121.90 |
| 31 | BA | 2286 | A | C8-N9-C4 | -5.13 | 103.75 | 105.80 |
| 31 | BA | 2481 | G | C8-N9-C4 | 5.13 | 108.45 | 106.40 |
| 31 | DA | 179 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |
| 31 | DA | 2048 | G | C8-N9-C4 | -5.13 | 104.35 | 106.40 |
| 1 | AA | 888 | G | C8-N9-C4 | 5.13 | 108.45 | 106.40 |
| 31 | BA | 1674 | G | N3-C4-C5 | -5.13 | 126.04 | 128.60 |
| 31 | BA | 2451 | A | C8-N9-C4 | -5.13 | 103.75 | 105.80 |
| 31 | DA | 1694 | C | C1'-O4'-C4' | -5.13 | 105.80 | 109.90 |
| 31 | BA | 1022 | G | N1-C2-N3 | 5.12 | 126.97 | 123.90 |
| 31 | BA | 2030 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 31 | BA | 2240 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 31 | BA | 2567 | G | N1-C6-O6 | 5.12 | 122.97 | 119.90 |
| 31 | DA | 2293 | C | C5-C6-N1 | -5.12 | 118.44 | 121.00 |
| 31 | BA | 133 | C | C2-N3-C4 | -5.12 | 117.34 | 119.90 |
| 31 | BA | 847 | U | N1-C2-N3 | 5.12 | 117.97 | 114.90 |
| 31 | BA | 1123 | C | C2-N3-C4 | -5.12 | 117.34 | 119.90 |
| 1 | CA | 1502 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 31 | DA | 1777 | U | C5-C6-N1 | -5.12 | 120.14 | 122.70 |
| 31 | BA | 737 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 31 | DA | 811 | U | C5-C4-O4 | 5.12 | 128.97 | 125.90 |
| 1 | CA | 1502 | A | C2-N3-C4 | -5.12 | 108.04 | 110.60 |
| 31 | DA | 739 | G | N7-C8-N9 | -5.12 | 110.54 | 113.10 |
| 31 | DA | 2067 | G | C5-C6-N1 | 5.12 | 114.06 | 111.50 |
| 1 | CA | 697 | U | C5-C6-N1 | -5.12 | 120.14 | 122.70 |
| 31 | BA | 697 | C | N1-C2-O2 | -5.12 | 115.83 | 118.90 |
| 31 | BA | 1196 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 41 | BP | 59 | LEU | CB-CG-CD1 | 5.12 | 119.69 | 111.00 |
| 31 | DA | 1333 | C | C2-N3-C4 | -5.12 | 117.34 | 119.90 |
| 31 | DA | 1828 | G | N1-C6-O6 | 5.12 | 122.97 | 119.90 |
| 31 | DA | 463 | G | N1-C6-O6 | -5.11 | 116.83 | 119.90 |
| 31 | DA | 1397 | U | N3-C4-O4 | -5.11 | 115.82 | 119.40 |
| 31 | BA | 1573 | G | N1-C6-O6 | 5.11 | 122.97 | 119.90 |
| 31 | BA | 1210 | A | N1-C6-N6 | 5.11 | 121.67 | 118.60 |
| 31 | BA | 186 | G | C5-C6-N1 | -5.11 | 108.95 | 111.50 |
| 31 | BA | 2267 | A | C2-N3-C4 | -5.11 | 108.05 | 110.60 |
| 31 | BA | 2609 | U | C2-N1-C1' | -5.11 | 111.57 | 117.70 |
| 31 | DA | 679 | C | N1-C2-O2 | -5.11 | 115.84 | 118.90 |
| 31 | DA | 753 | C | C6-N1-C2 | 5.11 | 122.34 | 120.30 |
| 31 | DA | 234 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | BA | 800 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 31 | BA | 1786 | A | N1-C2-N3 | 5.10 | 131.85 | 129.30 |
| 31 | BA | 2380 | C | C2-N3-C4 | -5.10 | 117.35 | 119.90 |
| 31 | DA | 204 | A | C8-N9-C4 | -5.10 | 103.76 | 105.80 |
| 31 | DA | 1021 | A | C4-C5-N7 | 5.10 | 113.25 | 110.70 |
| 31 | DA | 2518 | A | N7-C8-N9 | 5.10 | 116.35 | 113.80 |
| 31 | BA | 651 | G | C2-N3-C4 | 5.10 | 114.45 | 111.90 |
| 31 | BA | 1644 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 31 | DA | 242 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |
| 31 | DA | 482 | A | C8-N9-C4 | 5.10 | 107.84 | 105.80 |
| 31 | DA | 1314 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |
| 31 | DA | 1819 | A | C5-C6-N6 | 5.10 | 127.78 | 123.70 |
| 31 | BA | 1820 | U | C6-N1-C2 | 5.10 | 124.06 | 121.00 |
| 31 | BA | 2253 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 31 | DA | 453 | C | C5-C6-N1 | -5.10 | 118.45 | 121.00 |
| 31 | BA | 187 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 31 | BA | 586 | A | N1-C6-N6 | 5.10 | 121.66 | 118.60 |
| 31 | BA | 2827 | C | N1-C2-O2 | -5.10 | 115.84 | 118.90 |
| 1 | CA | 1499 | A | C8-N9-C4 | 5.10 | 107.84 | 105.80 |
| 31 | DA | 1204 | A | C3'-C2'-C1' | -5.10 | 97.42 | 101.50 |
| 31 | DA | 1600 | C | C2-N3-C4 | -5.10 | 117.35 | 119.90 |
| 31 | DA | 2240 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 31 | DA | 2547 | U | C6-N1-C2 | 5.10 | 124.06 | 121.00 |
| 31 | DA | 1021 | A | N3-C4-C5 | 5.10 | 130.37 | 126.80 |
| 31 | DA | 2563 | U | C5-C4-O4 | 5.10 | 128.96 | 125.90 |
| 31 | BA | 1616 | A | C2-N3-C4 | -5.09 | 108.05 | 110.60 |
| 31 | DA | 2540 | C | C6-N1-C2 | 5.09 | 122.34 | 120.30 |
| 31 | BA | 859 | G | N3-C4-N9 | -5.09 | 122.94 | 126.00 |
| 31 | BA | 745 | G | C6-N1-C2 | -5.09 | 122.05 | 125.10 |
| 31 | DA | 1308 | A | C2-N3-C4 | -5.09 | 108.05 | 110.60 |
| 31 | DA | 2085 | C | C5-C6-N1 | -5.09 | 118.45 | 121.00 |
| 31 | DA | 2680 | C | C5-C6-N1 | -5.09 | 118.45 | 121.00 |
| 31 | DA | 253 | C | N3-C2-O2 | 5.09 | 125.46 | 121.90 |
| 31 | DA | 1496 | A | C8-N9-C4 | -5.09 | 103.76 | 105.80 |
| 31 | DA | 2607 | G | C4-C5-C6 | 5.09 | 121.85 | 118.80 |
| 31 | DA | 808 | G | N1-C6-O6 | -5.09 | 116.85 | 119.90 |
| 31 | BA | 1656 | C | C6-N1-C2 | 5.09 | 122.33 | 120.30 |
| 31 | BA | 2758 | A | C8-N9-C4 | 5.09 | 107.83 | 105.80 |
| 31 | DA | 2472 | G | N1-C6-O6 | -5.09 | 116.85 | 119.90 |
| 31 | BA | 2456 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 31 | DA | 2823 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |
| 31 | BA | 1210 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | BA | 1493 | C | C6-N1-C1' | -5.08 | 114.70 | 120.80 |
| 31 | BA | 2810 | A | N1-C6-N6 | 5.08 | 121.65 | 118.60 |
| 32 | BB | 81 | G | N3-C2-N2 | 5.08 | 123.46 | 119.90 |
| 31 | DA | 32 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 31 | DA | 1663 | C | C5-C6-N1 | -5.08 | 118.46 | 121.00 |
| 31 | DA | 1827 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 31 | BA | 2487 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 31 | BA | 2569 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 31 | BA | 2618 | G | N9-C4-C5 | 5.08 | 107.43 | 105.40 |
| 31 | BA | 409 | C | N3-C2-O2 | 5.08 | 125.46 | 121.90 |
| 31 | BA | 995 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 31 | BA | 2330 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 31 | DA | 141 | A | N7-C8-N9 | 5.08 | 116.34 | 113.80 |
| 31 | DA | 995 | C | N1-C2-O2 | -5.08 | 115.85 | 118.90 |
| 31 | BA | 409 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 31 | DA | 1786 | A | N3-C4-C5 | 5.08 | 130.35 | 126.80 |
| 31 | BA | 1250 | G | N3-C4-C5 | -5.08 | 126.06 | 128.60 |
| 31 | BA | 2243 | U | C5-C4-O4 | -5.08 | 122.86 | 125.90 |
| 31 | DA | 36 | G | N9-C4-C5 | 5.08 | 107.43 | 105.40 |
| 31 | DA | 2070 | G | N1-C2-N3 | 5.08 | 126.95 | 123.90 |
| 31 | BA | 2497 | A | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 31 | BA | 2681 | C | N1-C2-O2 | -5.07 | 115.86 | 118.90 |
| 45 | DT | 80 | SER | N-CA-C | 5.07 | 124.69 | 111.00 |
| 31 | BA | 527 | C | N1-C2-O2 | -5.07 | 115.86 | 118.90 |
| 31 | BA | 843 | G | N3-C4-C5 | 5.07 | 131.13 | 128.60 |
| 31 | DA | 1786 | A | C5-C6-N6 | -5.07 | 119.64 | 123.70 |
| 31 | DA | 2741 | A | N9-C4-C5 | -5.07 | 103.77 | 105.80 |
| 31 | BA | 1001 | A | C8-N9-C4 | 5.07 | 107.83 | 105.80 |
| 30 | D8 | 33 | ASN | N-CA-C | -5.07 | 97.31 | 111.00 |
| 31 | BA | 859 | G | C4-N9-C1' | -5.07 | 119.91 | 126.50 |
| 31 | BA | 2503 | A | N1-C2-N3 | -5.07 | 126.77 | 129.30 |
| 31 | DA | 2346 | A | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 31 | BA | 2360 | A | C8-N9-C1' | -5.07 | 118.58 | 127.70 |
| 31 | DA | 1370 | C | C2-N1-C1' | -5.07 | 113.23 | 118.80 |
| 31 | BA | 2383 | G | N3-C4-C5 | -5.06 | 126.07 | 128.60 |
| 31 | DA | 339 | U | C6-N1-C2 | 5.06 | 124.04 | 121.00 |
| 31 | BA | 1158 | C | C4-C5-C6 | -5.06 | 114.87 | 117.40 |
| 31 | BA | 678 | C | N3-C2-O2 | 5.06 | 125.44 | 121.90 |
| 31 | DA | 1948 | G | N1-C2-N2 | 5.06 | 120.75 | 116.20 |
| 31 | DA | 2524 | G | N1-C6-O6 | 5.06 | 122.94 | 119.90 |
| 31 | BA | 584 | C | C6-N1-C2 | 5.06 | 122.32 | 120.30 |
| 31 | BA | 2377 | A | C2-N3-C4 | -5.06 | 108.07 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | DA | 676 | A | C6-C5-N7 | -5.06 | 128.76 | 132.30 |
| 31 | BA | 850 | C | C5-C6-N1 | -5.06 | 118.47 | 121.00 |
| 31 | DA | 2822 | G | C5-C6-O6 | -5.06 | 125.56 | 128.60 |
| 31 | BA | 732 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 31 | DA | 148 | C | C5-C6-N1 | -5.05 | 118.47 | 121.00 |
| 31 | DA | 1191 | G | C5-C6-N1 | 5.05 | 114.03 | 111.50 |
| 31 | DA | 2751 | G | C4-N9-C1' | 5.05 | 133.07 | 126.50 |
| 31 | BA | 678 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 31 | BA | 2496 | C | C6-N1-C2 | 5.05 | 122.32 | 120.30 |
| 31 | DA | 2422 | A | N1-C6-N6 | -5.05 | 115.57 | 118.60 |
| 31 | BA | 203 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 31 | BA | 2517 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 31 | BA | 2542 | A | C5-N7-C8 | -5.05 | 101.37 | 103.90 |
| 1 | CA | 1432 | G | N7-C8-N9 | 5.05 | 115.62 | 113.10 |
| 31 | BA | 2469 | A | C4-C5-C6 | 5.05 | 119.53 | 117.00 |
| 31 | BA | 2542 | A | C5-C6-N1 | -5.05 | 115.17 | 117.70 |
| 31 | DA | 516 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 31 | DA | 621 | A | C6-C5-N7 | -5.05 | 128.76 | 132.30 |
| 31 | DA | 1801 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 31 | DA | 2058 | A | N1-C2-N3 | 5.05 | 131.82 | 129.30 |
| 31 | BA | 1972 | A | C5-C6-N6 | -5.05 | 119.66 | 123.70 |
| 31 | BA | 2013 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 33 | BD | 237 | GLU | N-CA-C | 5.05 | 124.63 | 111.00 |
| 31 | DA | 1654 | A | C4-C5-C6 | -5.05 | 114.48 | 117.00 |
| 31 | DA | 210 | C | C4-C5-C6 | 5.04 | 119.92 | 117.40 |
| 31 | DA | 805 | G | C6-C5-N7 | -5.04 | 127.37 | 130.40 |
| 32 | DB | 71 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 1 | CA | 895 | G | C5-C6-O6 | -5.04 | 125.58 | 128.60 |
| 31 | BA | 371 | A | N1-C6-N6 | 5.04 | 121.62 | 118.60 |
| 31 | BA | 451 | C | N1-C2-O2 | -5.04 | 115.88 | 118.90 |
| 1 | CA | 896 | C | C6-N1-C2 | 5.04 | 122.31 | 120.30 |
| 31 | DA | 1313 | U | C5-C6-N1 | 5.04 | 125.22 | 122.70 |
| 31 | BA | 1332 | G | N7-C8-N9 | 5.03 | 115.62 | 113.10 |
| 31 | BA | 1955 | U | N1-C2-O2 | -5.03 | 119.28 | 122.80 |
| 31 | DA | 939 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 31 | DA | 1006 | C | C5-C6-N1 | -5.03 | 118.48 | 121.00 |
| 31 | DA | 671 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 31 | DA | 2502 | G | C4-C5-N7 | 5.03 | 112.81 | 110.80 |
| 31 | BA | 2617 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 31 | BA | 2059 | A | N9-C4-C5 | -5.03 | 103.79 | 105.80 |
| 31 | BA | 937 | U | C5-C6-N1 | -5.03 | 120.19 | 122.70 |
| 31 | DA | 772 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 31 | BA | 2440 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 31 | BA | 2508 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 31 | DA | 1157 | G | C8-N9-C4 | -5.03 | 104.39 | 106.40 |
| 31 | BA | 1332 | G | C4-C5-C6 | -5.02 | 115.78 | 118.80 |
| 31 | BA | 182 | A | N1-C6-N6 | 5.02 | 121.61 | 118.60 |
| 31 | BA | 1021 | A | N3-C4-N9 | -5.02 | 123.38 | 127.40 |
| 31 | DA | 630 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 31 | DA | 2612 | C | N3-C2-O2 | 5.02 | 125.42 | 121.90 |
| 31 | DA | 1496 | A | C8-N9-C1' | -5.02 | 118.66 | 127.70 |
| 31 | BA | 1682 | G | N9-C4-C5 | -5.02 | 103.39 | 105.40 |
| 31 | BA | 2040 | C | N3-C4-C5 | 5.02 | 123.91 | 121.90 |
| 31 | DA | 860 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 31 | DA | 1992 | G | C2-N3-C4 | 5.02 | 114.41 | 111.90 |
| 31 | BA | 2399 | G | C4-C5-C6 | 5.02 | 121.81 | 118.80 |
| 31 | DA | 76 | C | C2-N3-C4 | -5.02 | 117.39 | 119.90 |
| 31 | BA | 944 | G | N7-C8-N9 | 5.02 | 115.61 | 113.10 |
| 31 | DA | 552 | G | C5-C6-N1 | 5.02 | 114.01 | 111.50 |
| 31 | DA | 1543 | C | N1-C2-O2 | -5.02 | 115.89 | 118.90 |
| 31 | BA | 1306 | C | N3-C4-C5 | 5.01 | 123.91 | 121.90 |
| 31 | BA | 1632 | A | N1-C6-N6 | 5.01 | 121.61 | 118.60 |
| 31 | BA | 2271 | G | C4-N9-C1' | 5.01 | 133.02 | 126.50 |
| 31 | DA | 672 | C | C6-N1-C2 | 5.01 | 122.31 | 120.30 |
| 31 | DA | 2712(A) | A | N7-C8-N9 | 5.01 | 116.31 | 113.80 |
| 31 | BA | 672 | C | N1-C2-O2 | -5.01 | 115.89 | 118.90 |
| 31 | BA | 1350 | C | N3-C2-O2 | 5.01 | 125.41 | 121.90 |
| 31 | BA | 1485 | G | N3-C4-N9 | 5.01 | 129.00 | 126.00 |
| 31 | BA | 1681 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 31 | BA | 1951 | U | N3-C4-C5 | -5.01 | 111.59 | 114.60 |
| 31 | BA | 2374 | C | C6-N1-C2 | 5.01 | 122.30 | 120.30 |
| 31 | BA | 2742 | C | C2-N1-C1' | -5.01 | 113.29 | 118.80 |
| 31 | DA | 451 | C | C5-C6-N1 | -5.01 | 118.50 | 121.00 |
| 31 | DA | 928 | G | N9-C4-C5 | -5.01 | 103.40 | 105.40 |
| 31 | DA | 1029 | A | N1-C6-N6 | 5.01 | 121.61 | 118.60 |
| 28 | B6 | 10 | LEU | CA-CB-CG | 5.01 | 126.81 | 115.30 |
| 31 | BA | 376 | C | N1-C2-O2 | -5.01 | 115.90 | 118.90 |
| 31 | DA | 107 | C | C6-N1-C2 | 5.01 | 122.30 | 120.30 |
| 31 | DA | 191 | A | C5-N7-C8 | 5.01 | 106.40 | 103.90 |
| 31 | DA | 512 | G | O4'-C1'-N9 | 5.01 | 112.20 | 108.20 |
| 31 | DA | 1250 | G | N3-C4-C5 | -5.00 | 126.10 | 128.60 |
| 31 | DA | 2027 | G | N3-C4-C5 | -5.00 | 126.10 | 128.60 |
| 31 | DA | 2569 | G | C8-N9-C4 | 5.00 | 108.40 | 106.40 |
| 1 | AA | 569 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31 | BA | 1157 | G | C8-N9-C1' | -5.00 | 120.50 | 127.00 |
| 31 | BA | 1675 | C | N3-C4-C5 | 5.00 | 123.90 | 121.90 |
| 31 | DA | 1605 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |
| 31 | DA | 2223 | G | C8-N9-C4 | 5.00 | 108.40 | 106.40 |
| 31 | DA | 1261 | C | C2-N1-C1' | -5.00 | 113.30 | 118.80 |
| 31 | DA | 1771 | C | C4-C5-C6 | 5.00 | 119.90 | 117.40 |
| 31 | DA | 2010 | G | C6-C5-N7 | -5.00 | 127.40 | 130.40 |

All (42) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|-------------|
| 31 | BA | 100 | G | C1' |
| 31 | BA | 472 | A | C3' |
| 31 | BA | 669 | G | C4',C3',C1' |
| 31 | BA | 945 | A | C1' |
| 31 | BA | 1300 | U | C4',C3',C1' |
| 31 | BA | 1379 | A | C1' |
| 31 | BA | 1544 | A | C1' |
| 31 | BA | 1609 | A | C2' |
| 31 | BA | 1652 | A | C3' |
| 31 | BA | 1694 | C | C4',C3' |
| 31 | BA | 1934 | C | C3' |
| 31 | BA | 1962 | C | C4',C1' |
| 31 | BA | 2286 | A | C1' |
| 31 | BA | 2662 | A | C1' |
| 31 | BA | 2796 | U | C1' |
| 31 | DA | 100 | G | C1' |
| 31 | DA | 472 | A | C3' |
| 31 | DA | 669 | G | C4',C3',C1' |
| 31 | DA | 945 | A | C1' |
| 31 | DA | 1300 | U | C4',C3',C1' |
| 31 | DA | 1379 | A | C1' |
| 31 | DA | 1544 | A | C1' |
| 31 | DA | 1609 | A | C2' |
| 31 | DA | 1652 | A | C3' |
| 31 | DA | 1694 | C | C4',C3' |
| 31 | DA | 1934 | C | C3' |
| 31 | DA | 1962 | C | C4',C1' |
| 31 | DA | 2286 | A | C1' |
| 31 | DA | 2662 | A | C1' |
| 31 | DA | 2796 | U | C1' |

All (50) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 23 | B1 | 30 | VAL | Peptide |
| 27 | B5 | 51 | TYR | Peptide |
| 30 | B8 | 51 | ALA | Peptide |
| 33 | BD | 197 | GLY | Peptide |
| 33 | BD | 47 | GLY | Peptide |
| 34 | BE | 131 | ALA | Peptide |
| 34 | BE | 76 | ARG | Peptide |
| 37 | BH | 154 | PRO | Peptide |
| 37 | BH | 156 | ALA | Peptide |
| 41 | BP | 37 | GLY | Peptide |
| 41 | BP | 39 | LYS | Peptide |
| 41 | BP | 51 | PHE | Peptide |
| 41 | BP | 57 | THR | Peptide |
| 41 | BP | 9 | ASN | Peptide |
| 42 | BQ | 10 | ARG | Peptide |
| 43 | BR | 117 | VAL | Peptide |
| 43 | BR | 7 | GLY | Peptide |
| 44 | BS | 88 | ASP | Peptide |
| 45 | BT | 29 | ARG | Peptide |
| 46 | BU | 96 | ALA | Peptide |
| 47 | BV | 18 | LEU | Peptide |
| 49 | BX | 34 | ALA | Peptide |
| 49 | BX | 61 | GLY | Peptide |
| 49 | BX | 64 | LYS | Peptide |
| 49 | BX | 76 | ARG | Peptide |
| 49 | BX | 77 | LYS | Peptide |
| 23 | D1 | 30 | VAL | Peptide |
| 27 | D5 | 51 | TYR | Peptide |
| 30 | D8 | 51 | ALA | Peptide |
| 33 | DD | 197 | GLY | Peptide |
| 33 | DD | 47 | GLY | Peptide |
| 34 | DE | 131 | ALA | Peptide |
| 34 | DE | 76 | ARG | Peptide |
| 37 | DH | 154 | PRO | Peptide |
| 37 | DH | 156 | ALA | Peptide |
| 41 | DP | 51 | PHE | Peptide |
| 41 | DP | 57 | THR | Peptide |
| 41 | DP | 9 | ASN | Peptide |
| 42 | DQ | 10 | ARG | Peptide |
| 43 | DR | 117 | VAL | Peptide |
| 43 | DR | 7 | GLY | Peptide |
| 44 | DS | 88 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 45 | DT | 29 | ARG | Peptide |
| 46 | DU | 96 | ALA | Peptide |
| 47 | DV | 18 | LEU | Peptide |
| 49 | DX | 34 | ALA | Peptide |
| 49 | DX | 61 | GLY | Peptide |
| 49 | DX | 64 | LYS | Peptide |
| 49 | DX | 76 | ARG | Peptide |
| 49 | DX | 77 | LYS | 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 | 32329 | 0 | 16318 | 1467 | 0 |
| 1 | CA | 32329 | 0 | 16318 | 1441 | 0 |
| 2 | AB | 1901 | 0 | 1951 | 186 | 0 |
| 2 | CB | 1901 | 0 | 1951 | 185 | 0 |
| 3 | AC | 1613 | 0 | 1677 | 120 | 0 |
| 3 | CC | 1613 | 0 | 1677 | 126 | 0 |
| 4 | AD | 1703 | 0 | 1763 | 184 | 0 |
| 4 | CD | 1703 | 0 | 1764 | 184 | 0 |
| 5 | AE | 1147 | 0 | 1207 | 99 | 0 |
| 5 | CE | 1147 | 0 | 1207 | 103 | 0 |
| 6 | AF | 843 | 0 | 857 | 92 | 0 |
| 6 | CF | 843 | 0 | 857 | 92 | 0 |
| 7 | AG | 1257 | 0 | 1296 | 72 | 0 |
| 7 | CG | 1257 | 0 | 1296 | 77 | 0 |
| 8 | AH | 1116 | 0 | 1177 | 91 | 0 |
| 8 | CH | 1116 | 0 | 1177 | 95 | 0 |
| 9 | AI | 1011 | 0 | 1042 | 99 | 0 |
| 9 | CI | 1011 | 0 | 1042 | 96 | 0 |
| 10 | AJ | 795 | 0 | 840 | 88 | 0 |
| 10 | CJ | 795 | 0 | 840 | 85 | 0 |
| 11 | AK | 885 | 0 | 904 | 59 | 0 |
| 11 | CK | 885 | 0 | 904 | 65 | 0 |
| 12 | AL | 971 | 0 | 1057 | 102 | 0 |
| 12 | CL | 971 | 0 | 1057 | 103 | 0 |
| 13 | AM | 921 | 0 | 976 | 81 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13 | CM | 921 | 0 | 976 | 81 | 0 |
| 14 | AN | 492 | 0 | 530 | 44 | 0 |
| 14 | CN | 492 | 0 | 530 | 43 | 0 |
| 15 | AO | 734 | 0 | 771 | 49 | 0 |
| 15 | CO | 734 | 0 | 771 | 47 | 0 |
| 16 | AP | 701 | 0 | 720 | 78 | 0 |
| 16 | CP | 701 | 0 | 720 | 81 | 0 |
| 17 | AQ | 824 | 0 | 891 | 60 | 0 |
| 17 | CQ | 824 | 0 | 891 | 55 | 0 |
| 18 | AR | 574 | 0 | 644 | 61 | 0 |
| 18 | CR | 574 | 0 | 644 | 60 | 0 |
| 19 | AS | 630 | 0 | 652 | 38 | 0 |
| 19 | CS | 630 | 0 | 652 | 39 | 0 |
| 20 | AT | 763 | 0 | 861 | 84 | 0 |
| 20 | CT | 763 | 0 | 861 | 87 | 0 |
| 21 | AU | 209 | 0 | 221 | 9 | 0 |
| 21 | CU | 209 | 0 | 221 | 10 | 0 |
| 22 | B0 | 650 | 0 | 654 | 55 | 0 |
| 22 | D0 | 650 | 0 | 654 | 57 | 0 |
| 23 | B1 | 693 | 0 | 764 | 139 | 0 |
| 23 | D1 | 693 | 0 | 764 | 140 | 0 |
| 24 | B2 | 421 | 0 | 461 | 118 | 0 |
| 24 | D2 | 421 | 0 | 461 | 123 | 0 |
| 25 | B3 | 468 | 0 | 523 | 30 | 0 |
| 25 | D3 | 468 | 0 | 523 | 51 | 0 |
| 26 | B4 | 157 | 0 | 69 | 17 | 0 |
| 26 | D4 | 157 | 0 | 69 | 14 | 0 |
| 27 | B5 | 459 | 0 | 480 | 83 | 0 |
| 27 | D5 | 459 | 0 | 480 | 82 | 0 |
| 28 | B6 | 381 | 0 | 390 | 85 | 0 |
| 28 | D6 | 381 | 0 | 390 | 87 | 0 |
| 29 | B7 | 419 | 0 | 467 | 28 | 0 |
| 29 | D7 | 419 | 0 | 467 | 31 | 0 |
| 30 | B8 | 508 | 0 | 576 | 137 | 0 |
| 30 | D8 | 508 | 0 | 576 | 134 | 0 |
| 31 | BA | 58698 | 0 | 29591 | 2319 | 0 |
| 31 | DA | 58698 | 0 | 29590 | 2541 | 0 |
| 32 | BB | 2551 | 0 | 1295 | 128 | 0 |
| 32 | DB | 2551 | 0 | 1295 | 142 | 0 |
| 33 | BD | 2105 | 0 | 2182 | 298 | 0 |
| 33 | DD | 2105 | 0 | 2182 | 308 | 0 |
| 34 | BE | 1564 | 0 | 1629 | 206 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34 | DE | 1564 | 0 | 1629 | 213 | 0 |
| 35 | BF | 1624 | 0 | 1677 | 165 | 0 |
| 35 | DF | 1624 | 0 | 1677 | 173 | 0 |
| 36 | BG | 1474 | 0 | 1534 | 150 | 0 |
| 36 | DG | 1474 | 0 | 1534 | 149 | 0 |
| 37 | BH | 1223 | 0 | 1282 | 149 | 0 |
| 37 | DH | 1223 | 0 | 1282 | 141 | 0 |
| 38 | BI | 1132 | 0 | 1218 | 121 | 0 |
| 38 | DI | 1132 | 0 | 1218 | 118 | 0 |
| 39 | BN | 1105 | 0 | 1180 | 181 | 0 |
| 39 | DN | 1105 | 0 | 1180 | 188 | 0 |
| 40 | BO | 933 | 0 | 996 | 74 | 0 |
| 40 | DO | 933 | 0 | 996 | 69 | 0 |
| 41 | BP | 1114 | 0 | 1187 | 259 | 0 |
| 41 | DP | 1114 | 0 | 1187 | 245 | 0 |
| 42 | BQ | 1080 | 0 | 1127 | 142 | 0 |
| 42 | DQ | 1080 | 0 | 1127 | 151 | 0 |
| 43 | BR | 960 | 0 | 1021 | 106 | 0 |
| 43 | DR | 960 | 0 | 1021 | 116 | 0 |
| 44 | BS | 771 | 0 | 832 | 138 | 0 |
| 44 | DS | 771 | 0 | 832 | 143 | 0 |
| 45 | BT | 1100 | 0 | 1164 | 188 | 0 |
| 45 | DT | 1100 | 0 | 1164 | 182 | 0 |
| 46 | BU | 958 | 0 | 1015 | 128 | 0 |
| 46 | DU | 958 | 0 | 1015 | 123 | 0 |
| 47 | BV | 779 | 0 | 852 | 219 | 0 |
| 47 | DV | 779 | 0 | 852 | 215 | 0 |
| 48 | BW | 896 | 0 | 953 | 60 | 0 |
| 48 | DW | 896 | 0 | 953 | 69 | 0 |
| 49 | BX | 726 | 0 | 778 | 173 | 0 |
| 49 | DX | 726 | 0 | 778 | 176 | 0 |
| 50 | BY | 776 | 0 | 870 | 195 | 0 |
| 50 | DY | 776 | 0 | 870 | 194 | 0 |
| 51 | BZ | 1404 | 0 | 1432 | 152 | 0 |
| 51 | DZ | 1404 | 0 | 1432 | 154 | 0 |
| 52 | AA | 54 | 0 | 0 | 0 | 0 |
| 52 | B0 | 1 | 0 | 0 | 0 | 0 |
| 52 | B1 | 1 | 0 | 0 | 0 | 0 |
| 52 | B5 | 2 | 0 | 0 | 0 | 0 |
| 52 | BA | 362 | 0 | 0 | 0 | 0 |
| 52 | BB | 7 | 0 | 0 | 0 | 0 |
| 52 | BD | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 52 | BE | 1 | 0 | 0 | 0 | 0 |
| 52 | BF | 1 | 0 | 0 | 0 | 0 |
| 52 | BP | 3 | 0 | 0 | 0 | 0 |
| 52 | BQ | 2 | 0 | 0 | 0 | 0 |
| 52 | BR | 1 | 0 | 0 | 0 | 0 |
| 52 | BU | 1 | 0 | 0 | 0 | 0 |
| 52 | BX | 1 | 0 | 0 | 0 | 0 |
| 52 | CA | 50 | 0 | 0 | 0 | 0 |
| 52 | D0 | 1 | 0 | 0 | 0 | 0 |
| 52 | D3 | 1 | 0 | 0 | 0 | 0 |
| 52 | D5 | 1 | 0 | 0 | 0 | 0 |
| 52 | D7 | 1 | 0 | 0 | 0 | 0 |
| 52 | DA | 328 | 0 | 0 | 0 | 0 |
| 52 | DB | 3 | 0 | 0 | 0 | 0 |
| 52 | DE | 1 | 0 | 0 | 0 | 0 |
| 52 | DF | 1 | 0 | 0 | 0 | 0 |
| 52 | DP | 1 | 0 | 0 | 0 | 0 |
| 52 | DQ | 1 | 0 | 0 | 0 | 0 |
| 52 | DR | 1 | 0 | 0 | 0 | 0 |
| 52 | DU | 1 | 0 | 0 | 0 | 0 |
| 52 | DX | 1 | 0 | 0 | 0 | 0 |
| 53 | AD | 1 | 0 | 0 | 0 | 0 |
| 53 | AN | 1 | 0 | 0 | 0 | 0 |
| 53 | CD | 1 | 0 | 0 | 0 | 0 |
| 53 | CN | 1 | 0 | 0 | 0 | 0 |
| 54 | BA | 1 | 0 | 0 | 0 | 0 |
| 54 | DA | 1 | 0 | 0 | 0 | 0 |
| 55 | BA | 51 | 0 | 67 | 1 | 0 |
| 55 | DA | 51 | 0 | 67 | 2 | 0 |
| All | All | 278034 | 0 | 189242 | 17303 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (17303) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 42:BQ:81:VAL:O | 42:BQ:82:ARG:HD2 | 1.36 | 1.26 |
| 42:DQ:81:VAL:O | 42:DQ:82:ARG:HD2 | 1.37 | 1.22 |
| 33:BD:35:LYS:HD2 | 33:BD:104:TYR:CD1 | 1.78 | 1.19 |
| 50:BY:95:LYS:HD3 | 50:BY:100:ALA:HB1 | 1.21 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:AP:28:ARG:HG2 | 16:AP:28:ARG:HH11 | 1.06 | 1.18 |
| 31:DA:285:C:H2' | 31:DA:286:C:H5'' | 1.26 | 1.17 |
| 31:DA:102:G:C8 | 31:DA:102:G:H5'' | 1.79 | 1.17 |
| 51:DZ:53:ILE:HG22 | 51:DZ:71:VAL:HB | 1.27 | 1.17 |
| 33:DD:35:LYS:HD2 | 33:DD:104:TYR:CD1 | 1.80 | 1.17 |
| 34:DE:119:ARG:HG3 | 34:DE:119:ARG:HH11 | 1.07 | 1.16 |
| 39:BN:28:THR:HG22 | 39:BN:106:MET:HE1 | 1.22 | 1.16 |
| 31:BA:102:G:H5'' | 31:BA:102:G:C8 | 1.77 | 1.16 |
| 34:BE:119:ARG:HH11 | 34:BE:119:ARG:HG3 | 1.06 | 1.16 |
| 31:DA:2206:G:H21 | 31:DA:2207:G:H5' | 1.00 | 1.15 |
| 33:BD:65:ILE:HD11 | 33:BD:67:PHE:CE1 | 1.80 | 1.15 |
| 50:DY:95:LYS:HD3 | 50:DY:100:ALA:HB1 | 1.19 | 1.15 |
| 39:DN:28:THR:HG22 | 39:DN:106:MET:HE1 | 1.24 | 1.14 |
| 44:BS:34:HIS:HB3 | 44:BS:53:SER:HB3 | 1.29 | 1.14 |
| 31:DA:2206:G:N2 | 31:DA:2207:G:H5' | 1.63 | 1.14 |
| 23:B1:15:ALA:HA | 23:B1:46:LEU:HD21 | 1.26 | 1.14 |
| 39:BN:18:ALA:HB1 | 39:BN:21:LYS:HB2 | 1.28 | 1.13 |
| 50:DY:10:GLY:HA2 | 50:DY:27:VAL:HG13 | 1.31 | 1.13 |
| 31:BA:2317:C:C2' | 31:BA:2318:G:H5' | 1.78 | 1.13 |
| 51:BZ:53:ILE:HG22 | 51:BZ:71:VAL:HB | 1.26 | 1.12 |
| 33:DD:65:ILE:HD11 | 33:DD:67:PHE:CE1 | 1.84 | 1.12 |
| 44:DS:34:HIS:HB3 | 44:DS:53:SER:HB3 | 1.28 | 1.12 |
| 31:DA:2317:C:C2' | 31:DA:2318:G:H5' | 1.80 | 1.12 |
| 39:DN:18:ALA:HB1 | 39:DN:21:LYS:HB2 | 1.32 | 1.12 |
| 2:AB:111:ARG:HG2 | 2:AB:111:ARG:HH11 | 0.99 | 1.12 |
| 39:DN:18:ALA:HB3 | 39:DN:26:LEU:HD22 | 1.32 | 1.12 |
| 39:DN:42:TRP:HB3 | 46:DU:64:ARG:HH11 | 1.11 | 1.12 |
| 46:BU:64:ARG:CZ | 46:BU:64:ARG:HA | 1.80 | 1.12 |
| 31:BA:2206:G:N2 | 31:BA:2207:G:H5' | 1.63 | 1.11 |
| 50:BY:28:LYS:HB2 | 50:BY:37:VAL:HB | 1.29 | 1.11 |
| 45:DT:65:LYS:HE3 | 45:DT:66:VAL:H | 1.07 | 1.11 |
| 39:BN:42:TRP:HB3 | 46:BU:64:ARG:HH11 | 1.11 | 1.11 |
| 23:D1:47:GLN:HG2 | 31:DA:2230:G:H1' | 1.31 | 1.11 |
| 31:DA:2317:C:H2' | 31:DA:2318:G:H5' | 1.13 | 1.11 |
| 35:BF:22:ALA:O | 35:BF:26:ALA:HB2 | 1.51 | 1.11 |
| 27:D5:55:ARG:HD3 | 27:D5:56:LYS:H | 1.13 | 1.11 |
| 23:B1:41:ARG:HG3 | 23:B1:41:ARG:HH11 | 0.94 | 1.10 |
| 28:D6:46:HIS:HB2 | 28:D6:47:THR:N | 1.63 | 1.10 |
| 35:DF:53:THR:HG22 | 35:DF:55:GLY:H | 1.15 | 1.10 |
| 31:BA:285:C:H2' | 31:BA:286:C:H5'' | 1.27 | 1.10 |
| 35:DF:101:LEU:HD12 | 35:DF:102:PRO:HD2 | 1.32 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:AF:18:GLN:HA | 6:AF:21:LEU:HD23 | 1.33 | 1.10 |
| 41:DP:59:LEU:HA | 41:DP:61:ARG:NH1 | 1.67 | 1.10 |
| 28:B6:46:HIS:HB2 | 28:B6:47:THR:N | 1.65 | 1.10 |
| 37:BH:85:LYS:HD2 | 37:BH:141:VAL:HG13 | 1.30 | 1.10 |
| 23:D1:15:ALA:HA | 23:D1:46:LEU:HD21 | 1.27 | 1.10 |
| 47:DV:82:ARG:HG3 | 47:DV:82:ARG:HH11 | 1.06 | 1.09 |
| 31:BA:2317:C:H2' | 31:BA:2318:G:H5' | 1.11 | 1.09 |
| 47:BV:82:ARG:HG3 | 47:BV:82:ARG:HH11 | 1.08 | 1.09 |
| 50:BY:10:GLY:HA2 | 50:BY:27:VAL:HG13 | 1.21 | 1.09 |
| 41:BP:16:ARG:HD3 | 41:BP:18:ARG:HB2 | 1.12 | 1.09 |
| 24:D2:49:LYS:HD2 | 24:D2:53:LEU:HD13 | 1.11 | 1.09 |
| 34:BE:73:GLU:HG3 | 34:BE:74:PRO:HD2 | 1.27 | 1.09 |
| 45:BT:65:LYS:HE3 | 45:BT:66:VAL:H | 1.03 | 1.09 |
| 31:BA:2206:G:H21 | 31:BA:2207:G:H5' | 1.00 | 1.09 |
| 2:CB:111:ARG:HG2 | 2:CB:111:ARG:HH11 | 1.00 | 1.09 |
| 41:DP:16:ARG:HD3 | 41:DP:18:ARG:HB2 | 1.13 | 1.09 |
| 46:DU:64:ARG:HA | 46:DU:64:ARG:CZ | 1.82 | 1.09 |
| 49:BX:25:LYS:HG3 | 49:BX:26:TYR:H | 1.08 | 1.09 |
| 41:BP:59:LEU:HA | 41:BP:61:ARG:NH1 | 1.67 | 1.08 |
| 31:BA:1798:U:H5' | 33:BD:259:THR:HG22 | 1.10 | 1.08 |
| 22:D0:13:GLY:O | 22:D0:14:ARG:HB2 | 1.51 | 1.08 |
| 47:DV:19:LYS:HG3 | 47:DV:20:LEU:H | 1.15 | 1.08 |
| 25:D3:8:LEU:HD13 | 25:D3:31:LEU:HD23 | 1.36 | 1.08 |
| 37:DH:85:LYS:HD2 | 37:DH:141:VAL:HG13 | 1.35 | 1.08 |
| 44:BS:85:VAL:HG23 | 44:BS:106:ARG:HB2 | 1.34 | 1.07 |
| 50:DY:28:LYS:HB2 | 50:DY:37:VAL:HB | 1.31 | 1.07 |
| 27:B5:2:ALA:HA | 31:BA:2015:A:H1' | 1.35 | 1.07 |
| 31:DA:870:A:H5'' | 42:DQ:7:MET:HB2 | 1.34 | 1.07 |
| 31:DA:1798:U:H5' | 33:DD:259:THR:HG22 | 1.09 | 1.07 |
| 47:BV:19:LYS:HG3 | 47:BV:20:LEU:H | 1.07 | 1.07 |
| 12:AL:47:LYS:HB3 | 12:AL:48:PRO:HD3 | 1.36 | 1.07 |
| 47:DV:90:PRO:HG2 | 47:DV:91:TYR:H | 1.17 | 1.06 |
| 49:DX:25:LYS:HG3 | 49:DX:26:TYR:H | 1.05 | 1.06 |
| 2:AB:185:ILE:HG22 | 2:AB:199:TYR:HB2 | 1.34 | 1.06 |
| 33:BD:32:SER:O | 33:BD:33:LEU:HB2 | 1.53 | 1.06 |
| 31:BA:1696:G:H2' | 31:BA:1697:G:H5'' | 1.38 | 1.06 |
| 31:DA:1654:A:OP1 | 43:DR:3:HIS:HB2 | 1.53 | 1.06 |
| 4:AD:128:VAL:HG13 | 4:AD:129:ASN:HD22 | 1.20 | 1.06 |
| 31:DA:1899:G:H22 | 31:DA:1902:C:N4 | 1.51 | 1.06 |
| 31:DA:1696:G:H2' | 31:DA:1697:G:H5'' | 1.36 | 1.06 |
| 23:D1:41:ARG:HH11 | 23:D1:41:ARG:HG3 | 0.91 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:B1:17:SER:O | 23:B1:44:PRO:HD2 | 1.54 | 1.06 |
| 47:BV:19:LYS:CG | 47:BV:20:LEU:H | 1.68 | 1.06 |
| 43:DR:33:ARG:HG2 | 43:DR:115:GLU:HG3 | 1.38 | 1.06 |
| 6:CF:18:GLN:HA | 6:CF:21:LEU:HD23 | 1.33 | 1.05 |
| 33:DD:17:THR:HG22 | 33:DD:205:VAL:H | 0.95 | 1.05 |
| 34:DE:73:GLU:HG3 | 34:DE:74:PRO:HD2 | 1.31 | 1.05 |
| 24:B2:49:LYS:HD2 | 24:B2:53:LEU:HD13 | 1.07 | 1.05 |
| 31:BA:1654:A:OP1 | 43:BR:3:HIS:HB2 | 1.56 | 1.05 |
| 44:DS:85:VAL:HG23 | 44:DS:106:ARG:HB2 | 1.39 | 1.05 |
| 48:DW:4:LYS:HB2 | 48:DW:106:ILE:HG22 | 1.38 | 1.05 |
| 35:BF:101:LEU:HD12 | 35:BF:102:PRO:HD2 | 1.38 | 1.05 |
| 24:B2:46:GLN:HE21 | 24:B2:47:ASN:N | 1.51 | 1.05 |
| 39:DN:3:THR:HA | 39:DN:4:TYR:CE1 | 1.90 | 1.05 |
| 31:BA:102:G:H5'' | 31:BA:102:G:H8 | 0.88 | 1.05 |
| 47:BV:90:PRO:HG2 | 47:BV:91:TYR:H | 1.18 | 1.05 |
| 39:BN:3:THR:HA | 39:BN:4:TYR:CE1 | 1.92 | 1.05 |
| 49:BX:82:GLN:O | 49:BX:85:PRO:HD2 | 1.57 | 1.05 |
| 31:BA:1899:G:H22 | 31:BA:1902:C:N4 | 1.55 | 1.04 |
| 31:DA:145:G:H2' | 31:DA:146:G:H5'' | 1.39 | 1.04 |
| 15:CO:17:ARG:HG3 | 15:CO:17:ARG:HH11 | 1.19 | 1.04 |
| 31:BA:2287:A:N6 | 31:BA:2344:U:H3 | 1.54 | 1.04 |
| 27:D5:2:ALA:HA | 31:DA:2015:A:H1' | 1.38 | 1.04 |
| 31:DA:102:G:H8 | 31:DA:102:G:H5'' | 0.90 | 1.04 |
| 33:BD:17:THR:HG22 | 33:BD:205:VAL:N | 1.72 | 1.04 |
| 43:BR:33:ARG:HG2 | 43:BR:115:GLU:HG3 | 1.38 | 1.04 |
| 47:BV:82:ARG:CG | 47:BV:82:ARG:HH11 | 1.71 | 1.04 |
| 31:BA:870:A:H5'' | 42:BQ:7:MET:HB2 | 1.39 | 1.04 |
| 32:BB:74:U:H2' | 32:BB:75:G:H5'' | 1.40 | 1.04 |
| 39:BN:1:MET:HB3 | 47:BV:20:LEU:HD22 | 1.39 | 1.04 |
| 39:BN:18:ALA:HB3 | 39:BN:26:LEU:HD22 | 1.37 | 1.04 |
| 35:DF:22:ALA:O | 35:DF:26:ALA:HB2 | 1.56 | 1.04 |
| 12:CL:47:LYS:HB3 | 12:CL:48:PRO:HD3 | 1.35 | 1.04 |
| 33:BD:25:THR:HG21 | 33:BD:81:ALA:HB1 | 1.39 | 1.04 |
| 39:DN:65:LYS:HE2 | 39:DN:65:LYS:HA | 1.40 | 1.04 |
| 22:B0:13:GLY:O | 22:B0:14:ARG:HB2 | 1.53 | 1.03 |
| 31:BA:1592:C:C2' | 31:BA:1593:G:H5'' | 1.86 | 1.03 |
| 35:BF:24:LEU:HB3 | 35:BF:25:PRO:HD2 | 1.40 | 1.03 |
| 39:BN:65:LYS:HE2 | 39:BN:65:LYS:HA | 1.40 | 1.03 |
| 41:BP:140:ALA:HB1 | 25:D3:38:GLU:HG2 | 1.38 | 1.03 |
| 4:CD:128:VAL:HG13 | 4:CD:129:ASN:HD22 | 1.16 | 1.03 |
| 24:D2:46:GLN:HE21 | 24:D2:47:ASN:N | 1.56 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 39:BN:119:ARG:HH11 | 39:BN:119:ARG:HG3 | 1.23 | 1.03 |
| 5:AE:101:ILE:HD11 | 5:AE:119:LEU:HD23 | 1.39 | 1.03 |
| 43:BR:4:LEU:HD13 | 43:BR:4:LEU:O | 1.57 | 1.03 |
| 33:DD:17:THR:HG22 | 33:DD:205:VAL:N | 1.72 | 1.03 |
| 33:DD:32:SER:O | 33:DD:33:LEU:HB2 | 1.56 | 1.03 |
| 31:BA:2068:U:H3 | 31:BA:2430:A:H2 | 1.06 | 1.03 |
| 23:B1:46:LEU:H | 23:B1:46:LEU:HD12 | 1.23 | 1.03 |
| 27:B5:16:ARG:HG2 | 27:B5:16:ARG:HH11 | 1.23 | 1.03 |
| 33:BD:35:LYS:NZ | 33:BD:104:TYR:HB2 | 1.73 | 1.03 |
| 47:BV:85:LYS:O | 47:BV:87:HIS:N | 1.90 | 1.03 |
| 31:DA:330:A:H2 | 31:DA:1210:A:H2' | 1.24 | 1.03 |
| 41:DP:85:LEU:HD23 | 41:DP:85:LEU:H | 1.20 | 1.03 |
| 35:BF:46:ARG:HH11 | 35:BF:46:ARG:HG2 | 1.17 | 1.03 |
| 13:CM:3:ARG:HH22 | 36:DG:139:LEU:HD13 | 1.22 | 1.03 |
| 41:BP:141:ALA:HB3 | 25:D3:1:MET:SD | 1.99 | 1.02 |
| 32:DB:74:U:H2' | 32:DB:75:G:H5'' | 1.38 | 1.02 |
| 15:AO:17:ARG:HH11 | 15:AO:17:ARG:HG3 | 1.22 | 1.02 |
| 38:BI:130:TYR:HB3 | 38:BI:136:VAL:HG13 | 1.41 | 1.02 |
| 28:B6:15:GLU:HG2 | 28:B6:18:ARG:HE | 1.20 | 1.02 |
| 49:BX:77:LYS:HG2 | 49:BX:78:LYS:HG3 | 1.40 | 1.02 |
| 5:CE:101:ILE:HD11 | 5:CE:119:LEU:HD23 | 1.41 | 1.02 |
| 47:DV:62:LEU:HD22 | 47:DV:98:GLU:HB2 | 1.40 | 1.02 |
| 2:AB:91:PRO:HG3 | 2:AB:154:LEU:HB2 | 1.41 | 1.02 |
| 41:BP:47:ASP:HB3 | 41:BP:48:PRO:O | 1.60 | 1.02 |
| 46:BU:83:LEU:HG | 46:BU:88:ILE:HG12 | 1.38 | 1.02 |
| 1:CA:626:U:H2' | 1:CA:627:G:H8 | 1.23 | 1.02 |
| 2:CB:185:ILE:HG22 | 2:CB:199:TYR:HB2 | 1.35 | 1.02 |
| 33:DD:27:THR:HG21 | 33:DD:83:GLU:HG2 | 1.40 | 1.02 |
| 31:DA:1210:A:H5' | 31:DA:1210:A:H8 | 1.20 | 1.02 |
| 31:BA:1592:C:H2' | 31:BA:1593:G:H5'' | 1.38 | 1.02 |
| 35:BF:53:THR:HG22 | 35:BF:55:GLY:H | 1.18 | 1.02 |
| 16:CP:28:ARG:HH11 | 16:CP:28:ARG:HG2 | 1.14 | 1.02 |
| 33:BD:17:THR:HG22 | 33:BD:205:VAL:H | 0.91 | 1.01 |
| 31:BA:145:G:H2' | 31:BA:146:G:H5'' | 1.40 | 1.01 |
| 28:D6:15:GLU:HG2 | 28:D6:18:ARG:HE | 1.24 | 1.01 |
| 31:BA:1019:U:H3 | 31:BA:1142(A):A:H62 | 1.03 | 1.01 |
| 31:DA:1798:U:H5' | 33:DD:259:THR:CG2 | 1.91 | 1.01 |
| 31:DA:2334:G:H21 | 44:DS:18:ILE:HD11 | 1.20 | 1.01 |
| 39:DN:119:ARG:HG3 | 39:DN:119:ARG:HH11 | 1.25 | 1.01 |
| 27:B5:55:ARG:HD3 | 27:B5:56:LYS:H | 1.19 | 1.01 |
| 47:BV:19:LYS:HG3 | 47:BV:20:LEU:N | 1.73 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 49:BX:36:LYS:NZ | 49:BX:38:GLU:O | 1.94 | 1.01 |
| 50:BY:28:LYS:HE2 | 50:BY:30:VAL:HG22 | 1.43 | 1.01 |
| 47:DV:2:PHE:HB2 | 47:DV:42:GLY:HA2 | 1.42 | 1.01 |
| 1:CA:1442:G:O2' | 1:CA:1442(A):G:H5'' | 1.61 | 1.01 |
| 33:DD:25:THR:HG21 | 33:DD:81:ALA:HB1 | 1.41 | 1.01 |
| 25:B3:8:LEU:HD13 | 25:B3:31:LEU:HD23 | 1.39 | 1.00 |
| 41:BP:30:THR:HG22 | 41:BP:31:ALA:H | 1.26 | 1.00 |
| 29:D7:8:ASN:ND2 | 29:D7:11:LYS:H | 1.59 | 1.00 |
| 35:DF:46:ARG:HG2 | 35:DF:46:ARG:HH11 | 1.19 | 1.00 |
| 49:DX:82:GLN:O | 49:DX:85:PRO:HD2 | 1.61 | 1.00 |
| 31:BA:676:A:H8 | 31:BA:2069:G:H21 | 1.02 | 1.00 |
| 31:BA:2334:G:H21 | 44:BS:18:ILE:HD11 | 1.22 | 1.00 |
| 42:DQ:9:TYR:O | 42:DQ:9:TYR:HD2 | 1.45 | 1.00 |
| 1:AA:626:U:H2' | 1:AA:627:G:H8 | 1.26 | 1.00 |
| 34:BE:38:THR:HG22 | 34:BE:40:GLU:H | 1.27 | 1.00 |
| 27:D5:16:ARG:HG2 | 27:D5:16:ARG:HH11 | 1.19 | 1.00 |
| 46:DU:83:LEU:HG | 46:DU:88:ILE:HG12 | 1.40 | 1.00 |
| 42:BQ:22:LYS:HE2 | 42:BQ:22:LYS:HA | 1.42 | 1.00 |
| 38:DI:130:TYR:HB3 | 38:DI:136:VAL:HG13 | 1.41 | 1.00 |
| 39:DN:1:MET:HB3 | 47:DV:20:LEU:HD22 | 1.39 | 1.00 |
| 2:CB:91:PRO:HG3 | 2:CB:154:LEU:HB2 | 1.41 | 1.00 |
| 23:B1:47:GLN:HG2 | 31:BA:2230:G:H1' | 1.41 | 1.00 |
| 23:D1:46:LEU:H | 23:D1:46:LEU:HD12 | 1.23 | 1.00 |
| 30:B8:32:LEU:O | 30:B8:33:ASN:HB3 | 1.60 | 0.99 |
| 30:B8:32:LEU:HB3 | 30:B8:34:TRP:HB3 | 1.42 | 0.99 |
| 35:BF:18:ARG:HG2 | 35:BF:19:GLU:H | 1.27 | 0.99 |
| 30:D8:32:LEU:O | 30:D8:33:ASN:HB3 | 1.62 | 0.99 |
| 49:DX:76:ARG:HG2 | 49:DX:76:ARG:HH11 | 1.19 | 0.99 |
| 31:DA:1592:C:C2' | 31:DA:1593:G:H5'' | 1.92 | 0.99 |
| 31:DA:2287:A:N6 | 31:DA:2344:U:H3 | 1.58 | 0.99 |
| 40:DO:10:VAL:HG21 | 40:DO:16:ALA:O | 1.61 | 0.99 |
| 50:DY:28:LYS:HE2 | 50:DY:30:VAL:HG22 | 1.43 | 0.99 |
| 23:D1:17:SER:O | 23:D1:44:PRO:HD2 | 1.63 | 0.99 |
| 23:B1:10:LYS:HD3 | 23:B1:14:VAL:HA | 1.44 | 0.99 |
| 30:B8:46:ARG:HH22 | 41:BP:65:ARG:NH2 | 1.60 | 0.99 |
| 31:BA:1798:U:H5' | 33:BD:259:THR:CG2 | 1.92 | 0.99 |
| 39:BN:47:ALA:HB2 | 39:BN:112:LEU:HD11 | 1.45 | 0.99 |
| 35:DF:24:LEU:HB3 | 35:DF:25:PRO:HD2 | 1.41 | 0.99 |
| 50:BY:96:ILE:HD12 | 50:BY:99:CYS:SG | 2.03 | 0.99 |
| 30:D8:32:LEU:HB3 | 30:D8:34:TRP:HB3 | 1.45 | 0.98 |
| 47:DV:75:PHE:CE1 | 47:DV:89:GLN:HB3 | 1.97 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 23:D1:41:ARG:NH1 | 23:D1:41:ARG:HG3 | 1.70 | 0.98 |
| 31:DA:1494:A:H4' | 31:DA:1495:A:OP1 | 1.62 | 0.98 |
| 34:BE:36:ARG:NH2 | 34:BE:88:GLY:HA2 | 1.78 | 0.98 |
| 48:BW:64:MET:O | 48:BW:65:LEU:HB2 | 1.61 | 0.98 |
| 2:CB:84:GLU:HB3 | 2:CB:219:VAL:HG21 | 1.43 | 0.98 |
| 50:DY:96:ILE:HD12 | 50:DY:99:CYS:SG | 2.04 | 0.98 |
| 47:BV:75:PHE:CE1 | 47:BV:89:GLN:HB3 | 1.98 | 0.98 |
| 31:BA:1494:A:H4' | 31:BA:1495:A:OP1 | 1.62 | 0.98 |
| 43:BR:118:GLU:HA | 43:BR:118:GLU:OE1 | 1.61 | 0.98 |
| 33:DD:35:LYS:HB3 | 33:DD:63:ARG:HA | 1.43 | 0.98 |
| 31:DA:71:A:C2 | 49:DX:31:HIS:HE1 | 1.82 | 0.98 |
| 34:DE:152:LYS:HG2 | 39:DN:78:TYR:CD2 | 1.99 | 0.98 |
| 43:BR:67:LEU:HD13 | 43:BR:76:VAL:HG21 | 1.46 | 0.97 |
| 1:CA:1090:U:H2' | 1:CA:1091:U:H6 | 1.28 | 0.97 |
| 35:DF:18:ARG:HG2 | 35:DF:19:GLU:H | 1.27 | 0.97 |
| 45:DT:53:ARG:HG3 | 45:DT:53:ARG:HH11 | 1.26 | 0.97 |
| 31:BA:2681:C:H5 | 31:BA:2725:A:H62 | 0.99 | 0.97 |
| 43:DR:118:GLU:HA | 43:DR:118:GLU:OE1 | 1.63 | 0.97 |
| 47:DV:19:LYS:CG | 47:DV:20:LEU:H | 1.75 | 0.97 |
| 31:BA:102:G:O2' | 31:BA:103:A:OP2 | 1.81 | 0.97 |
| 33:BD:35:LYS:HB3 | 33:BD:63:ARG:HA | 1.43 | 0.97 |
| 8:CH:86:ILE:HG21 | 8:CH:133:LEU:HD13 | 1.40 | 0.97 |
| 1:AA:1442:G:O2' | 1:AA:1442(A):G:H5'' | 1.65 | 0.97 |
| 31:BA:2359:C:H2' | 31:BA:2360:A:H5' | 1.45 | 0.97 |
| 31:BA:71:A:H2 | 49:BX:31:HIS:HE1 | 1.12 | 0.97 |
| 31:DA:2787:C:H1' | 34:DE:61:ARG:HB2 | 1.45 | 0.97 |
| 33:DD:186:HIS:CD2 | 33:DD:188:GLU:H | 1.82 | 0.97 |
| 42:BQ:8:LYS:HG3 | 42:BQ:9:TYR:H | 1.28 | 0.97 |
| 30:B8:46:ARG:HH22 | 41:BP:65:ARG:HH22 | 1.10 | 0.97 |
| 43:DR:67:LEU:HD13 | 43:DR:76:VAL:HG21 | 1.47 | 0.97 |
| 31:BA:154:G:H1 | 31:BA:172:C:N4 | 1.62 | 0.97 |
| 33:BD:235:GLY:O | 33:BD:237:GLU:HG2 | 1.64 | 0.97 |
| 47:BV:15:GLU:HB3 | 47:BV:16:PRO:HD2 | 1.45 | 0.97 |
| 16:CP:4:ILE:HG13 | 16:CP:21:VAL:HG12 | 1.46 | 0.97 |
| 49:DX:77:LYS:HG2 | 49:DX:78:LYS:HG3 | 1.44 | 0.97 |
| 23:B1:19:GLN:HE21 | 31:BA:379:G:H21 | 1.02 | 0.97 |
| 23:B1:41:ARG:HG3 | 23:B1:41:ARG:NH1 | 1.74 | 0.97 |
| 30:B8:32:LEU:HD13 | 30:B8:32:LEU:H | 1.27 | 0.97 |
| 31:BA:1210:A:H8 | 31:BA:1210:A:H5' | 1.24 | 0.97 |
| 44:BS:30:ARG:HH22 | 44:BS:62:LYS:HD2 | 1.26 | 0.97 |
| 31:DA:2359:C:H2' | 31:DA:2360:A:H5' | 1.45 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 42:DQ:140:ALA:HB3 | 51:DZ:53:ILE:HG13 | 1.47 | 0.97 |
| 41:BP:64:LYS:C | 41:BP:66:GLY:H | 1.69 | 0.96 |
| 31:DA:676:A:H8 | 31:DA:2069:G:H21 | 0.98 | 0.96 |
| 31:DA:2475:C:H5' | 31:DA:2476:A:OP2 | 1.65 | 0.96 |
| 31:BA:2523:G:H2' | 31:BA:2524:G:H5'' | 1.44 | 0.96 |
| 42:BQ:140:ALA:HB3 | 51:BZ:53:ILE:HG13 | 1.47 | 0.96 |
| 31:DA:102:G:O2' | 31:DA:103:A:OP2 | 1.82 | 0.96 |
| 33:DD:35:LYS:NZ | 33:DD:104:TYR:HB2 | 1.78 | 0.96 |
| 49:DX:36:LYS:HD2 | 49:DX:36:LYS:O | 1.65 | 0.96 |
| 31:BA:2475:C:H5' | 31:BA:2476:A:OP2 | 1.65 | 0.96 |
| 47:BV:2:PHE:HB2 | 47:BV:42:GLY:HA2 | 1.47 | 0.96 |
| 31:DA:1019:U:H3 | 31:DA:1142(A):A:H62 | 1.02 | 0.96 |
| 36:DG:82:LEU:HB3 | 36:DG:87:PRO:HG3 | 1.47 | 0.96 |
| 44:DS:30:ARG:HH22 | 44:DS:62:LYS:HD2 | 1.26 | 0.96 |
| 41:BP:85:LEU:H | 41:BP:85:LEU:HD23 | 1.28 | 0.96 |
| 31:DA:1021:A:H62 | 31:DA:1141:U:H3 | 1.13 | 0.96 |
| 31:DA:1592:C:H2' | 31:DA:1593:G:H5'' | 1.48 | 0.96 |
| 41:DP:47:ASP:HB3 | 41:DP:48:PRO:O | 1.65 | 0.96 |
| 33:BD:108:PRO:HB3 | 33:BD:143:HIS:HE1 | 1.29 | 0.96 |
| 31:DA:607:U:H3 | 31:DA:621:A:H2 | 1.11 | 0.96 |
| 45:DT:83:ILE:HG13 | 45:DT:84:GLN:H | 1.30 | 0.96 |
| 23:B1:34:THR:HG23 | 31:BA:388:G:OP1 | 1.66 | 0.96 |
| 36:BG:82:LEU:HB3 | 36:BG:87:PRO:HG3 | 1.46 | 0.96 |
| 30:D8:62:LEU:HD13 | 31:DA:242:G:H5'' | 1.47 | 0.96 |
| 34:DE:38:THR:HG22 | 34:DE:40:GLU:H | 1.27 | 0.96 |
| 31:DA:2523:G:H2' | 31:DA:2524:G:H5'' | 1.43 | 0.96 |
| 35:DF:178:PRO:HB2 | 35:DF:201:VAL:HG11 | 1.47 | 0.96 |
| 31:DA:911:A:H2' | 42:DQ:9:TYR:OH | 1.64 | 0.96 |
| 39:BN:17:ASP:OD2 | 39:BN:19:GLU:HB3 | 1.65 | 0.96 |
| 30:B8:31:HIS:CG | 31:BA:2419:U:O4 | 2.19 | 0.96 |
| 23:D1:34:THR:HG23 | 31:DA:388:G:OP1 | 1.66 | 0.96 |
| 31:DA:171:G:H2' | 31:DA:172:C:O4' | 1.66 | 0.96 |
| 34:DE:36:ARG:NH2 | 34:DE:88:GLY:HA2 | 1.80 | 0.95 |
| 41:BP:59:LEU:HA | 41:BP:61:ARG:HH11 | 1.21 | 0.95 |
| 45:BT:17:THR:O | 45:BT:18:ASP:HB3 | 1.66 | 0.95 |
| 30:D8:32:LEU:HD13 | 30:D8:32:LEU:H | 1.27 | 0.95 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:H6 | 1.28 | 0.95 |
| 30:D8:46:ARG:HH22 | 41:DP:65:ARG:NH2 | 1.61 | 0.95 |
| 16:AP:4:ILE:HG13 | 16:AP:21:VAL:HG12 | 1.46 | 0.95 |
| 39:DN:17:ASP:OD2 | 39:DN:19:GLU:HB3 | 1.66 | 0.95 |
| 31:BA:607:U:H3 | 31:BA:621:A:H2 | 1.12 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:D5:55:ARG:HD3 | 27:D5:56:LYS:N | 1.81 | 0.95 |
| 31:DA:2469:A:H2 | 31:DA:2481:G:H21 | 1.09 | 0.95 |
| 50:DY:27:VAL:HG12 | 50:DY:29:GLU:H | 1.28 | 0.95 |
| 46:DU:87:GLY:HA3 | 47:DV:52:VAL:HG13 | 1.47 | 0.95 |
| 1:AA:386:C:C2' | 1:AA:387:U:H5' | 1.97 | 0.95 |
| 47:DV:15:GLU:HB3 | 47:DV:16:PRO:HD2 | 1.46 | 0.95 |
| 39:BN:42:TRP:HA | 39:BN:48:MET:HE1 | 1.47 | 0.95 |
| 41:DP:97:PRO:O | 41:DP:98:GLU:HB3 | 1.63 | 0.95 |
| 49:BX:76:ARG:HH11 | 49:BX:76:ARG:HG2 | 1.29 | 0.95 |
| 47:DV:69:LYS:HG3 | 47:DV:70:ILE:H | 1.31 | 0.95 |
| 30:B8:32:LEU:CB | 30:B8:35:GLN:H | 1.80 | 0.94 |
| 31:DA:154:G:H1 | 31:DA:172:C:N4 | 1.63 | 0.94 |
| 31:DA:2681:C:H5 | 31:DA:2725:A:N6 | 1.63 | 0.94 |
| 49:DX:25:LYS:HG3 | 49:DX:26:TYR:N | 1.81 | 0.94 |
| 41:BP:62:LEU:HD22 | 41:BP:62:LEU:H | 1.29 | 0.94 |
| 44:BS:92:TYR:HD1 | 44:BS:93:LYS:H | 0.99 | 0.94 |
| 47:DV:75:PHE:HE1 | 47:DV:89:GLN:HB3 | 1.31 | 0.94 |
| 31:DA:1300:U:H3' | 31:DA:1301:A:H5'' | 1.49 | 0.94 |
| 47:DV:19:LYS:HG3 | 47:DV:20:LEU:N | 1.81 | 0.94 |
| 49:DX:36:LYS:NZ | 49:DX:38:GLU:O | 2.00 | 0.94 |
| 31:BA:1822:G:H5' | 31:BA:1822:G:H8 | 1.29 | 0.94 |
| 31:BA:330:A:H2 | 31:BA:1210:A:H2' | 1.30 | 0.94 |
| 31:BA:620:G:H4' | 31:BA:621:A:H5'' | 1.48 | 0.94 |
| 30:D8:32:LEU:HB2 | 30:D8:35:GLN:H | 1.31 | 0.94 |
| 31:DA:145:G:C2' | 31:DA:146:G:H5'' | 1.96 | 0.94 |
| 47:DV:72:VAL:HG13 | 47:DV:88:ARG:HH22 | 1.32 | 0.94 |
| 50:BY:27:VAL:HG12 | 50:BY:29:GLU:H | 1.31 | 0.94 |
| 31:BA:2787:C:H1' | 34:BE:61:ARG:HB2 | 1.47 | 0.94 |
| 45:BT:29:ARG:HG3 | 45:BT:30:VAL:HG13 | 1.50 | 0.94 |
| 48:BW:4:LYS:HB2 | 48:BW:106:ILE:HG22 | 1.49 | 0.94 |
| 31:DA:1822:G:H8 | 31:DA:1822:G:H5' | 1.32 | 0.94 |
| 1:AA:445:G:H2' | 1:AA:446:G:H8 | 1.30 | 0.94 |
| 27:B5:55:ARG:HD3 | 27:B5:56:LYS:N | 1.81 | 0.94 |
| 31:BA:1300:U:H3' | 31:BA:1301:A:H5'' | 1.50 | 0.94 |
| 47:BV:62:LEU:HD22 | 47:BV:98:GLU:HB2 | 1.47 | 0.94 |
| 36:DG:63:ILE:HA | 36:DG:143:GLU:HG3 | 1.50 | 0.94 |
| 31:BA:171:G:H2' | 31:BA:172:C:O4' | 1.66 | 0.94 |
| 31:DA:2415:G:H4' | 41:DP:67:MET:N | 1.83 | 0.94 |
| 24:B2:49:LYS:HD2 | 24:B2:53:LEU:CD1 | 1.98 | 0.94 |
| 29:B7:8:ASN:ND2 | 29:B7:11:LYS:H | 1.64 | 0.94 |
| 30:B8:62:LEU:HD13 | 31:BA:242:G:H5'' | 1.48 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:542:C:N4 | 31:BA:543:C:N4 | 2.16 | 0.94 |
| 47:BV:90:PRO:CG | 47:BV:91:TYR:H | 1.80 | 0.94 |
| 31:DA:587:C:H4' | 31:DA:588:U:OP2 | 1.67 | 0.94 |
| 35:BF:178:PRO:HB2 | 35:BF:201:VAL:HG11 | 1.50 | 0.93 |
| 42:BQ:9:TYR:HD2 | 42:BQ:9:TYR:O | 1.50 | 0.93 |
| 49:DX:25:LYS:CG | 49:DX:26:TYR:H | 1.80 | 0.93 |
| 30:D8:32:LEU:CB | 30:D8:35:GLN:H | 1.81 | 0.93 |
| 31:DA:1024:G:H3' | 31:DA:1025:G:H5'' | 1.50 | 0.93 |
| 31:DA:1779:U:H5 | 31:DA:1784:A:N7 | 1.64 | 0.93 |
| 31:BA:911:A:H2' | 42:BQ:9:TYR:OH | 1.68 | 0.93 |
| 1:CA:626:U:H2' | 1:CA:627:G:C8 | 2.03 | 0.93 |
| 45:BT:83:ILE:HG13 | 45:BT:84:GLN:H | 1.31 | 0.93 |
| 4:AD:12:CYS:HA | 4:AD:19:LEU:HD12 | 1.49 | 0.93 |
| 31:BA:1779:U:H5 | 31:BA:1784:A:N7 | 1.67 | 0.93 |
| 41:DP:59:LEU:HA | 41:DP:61:ARG:HH11 | 1.23 | 0.93 |
| 41:DP:75:ILE:H | 41:DP:75:ILE:HD13 | 1.31 | 0.93 |
| 47:DV:82:ARG:CG | 47:DV:82:ARG:HH11 | 1.79 | 0.93 |
| 34:DE:111:ARG:NH1 | 43:DR:2:ARG:HH21 | 1.66 | 0.93 |
| 23:B1:49:VAL:HG11 | 31:BA:2091:U:O2' | 1.68 | 0.93 |
| 31:BA:571:A:H5' | 31:BA:2030:A:H62 | 1.31 | 0.93 |
| 39:BN:3:THR:HG22 | 39:BN:4:TYR:H | 1.33 | 0.93 |
| 41:BP:115:LEU:HA | 41:BP:134:ALA:HB2 | 1.51 | 0.93 |
| 1:CA:386:C:C2' | 1:CA:387:U:H5' | 1.98 | 0.93 |
| 31:BA:993:G:H5'' | 47:BV:75:PHE:CE2 | 2.03 | 0.93 |
| 33:BD:35:LYS:CD | 33:BD:104:TYR:CD1 | 2.52 | 0.93 |
| 8:CH:102:ARG:H | 8:CH:102:ARG:HE | 1.16 | 0.93 |
| 41:DP:24:GLY:HA3 | 41:DP:33:ARG:HH21 | 1.34 | 0.93 |
| 41:DP:30:THR:HG22 | 41:DP:31:ALA:H | 1.34 | 0.93 |
| 4:AD:8:VAL:HB | 4:AD:21:LEU:HD12 | 1.51 | 0.93 |
| 23:D1:10:LYS:HD3 | 23:D1:14:VAL:HA | 1.48 | 0.93 |
| 1:CA:445:G:H2' | 1:CA:446:G:H8 | 1.31 | 0.93 |
| 10:CJ:29:ARG:HH22 | 10:CJ:84:GLN:HG2 | 1.31 | 0.93 |
| 28:D6:10:LEU:HD12 | 30:D8:35:GLN:HE22 | 1.33 | 0.93 |
| 30:D8:46:ARG:HH22 | 41:DP:65:ARG:HH22 | 1.12 | 0.93 |
| 1:AA:626:U:H2' | 1:AA:627:G:C8 | 2.05 | 0.92 |
| 2:AB:84:GLU:HB3 | 2:AB:219:VAL:HG21 | 1.48 | 0.92 |
| 10:AJ:29:ARG:HH22 | 10:AJ:84:GLN:HG2 | 1.32 | 0.92 |
| 28:B6:15:GLU:OE2 | 28:B6:43:CYS:SG | 2.27 | 0.92 |
| 41:BP:97:PRO:O | 41:BP:98:GLU:HB3 | 1.66 | 0.92 |
| 42:DQ:22:LYS:HA | 42:DQ:22:LYS:HE2 | 1.50 | 0.92 |
| 8:AH:86:ILE:HG21 | 8:AH:133:LEU:HD13 | 1.47 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:B2:41:ILE:O | 24:B2:42:GLY:C | 2.06 | 0.92 |
| 33:BD:186:HIS:CD2 | 33:BD:188:GLU:H | 1.87 | 0.92 |
| 36:BG:63:ILE:HA | 36:BG:143:GLU:HG3 | 1.50 | 0.92 |
| 4:CD:12:CYS:HA | 4:CD:19:LEU:HD12 | 1.50 | 0.92 |
| 24:D2:56:GLN:H | 24:D2:56:GLN:NE2 | 1.68 | 0.92 |
| 31:DA:2068:U:H3 | 31:DA:2430:A:H2 | 1.08 | 0.92 |
| 33:DD:235:GLY:O | 33:DD:237:GLU:HG2 | 1.68 | 0.92 |
| 35:BF:66:PRO:O | 35:BF:67:GLN:HB3 | 1.69 | 0.92 |
| 49:BX:25:LYS:CG | 49:BX:26:TYR:H | 1.82 | 0.92 |
| 31:BA:71:A:C2 | 49:BX:31:HIS:HE1 | 1.86 | 0.92 |
| 49:BX:36:LYS:HD2 | 49:BX:36:LYS:O | 1.69 | 0.92 |
| 31:DA:1899:G:N2 | 31:DA:1902:C:H41 | 1.65 | 0.92 |
| 31:DA:997:G:OP1 | 46:DU:93:LYS:HD3 | 1.70 | 0.92 |
| 43:DR:4:LEU:HD13 | 43:DR:4:LEU:O | 1.69 | 0.92 |
| 31:BA:145:G:C2' | 31:BA:146:G:H5'' | 2.00 | 0.92 |
| 39:DN:47:ALA:HB2 | 39:DN:112:LEU:HD11 | 1.52 | 0.92 |
| 41:DP:115:LEU:HA | 41:DP:134:ALA:HB2 | 1.51 | 0.92 |
| 47:DV:72:VAL:HA | 47:DV:88:ARG:HH12 | 1.34 | 0.92 |
| 44:BS:92:TYR:CD1 | 44:BS:93:LYS:N | 2.38 | 0.92 |
| 49:BX:60:ARG:HE | 49:BX:74:PRO:HG2 | 1.33 | 0.92 |
| 42:DQ:35:VAL:HG13 | 42:DQ:130:LYS:HB3 | 1.52 | 0.92 |
| 31:BA:84:A:H61 | 31:BA:102:G:H1' | 1.34 | 0.92 |
| 33:BD:35:LYS:CD | 33:BD:104:TYR:HD1 | 1.81 | 0.92 |
| 42:BQ:24:GLY:HA3 | 51:BZ:78:LYS:HB3 | 1.50 | 0.92 |
| 31:DA:71:A:H2 | 49:DX:31:HIS:HE1 | 1.07 | 0.92 |
| 31:BA:1169:G:H1 | 31:BA:1180:C:H42 | 1.12 | 0.92 |
| 31:BA:2317:C:H2' | 31:BA:2318:G:C5' | 1.99 | 0.92 |
| 41:BP:62:LEU:N | 41:BP:62:LEU:HD22 | 1.83 | 0.92 |
| 50:BY:76:CYS:SG | 50:BY:77:PRO:HD2 | 2.09 | 0.92 |
| 23:D1:19:GLN:HE21 | 31:DA:379:G:H21 | 1.11 | 0.92 |
| 31:DA:993:G:H5'' | 47:DV:75:PHE:CE2 | 2.04 | 0.92 |
| 35:DF:66:PRO:O | 35:DF:67:GLN:HB3 | 1.67 | 0.92 |
| 47:DV:85:LYS:O | 47:DV:87:HIS:N | 2.01 | 0.92 |
| 31:BA:2020:A:O2' | 31:BA:2021:C:H5' | 1.70 | 0.92 |
| 4:CD:18:LYS:HE3 | 4:CD:31:CYS:SG | 2.09 | 0.92 |
| 33:DD:35:LYS:CD | 33:DD:104:TYR:HD1 | 1.83 | 0.92 |
| 41:DP:64:LYS:C | 41:DP:66:GLY:H | 1.71 | 0.92 |
| 44:DS:92:TYR:CD1 | 44:DS:93:LYS:N | 2.37 | 0.92 |
| 36:DG:47:LYS:HD3 | 36:DG:81:LYS:HD2 | 1.50 | 0.92 |
| 31:BA:286:C:C2' | 31:BA:287:C:H5' | 2.01 | 0.91 |
| 49:BX:25:LYS:HG3 | 49:BX:26:TYR:N | 1.83 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DN:42:TRP:HB3 | 46:DU:64:ARG:NH1 | 1.85 | 0.91 |
| 47:DV:15:GLU:HB3 | 47:DV:16:PRO:CD | 2.00 | 0.91 |
| 34:DE:132:HIS:CD2 | 34:DE:135:HIS:NE2 | 2.39 | 0.91 |
| 39:DN:24:GLY:O | 39:DN:28:THR:HG23 | 1.69 | 0.91 |
| 40:BO:10:VAL:HG21 | 40:BO:16:ALA:O | 1.71 | 0.91 |
| 35:DF:53:THR:HG22 | 35:DF:55:GLY:N | 1.84 | 0.91 |
| 37:DH:41:MET:HA | 37:DH:41:MET:CE | 2.00 | 0.91 |
| 38:DI:72:LEU:HD12 | 38:DI:138:ILE:HG23 | 1.51 | 0.91 |
| 41:DP:112:LEU:HD22 | 41:DP:113:LYS:H | 1.36 | 0.91 |
| 45:DT:17:THR:O | 45:DT:18:ASP:HB3 | 1.68 | 0.91 |
| 47:DV:90:PRO:CG | 47:DV:91:TYR:H | 1.79 | 0.91 |
| 47:BV:72:VAL:HG13 | 47:BV:88:ARG:HH22 | 1.34 | 0.91 |
| 1:CA:266:G:H5'' | 1:CA:268:C:H41 | 1.35 | 0.91 |
| 31:DA:811:U:O2 | 31:DA:1250:G:H3' | 1.70 | 0.91 |
| 34:BE:152:LYS:HG2 | 39:BN:78:TYR:CD2 | 2.05 | 0.91 |
| 1:CA:1030(A):G:H1' | 1:CA:1031:G:H22 | 1.35 | 0.91 |
| 1:AA:250:A:H4' | 1:AA:251:G:O5' | 1.68 | 0.91 |
| 19:AS:40:ILE:HD13 | 19:AS:62:ILE:HD11 | 1.52 | 0.91 |
| 36:BG:47:LYS:HD3 | 36:BG:81:LYS:HD2 | 1.49 | 0.91 |
| 41:BP:24:GLY:HA3 | 41:BP:33:ARG:HH21 | 1.32 | 0.91 |
| 31:DA:2206:G:H21 | 31:DA:2207:G:C5' | 1.84 | 0.91 |
| 46:BU:87:GLY:HA3 | 47:BV:52:VAL:HG13 | 1.50 | 0.91 |
| 45:DT:53:ARG:HG3 | 45:DT:53:ARG:NH1 | 1.83 | 0.91 |
| 1:AA:353:A:H5' | 1:AA:353:A:H8 | 1.34 | 0.91 |
| 24:B2:56:GLN:NE2 | 24:B2:56:GLN:H | 1.68 | 0.91 |
| 30:D8:32:LEU:C | 30:D8:34:TRP:H | 1.73 | 0.91 |
| 31:DA:2020:A:O2' | 31:DA:2021:C:H5' | 1.71 | 0.91 |
| 44:DS:92:TYR:HD1 | 44:DS:93:LYS:H | 0.99 | 0.91 |
| 31:BA:529:A:H62 | 31:BA:2041:U:H3 | 1.14 | 0.91 |
| 41:BP:64:LYS:O | 41:BP:66:GLY:N | 2.03 | 0.91 |
| 47:BV:19:LYS:HB3 | 47:BV:96:ILE:O | 1.71 | 0.91 |
| 47:BV:72:VAL:HA | 47:BV:88:ARG:HH12 | 1.33 | 0.91 |
| 31:DA:2463:C:C2' | 31:DA:2464:C:H5' | 2.02 | 0.91 |
| 2:AB:87:ARG:HE | 2:AB:233:SER:HB3 | 1.36 | 0.90 |
| 24:B2:26:ARG:CZ | 24:B2:29:LYS:HE2 | 2.01 | 0.90 |
| 46:BU:64:ARG:NH2 | 46:BU:64:ARG:HA | 1.86 | 0.90 |
| 22:D0:72:ARG:HB2 | 22:D0:75:LEU:HB2 | 1.52 | 0.90 |
| 48:DW:9:TYR:H | 48:DW:102:HIS:HD2 | 1.19 | 0.90 |
| 31:BA:1899:G:N2 | 31:BA:1902:C:H41 | 1.69 | 0.90 |
| 31:BA:2394:C:OP1 | 41:BP:63:PRO:HD2 | 1.70 | 0.90 |
| 4:CD:8:VAL:HB | 4:CD:21:LEU:HD12 | 1.53 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DD:93:ALA:HB3 | 33:DD:105:ILE:HG22 | 1.53 | 0.90 |
| 28:B6:43:CYS:SG | 28:B6:43:CYS:O | 2.29 | 0.90 |
| 38:BI:38:LEU:HD12 | 38:BI:38:LEU:H | 1.36 | 0.90 |
| 42:BQ:23:GLY:O | 42:BQ:100:GLY:HA3 | 1.71 | 0.90 |
| 47:BV:22:VAL:O | 47:BV:23:GLU:HB2 | 1.69 | 0.90 |
| 13:CM:10:PRO:HB2 | 13:CM:18:ALA:HB1 | 1.53 | 0.90 |
| 31:DA:2463:C:H2' | 31:DA:2464:C:H5' | 1.53 | 0.90 |
| 31:DA:542:C:N4 | 31:DA:543:C:N4 | 2.19 | 0.90 |
| 47:DV:22:VAL:O | 47:DV:23:GLU:HB2 | 1.70 | 0.90 |
| 28:B6:15:GLU:CD | 28:B6:43:CYS:SG | 2.50 | 0.90 |
| 23:D1:41:ARG:HH11 | 23:D1:41:ARG:CG | 1.84 | 0.90 |
| 31:DA:71:A:H2 | 49:DX:31:HIS:CE1 | 1.88 | 0.90 |
| 41:DP:62:LEU:H | 41:DP:62:LEU:HD22 | 1.36 | 0.90 |
| 8:AH:102:ARG:H | 8:AH:102:ARG:HE | 1.19 | 0.90 |
| 31:DA:286:C:C2' | 31:DA:287:C:H5' | 2.00 | 0.90 |
| 41:BP:75:ILE:HD13 | 41:BP:75:ILE:H | 1.35 | 0.90 |
| 33:DD:35:LYS:CD | 33:DD:104:TYR:CD1 | 2.54 | 0.90 |
| 1:AA:1030(A):G:H1' | 1:AA:1031:G:H22 | 1.35 | 0.90 |
| 30:B8:32:LEU:C | 30:B8:34:TRP:H | 1.70 | 0.90 |
| 31:BA:1024:G:H3' | 31:BA:1025:G:H5'' | 1.54 | 0.90 |
| 31:BA:2712:U:O2 | 31:BA:2712:U:H5'' | 1.72 | 0.90 |
| 41:BP:16:ARG:HD3 | 41:BP:18:ARG:CB | 2.00 | 0.90 |
| 50:BY:17:SER:HB2 | 50:BY:71:LYS:HD2 | 1.53 | 0.90 |
| 50:BY:10:GLY:HA2 | 50:BY:27:VAL:CG1 | 2.01 | 0.90 |
| 31:DA:2524:G:H8 | 31:DA:2524:G:H5' | 1.35 | 0.90 |
| 42:DQ:24:GLY:HA3 | 51:DZ:78:LYS:HB3 | 1.50 | 0.90 |
| 42:DQ:8:LYS:HG3 | 42:DQ:9:TYR:H | 1.35 | 0.90 |
| 41:BP:16:ARG:CD | 41:BP:18:ARG:HB2 | 2.01 | 0.90 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:C8 | 2.07 | 0.90 |
| 30:D8:31:HIS:CG | 31:DA:2419:U:O4 | 2.25 | 0.90 |
| 28:B6:10:LEU:HD12 | 30:B8:35:GLN:HE22 | 1.35 | 0.90 |
| 31:BA:1697:G:H5' | 31:BA:1697:G:H8 | 1.36 | 0.90 |
| 33:BD:35:LYS:CE | 33:BD:104:TYR:HB2 | 2.02 | 0.90 |
| 37:BH:41:MET:CE | 37:BH:41:MET:HA | 1.99 | 0.90 |
| 31:DA:1652:A:H2' | 31:DA:1653:G:H5' | 1.53 | 0.90 |
| 32:BB:20:C:H2' | 32:BB:21:G:H5' | 1.54 | 0.89 |
| 2:CB:87:ARG:HE | 2:CB:233:SER:HB3 | 1.37 | 0.89 |
| 23:D1:10:LYS:HB2 | 23:D1:14:VAL:H | 1.34 | 0.89 |
| 2:AB:111:ARG:NH1 | 2:AB:111:ARG:HG2 | 1.79 | 0.89 |
| 33:BD:27:THR:HG21 | 33:BD:83:GLU:HG2 | 1.50 | 0.89 |
| 31:BA:1658:C:OP1 | 34:BE:132:HIS:CE1 | 2.24 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:1430:C:H2' | 31:DA:1431:U:C6 | 2.08 | 0.89 |
| 31:DA:1771:C:HO2' | 31:DA:1786:A:H8 | 0.97 | 0.89 |
| 31:DA:1821:A:H2' | 31:DA:1822:G:H5'' | 1.55 | 0.89 |
| 46:DU:64:ARG:HA | 46:DU:64:ARG:NH2 | 1.87 | 0.89 |
| 49:DX:60:ARG:HE | 49:DX:74:PRO:HG2 | 1.36 | 0.89 |
| 27:B5:40:LYS:HD3 | 27:B5:46:CYS:HB3 | 1.53 | 0.89 |
| 31:BA:875:G:H4' | 51:BZ:170:THR:HG21 | 1.54 | 0.89 |
| 41:DP:64:LYS:O | 41:DP:66:GLY:N | 2.05 | 0.89 |
| 44:DS:34:HIS:HB3 | 44:DS:53:SER:CB | 2.02 | 0.89 |
| 13:AM:10:PRO:HB2 | 13:AM:18:ALA:HB1 | 1.54 | 0.89 |
| 34:BE:132:HIS:CD2 | 34:BE:135:HIS:NE2 | 2.40 | 0.89 |
| 33:DD:186:HIS:HD2 | 33:DD:188:GLU:H | 1.15 | 0.89 |
| 31:DA:875:G:H4' | 51:DZ:170:THR:HG21 | 1.52 | 0.89 |
| 1:AA:503:C:OP2 | 12:AL:116:SER:HB3 | 1.73 | 0.89 |
| 31:BA:1379:A:O2' | 31:BA:1380:G:OP1 | 1.90 | 0.89 |
| 31:BA:2307:G:N2 | 31:BA:2308:G:H5' | 1.87 | 0.89 |
| 31:BA:2415:G:H4' | 41:BP:67:MET:N | 1.87 | 0.89 |
| 45:BT:65:LYS:HE3 | 45:BT:66:VAL:N | 1.87 | 0.89 |
| 49:BX:72:LYS:HG3 | 49:BX:73:ARG:H | 1.38 | 0.89 |
| 1:CA:503:C:OP2 | 12:CL:116:SER:HB3 | 1.73 | 0.89 |
| 31:DA:620:G:H4' | 31:DA:621:A:H5'' | 1.52 | 0.89 |
| 31:DA:786:C:C2' | 31:DA:787:U:H5' | 2.02 | 0.89 |
| 23:B1:10:LYS:HB2 | 23:B1:14:VAL:H | 1.34 | 0.89 |
| 31:BA:1652:A:H2' | 31:BA:1653:G:H5' | 1.52 | 0.89 |
| 35:BF:53:THR:HG22 | 35:BF:55:GLY:N | 1.87 | 0.89 |
| 41:DP:16:ARG:HD3 | 41:DP:18:ARG:CB | 2.02 | 0.89 |
| 34:BE:119:ARG:HG3 | 34:BE:119:ARG:NH1 | 1.86 | 0.89 |
| 31:DA:1169:G:H1 | 31:DA:1180:C:H42 | 1.11 | 0.89 |
| 31:DA:2688:U:H5 | 31:DA:2720:U:OP2 | 1.56 | 0.89 |
| 1:AA:624:C:H4' | 16:AP:10:GLY:HA2 | 1.54 | 0.89 |
| 41:BP:120:ALA:HB1 | 41:BP:138:LEU:HB3 | 1.55 | 0.89 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:H8 | 1.36 | 0.89 |
| 5:CE:51:VAL:HB | 5:CE:52:PRO:HD3 | 1.55 | 0.89 |
| 31:DA:529:A:H62 | 31:DA:2041:U:H3 | 1.13 | 0.89 |
| 34:DE:116:VAL:O | 34:DE:117:MET:HB3 | 1.71 | 0.89 |
| 1:AA:266:G:H5'' | 1:AA:268:C:H41 | 1.35 | 0.89 |
| 31:BA:1464:C:HO2' | 31:BA:1528:A:H8 | 0.90 | 0.89 |
| 31:BA:2206:G:H21 | 31:BA:2207:G:C5' | 1.83 | 0.89 |
| 41:BP:21:ARG:HG2 | 41:BP:21:ARG:O | 1.71 | 0.89 |
| 47:BV:69:LYS:HG3 | 47:BV:70:ILE:H | 1.36 | 0.89 |
| 31:DA:796:C:H2' | 31:DA:797:C:C6 | 2.08 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:DB:44:G:H5'' | 32:DB:45:A:OP1 | 1.73 | 0.89 |
| 43:DR:10:LEU:HB3 | 43:DR:17:ARG:NE | 1.87 | 0.89 |
| 15:AO:39:LEU:HD12 | 15:AO:56:LEU:HB2 | 1.55 | 0.88 |
| 23:B1:13:ILE:HG12 | 23:B1:14:VAL:N | 1.88 | 0.88 |
| 30:B8:32:LEU:HB2 | 30:B8:35:GLN:H | 1.35 | 0.88 |
| 31:BA:811:U:O2 | 31:BA:1250:G:H3' | 1.71 | 0.88 |
| 31:BA:1430:C:H2' | 31:BA:1431:U:C6 | 2.08 | 0.88 |
| 39:BN:42:TRP:HB3 | 46:BU:64:ARG:NH1 | 1.86 | 0.88 |
| 50:BY:96:ILE:HG13 | 50:BY:99:CYS:O | 1.72 | 0.88 |
| 1:CA:1256:A:H61 | 1:CA:1278:U:H1' | 1.37 | 0.88 |
| 28:D6:43:CYS:O | 28:D6:43:CYS:SG | 2.30 | 0.88 |
| 31:BA:786:C:C2' | 31:BA:787:U:H5' | 2.03 | 0.88 |
| 23:D1:13:ILE:HG12 | 23:D1:14:VAL:N | 1.87 | 0.88 |
| 23:D1:47:GLN:HB2 | 31:DA:397:G:H5'' | 1.55 | 0.88 |
| 39:DN:16:ILE:HD11 | 39:DN:26:LEU:HD11 | 1.54 | 0.88 |
| 1:AA:1432:G:OP1 | 45:BT:107:ASP:HB2 | 1.73 | 0.88 |
| 24:D2:26:ARG:CZ | 24:D2:29:LYS:HE2 | 2.02 | 0.88 |
| 31:DA:669:G:H4' | 31:DA:670:A:OP2 | 1.71 | 0.88 |
| 50:DY:76:CYS:SG | 50:DY:77:PRO:HD2 | 2.13 | 0.88 |
| 31:BA:2524:G:H8 | 31:BA:2524:G:H5' | 1.34 | 0.88 |
| 33:BD:108:PRO:HB3 | 33:BD:143:HIS:CE1 | 2.07 | 0.88 |
| 1:CA:386:C:H2' | 1:CA:387:U:H5' | 1.55 | 0.88 |
| 29:D7:8:ASN:C | 29:D7:8:ASN:HD22 | 1.76 | 0.88 |
| 33:DD:35:LYS:HD3 | 33:DD:63:ARG:HB3 | 1.55 | 0.88 |
| 45:DT:3:ARG:HB2 | 45:DT:6:LEU:HB3 | 1.56 | 0.88 |
| 51:DZ:7:ALA:HB3 | 51:DZ:61:LEU:HD23 | 1.55 | 0.88 |
| 37:BH:41:MET:HE2 | 37:BH:41:MET:HA | 1.53 | 0.88 |
| 1:CA:1003:G:H2' | 1:CA:1004:A:H4' | 1.55 | 0.88 |
| 31:DA:84:A:H61 | 31:DA:102:G:H1' | 1.36 | 0.88 |
| 31:BA:1697:G:H5' | 31:BA:1697:G:C8 | 2.09 | 0.88 |
| 38:BI:1:MET:HG3 | 38:BI:23:PRO:HA | 1.56 | 0.88 |
| 49:BX:72:LYS:HG3 | 49:BX:74:PRO:HD3 | 1.54 | 0.88 |
| 50:BY:8:LYS:HZ1 | 50:BY:73:ARG:HA | 1.38 | 0.88 |
| 31:DA:751:A:H5' | 48:DW:90:ARG:HA | 1.54 | 0.88 |
| 32:DB:20:C:H2' | 32:DB:21:G:H5' | 1.53 | 0.88 |
| 38:DI:38:LEU:H | 38:DI:38:LEU:HD12 | 1.38 | 0.88 |
| 10:AJ:40:LEU:HB2 | 10:AJ:41:PRO:HD2 | 1.54 | 0.88 |
| 28:B6:9:LEU:HD22 | 28:B6:10:LEU:H | 1.38 | 0.88 |
| 31:BA:1882:C:H5' | 31:BA:1883:G:OP2 | 1.73 | 0.88 |
| 45:BT:53:ARG:HH11 | 45:BT:53:ARG:HG3 | 1.38 | 0.88 |
| 47:BV:15:GLU:HB3 | 47:BV:16:PRO:CD | 2.01 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:BY:75:ILE:HD11 | 50:BY:79:CYS:CA | 2.04 | 0.88 |
| 31:DA:2523:G:C2' | 31:DA:2524:G:H5'' | 2.02 | 0.88 |
| 31:DA:271(L):U:H4' | 31:DA:271(M):G:C5 | 2.08 | 0.88 |
| 31:DA:285:C:C2' | 31:DA:286:C:H5'' | 2.04 | 0.88 |
| 38:DI:1:MET:HG3 | 38:DI:23:PRO:HA | 1.56 | 0.88 |
| 40:DO:115:VAL:HG13 | 40:DO:121:VAL:HG21 | 1.56 | 0.88 |
| 31:BA:2036:C:H6 | 31:BA:2036:C:H5' | 1.38 | 0.88 |
| 47:BV:75:PHE:HE1 | 47:BV:89:GLN:HB3 | 1.35 | 0.88 |
| 6:CF:11:ASN:HB3 | 6:CF:14:LEU:HG | 1.55 | 0.88 |
| 10:CJ:40:LEU:HB2 | 10:CJ:41:PRO:HD2 | 1.53 | 0.88 |
| 31:DA:1821:A:C2' | 31:DA:1822:G:H5'' | 2.03 | 0.88 |
| 38:DI:133:HIS:ND1 | 38:DI:134:PRO:HD2 | 1.87 | 0.88 |
| 1:AA:1003:G:H2' | 1:AA:1004:A:H4' | 1.55 | 0.88 |
| 1:AA:200:G:H1 | 1:AA:217:C:H42 | 1.20 | 0.88 |
| 31:BA:271(L):U:H4' | 31:BA:271(M):G:C5 | 2.09 | 0.88 |
| 19:CS:40:ILE:HD13 | 19:CS:62:ILE:HD11 | 1.54 | 0.88 |
| 31:DA:1022:G:H22 | 31:DA:1142(A):A:H2 | 1.21 | 0.88 |
| 33:BD:63:ARG:HH11 | 33:BD:63:ARG:HG3 | 1.39 | 0.88 |
| 14:CN:4:LYS:O | 14:CN:7:ILE:HG12 | 1.74 | 0.88 |
| 31:DA:1278:A:OP1 | 43:DR:36:THR:HG22 | 1.74 | 0.88 |
| 34:DE:119:ARG:HG3 | 34:DE:119:ARG:NH1 | 1.87 | 0.88 |
| 31:DA:1006:C:H1' | 39:DN:106:MET:HE3 | 1.53 | 0.88 |
| 50:DY:75:ILE:HD11 | 50:DY:79:CYS:C | 1.93 | 0.88 |
| 14:AN:4:LYS:O | 14:AN:7:ILE:HG12 | 1.74 | 0.87 |
| 31:BA:2523:G:C2' | 31:BA:2524:G:H5'' | 2.04 | 0.87 |
| 31:BA:2850:A:OP2 | 31:BA:2866:U:H5 | 1.57 | 0.87 |
| 1:CA:954:G:H21 | 1:CA:1227:A:H62 | 1.22 | 0.87 |
| 24:D2:41:ILE:O | 24:D2:42:GLY:C | 2.12 | 0.87 |
| 31:DA:2850:A:OP2 | 31:DA:2866:U:H5 | 1.55 | 0.87 |
| 31:DA:542:C:C4 | 31:DA:543:C:N4 | 2.42 | 0.87 |
| 46:DU:55:ARG:HA | 46:DU:58:ARG:HD2 | 1.55 | 0.87 |
| 50:DY:96:ILE:HG21 | 50:DY:99:CYS:SG | 2.14 | 0.87 |
| 51:DZ:101:PRO:O | 51:DZ:102:LEU:HD23 | 1.74 | 0.87 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:H8 | 1.37 | 0.87 |
| 42:BQ:8:LYS:CG | 42:BQ:9:TYR:H | 1.87 | 0.87 |
| 1:CA:735:C:H2' | 1:CA:736:C:H6 | 1.40 | 0.87 |
| 31:DA:1697:G:H5' | 31:DA:1697:G:C8 | 2.08 | 0.87 |
| 31:DA:1697:G:H5' | 31:DA:1697:G:H8 | 1.36 | 0.87 |
| 41:DP:21:ARG:HG2 | 41:DP:21:ARG:O | 1.73 | 0.87 |
| 1:AA:1256:A:H61 | 1:AA:1278:U:H1' | 1.38 | 0.87 |
| 43:BR:10:LEU:HB3 | 43:BR:17:ARG:NE | 1.90 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:BS:34:HIS:HB3 | 44:BS:53:SER:CB | 2.03 | 0.87 |
| 28:D6:15:GLU:OE2 | 28:D6:41:PRO:HG3 | 1.74 | 0.87 |
| 41:DP:120:ALA:HB1 | 41:DP:138:LEU:HB3 | 1.55 | 0.87 |
| 30:D8:25:MET:HB2 | 41:DP:62:LEU:HD23 | 1.55 | 0.87 |
| 28:B6:46:HIS:CB | 28:B6:47:THR:N | 2.36 | 0.87 |
| 39:BN:18:ALA:HB1 | 39:BN:21:LYS:CB | 2.05 | 0.87 |
| 39:DN:42:TRP:HA | 39:DN:48:MET:HE1 | 1.55 | 0.87 |
| 45:DT:29:ARG:HG3 | 45:DT:30:VAL:HG13 | 1.55 | 0.87 |
| 28:B6:28:ARG:HA | 28:B6:32:ASN:HD22 | 1.37 | 0.87 |
| 31:BA:1021:A:H62 | 31:BA:1141:U:H3 | 1.14 | 0.87 |
| 39:BN:24:GLY:O | 39:BN:28:THR:HG23 | 1.74 | 0.87 |
| 45:BT:3:ARG:HB2 | 45:BT:6:LEU:HB3 | 1.56 | 0.87 |
| 31:DA:1379:A:O2' | 31:DA:1380:G:OP1 | 1.92 | 0.87 |
| 31:BA:1821:A:H2' | 31:BA:1822:G:H5'' | 1.57 | 0.87 |
| 31:BA:542:C:C4 | 31:BA:543:C:N4 | 2.42 | 0.87 |
| 1:CA:624:C:H4' | 16:CP:10:GLY:HA2 | 1.55 | 0.87 |
| 31:DA:2476:A:N3 | 31:DA:2477:C:H5'' | 1.90 | 0.87 |
| 33:DD:35:LYS:CE | 33:DD:104:TYR:HB2 | 2.04 | 0.87 |
| 50:DY:45:VAL:HG13 | 50:DY:62:GLU:HB2 | 1.55 | 0.87 |
| 10:AJ:51:ARG:HE | 10:AJ:61:GLU:HB2 | 1.40 | 0.87 |
| 31:BA:146:G:H5' | 31:BA:146:G:H8 | 1.39 | 0.87 |
| 30:B8:6:THR:HG22 | 30:B8:63:PRO:HD3 | 1.55 | 0.87 |
| 31:BA:1899:G:H22 | 31:BA:1902:C:H41 | 0.91 | 0.87 |
| 38:BI:72:LEU:HD12 | 38:BI:138:ILE:HG23 | 1.54 | 0.87 |
| 43:BR:11:ASN:OD1 | 43:BR:12:ARG:N | 2.08 | 0.87 |
| 31:DA:146:G:H5' | 31:DA:146:G:H8 | 1.37 | 0.87 |
| 1:AA:445:G:H2' | 1:AA:446:G:C8 | 2.10 | 0.87 |
| 3:AC:20:SER:HB2 | 3:AC:40:ARG:HH22 | 1.39 | 0.87 |
| 33:BD:35:LYS:HE3 | 33:BD:64:ILE:C | 1.96 | 0.87 |
| 49:DX:63:LYS:HE3 | 49:DX:70:LEU:HD22 | 1.57 | 0.87 |
| 28:B6:15:GLU:OE2 | 28:B6:41:PRO:HG3 | 1.74 | 0.86 |
| 31:BA:2688:U:H5 | 31:BA:2720:U:OP2 | 1.58 | 0.86 |
| 1:CA:200:G:H1 | 1:CA:217:C:H42 | 1.22 | 0.86 |
| 27:D5:40:LYS:HD3 | 27:D5:46:CYS:HB3 | 1.57 | 0.86 |
| 29:D7:16:HIS:HB2 | 29:D7:44:PRO:HG2 | 1.54 | 0.86 |
| 1:AA:386:C:H2' | 1:AA:387:U:H5' | 1.55 | 0.86 |
| 29:B7:8:ASN:HD22 | 29:B7:8:ASN:C | 1.77 | 0.86 |
| 31:BA:2068:U:N3 | 31:BA:2430:A:H2 | 1.72 | 0.86 |
| 39:BN:45:ASN:HD22 | 39:BN:45:ASN:H | 1.22 | 0.86 |
| 50:BY:96:ILE:HG21 | 50:BY:99:CYS:SG | 2.14 | 0.86 |
| 4:CD:126:ILE:HG22 | 4:CD:127:THR:H | 1.40 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:CL:82:VAL:HG12 | 12:CL:83:VAL:H | 1.39 | 0.86 |
| 48:DW:64:MET:O | 48:DW:65:LEU:HB2 | 1.74 | 0.86 |
| 31:BA:1821:A:C2' | 31:BA:1822:G:H5'' | 2.05 | 0.86 |
| 31:BA:587:C:C5 | 41:BP:33:ARG:HG2 | 2.09 | 0.86 |
| 47:BV:47:VAL:HG13 | 47:BV:48:GLY:H | 1.39 | 0.86 |
| 1:CA:250:A:H4' | 1:CA:251:G:O5' | 1.72 | 0.86 |
| 1:CA:353:A:H5' | 1:CA:353:A:H8 | 1.36 | 0.86 |
| 1:CA:532:A:H61 | 3:CC:193:TYR:HB3 | 1.40 | 0.86 |
| 50:DY:71:LYS:HB2 | 50:DY:71:LYS:NZ | 1.88 | 0.86 |
| 50:DY:75:ILE:HD11 | 50:DY:79:CYS:CA | 2.05 | 0.86 |
| 50:DY:96:ILE:HG13 | 50:DY:99:CYS:O | 1.76 | 0.86 |
| 51:DZ:53:ILE:CG2 | 51:DZ:71:VAL:HB | 2.05 | 0.86 |
| 1:AA:1065:U:H1' | 1:AA:1066:C:OP2 | 1.75 | 0.86 |
| 31:BA:2577:A:H5'' | 31:BA:2578:G:H5' | 1.57 | 0.86 |
| 31:BA:71:A:H2 | 49:BX:31:HIS:CE1 | 1.91 | 0.86 |
| 24:D2:33:MET:HG2 | 49:DX:11:PRO:HD2 | 1.57 | 0.86 |
| 31:DA:1882:C:H5' | 31:DA:1883:G:OP2 | 1.76 | 0.86 |
| 50:DY:28:LYS:O | 50:DY:38:ILE:HB | 1.75 | 0.86 |
| 2:CB:111:ARG:NH1 | 2:CB:111:ARG:HG2 | 1.80 | 0.86 |
| 33:DD:30:GLU:HG3 | 33:DD:63:ARG:CZ | 2.05 | 0.86 |
| 31:DA:2394:C:OP1 | 41:DP:63:PRO:HD2 | 1.74 | 0.86 |
| 29:B7:8:ASN:HD21 | 29:B7:11:LYS:H | 1.24 | 0.86 |
| 31:BA:2463:C:C2' | 31:BA:2464:C:H5' | 2.06 | 0.86 |
| 51:BZ:101:PRO:O | 51:BZ:102:LEU:HD23 | 1.76 | 0.86 |
| 31:DA:571:A:H5' | 31:DA:2030:A:H62 | 1.39 | 0.86 |
| 50:DY:8:LYS:HZ1 | 50:DY:73:ARG:HA | 1.39 | 0.86 |
| 51:BZ:53:ILE:CG2 | 51:BZ:71:VAL:HB | 2.06 | 0.86 |
| 1:CA:975:A:H4' | 1:CA:976:G:H5'' | 1.57 | 0.86 |
| 10:CJ:51:ARG:HE | 10:CJ:61:GLU:HB2 | 1.41 | 0.86 |
| 31:BA:285:C:C2' | 31:BA:286:C:H5'' | 2.05 | 0.86 |
| 34:BE:116:VAL:O | 34:BE:117:MET:HB3 | 1.73 | 0.86 |
| 38:BI:133:HIS:ND1 | 38:BI:134:PRO:HD2 | 1.90 | 0.86 |
| 11:CK:22:HIS:HB3 | 11:CK:29:ILE:HG23 | 1.54 | 0.86 |
| 33:DD:228:PRO:HD3 | 33:DD:235:GLY:HA3 | 1.55 | 0.86 |
| 39:DN:40:PRO:HA | 46:DU:64:ARG:HH22 | 1.41 | 0.86 |
| 45:DT:25:GLY:O | 45:DT:26:ASP:HB2 | 1.74 | 0.86 |
| 49:DX:72:LYS:HG3 | 49:DX:73:ARG:H | 1.41 | 0.86 |
| 49:DX:72:LYS:HG3 | 49:DX:74:PRO:HD3 | 1.56 | 0.86 |
| 12:AL:82:VAL:HG12 | 12:AL:83:VAL:H | 1.41 | 0.86 |
| 24:B2:25:VAL:HG13 | 24:B2:26:ARG:HD2 | 1.58 | 0.86 |
| 31:BA:1970:A:H5' | 31:BA:1972:A:H1' | 1.58 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BD:8:PRO:HB3 | 33:BD:14:ARG:HB2 | 1.57 | 0.86 |
| 41:BP:47:ASP:HB3 | 41:BP:48:PRO:C | 1.95 | 0.86 |
| 31:DA:2317:C:H2' | 31:DA:2318:G:C5' | 2.02 | 0.86 |
| 39:DN:45:ASN:HD22 | 39:DN:45:ASN:H | 1.24 | 0.86 |
| 1:AA:975:A:H4' | 1:AA:976:G:H5'' | 1.57 | 0.86 |
| 36:DG:85:GLY:O | 36:DG:87:PRO:HD2 | 1.76 | 0.86 |
| 3:AC:70:VAL:HG12 | 3:AC:72:LYS:H | 1.40 | 0.85 |
| 31:BA:1697:G:C5' | 31:BA:1697:G:H8 | 1.89 | 0.85 |
| 39:DN:3:THR:HG22 | 39:DN:4:TYR:H | 1.39 | 0.85 |
| 42:DQ:23:GLY:O | 42:DQ:100:GLY:HA3 | 1.76 | 0.85 |
| 45:DT:29:ARG:HD3 | 45:DT:86:ILE:HG22 | 1.58 | 0.85 |
| 1:AA:954:G:H21 | 1:AA:1227:A:H62 | 1.24 | 0.85 |
| 33:BD:186:HIS:HD2 | 33:BD:188:GLU:H | 1.21 | 0.85 |
| 13:CM:49:THR:HG22 | 13:CM:51:ALA:H | 1.39 | 0.85 |
| 31:DA:1116:C:H2' | 31:DA:1117:G:H5' | 1.58 | 0.85 |
| 31:DA:2712:U:O2 | 31:DA:2712:U:H5'' | 1.75 | 0.85 |
| 31:DA:286:C:H42 | 31:DA:355:G:H1 | 1.22 | 0.85 |
| 11:AK:22:HIS:HB3 | 11:AK:29:ILE:HG23 | 1.56 | 0.85 |
| 30:B8:32:LEU:HD23 | 30:B8:35:GLN:HA | 1.58 | 0.85 |
| 31:BA:587:C:H4' | 31:BA:588:U:OP2 | 1.75 | 0.85 |
| 23:D1:40:ARG:HD3 | 23:D1:41:ARG:H | 1.42 | 0.85 |
| 31:DA:1464:C:HO2' | 31:DA:1528:A:H8 | 0.86 | 0.85 |
| 31:BA:2469:A:H2 | 31:BA:2481:G:H21 | 1.18 | 0.85 |
| 1:CA:1065:U:H1' | 1:CA:1066:C:OP2 | 1.75 | 0.85 |
| 31:DA:1448:G:H1' | 31:DA:1528:A:N6 | 1.91 | 0.85 |
| 35:DF:53:THR:CG2 | 35:DF:55:GLY:H | 1.88 | 0.85 |
| 36:DG:41:GLN:HG2 | 36:DG:155:MET:HB3 | 1.57 | 0.85 |
| 41:DP:47:ASP:HB3 | 41:DP:48:PRO:C | 1.96 | 0.85 |
| 6:AF:69:GLU:O | 6:AF:72:VAL:HG12 | 1.76 | 0.85 |
| 31:BA:1497:U:H5' | 31:BA:1498:C:H5 | 1.41 | 0.85 |
| 31:BA:2463:C:H2' | 31:BA:2464:C:H5' | 1.56 | 0.85 |
| 41:BP:64:LYS:C | 41:BP:66:GLY:N | 2.28 | 0.85 |
| 20:CT:50:GLU:HB3 | 20:CT:100:ILE:HG12 | 1.58 | 0.85 |
| 24:D2:49:LYS:HD2 | 24:D2:53:LEU:CD1 | 2.03 | 0.85 |
| 1:AA:1281:U:H4' | 1:AA:1282:C:OP2 | 1.76 | 0.85 |
| 31:BA:1494:A:C4' | 31:BA:1495:A:OP1 | 2.24 | 0.85 |
| 30:B8:25:MET:HB2 | 41:BP:62:LEU:HD23 | 1.58 | 0.85 |
| 1:CA:1281:U:H4' | 1:CA:1282:C:OP2 | 1.76 | 0.85 |
| 28:D6:46:HIS:CB | 28:D6:47:THR:N | 2.39 | 0.85 |
| 31:DA:2068:U:N3 | 31:DA:2430:A:H2 | 1.74 | 0.85 |
| 47:DV:47:VAL:HG13 | 47:DV:48:GLY:H | 1.38 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:BD:35:LYS:HD3 | 33:BD:63:ARG:C | 1.96 | 0.85 |
| 37:BH:89:ILE:O | 37:BH:90:LYS:HG2 | 1.76 | 0.85 |
| 31:DA:1696:G:C2' | 31:DA:1697:G:H5'' | 2.07 | 0.85 |
| 44:DS:17:ARG:HA | 44:DS:20:ARG:HG2 | 1.57 | 0.85 |
| 45:DT:53:ARG:CG | 45:DT:53:ARG:HH11 | 1.90 | 0.85 |
| 24:B2:49:LYS:CD | 24:B2:53:LEU:HD13 | 2.01 | 0.85 |
| 31:DA:2307:G:N2 | 31:DA:2308:G:H5' | 1.91 | 0.85 |
| 34:DE:59:VAL:HG22 | 34:DE:63:LEU:HA | 1.58 | 0.85 |
| 45:DT:65:LYS:HE3 | 45:DT:66:VAL:N | 1.90 | 0.85 |
| 27:B5:4:HIS:HB3 | 27:B5:5:PRO:HD3 | 1.59 | 0.85 |
| 31:BA:2030:A:H5'' | 31:BA:2031:A:OP1 | 1.76 | 0.85 |
| 43:BR:71:GLN:HE21 | 43:BR:71:GLN:HA | 1.42 | 0.85 |
| 1:CA:240:C:H2' | 1:CA:241:C:H6 | 1.42 | 0.85 |
| 31:DA:102:G:C5' | 31:DA:102:G:H8 | 1.84 | 0.85 |
| 31:DA:2287:A:C2 | 31:DA:2346:A:H2 | 1.95 | 0.85 |
| 32:DB:82:G:C2' | 32:DB:83:G:H5' | 2.07 | 0.85 |
| 50:DY:17:SER:HB2 | 50:DY:71:LYS:HD2 | 1.55 | 0.85 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.11 | 0.84 |
| 31:BA:1006:C:H1' | 39:BN:106:MET:HE3 | 1.58 | 0.84 |
| 39:BN:16:ILE:HD11 | 39:BN:26:LEU:HD11 | 1.57 | 0.84 |
| 37:DH:44:VAL:HG12 | 37:DH:45:VAL:H | 1.42 | 0.84 |
| 41:DP:62:LEU:N | 41:DP:62:LEU:HD22 | 1.92 | 0.84 |
| 47:DV:18:LEU:HD22 | 47:DV:19:LYS:HA | 1.57 | 0.84 |
| 4:AD:18:LYS:HE3 | 4:AD:31:CYS:SG | 2.17 | 0.84 |
| 41:BP:143:GLY:C | 41:BP:145:PRO:HD3 | 1.97 | 0.84 |
| 30:D8:6:THR:HG22 | 30:D8:63:PRO:HD3 | 1.59 | 0.84 |
| 31:DA:141:A:C8 | 31:DA:1408:C:O2' | 2.30 | 0.84 |
| 51:DZ:126:VAL:HG12 | 51:DZ:163:LEU:HA | 1.59 | 0.84 |
| 13:AM:49:THR:HG22 | 13:AM:51:ALA:H | 1.41 | 0.84 |
| 34:BE:59:VAL:HG22 | 34:BE:63:LEU:HA | 1.59 | 0.84 |
| 36:BG:41:GLN:HG2 | 36:BG:155:MET:HB3 | 1.57 | 0.84 |
| 50:BY:75:ILE:HD11 | 50:BY:79:CYS:HA | 1.59 | 0.84 |
| 31:DA:1019:U:HO2' | 31:DA:1021:A:H2 | 0.85 | 0.84 |
| 31:DA:1678:G:N2 | 31:DA:1989:G:H22 | 1.75 | 0.84 |
| 44:DS:34:HIS:CE1 | 44:DS:54:LEU:HB3 | 2.12 | 0.84 |
| 1:AA:627:G:H2' | 1:AA:628:G:H8 | 1.41 | 0.84 |
| 29:B7:16:HIS:HB2 | 29:B7:44:PRO:HG2 | 1.59 | 0.84 |
| 31:BA:286:C:H42 | 31:BA:355:G:H1 | 1.23 | 0.84 |
| 3:CC:20:SER:HB2 | 3:CC:40:ARG:HH22 | 1.39 | 0.84 |
| 8:CH:7:ALA:HB2 | 8:CH:85:ARG:HD3 | 1.60 | 0.84 |
| 31:DA:1970:A:H5' | 31:DA:1972:A:H1' | 1.58 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:D1:49:VAL:HG11 | 31:DA:2091:U:O2' | 1.76 | 0.84 |
| 16:AP:28:ARG:HH11 | 16:AP:28:ARG:CG | 1.88 | 0.84 |
| 31:BA:2476:A:N3 | 31:BA:2477:C:H5'' | 1.93 | 0.84 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:N1 | 1.75 | 0.84 |
| 43:DR:55:ALA:HB2 | 43:DR:79:LEU:HD13 | 1.57 | 0.84 |
| 1:CA:627:G:H2' | 1:CA:628:G:H8 | 1.42 | 0.84 |
| 31:DA:1884:A:C2' | 31:DA:1885:A:H5'' | 2.07 | 0.84 |
| 31:DA:65:C:H2' | 31:DA:66:C:H6 | 1.40 | 0.84 |
| 1:AA:598:U:H4' | 8:AH:94:TYR:CD2 | 2.13 | 0.84 |
| 20:AT:50:GLU:HB3 | 20:AT:100:ILE:HG12 | 1.59 | 0.84 |
| 24:B2:46:GLN:NE2 | 24:B2:47:ASN:N | 2.25 | 0.84 |
| 31:BA:2681:C:H5 | 31:BA:2725:A:N6 | 1.75 | 0.84 |
| 3:CC:47:LEU:HD21 | 3:CC:68:VAL:HG11 | 1.59 | 0.84 |
| 31:DA:2287:A:H2 | 31:DA:2346:A:C2 | 1.94 | 0.84 |
| 46:DU:102:GLU:HG3 | 47:DV:2:PHE:CZ | 2.12 | 0.84 |
| 49:DX:62:LYS:HB2 | 49:DX:69:TYR:H | 1.39 | 0.84 |
| 5:AE:78:HIS:HE1 | 5:AE:142:LEU:HA | 1.43 | 0.84 |
| 24:B2:45:SER:O | 24:B2:48:HIS:HB3 | 1.78 | 0.84 |
| 31:BA:1116:C:H2' | 31:BA:1117:G:H5' | 1.58 | 0.84 |
| 31:BA:154:G:H1 | 31:BA:172:C:H42 | 0.88 | 0.84 |
| 31:BA:671:C:H5' | 31:BA:671:C:H6 | 1.40 | 0.84 |
| 44:BS:34:HIS:CE1 | 44:BS:54:LEU:HB3 | 2.13 | 0.84 |
| 50:BY:45:VAL:HG13 | 50:BY:62:GLU:HB2 | 1.57 | 0.84 |
| 24:D2:45:SER:O | 24:D2:48:HIS:HB3 | 1.76 | 0.84 |
| 3:AC:47:LEU:HD21 | 3:AC:68:VAL:HG11 | 1.60 | 0.84 |
| 44:BS:17:ARG:HA | 44:BS:20:ARG:HG2 | 1.56 | 0.84 |
| 31:DA:1497:U:H5' | 31:DA:1498:C:H5 | 1.42 | 0.84 |
| 31:DA:1899:G:H22 | 31:DA:1902:C:H41 | 0.86 | 0.84 |
| 33:DD:35:LYS:HE3 | 33:DD:64:ILE:C | 1.97 | 0.84 |
| 50:DY:10:GLY:HA2 | 50:DY:27:VAL:CG1 | 2.07 | 0.84 |
| 31:BA:1019:U:HO2' | 31:BA:1021:A:H2 | 0.86 | 0.84 |
| 39:BN:40:PRO:HA | 46:BU:64:ARG:HH22 | 1.43 | 0.83 |
| 24:D2:46:GLN:NE2 | 24:D2:47:ASN:N | 2.26 | 0.83 |
| 41:DP:16:ARG:CD | 41:DP:18:ARG:HB2 | 2.04 | 0.83 |
| 48:DW:9:TYR:H | 48:DW:102:HIS:CD2 | 1.96 | 0.83 |
| 1:AA:1442(A):G:H3' | 1:AA:1442(B):A:C5' | 2.08 | 0.83 |
| 28:B6:9:LEU:HD22 | 28:B6:10:LEU:N | 1.92 | 0.83 |
| 33:BD:93:ALA:HB3 | 33:BD:105:ILE:HG22 | 1.58 | 0.83 |
| 51:BZ:126:VAL:HG12 | 51:BZ:163:LEU:HA | 1.59 | 0.83 |
| 31:DA:1210:A:C8 | 31:DA:1210:A:H5' | 2.11 | 0.83 |
| 29:D7:19:ARG:HD3 | 31:DA:125:G:H5'' | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:142:A:H8 | 31:DA:1595:G:H21 | 1.23 | 0.83 |
| 31:DA:2393:A:H5' | 41:DP:62:LEU:HB3 | 1.60 | 0.83 |
| 47:DV:19:LYS:HB3 | 47:DV:96:ILE:O | 1.78 | 0.83 |
| 1:AA:748:C:H4' | 1:AA:749:C:O5' | 1.77 | 0.83 |
| 24:B2:33:MET:HG2 | 49:BX:11:PRO:HD2 | 1.59 | 0.83 |
| 41:BP:58:THR:O | 41:BP:61:ARG:CZ | 2.27 | 0.83 |
| 31:BA:2393:A:H5' | 41:BP:62:LEU:HB3 | 1.58 | 0.83 |
| 31:DA:154:G:H1 | 31:DA:172:C:H42 | 0.89 | 0.83 |
| 31:BA:997:G:OP1 | 46:BU:93:LYS:HD3 | 1.77 | 0.83 |
| 49:BX:62:LYS:HB2 | 49:BX:69:TYR:H | 1.42 | 0.83 |
| 50:BY:75:ILE:HD11 | 50:BY:79:CYS:C | 1.97 | 0.83 |
| 35:DF:20:LEU:HD22 | 35:DF:203:GLN:HE22 | 1.42 | 0.83 |
| 31:DA:2334:G:N2 | 44:DS:18:ILE:HD11 | 1.94 | 0.83 |
| 47:DV:82:ARG:HG3 | 47:DV:82:ARG:NH1 | 1.88 | 0.83 |
| 50:DY:8:LYS:HZ1 | 50:DY:74:PRO:HD3 | 1.42 | 0.83 |
| 31:BA:1158:C:O2' | 31:BA:1159:U:P | 2.36 | 0.83 |
| 31:BA:669:G:H4' | 31:BA:670:A:OP2 | 1.78 | 0.83 |
| 31:DA:719:C:H2' | 31:DA:720:C:H6 | 1.43 | 0.83 |
| 41:DP:58:THR:O | 41:DP:61:ARG:CZ | 2.26 | 0.83 |
| 41:DP:64:LYS:C | 41:DP:66:GLY:N | 2.30 | 0.83 |
| 1:AA:735:C:H2' | 1:AA:736:C:H6 | 1.42 | 0.83 |
| 1:AA:992:U:H1' | 1:AA:993:G:OP2 | 1.78 | 0.83 |
| 2:AB:115:LEU:HD13 | 2:AB:145:LEU:HB3 | 1.61 | 0.83 |
| 1:CA:445:G:H2' | 1:CA:446:G:C8 | 2.12 | 0.83 |
| 2:CB:115:LEU:HD13 | 2:CB:145:LEU:HB3 | 1.61 | 0.83 |
| 8:CH:58:TYR:O | 8:CH:59:LEU:HD23 | 1.77 | 0.83 |
| 28:D6:16:CYS:O | 28:D6:17:LYS:HB2 | 1.76 | 0.83 |
| 28:D6:28:ARG:HA | 28:D6:32:ASN:HD22 | 1.41 | 0.83 |
| 31:BA:1771:C:HO2' | 31:BA:1786:A:H8 | 0.84 | 0.83 |
| 35:BF:78:ILE:H | 35:BF:78:ILE:HD13 | 1.43 | 0.83 |
| 37:BH:30:LYS:NZ | 37:BH:81:GLU:HA | 1.94 | 0.83 |
| 45:BT:50:ILE:HD11 | 45:BT:102:ILE:HD11 | 1.59 | 0.83 |
| 5:CE:78:HIS:HE1 | 5:CE:142:LEU:HA | 1.44 | 0.83 |
| 31:DA:84:A:N6 | 31:DA:102:G:H1' | 1.94 | 0.83 |
| 31:DA:1902:C:H1' | 33:DD:244:ARG:HD3 | 1.60 | 0.83 |
| 31:DA:2580:U:H5' | 34:DE:131:ALA:CB | 2.08 | 0.83 |
| 31:BA:141:A:C8 | 31:BA:1408:C:O2' | 2.31 | 0.83 |
| 33:BD:222:ARG:O | 33:BD:225:ALA:HB3 | 1.79 | 0.83 |
| 48:BW:9:TYR:H | 48:BW:102:HIS:HD2 | 1.23 | 0.83 |
| 51:BZ:7:ALA:HB3 | 51:BZ:61:LEU:HD23 | 1.60 | 0.83 |
| 28:D6:15:GLU:OE2 | 28:D6:43:CYS:SG | 2.37 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:2287:A:H62 | 31:DA:2344:U:H3 | 1.26 | 0.83 |
| 31:DA:993:G:H5'' | 47:DV:75:PHE:CZ | 2.14 | 0.83 |
| 33:DD:8:PRO:HB3 | 33:DD:14:ARG:HB2 | 1.61 | 0.83 |
| 42:DQ:75:THR:HA | 42:DQ:88:GLY:HA2 | 1.60 | 0.83 |
| 1:AA:1281:U:H5' | 1:AA:1282:C:H5 | 1.43 | 0.83 |
| 31:BA:1947:C:H2' | 31:BA:1948:G:H5' | 1.61 | 0.83 |
| 24:D2:30:ARG:HH11 | 24:D2:30:ARG:HG3 | 1.43 | 0.83 |
| 23:B1:19:GLN:NE2 | 31:BA:379:G:H21 | 1.76 | 0.83 |
| 33:BD:34:VAL:HG21 | 33:BD:103:ARG:HA | 1.60 | 0.83 |
| 34:BE:111:ARG:NH1 | 43:BR:2:ARG:HH21 | 1.77 | 0.83 |
| 42:BQ:110:THR:OG1 | 42:BQ:113:GLN:HG3 | 1.79 | 0.83 |
| 46:DU:31:SER:O | 46:DU:33:ARG:N | 2.10 | 0.83 |
| 49:DX:76:ARG:HG2 | 49:DX:76:ARG:NH1 | 1.88 | 0.83 |
| 50:DY:7:VAL:HB | 50:DY:8:LYS:HZ2 | 1.44 | 0.83 |
| 8:AH:7:ALA:HB2 | 8:AH:85:ARG:HD3 | 1.60 | 0.82 |
| 31:BA:1448:G:H1' | 31:BA:1528:A:N6 | 1.94 | 0.82 |
| 31:BA:2287:A:H62 | 31:BA:2344:U:H3 | 1.22 | 0.82 |
| 33:BD:35:LYS:HD3 | 33:BD:63:ARG:HB3 | 1.59 | 0.82 |
| 31:DA:587:C:C5 | 41:DP:33:ARG:HG2 | 2.14 | 0.82 |
| 35:DF:158:THR:HG23 | 35:DF:160:ASN:H | 1.44 | 0.82 |
| 37:DH:30:LYS:NZ | 37:DH:81:GLU:HA | 1.94 | 0.82 |
| 39:DN:82:LEU:H | 39:DN:82:LEU:HD12 | 1.42 | 0.82 |
| 35:BF:53:THR:CG2 | 35:BF:55:GLY:H | 1.91 | 0.82 |
| 18:CR:73:ALA:HB3 | 18:CR:79:LEU:HD12 | 1.61 | 0.82 |
| 23:D1:85:LEU:C | 23:D1:87:PRO:HD3 | 1.98 | 0.82 |
| 31:DA:954:G:H5'' | 42:DQ:13:GLN:HG2 | 1.59 | 0.82 |
| 5:AE:51:VAL:HB | 5:AE:52:PRO:HD3 | 1.60 | 0.82 |
| 37:BH:137:ASP:O | 37:BH:138:LYS:HB2 | 1.77 | 0.82 |
| 45:BT:25:GLY:O | 45:BT:26:ASP:HB2 | 1.77 | 0.82 |
| 27:D5:46:CYS:SG | 27:D5:47:PRO:HD2 | 2.18 | 0.82 |
| 30:D8:52:LYS:H | 30:D8:54:GLU:HG2 | 1.43 | 0.82 |
| 31:DA:1403:C:H5'' | 31:DA:1471:A:H1' | 1.59 | 0.82 |
| 31:DA:1494:A:C4' | 31:DA:1495:A:OP1 | 2.26 | 0.82 |
| 38:DI:81:VAL:HG11 | 38:DI:88:ILE:HG23 | 1.60 | 0.82 |
| 2:AB:54:THR:HG21 | 2:AB:201:ILE:HD11 | 1.59 | 0.82 |
| 30:B8:30:ARG:O | 30:B8:31:HIS:C | 2.18 | 0.82 |
| 31:BA:1678:G:N2 | 31:BA:1989:G:H22 | 1.76 | 0.82 |
| 39:BN:73:THR:O | 39:BN:75:TYR:N | 2.12 | 0.82 |
| 1:CA:1281:U:H5' | 1:CA:1282:C:H5 | 1.42 | 0.82 |
| 22:D0:41:ARG:HD2 | 22:D0:41:ARG:H | 1.44 | 0.82 |
| 31:DA:1158:C:O2' | 31:DA:1159:U:O5' | 1.98 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DH:153:LYS:H | 37:DH:153:LYS:HD3 | 1.42 | 0.82 |
| 46:DU:92:ARG:HD3 | 46:DU:94:ASN:HB3 | 1.60 | 0.82 |
| 31:BA:786:C:H2' | 31:BA:787:U:H5' | 1.62 | 0.82 |
| 45:BT:29:ARG:HD3 | 45:BT:86:ILE:HG22 | 1.59 | 0.82 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:H1 | 1.26 | 0.82 |
| 33:DD:186:HIS:HD2 | 33:DD:188:GLU:N | 1.77 | 0.82 |
| 35:DF:78:ILE:H | 35:DF:78:ILE:HD13 | 1.43 | 0.82 |
| 35:BF:20:LEU:HD23 | 35:BF:23:ASP:OD2 | 1.80 | 0.82 |
| 42:BQ:35:VAL:HG13 | 42:BQ:130:LYS:HB3 | 1.60 | 0.82 |
| 43:BR:55:ALA:HB2 | 43:BR:79:LEU:HD13 | 1.59 | 0.82 |
| 44:BS:33:LYS:HB3 | 44:BS:34:HIS:CD2 | 2.15 | 0.82 |
| 6:CF:69:GLU:O | 6:CF:72:VAL:HG12 | 1.79 | 0.82 |
| 33:DD:108:PRO:HB3 | 33:DD:143:HIS:HE1 | 1.42 | 0.82 |
| 35:DF:101:LEU:HD12 | 35:DF:102:PRO:CD | 2.08 | 0.82 |
| 40:BO:115:VAL:HG13 | 40:BO:121:VAL:HG21 | 1.62 | 0.82 |
| 49:BX:33:LYS:O | 49:BX:35:THR:N | 2.13 | 0.82 |
| 31:DA:309:G:O3' | 50:DY:18:GLY:HA2 | 1.80 | 0.82 |
| 41:DP:105:LEU:O | 41:DP:106:LEU:HB2 | 1.79 | 0.82 |
| 42:DQ:20:ALA:HB2 | 42:DQ:99:PRO:HD2 | 1.61 | 0.82 |
| 47:DV:66:ARG:HG2 | 47:DV:94:LEU:HG | 1.60 | 0.82 |
| 6:AF:11:ASN:HB3 | 6:AF:14:LEU:HG | 1.61 | 0.82 |
| 31:BA:2845:G:O2' | 31:BA:2846:G:H5' | 1.80 | 0.82 |
| 31:BA:287:C:H42 | 31:BA:354:G:H1 | 1.28 | 0.82 |
| 31:BA:2580:U:H5' | 34:BE:131:ALA:CB | 2.09 | 0.82 |
| 46:BU:55:ARG:HA | 46:BU:58:ARG:HD2 | 1.61 | 0.82 |
| 1:CA:748:C:H4' | 1:CA:749:C:O5' | 1.78 | 0.82 |
| 1:CA:992:U:H1' | 1:CA:993:G:OP2 | 1.79 | 0.82 |
| 23:B1:85:LEU:C | 23:B1:87:PRO:HD3 | 2.00 | 0.82 |
| 49:BX:76:ARG:HG2 | 49:BX:76:ARG:NH1 | 1.94 | 0.82 |
| 1:CA:1442(A):G:H3' | 1:CA:1442(B):A:C5' | 2.09 | 0.82 |
| 15:CO:17:ARG:HH11 | 15:CO:17:ARG:CG | 1.93 | 0.82 |
| 25:D3:19:GLN:NE2 | 25:D3:52:HIS:HE1 | 1.78 | 0.82 |
| 31:DA:1697:G:C5' | 31:DA:1697:G:H8 | 1.91 | 0.82 |
| 31:DA:2562:U:H1' | 40:DO:23:ARG:HH11 | 1.45 | 0.82 |
| 33:DD:34:VAL:HG21 | 33:DD:103:ARG:HA | 1.60 | 0.82 |
| 39:DN:18:ALA:HB1 | 39:DN:21:LYS:CB | 2.10 | 0.82 |
| 1:AA:1106:G:H5'' | 3:AC:172:ARG:HG2 | 1.62 | 0.82 |
| 31:BA:84:A:N6 | 31:BA:102:G:H1' | 1.95 | 0.82 |
| 31:BA:1696:G:C2' | 31:BA:1697:G:H5'' | 2.10 | 0.82 |
| 37:BH:20:ALA:HB1 | 37:BH:21:PRO:HD2 | 1.62 | 0.82 |
| 50:BY:71:LYS:NZ | 50:BY:71:LYS:HB2 | 1.93 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1169:A:H2' | 1:CA:1170:A:C8 | 2.15 | 0.82 |
| 1:CA:1201:A:H1' | 1:CA:1202:G:OP2 | 1.80 | 0.82 |
| 3:CC:70:VAL:HG12 | 3:CC:72:LYS:H | 1.42 | 0.82 |
| 31:DA:330:A:C2 | 31:DA:1210:A:H2' | 2.14 | 0.82 |
| 31:DA:2036:C:H6 | 31:DA:2036:C:H5' | 1.44 | 0.82 |
| 31:DA:2287:A:C2 | 31:DA:2346:A:C2 | 2.67 | 0.82 |
| 31:DA:287:C:H42 | 31:DA:354:G:H1 | 1.28 | 0.82 |
| 32:DB:52:A:N7 | 44:DS:33:LYS:HE3 | 1.94 | 0.82 |
| 1:AA:976:G:H5' | 1:AA:1358:U:O2' | 1.79 | 0.81 |
| 1:AA:240:C:H2' | 1:AA:241:C:H6 | 1.45 | 0.81 |
| 41:BP:112:LEU:HD22 | 41:BP:113:LYS:H | 1.41 | 0.81 |
| 1:CA:976:G:H5' | 1:CA:1358:U:O2' | 1.80 | 0.81 |
| 12:CL:47:LYS:HB3 | 12:CL:48:PRO:CD | 2.10 | 0.81 |
| 31:DA:1884:A:H2' | 31:DA:1885:A:C5' | 2.10 | 0.81 |
| 31:DA:2030:A:H5'' | 31:DA:2031:A:OP1 | 1.80 | 0.81 |
| 31:DA:2262:U:C2' | 31:DA:2263:C:H5'' | 2.10 | 0.81 |
| 31:BA:2562:U:H1' | 40:BO:23:ARG:HH11 | 1.43 | 0.81 |
| 32:BB:52:A:N7 | 44:BS:33:LYS:HE3 | 1.95 | 0.81 |
| 27:D5:57:VAL:HG23 | 27:D5:58:LEU:H | 1.44 | 0.81 |
| 31:DA:2327:A:H2' | 31:DA:2328:A:C8 | 2.15 | 0.81 |
| 47:DV:5:VAL:HG23 | 47:DV:36:PRO:HB2 | 1.59 | 0.81 |
| 31:BA:2287:A:H2 | 31:BA:2346:A:C2 | 1.97 | 0.81 |
| 35:BF:46:ARG:HH11 | 35:BF:46:ARG:CG | 1.94 | 0.81 |
| 31:BA:2469:A:O2' | 42:BQ:56:ARG:HG2 | 1.80 | 0.81 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C6 | 2.15 | 0.81 |
| 1:CA:450:G:H5'' | 16:CP:41:PRO:O | 1.80 | 0.81 |
| 31:DA:2688:U:C5 | 31:DA:2720:U:OP2 | 2.33 | 0.81 |
| 42:DQ:9:TYR:CD2 | 42:DQ:9:TYR:O | 2.31 | 0.81 |
| 1:AA:685:G:O2' | 1:AA:686:U:H5' | 1.80 | 0.81 |
| 31:BA:1884:A:C2' | 31:BA:1885:A:H5'' | 2.10 | 0.81 |
| 31:BA:814:C:C5 | 41:BP:27:HIS:NE2 | 2.48 | 0.81 |
| 31:BA:674:G:O2' | 35:BF:74:ARG:HG3 | 1.81 | 0.81 |
| 36:BG:76:SER:HB2 | 36:BG:83:ARG:HB3 | 1.61 | 0.81 |
| 31:DA:1778:U:H2' | 31:DA:1784:A:N6 | 1.95 | 0.81 |
| 44:DS:33:LYS:HB3 | 44:DS:34:HIS:CD2 | 2.15 | 0.81 |
| 1:AA:1169:A:H2' | 1:AA:1170:A:C8 | 2.16 | 0.81 |
| 1:AA:955:U:H1' | 1:AA:1227:A:H61 | 1.44 | 0.81 |
| 31:BA:2660:A:H5'' | 31:BA:2661:G:N3 | 1.95 | 0.81 |
| 42:BQ:75:THR:HA | 42:BQ:88:GLY:HA2 | 1.61 | 0.81 |
| 50:DY:75:ILE:HD11 | 50:DY:79:CYS:HA | 1.62 | 0.81 |
| 18:AR:73:ALA:HB3 | 18:AR:79:LEU:HD12 | 1.63 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:90:U:H2' | 31:BA:90:U:O2 | 1.78 | 0.81 |
| 1:CA:1106:G:H5'' | 3:CC:172:ARG:HG2 | 1.62 | 0.81 |
| 33:DD:71:ASP:HB3 | 33:DD:103:ARG:HH22 | 1.46 | 0.81 |
| 35:DF:183:VAL:O | 35:DF:187:VAL:HG23 | 1.81 | 0.81 |
| 39:DN:130:HIS:CG | 39:DN:130:HIS:O | 2.33 | 0.81 |
| 31:DA:2469:A:O2' | 42:DQ:56:ARG:HG2 | 1.79 | 0.81 |
| 42:DQ:8:LYS:CG | 42:DQ:9:TYR:H | 1.93 | 0.81 |
| 47:DV:2:PHE:CB | 47:DV:42:GLY:HA2 | 2.10 | 0.81 |
| 31:BA:780:G:H21 | 31:BA:783:A:H62 | 1.28 | 0.81 |
| 39:BN:82:LEU:H | 39:BN:82:LEU:HD12 | 1.44 | 0.81 |
| 40:BO:2:ILE:HG13 | 40:BO:8:LEU:HD11 | 1.62 | 0.81 |
| 31:DA:2199:A:H3' | 31:DA:2200:C:H6 | 1.45 | 0.81 |
| 32:DB:66:A:H61 | 32:DB:108:U:H2' | 1.44 | 0.81 |
| 37:DH:148:ILE:O | 37:DH:151:ILE:HG12 | 1.79 | 0.81 |
| 22:B0:72:ARG:HB2 | 22:B0:75:LEU:HB2 | 1.62 | 0.81 |
| 33:BD:228:PRO:HD3 | 33:BD:235:GLY:HA3 | 1.62 | 0.81 |
| 33:BD:30:GLU:HG3 | 33:BD:63:ARG:CZ | 2.10 | 0.81 |
| 37:BH:157:TYR:CE1 | 37:BH:171:LEU:N | 2.49 | 0.81 |
| 45:BT:29:ARG:CB | 45:BT:85:LYS:HA | 2.11 | 0.81 |
| 47:BV:18:LEU:HD22 | 47:BV:19:LYS:HA | 1.61 | 0.81 |
| 50:BY:8:LYS:CE | 50:BY:72:VAL:HG23 | 2.11 | 0.81 |
| 24:D2:25:VAL:HG13 | 24:D2:26:ARG:HD2 | 1.62 | 0.81 |
| 30:D8:25:MET:HB2 | 41:DP:62:LEU:CD2 | 2.11 | 0.81 |
| 2:AB:29:ALA:O | 2:AB:32:ILE:HG22 | 1.81 | 0.81 |
| 35:BF:101:LEU:HD12 | 35:BF:102:PRO:CD | 2.10 | 0.81 |
| 1:CA:598:U:H4' | 8:CH:94:TYR:CD2 | 2.15 | 0.81 |
| 13:CM:34:LEU:HD13 | 13:CM:41:PRO:HG3 | 1.60 | 0.81 |
| 31:DA:1658:C:OP1 | 34:DE:132:HIS:CE1 | 2.34 | 0.81 |
| 31:DA:1779:U:C5 | 31:DA:1784:A:N7 | 2.47 | 0.81 |
| 33:DD:222:ARG:O | 33:DD:225:ALA:HB3 | 1.80 | 0.81 |
| 33:DD:35:LYS:HD3 | 33:DD:63:ARG:C | 2.00 | 0.81 |
| 36:DG:76:SER:HB2 | 36:DG:83:ARG:HB3 | 1.61 | 0.81 |
| 24:B2:15:LYS:O | 24:B2:16:LEU:HB3 | 1.81 | 0.81 |
| 27:B5:46:CYS:SG | 27:B5:47:PRO:HD2 | 2.21 | 0.81 |
| 31:BA:142:A:H8 | 31:BA:1595:G:H21 | 1.27 | 0.81 |
| 37:BH:43:VAL:HG23 | 37:BH:43:VAL:O | 1.81 | 0.81 |
| 48:BW:9:TYR:H | 48:BW:102:HIS:CD2 | 1.97 | 0.81 |
| 9:CI:4:TYR:HB2 | 9:CI:19:LEU:HB2 | 1.61 | 0.81 |
| 31:BA:1022:G:O2' | 31:BA:1023:U:OP2 | 1.99 | 0.81 |
| 31:DA:2577:A:H5'' | 31:DA:2578:G:H5' | 1.62 | 0.81 |
| 32:DB:15:A:H5' | 32:DB:16:G:C8 | 2.17 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:DV:62:LEU:HB3 | 47:DV:98:GLU:HA | 1.62 | 0.81 |
| 31:BA:1278:A:OP1 | 43:BR:36:THR:HG22 | 1.81 | 0.80 |
| 1:AA:1423:G:C5' | 40:BO:49:ARG:HH22 | 1.93 | 0.80 |
| 1:AA:1423:G:H5' | 40:BO:49:ARG:HH22 | 1.44 | 0.80 |
| 31:BA:993:G:H5'' | 47:BV:75:PHE:CZ | 2.15 | 0.80 |
| 2:CB:69:LEU:HB3 | 2:CB:162:ILE:HG22 | 1.64 | 0.80 |
| 15:CO:39:LEU:HD12 | 15:CO:56:LEU:HB2 | 1.63 | 0.80 |
| 31:DA:2660:A:H5'' | 31:DA:2661:G:N3 | 1.95 | 0.80 |
| 31:DA:90:U:H2' | 31:DA:90:U:O2 | 1.79 | 0.80 |
| 33:DD:44:ASN:HB3 | 33:DD:49:ILE:HA | 1.61 | 0.80 |
| 1:AA:662:G:H2' | 1:AA:663:A:C8 | 2.16 | 0.80 |
| 31:BA:7:G:H2' | 31:BA:8:A:O4' | 1.80 | 0.80 |
| 33:BD:71:ASP:HB3 | 33:BD:103:ARG:HH22 | 1.44 | 0.80 |
| 49:BX:63:LYS:HE3 | 49:BX:70:LEU:HD22 | 1.61 | 0.80 |
| 31:DA:863:A:O2' | 31:DA:864:G:H5' | 1.81 | 0.80 |
| 31:DA:1798:U:C5' | 33:DD:259:THR:HG22 | 2.04 | 0.80 |
| 13:AM:34:LEU:HD13 | 13:AM:41:PRO:HG3 | 1.61 | 0.80 |
| 32:BB:82:G:C2' | 32:BB:83:G:H5' | 2.11 | 0.80 |
| 37:BH:153:LYS:H | 37:BH:153:LYS:HD3 | 1.44 | 0.80 |
| 47:BV:82:ARG:HG3 | 47:BV:82:ARG:NH1 | 1.90 | 0.80 |
| 31:DA:2712:U:H1' | 31:DA:2712(A):A:C8 | 2.16 | 0.80 |
| 31:DA:2681:C:H5 | 31:DA:2725:A:H62 | 0.86 | 0.80 |
| 9:AI:4:TYR:HB2 | 9:AI:19:LEU:HB2 | 1.62 | 0.80 |
| 12:AL:47:LYS:HB3 | 12:AL:48:PRO:CD | 2.10 | 0.80 |
| 31:BA:2307:G:H21 | 31:BA:2308:G:H5' | 1.47 | 0.80 |
| 33:BD:44:ASN:HB3 | 33:BD:49:ILE:HA | 1.63 | 0.80 |
| 46:BU:31:SER:O | 46:BU:33:ARG:N | 2.14 | 0.80 |
| 31:DA:1464:C:O2' | 31:DA:1528:A:H8 | 1.64 | 0.80 |
| 37:DH:89:ILE:O | 37:DH:90:LYS:HG2 | 1.82 | 0.80 |
| 41:DP:38:GLN:HG3 | 41:DP:39:LYS:H | 1.45 | 0.80 |
| 49:DX:35:THR:HB | 49:DX:75:ASP:OD2 | 1.81 | 0.80 |
| 50:DY:8:LYS:CE | 50:DY:72:VAL:HG23 | 2.11 | 0.80 |
| 13:AM:81:LEU:HB3 | 13:AM:89:GLY:HA2 | 1.63 | 0.80 |
| 31:BA:1884:A:H2' | 31:BA:1885:A:C5' | 2.12 | 0.80 |
| 31:BA:2287:A:C2 | 31:BA:2346:A:H2 | 1.98 | 0.80 |
| 34:BE:203:LYS:O | 34:BE:203:LYS:HD2 | 1.81 | 0.80 |
| 1:CA:973:G:H3' | 1:CA:974:A:H5'' | 1.64 | 0.80 |
| 12:CL:90:VAL:O | 12:CL:92:ASP:N | 2.14 | 0.80 |
| 41:DP:85:LEU:HD12 | 41:DP:120:ALA:HB2 | 1.64 | 0.80 |
| 31:DA:1341:U:C2 | 49:DX:77:LYS:HE2 | 2.16 | 0.80 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C6 | 2.17 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AD:126:ILE:HG22 | 4:AD:127:THR:H | 1.46 | 0.80 |
| 32:BB:44:G:H5'' | 32:BB:45:A:OP1 | 1.82 | 0.80 |
| 41:BP:51:PHE:HB3 | 41:BP:52:GLU:OE2 | 1.82 | 0.80 |
| 45:BT:53:ARG:NH1 | 45:BT:53:ARG:HG3 | 1.94 | 0.80 |
| 2:CB:54:THR:HG21 | 2:CB:201:ILE:HD11 | 1.62 | 0.80 |
| 10:CJ:30:SER:OG | 10:CJ:81:THR:HG22 | 1.82 | 0.80 |
| 25:D3:6:VAL:CG1 | 25:D3:54:VAL:HG11 | 2.11 | 0.80 |
| 37:DH:149:ARG:HA | 37:DH:162:ILE:HG13 | 1.63 | 0.80 |
| 1:AA:1201:A:H1' | 1:AA:1202:G:OP2 | 1.80 | 0.80 |
| 47:BV:5:VAL:HG23 | 47:BV:36:PRO:HB2 | 1.63 | 0.80 |
| 31:DA:1434:A:O2' | 31:DA:1435:G:H5' | 1.80 | 0.80 |
| 10:AJ:30:SER:OG | 10:AJ:81:THR:HG22 | 1.80 | 0.80 |
| 23:B1:47:GLN:HB2 | 31:BA:397:G:H5'' | 1.64 | 0.80 |
| 31:BA:2287:A:C2 | 31:BA:2346:A:C2 | 2.70 | 0.80 |
| 31:BA:2334:G:N2 | 44:BS:18:ILE:HD11 | 1.96 | 0.80 |
| 13:CM:81:LEU:HB3 | 13:CM:89:GLY:HA2 | 1.63 | 0.80 |
| 27:D5:4:HIS:HB3 | 27:D5:5:PRO:HD3 | 1.61 | 0.80 |
| 31:DA:1430:C:H2' | 31:DA:1431:U:H6 | 1.44 | 0.80 |
| 31:DA:145:G:H2' | 31:DA:146:G:C5' | 2.11 | 0.80 |
| 31:DA:2656:U:H3 | 31:DA:2665:A:H2 | 1.28 | 0.80 |
| 31:DA:7:G:H2' | 31:DA:8:A:O4' | 1.82 | 0.80 |
| 38:DI:2:LYS:HB2 | 38:DI:39:ALA:HB3 | 1.64 | 0.80 |
| 41:DP:143:GLY:C | 41:DP:145:PRO:HD3 | 2.01 | 0.80 |
| 31:BA:2199:A:H3' | 31:BA:2200:C:H6 | 1.47 | 0.80 |
| 33:BD:35:LYS:HE2 | 33:BD:104:TYR:HB2 | 1.62 | 0.80 |
| 36:BG:85:GLY:O | 36:BG:87:PRO:HD2 | 1.81 | 0.80 |
| 28:D6:15:GLU:CD | 28:D6:43:CYS:SG | 2.61 | 0.80 |
| 28:D6:9:LEU:HD22 | 28:D6:10:LEU:H | 1.45 | 0.80 |
| 31:DA:2845:G:O2' | 31:DA:2846:G:H5' | 1.82 | 0.80 |
| 31:DA:806:C:OP2 | 41:DP:39:LYS:CD | 2.30 | 0.80 |
| 31:DA:1396:U:H2' | 31:DA:1396:U:O2 | 1.82 | 0.80 |
| 31:DA:2415:G:H4' | 41:DP:67:MET:H | 1.44 | 0.80 |
| 1:AA:450:G:H5'' | 16:AP:41:PRO:O | 1.82 | 0.79 |
| 31:BA:863:A:O2' | 31:BA:864:G:H5' | 1.82 | 0.79 |
| 33:BD:137:PRO:HB2 | 33:BD:140:THR:HG23 | 1.61 | 0.79 |
| 33:BD:137:PRO:HB2 | 33:BD:140:THR:CG2 | 2.13 | 0.79 |
| 39:BN:47:ALA:HB2 | 39:BN:112:LEU:CD1 | 2.12 | 0.79 |
| 46:BU:102:GLU:HG3 | 47:BV:2:PHE:CZ | 2.18 | 0.79 |
| 49:DX:33:LYS:C | 49:DX:35:THR:H | 1.86 | 0.79 |
| 31:BA:1902:C:H1' | 33:BD:244:ARG:HD3 | 1.61 | 0.79 |
| 37:BH:44:VAL:HG12 | 37:BH:45:VAL:H | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DD:172:TYR:CE1 | 33:DD:186:HIS:HB2 | 2.18 | 0.79 |
| 40:DO:13:ASN:HD21 | 40:DO:96:THR:H | 1.28 | 0.79 |
| 42:DQ:89:ASN:O | 42:DQ:91:GLU:N | 2.14 | 0.79 |
| 31:BA:1210:A:H8 | 31:BA:1210:A:C5' | 1.94 | 0.79 |
| 35:BF:20:LEU:HD22 | 35:BF:203:GLN:HE22 | 1.46 | 0.79 |
| 35:BF:53:THR:HB | 35:BF:56:GLU:OE1 | 1.83 | 0.79 |
| 50:BY:8:LYS:HZ1 | 50:BY:74:PRO:HD3 | 1.47 | 0.79 |
| 24:D2:49:LYS:CD | 24:D2:53:LEU:HD13 | 2.04 | 0.79 |
| 30:D8:32:LEU:HD23 | 30:D8:35:GLN:HA | 1.63 | 0.79 |
| 31:DA:1022:G:N2 | 31:DA:1142(A):A:C2 | 2.50 | 0.79 |
| 31:DA:1300:U:H3' | 31:DA:1301:A:C5' | 2.12 | 0.79 |
| 31:DA:588:U:H6 | 31:DA:588:U:OP2 | 1.64 | 0.79 |
| 31:DA:925:C:H2' | 31:DA:926:A:H5'' | 1.64 | 0.79 |
| 32:DB:74:U:C2' | 32:DB:75:G:H5'' | 2.11 | 0.79 |
| 37:DH:41:MET:SD | 37:DH:55:PRO:HD3 | 2.22 | 0.79 |
| 41:DP:84:ASN:OD1 | 41:DP:117:GLU:HB2 | 1.82 | 0.79 |
| 8:AH:58:TYR:O | 8:AH:59:LEU:HD23 | 1.82 | 0.79 |
| 41:BP:105:LEU:O | 41:BP:106:LEU:HB2 | 1.83 | 0.79 |
| 16:CP:28:ARG:HH11 | 16:CP:28:ARG:CG | 1.95 | 0.79 |
| 31:DA:1158:C:O2' | 31:DA:1159:U:P | 2.40 | 0.79 |
| 31:DA:142:A:C8 | 31:DA:1408:C:H1' | 2.17 | 0.79 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:N1 | 1.79 | 0.79 |
| 41:BP:16:ARG:HG3 | 41:BP:17:LYS:N | 1.95 | 0.79 |
| 42:BQ:9:TYR:CD2 | 42:BQ:9:TYR:O | 2.33 | 0.79 |
| 50:BY:7:VAL:HB | 50:BY:8:LYS:HZ2 | 1.47 | 0.79 |
| 1:CA:1279:A:H5'' | 1:CA:1280:A:OP1 | 1.81 | 0.79 |
| 1:CA:322:C:H5 | 1:CA:328:C:H5 | 1.30 | 0.79 |
| 31:DA:2808:U:H5' | 31:DA:2891:G:O6 | 1.83 | 0.79 |
| 35:DF:89:VAL:HG12 | 35:DF:90:PHE:N | 1.96 | 0.79 |
| 12:AL:90:VAL:O | 12:AL:92:ASP:N | 2.15 | 0.79 |
| 31:BA:1779:U:C5 | 31:BA:1784:A:N7 | 2.51 | 0.79 |
| 50:BY:60:PHE:HA | 50:BY:62:GLU:OE2 | 1.83 | 0.79 |
| 1:CA:685:G:O2' | 1:CA:686:U:H5' | 1.82 | 0.79 |
| 2:CB:29:ALA:O | 2:CB:32:ILE:HG22 | 1.83 | 0.79 |
| 33:DD:108:PRO:HB3 | 33:DD:143:HIS:CE1 | 2.16 | 0.79 |
| 35:DF:46:ARG:HH11 | 35:DF:46:ARG:CG | 1.95 | 0.79 |
| 36:DG:33:ARG:H | 36:DG:162:THR:HB | 1.48 | 0.79 |
| 37:DH:137:ASP:O | 37:DH:138:LYS:HB2 | 1.82 | 0.79 |
| 44:DS:87:PHE:HE2 | 44:DS:97:ARG:HH21 | 1.29 | 0.79 |
| 49:DX:33:LYS:O | 49:DX:35:THR:N | 2.16 | 0.79 |
| 1:CA:1063:C:H3' | 1:CA:1064:G:H2' | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DD:35:LYS:HE2 | 33:DD:104:TYR:HB2 | 1.62 | 0.79 |
| 51:DZ:109:ALA:HB1 | 51:DZ:145:GLU:OE2 | 1.83 | 0.79 |
| 5:AE:102:ALA:HB1 | 5:AE:106:PRO:HG2 | 1.65 | 0.79 |
| 31:BA:2808:U:H5' | 31:BA:2891:G:O6 | 1.83 | 0.79 |
| 31:BA:615:G:OP1 | 35:BF:40:GLN:NE2 | 2.16 | 0.79 |
| 38:BI:1:MET:HB2 | 38:BI:21:VAL:O | 1.81 | 0.79 |
| 42:BQ:89:ASN:O | 42:BQ:91:GLU:N | 2.15 | 0.79 |
| 23:D1:12:PRO:HD2 | 23:D1:62:VAL:HG23 | 1.65 | 0.79 |
| 42:DQ:110:THR:OG1 | 42:DQ:113:GLN:HG3 | 1.83 | 0.79 |
| 1:AA:382:A:H2' | 1:AA:383:A:H8 | 1.47 | 0.79 |
| 30:B8:52:LYS:N | 30:B8:53:PRO:HD2 | 1.98 | 0.79 |
| 30:B8:4:MET:SD | 30:B8:61:LEU:HD12 | 2.22 | 0.79 |
| 33:BD:186:HIS:HD2 | 33:BD:188:GLU:N | 1.80 | 0.79 |
| 44:BS:36:TYR:HD1 | 44:BS:36:TYR:N | 1.80 | 0.79 |
| 49:BX:33:LYS:C | 49:BX:35:THR:H | 1.86 | 0.79 |
| 31:BA:139(A):G:N2 | 49:BX:44:GLU:OE1 | 2.15 | 0.79 |
| 50:BY:28:LYS:CB | 50:BY:37:VAL:HB | 2.12 | 0.79 |
| 31:DA:1210:A:C5' | 31:DA:1210:A:H8 | 1.94 | 0.79 |
| 31:DA:786:C:H2' | 31:DA:787:U:H5' | 1.64 | 0.79 |
| 33:DD:172:TYR:CD1 | 33:DD:186:HIS:HA | 2.18 | 0.79 |
| 37:DH:157:TYR:CE1 | 37:DH:171:LEU:N | 2.50 | 0.79 |
| 50:DY:60:PHE:HA | 50:DY:62:GLU:OE2 | 1.82 | 0.79 |
| 16:AP:76:GLN:HG2 | 16:AP:76:GLN:O | 1.83 | 0.79 |
| 31:BA:142:A:C8 | 31:BA:1408:C:H1' | 2.18 | 0.79 |
| 31:BA:751:A:H5' | 48:BW:90:ARG:HA | 1.63 | 0.79 |
| 31:BA:1798:U:C5' | 33:BD:259:THR:HG22 | 2.04 | 0.79 |
| 31:DA:1163:G:H5' | 47:DV:92:THR:HG21 | 1.64 | 0.79 |
| 15:AO:17:ARG:CG | 15:AO:17:ARG:HH11 | 1.95 | 0.78 |
| 24:B2:14:ARG:O | 24:B2:18:PRO:HD3 | 1.83 | 0.78 |
| 41:BP:84:ASN:OD1 | 41:BP:117:GLU:HB2 | 1.83 | 0.78 |
| 49:BX:35:THR:HB | 49:BX:75:ASP:OD2 | 1.81 | 0.78 |
| 39:DN:3:THR:C | 39:DN:4:TYR:CD1 | 2.57 | 0.78 |
| 31:DA:662:G:OP1 | 41:DP:18:ARG:HD2 | 1.83 | 0.78 |
| 41:DP:30:THR:HG22 | 41:DP:31:ALA:N | 1.97 | 0.78 |
| 43:DR:11:ASN:OD1 | 43:DR:12:ARG:N | 2.14 | 0.78 |
| 28:B6:44:ARG:O | 28:B6:45:LYS:HG2 | 1.82 | 0.78 |
| 31:BA:1592:C:H2' | 31:BA:1593:G:C5' | 2.13 | 0.78 |
| 44:BS:101:LEU:HD13 | 44:BS:102:ALA:O | 1.83 | 0.78 |
| 44:BS:87:PHE:HE2 | 44:BS:97:ARG:HH21 | 1.29 | 0.78 |
| 1:CA:929:G:H1 | 1:CA:1388:C:H42 | 1.29 | 0.78 |
| 4:CD:128:VAL:HG13 | 4:CD:129:ASN:ND2 | 1.97 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:D6:9:LEU:HD22 | 28:D6:10:LEU:N | 1.98 | 0.78 |
| 31:DA:1019:U:O2' | 31:DA:1021:A:H2 | 1.66 | 0.78 |
| 31:DA:128:C:H6 | 31:DA:128:C:H5'' | 1.45 | 0.78 |
| 38:DI:82:ARG:HG2 | 38:DI:89:TYR:CD2 | 2.18 | 0.78 |
| 41:DP:71:VAL:HG12 | 41:DP:72:PRO:HD3 | 1.65 | 0.78 |
| 1:AA:194:C:H2' | 1:AA:195:A:H5'' | 1.65 | 0.78 |
| 1:AA:322:C:H5 | 1:AA:328:C:H5 | 1.31 | 0.78 |
| 23:B1:16:ASN:HB3 | 23:B1:46:LEU:CD1 | 2.13 | 0.78 |
| 30:B8:52:LYS:H | 30:B8:54:GLU:HG2 | 1.47 | 0.78 |
| 31:BA:1204:A:H2 | 31:BA:1241:A:N1 | 1.80 | 0.78 |
| 40:BO:66:LYS:H | 40:BO:82:ASN:ND2 | 1.81 | 0.78 |
| 47:BV:83:ARG:CG | 47:BV:83:ARG:HH11 | 1.96 | 0.78 |
| 8:CH:102:ARG:N | 8:CH:102:ARG:HE | 1.80 | 0.78 |
| 31:DA:1899:G:N2 | 31:DA:1902:C:C5 | 2.52 | 0.78 |
| 34:DE:203:LYS:HD2 | 34:DE:203:LYS:O | 1.83 | 0.78 |
| 36:DG:127:GLY:HA2 | 36:DG:166:ASP:HB3 | 1.66 | 0.78 |
| 31:DA:1654:A:OP1 | 43:DR:3:HIS:CB | 2.30 | 0.78 |
| 1:AA:1063:C:H3' | 1:AA:1064:G:H2' | 1.64 | 0.78 |
| 31:BA:1341:U:C2 | 49:BX:77:LYS:HE2 | 2.19 | 0.78 |
| 31:BA:1899:G:N2 | 31:BA:1902:C:C5 | 2.51 | 0.78 |
| 31:BA:2688:U:C5 | 31:BA:2720:U:OP2 | 2.37 | 0.78 |
| 33:BD:267:SER:C | 33:BD:269:PHE:H | 1.83 | 0.78 |
| 39:BN:3:THR:C | 39:BN:4:TYR:CD1 | 2.57 | 0.78 |
| 31:DA:615:G:OP1 | 35:DF:40:GLN:NE2 | 2.16 | 0.78 |
| 39:DN:73:THR:O | 39:DN:75:TYR:N | 2.16 | 0.78 |
| 45:DT:29:ARG:CB | 45:DT:85:LYS:HA | 2.12 | 0.78 |
| 49:DX:23:GLU:HG3 | 49:DX:24:GLY:H | 1.48 | 0.78 |
| 6:AF:99:ALA:HB1 | 18:AR:23:LYS:HZ2 | 1.47 | 0.78 |
| 22:B0:41:ARG:H | 22:B0:41:ARG:HD2 | 1.48 | 0.78 |
| 31:BA:796:C:H2' | 31:BA:797:C:C6 | 2.18 | 0.78 |
| 41:BP:17:LYS:O | 41:BP:19:VAL:N | 2.16 | 0.78 |
| 45:BT:23:ARG:HB2 | 45:BT:24:PRO:HD2 | 1.66 | 0.78 |
| 50:BY:28:LYS:HB2 | 50:BY:37:VAL:CB | 2.12 | 0.78 |
| 31:DA:1973:G:H2' | 31:DA:1974:C:H6 | 1.49 | 0.78 |
| 31:DA:2781:A:H5'' | 31:DA:2782:G:H5' | 1.64 | 0.78 |
| 37:DH:20:ALA:HB1 | 37:DH:21:PRO:HD2 | 1.65 | 0.78 |
| 23:B1:15:ALA:CA | 23:B1:46:LEU:HD21 | 2.13 | 0.78 |
| 51:BZ:151:HIS:CD2 | 51:BZ:151:HIS:N | 2.50 | 0.78 |
| 1:CA:1285:A:H1' | 1:CA:1286:A:OP2 | 1.84 | 0.78 |
| 24:D2:15:LYS:O | 24:D2:16:LEU:HB3 | 1.81 | 0.78 |
| 1:CA:102:G:H2' | 1:CA:103:C:H6 | 1.49 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:955:U:H1' | 1:CA:1227:A:H61 | 1.45 | 0.78 |
| 16:CP:39:TYR:HA | 16:CP:48:TRP:O | 1.84 | 0.78 |
| 17:CQ:45:HIS:CD2 | 17:CQ:47:PRO:HD3 | 2.18 | 0.78 |
| 24:D2:41:ILE:HG21 | 31:DA:95:G:H21 | 1.49 | 0.78 |
| 33:DD:137:PRO:HB2 | 33:DD:140:THR:HG23 | 1.65 | 0.78 |
| 31:DA:308:G:O2' | 50:DY:19:LYS:HE3 | 1.84 | 0.78 |
| 2:AB:69:LEU:HB3 | 2:AB:162:ILE:HG22 | 1.63 | 0.78 |
| 31:BA:1300:U:H3' | 31:BA:1301:A:C5' | 2.13 | 0.78 |
| 31:BA:1744:C:H2' | 31:BA:1745:C:H5' | 1.64 | 0.78 |
| 32:BB:66:A:H61 | 32:BB:108:U:H2' | 1.49 | 0.78 |
| 1:CA:382:A:H2' | 1:CA:383:A:H8 | 1.49 | 0.78 |
| 23:D1:37:ILE:HD11 | 31:DA:2079:U:H4' | 1.66 | 0.78 |
| 31:DA:676:A:H8 | 31:DA:2069:G:N2 | 1.81 | 0.78 |
| 35:DF:164:ARG:HG2 | 35:DF:164:ARG:HH11 | 1.49 | 0.78 |
| 41:DP:112:LEU:HD22 | 41:DP:113:LYS:N | 1.99 | 0.78 |
| 31:DA:661:C:H4' | 41:DP:16:ARG:NH1 | 1.99 | 0.78 |
| 50:DY:42:VAL:HB | 50:DY:65:ALA:HB3 | 1.63 | 0.78 |
| 1:CA:1392:G:N2 | 1:CA:1502:A:H8 | 1.82 | 0.78 |
| 31:DA:1744:C:H2' | 31:DA:1745:C:H5' | 1.66 | 0.78 |
| 31:DA:2631:G:N2 | 34:DE:61:ARG:HH12 | 1.80 | 0.78 |
| 32:DB:88:C:H2' | 32:DB:89:G:C8 | 2.19 | 0.78 |
| 33:DD:71:ASP:CB | 33:DD:103:ARG:HH22 | 1.97 | 0.78 |
| 42:DQ:141:GLN:HG3 | 51:DZ:72:ARG:HD3 | 1.65 | 0.78 |
| 44:DS:36:TYR:HD1 | 44:DS:36:TYR:N | 1.81 | 0.78 |
| 46:DU:83:LEU:HB3 | 46:DU:88:ILE:HD11 | 1.66 | 0.78 |
| 47:DV:69:LYS:HG3 | 47:DV:70:ILE:N | 1.99 | 0.78 |
| 51:DZ:151:HIS:N | 51:DZ:151:HIS:CD2 | 2.52 | 0.78 |
| 27:B5:57:VAL:HG23 | 27:B5:58:LEU:H | 1.49 | 0.78 |
| 31:BA:719:C:H2' | 31:BA:720:C:H6 | 1.48 | 0.78 |
| 38:BI:81:VAL:HG11 | 38:BI:88:ILE:HG23 | 1.66 | 0.78 |
| 1:CA:38:G:C2 | 1:CA:397:A:C2 | 2.72 | 0.78 |
| 22:D0:43:THR:H | 31:DA:2331:G:H4' | 1.48 | 0.78 |
| 50:DY:37:VAL:HG13 | 50:DY:69:ALA:HA | 1.66 | 0.78 |
| 23:B1:40:ARG:HD3 | 23:B1:41:ARG:H | 1.46 | 0.77 |
| 49:BX:23:GLU:HG3 | 49:BX:24:GLY:H | 1.47 | 0.77 |
| 46:DU:93:LYS:HD3 | 46:DU:93:LYS:H | 1.47 | 0.77 |
| 1:AA:667:G:H4' | 15:AO:51:HIS:CE1 | 2.20 | 0.77 |
| 31:BA:1108:U:H2' | 31:BA:1109:C:H5' | 1.66 | 0.77 |
| 31:BA:1778:U:H2' | 31:BA:1784:A:N6 | 1.99 | 0.77 |
| 31:BA:2305:A:H5'' | 36:BG:134:GLY:HA3 | 1.66 | 0.77 |
| 33:BD:25:THR:HG23 | 33:BD:27:THR:HB | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BG:43:LEU:HD12 | 36:BG:153:ARG:HD2 | 1.67 | 0.77 |
| 39:BN:78:TYR:HD1 | 39:BN:79:PRO:CD | 1.98 | 0.77 |
| 31:DA:2850:A:OP2 | 31:DA:2866:U:C5 | 2.36 | 0.77 |
| 45:DT:50:ILE:HD11 | 45:DT:102:ILE:HD11 | 1.65 | 0.77 |
| 49:DX:26:TYR:OH | 49:DX:89:ILE:HG21 | 1.85 | 0.77 |
| 50:DY:28:LYS:HB2 | 50:DY:37:VAL:CB | 2.14 | 0.77 |
| 50:DY:8:LYS:HE2 | 50:DY:72:VAL:HG23 | 1.65 | 0.77 |
| 7:AG:146:GLU:HA | 7:AG:149:ARG:HB2 | 1.66 | 0.77 |
| 31:BA:1332:G:C8 | 31:BA:1332:G:H5' | 2.18 | 0.77 |
| 39:BN:130:HIS:O | 39:BN:130:HIS:CG | 2.35 | 0.77 |
| 4:CD:49:ARG:HE | 4:CD:49:ARG:HA | 1.49 | 0.77 |
| 23:D1:19:GLN:OE1 | 23:D1:44:PRO:HB3 | 1.84 | 0.77 |
| 28:D6:13:CYS:HB3 | 28:D6:49:HIS:HB3 | 1.66 | 0.77 |
| 31:DA:2580:U:C5' | 34:DE:131:ALA:H | 1.97 | 0.77 |
| 1:AA:1279:A:H5'' | 1:AA:1280:A:OP1 | 1.83 | 0.77 |
| 4:CD:18:LYS:HD2 | 4:CD:33:MET:HG2 | 1.66 | 0.77 |
| 20:CT:16:HIS:O | 20:CT:19:SER:HB3 | 1.84 | 0.77 |
| 33:DD:131:LEU:HB2 | 33:DD:136:ILE:HD11 | 1.64 | 0.77 |
| 14:AN:29:ARG:HD3 | 14:AN:40:CYS:SG | 2.24 | 0.77 |
| 42:BQ:141:GLN:HG3 | 51:BZ:72:ARG:HD3 | 1.65 | 0.77 |
| 50:BY:17:SER:OG | 50:BY:18:GLY:N | 2.18 | 0.77 |
| 31:DA:1204:A:N1 | 31:DA:1241:A:H2 | 1.82 | 0.77 |
| 31:DA:1884:A:H2' | 31:DA:1885:A:H5'' | 1.64 | 0.77 |
| 31:DA:510:C:C2' | 31:DA:511:U:H5' | 2.15 | 0.77 |
| 31:DA:588:U:H2' | 31:DA:589:C:C6 | 2.20 | 0.77 |
| 1:AA:353:A:H5' | 1:AA:353:A:C8 | 2.19 | 0.77 |
| 31:BA:1047:G:H21 | 31:BA:1111:A:H62 | 1.30 | 0.77 |
| 31:BA:1163:G:H5' | 47:BV:92:THR:HG21 | 1.67 | 0.77 |
| 32:BB:88:C:H2' | 32:BB:89:G:C8 | 2.20 | 0.77 |
| 33:BD:131:LEU:HB2 | 33:BD:136:ILE:HD11 | 1.67 | 0.77 |
| 1:CA:17:U:H2' | 1:CA:18:C:C6 | 2.20 | 0.77 |
| 31:DA:2810:A:H2' | 34:DE:61:ARG:NH2 | 2.00 | 0.77 |
| 35:DF:20:LEU:HD23 | 35:DF:23:ASP:OD2 | 1.82 | 0.77 |
| 4:AD:49:ARG:HE | 4:AD:49:ARG:HA | 1.47 | 0.77 |
| 8:AH:102:ARG:N | 8:AH:102:ARG:HE | 1.83 | 0.77 |
| 31:BA:71:A:H3' | 31:BA:71:A:OP2 | 1.84 | 0.77 |
| 31:BA:954:G:H5'' | 42:BQ:13:GLN:HG2 | 1.67 | 0.77 |
| 50:BY:28:LYS:O | 50:BY:38:ILE:HB | 1.82 | 0.77 |
| 1:CA:1226:C:C4 | 13:CM:104:ARG:HB2 | 2.20 | 0.77 |
| 2:CB:44:LEU:H | 2:CB:44:LEU:HD12 | 1.48 | 0.77 |
| 31:DA:1108:U:H2' | 31:DA:1109:C:H5' | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:1405:U:H2' | 31:DA:1406:U:C6 | 2.20 | 0.77 |
| 33:DD:255:LYS:HZ1 | 33:DD:255:LYS:H | 1.33 | 0.77 |
| 31:DA:806:C:OP2 | 41:DP:39:LYS:HD2 | 1.85 | 0.77 |
| 1:AA:353:A:H8 | 1:AA:353:A:C5' | 1.98 | 0.77 |
| 1:AA:973:G:H3' | 1:AA:974:A:H5'' | 1.66 | 0.77 |
| 32:BB:74:U:C2' | 32:BB:75:G:H5'' | 2.14 | 0.77 |
| 35:BF:158:THR:HG23 | 35:BF:160:ASN:H | 1.50 | 0.77 |
| 38:BI:133:HIS:HB2 | 38:BI:134:PRO:CD | 2.14 | 0.77 |
| 49:BX:59:VAL:HG23 | 49:BX:60:ARG:H | 1.48 | 0.77 |
| 49:BX:60:ARG:NE | 49:BX:74:PRO:HG2 | 1.99 | 0.77 |
| 50:BY:7:VAL:HB | 50:BY:8:LYS:NZ | 1.99 | 0.77 |
| 31:DA:2287:A:H2 | 31:DA:2346:A:H2 | 1.30 | 0.77 |
| 31:DA:2359:C:C2' | 31:DA:2360:A:H5' | 2.13 | 0.77 |
| 31:DA:2567:G:H2' | 31:DA:2568:C:C6 | 2.19 | 0.77 |
| 41:DP:58:THR:O | 41:DP:61:ARG:NE | 2.17 | 0.77 |
| 1:AA:339:C:OP2 | 40:BO:97:ARG:NH1 | 2.17 | 0.77 |
| 1:AA:38:G:C2 | 1:AA:397:A:C2 | 2.72 | 0.77 |
| 2:AB:17:PHE:HD1 | 2:AB:44:LEU:HD11 | 1.50 | 0.77 |
| 2:AB:44:LEU:HD12 | 2:AB:44:LEU:H | 1.48 | 0.77 |
| 31:BA:94:C:H5' | 31:BA:94(A):G:OP2 | 1.85 | 0.77 |
| 50:BY:8:LYS:HE2 | 50:BY:72:VAL:HG23 | 1.65 | 0.77 |
| 1:CA:472:A:H4' | 16:CP:82:GLN:HE22 | 1.50 | 0.77 |
| 20:CT:89:ARG:HB2 | 20:CT:104:LEU:HD11 | 1.67 | 0.77 |
| 23:D1:16:ASN:HB3 | 23:D1:46:LEU:CD1 | 2.14 | 0.77 |
| 31:DA:1495:A:N3 | 31:DA:1496:A:C2 | 2.53 | 0.77 |
| 31:DA:847:U:H5 | 31:DA:933:A:H62 | 1.33 | 0.77 |
| 31:DA:674:G:O2' | 35:DF:74:ARG:HG3 | 1.84 | 0.77 |
| 35:DF:65:TRP:CZ3 | 35:DF:75:HIS:HD2 | 2.03 | 0.77 |
| 43:DR:71:GLN:HE21 | 43:DR:71:GLN:HA | 1.49 | 0.77 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:H1 | 1.30 | 0.77 |
| 2:AB:111:ARG:HH11 | 2:AB:111:ARG:CG | 1.91 | 0.77 |
| 31:BA:1396:U:H2' | 31:BA:1396:U:O2 | 1.84 | 0.77 |
| 31:DA:1607:C:H4' | 31:DA:1608:A:O5' | 1.85 | 0.77 |
| 33:DD:35:LYS:HZ1 | 33:DD:104:TYR:HB2 | 1.48 | 0.77 |
| 34:DE:34:VAL:HG22 | 34:DE:48:GLN:HE21 | 1.50 | 0.77 |
| 31:BA:1590:U:H2' | 31:BA:1591:G:H5'' | 1.67 | 0.76 |
| 31:BA:2287:A:H2 | 31:BA:2346:A:H2 | 1.33 | 0.76 |
| 31:BA:2712:U:H1' | 31:BA:2712(A):A:C8 | 2.19 | 0.76 |
| 34:BE:61:ARG:H | 34:BE:62:PRO:HD2 | 1.50 | 0.76 |
| 36:BG:33:ARG:H | 36:BG:162:THR:HB | 1.51 | 0.76 |
| 39:BN:3:THR:C | 39:BN:4:TYR:CG | 2.59 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 41:BP:85:LEU:HD12 | 41:BP:120:ALA:HB2 | 1.67 | 0.76 |
| 42:BQ:81:VAL:O | 42:BQ:82:ARG:CD | 2.29 | 0.76 |
| 47:BV:2:PHE:CB | 47:BV:42:GLY:HA2 | 2.14 | 0.76 |
| 1:CA:662:G:H2' | 1:CA:663:A:C8 | 2.20 | 0.76 |
| 4:CD:31:CYS:C | 4:CD:33:MET:H | 1.87 | 0.76 |
| 5:CE:102:ALA:HB1 | 5:CE:106:PRO:HG2 | 1.66 | 0.76 |
| 16:CP:28:ARG:NH1 | 16:CP:28:ARG:HG2 | 1.94 | 0.76 |
| 28:D6:10:LEU:HD12 | 30:D8:35:GLN:NE2 | 2.00 | 0.76 |
| 50:DY:7:VAL:HB | 50:DY:8:LYS:NZ | 2.00 | 0.76 |
| 48:BW:18:ARG:HG2 | 48:BW:18:ARG:HH11 | 1.49 | 0.76 |
| 1:CA:1096:C:H2' | 1:CA:1097:C:H6 | 1.49 | 0.76 |
| 1:CA:194:C:H2' | 1:CA:195:A:H5'' | 1.65 | 0.76 |
| 23:D1:15:ALA:CA | 23:D1:46:LEU:HD21 | 2.12 | 0.76 |
| 28:D6:10:LEU:CD1 | 30:D8:35:GLN:HE22 | 1.98 | 0.76 |
| 31:DA:1022:G:O2' | 31:DA:1023:U:OP2 | 2.02 | 0.76 |
| 47:DV:72:VAL:HG13 | 47:DV:88:ARG:NH2 | 1.99 | 0.76 |
| 4:AD:18:LYS:HD2 | 4:AD:33:MET:HG2 | 1.67 | 0.76 |
| 17:AQ:45:HIS:CD2 | 17:AQ:47:PRO:HD3 | 2.20 | 0.76 |
| 31:BA:102:G:H8 | 31:BA:102:G:C5' | 1.83 | 0.76 |
| 31:BA:1899:G:N2 | 31:BA:1902:C:H5 | 1.82 | 0.76 |
| 31:BA:1973:G:H2' | 31:BA:1974:C:H6 | 1.50 | 0.76 |
| 35:BF:65:TRP:CZ3 | 35:BF:75:HIS:HD2 | 2.02 | 0.76 |
| 37:BH:148:ILE:O | 37:BH:151:ILE:HG12 | 1.84 | 0.76 |
| 46:BU:83:LEU:HB3 | 46:BU:88:ILE:HD11 | 1.67 | 0.76 |
| 47:BV:64:HIS:O | 47:BV:64:HIS:CG | 2.36 | 0.76 |
| 50:BY:39:VAL:HG12 | 50:BY:40:GLU:N | 2.00 | 0.76 |
| 18:CR:50:ILE:HD11 | 18:CR:70:ILE:HG21 | 1.66 | 0.76 |
| 31:DA:1204:A:H2 | 31:DA:1241:A:N1 | 1.83 | 0.76 |
| 38:DI:133:HIS:HB2 | 38:DI:134:PRO:CD | 2.14 | 0.76 |
| 41:DP:71:VAL:CG1 | 41:DP:72:PRO:HD3 | 2.15 | 0.76 |
| 41:DP:6:LEU:HG | 41:DP:8:PRO:O | 1.85 | 0.76 |
| 51:DZ:149:SER:HB2 | 51:DZ:172:ALA:O | 1.84 | 0.76 |
| 1:AA:1442(A):G:H3' | 1:AA:1442(B):A:H5'' | 1.66 | 0.76 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.21 | 0.76 |
| 23:B1:37:ILE:HD11 | 31:BA:2079:U:H4' | 1.67 | 0.76 |
| 31:BA:2850:A:OP2 | 31:BA:2866:U:C5 | 2.38 | 0.76 |
| 36:BG:127:GLY:HA2 | 36:BG:166:ASP:HB3 | 1.67 | 0.76 |
| 41:BP:30:THR:HG22 | 41:BP:31:ALA:N | 1.98 | 0.76 |
| 41:BP:51:PHE:O | 41:BP:52:GLU:HB2 | 1.84 | 0.76 |
| 49:BX:53:LYS:H | 49:BX:80:ILE:HG22 | 1.49 | 0.76 |
| 1:CA:949:A:H61 | 1:CA:1232:U:H3 | 1.33 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:1484:G:H22 | 31:DA:1505:C:H5 | 1.33 | 0.76 |
| 34:DE:3:GLY:HA3 | 34:DE:81:ILE:HG13 | 1.67 | 0.76 |
| 1:AA:247:G:OP2 | 17:AQ:100:LYS:HG2 | 1.84 | 0.76 |
| 27:B5:54:GLY:O | 27:B5:56:LYS:NZ | 2.18 | 0.76 |
| 29:B7:19:ARG:HD3 | 31:BA:125:G:H5'' | 1.66 | 0.76 |
| 31:BA:1204:A:N1 | 31:BA:1241:A:H2 | 1.83 | 0.76 |
| 31:BA:2262:U:C2' | 31:BA:2263:C:H5'' | 2.16 | 0.76 |
| 31:BA:588:U:H6 | 31:BA:588:U:OP2 | 1.68 | 0.76 |
| 33:BD:32:SER:O | 33:BD:33:LEU:CB | 2.32 | 0.76 |
| 37:BH:41:MET:SD | 37:BH:55:PRO:HD3 | 2.26 | 0.76 |
| 46:BU:92:ARG:HD3 | 46:BU:94:ASN:HB3 | 1.66 | 0.76 |
| 3:CC:150:LYS:HB3 | 3:CC:201:TYR:HB2 | 1.68 | 0.76 |
| 30:D8:59:LYS:HD3 | 41:DP:50:ARG:HB3 | 1.67 | 0.76 |
| 31:DA:1332:G:N2 | 31:DA:1610:A:H8 | 1.84 | 0.76 |
| 31:DA:1639:U:H2' | 31:DA:1640:C:H5'' | 1.66 | 0.76 |
| 1:AA:1285:A:H1' | 1:AA:1286:A:OP2 | 1.85 | 0.76 |
| 31:BA:2068:U:N3 | 31:BA:2430:A:C2 | 2.50 | 0.76 |
| 42:BQ:6:ARG:O | 42:BQ:7:MET:HG2 | 1.85 | 0.76 |
| 47:BV:72:VAL:HG13 | 47:BV:88:ARG:NH2 | 1.99 | 0.76 |
| 1:CA:328:C:H2' | 1:CA:328:C:O2 | 1.86 | 0.76 |
| 30:D8:52:LYS:N | 30:D8:53:PRO:HD2 | 2.00 | 0.76 |
| 31:DA:2572:A:N7 | 34:DE:144:ARG:HD2 | 2.01 | 0.76 |
| 31:BA:2660:A:C5' | 31:BA:2661:G:H21 | 1.99 | 0.76 |
| 33:BD:71:ASP:CB | 33:BD:103:ARG:HH22 | 1.97 | 0.76 |
| 35:BF:22:ALA:HB1 | 35:BF:26:ALA:HB1 | 1.67 | 0.76 |
| 41:BP:58:THR:O | 41:BP:61:ARG:NE | 2.18 | 0.76 |
| 7:CG:146:GLU:HA | 7:CG:149:ARG:HB2 | 1.66 | 0.76 |
| 22:D0:71:ASP:C | 22:D0:72:ARG:HG2 | 2.05 | 0.76 |
| 35:DF:53:THR:HB | 35:DF:56:GLU:OE1 | 1.86 | 0.76 |
| 50:DY:15:VAL:HG12 | 50:DY:17:SER:H | 1.51 | 0.76 |
| 1:AA:594:G:H1 | 1:AA:645:C:H42 | 1.34 | 0.76 |
| 2:AB:217:ARG:HA | 2:AB:220:ASP:HB2 | 1.68 | 0.76 |
| 13:AM:61:GLU:HA | 13:AM:66:LEU:HD11 | 1.66 | 0.76 |
| 28:B6:36:LEU:HD13 | 28:B6:50:ARG:CZ | 2.16 | 0.76 |
| 31:BA:157:U:H5' | 31:BA:171:G:H22 | 1.50 | 0.76 |
| 31:BA:2094:G:C2' | 31:BA:2095:C:H5' | 2.15 | 0.76 |
| 33:BD:35:LYS:HZ1 | 33:BD:104:TYR:HB2 | 1.47 | 0.76 |
| 34:BE:95:ILE:HD12 | 34:BE:95:ILE:H | 1.49 | 0.76 |
| 42:BQ:134:ARG:HH21 | 51:BZ:122:ARG:HD2 | 1.50 | 0.76 |
| 36:DG:43:LEU:HD12 | 36:DG:153:ARG:HD2 | 1.67 | 0.76 |
| 39:DN:3:THR:C | 39:DN:4:TYR:CG | 2.59 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 47:DV:82:ARG:CG | 47:DV:82:ARG:NH1 | 2.45 | 0.76 |
| 1:AA:1226:C:C4 | 13:AM:104:ARG:HB2 | 2.20 | 0.76 |
| 28:B6:10:LEU:CD1 | 30:B8:35:GLN:HE22 | 1.99 | 0.76 |
| 31:BA:2359:C:C2' | 31:BA:2360:A:H5' | 2.15 | 0.76 |
| 34:BE:34:VAL:HG22 | 34:BE:48:GLN:HE21 | 1.50 | 0.76 |
| 42:BQ:140:ALA:HA | 51:BZ:99:TYR:CD2 | 2.21 | 0.76 |
| 1:CA:1442(A):G:H3' | 1:CA:1442(B):A:H5'' | 1.66 | 0.76 |
| 16:CP:72:ARG:HH21 | 16:CP:73:LEU:HD21 | 1.51 | 0.76 |
| 25:D3:19:GLN:HE22 | 25:D3:52:HIS:HE1 | 1.32 | 0.76 |
| 44:DS:101:LEU:HD13 | 44:DS:102:ALA:O | 1.86 | 0.76 |
| 31:BA:145:G:H2' | 31:BA:146:G:C5' | 2.16 | 0.76 |
| 46:BU:93:LYS:H | 46:BU:93:LYS:HD3 | 1.50 | 0.76 |
| 3:CC:52:LEU:H | 3:CC:52:LEU:HD23 | 1.50 | 0.76 |
| 11:CK:111:ASP:HA | 18:CR:84:LYS:HG3 | 1.67 | 0.76 |
| 31:DA:2223:G:H2' | 31:DA:2224:G:H5' | 1.68 | 0.76 |
| 32:DB:75:G:H5' | 32:DB:75:G:H8 | 1.50 | 0.76 |
| 45:DT:23:ARG:HB2 | 45:DT:24:PRO:HD2 | 1.68 | 0.76 |
| 49:DX:60:ARG:NE | 49:DX:74:PRO:HG2 | 2.01 | 0.76 |
| 1:AA:929:G:H1 | 1:AA:1388:C:H42 | 1.29 | 0.75 |
| 47:BV:62:LEU:HB3 | 47:BV:98:GLU:HA | 1.67 | 0.75 |
| 31:DA:322:A:H5' | 31:DA:340:A:H1' | 1.68 | 0.75 |
| 1:AA:737:A:H2' | 1:AA:738:C:C6 | 2.22 | 0.75 |
| 31:BA:1884:A:H2' | 31:BA:1885:A:H5'' | 1.69 | 0.75 |
| 45:BT:53:ARG:HH11 | 45:BT:53:ARG:CG | 1.97 | 0.75 |
| 47:BV:73:SER:OG | 47:BV:74:LYS:N | 2.19 | 0.75 |
| 51:BZ:109:ALA:HB1 | 51:BZ:145:GLU:OE2 | 1.86 | 0.75 |
| 1:CA:920:U:H1' | 1:CA:1080:A:C2 | 2.20 | 0.75 |
| 2:CB:17:PHE:HD1 | 2:CB:44:LEU:HD11 | 1.51 | 0.75 |
| 9:CI:112:LYS:HE3 | 9:CI:116:LYS:O | 1.86 | 0.75 |
| 33:DD:32:SER:O | 33:DD:33:LEU:CB | 2.34 | 0.75 |
| 38:DI:133:HIS:CG | 38:DI:134:PRO:HD2 | 2.19 | 0.75 |
| 45:DT:51:ARG:HG3 | 45:DT:98:LYS:HE2 | 1.66 | 0.75 |
| 47:DV:83:ARG:HH11 | 47:DV:83:ARG:CG | 1.99 | 0.75 |
| 1:AA:545:C:O2' | 1:AA:546:G:H5' | 1.87 | 0.75 |
| 16:AP:39:TYR:HA | 16:AP:48:TRP:O | 1.85 | 0.75 |
| 27:B5:55:ARG:CD | 27:B5:56:LYS:H | 1.98 | 0.75 |
| 30:B8:4:MET:HE1 | 31:BA:593:G:H1' | 1.68 | 0.75 |
| 31:BA:661:C:H4' | 41:BP:18:ARG:HG2 | 1.68 | 0.75 |
| 41:BP:38:GLN:HG3 | 41:BP:39:LYS:H | 1.50 | 0.75 |
| 46:BU:88:ILE:C | 46:BU:90:VAL:H | 1.88 | 0.75 |
| 1:CA:409:G:H2' | 1:CA:410:G:H5' | 1.66 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:1948:G:H5' | 31:DA:1948:G:H8 | 1.51 | 0.75 |
| 31:DA:671:C:H5' | 31:DA:671:C:H6 | 1.49 | 0.75 |
| 31:DA:71:A:OP2 | 31:DA:71:A:H3' | 1.87 | 0.75 |
| 41:DP:48:PRO:HG2 | 41:DP:49:ARG:H | 1.52 | 0.75 |
| 41:DP:75:ILE:N | 41:DP:75:ILE:HD13 | 2.00 | 0.75 |
| 31:DA:910:A:H62 | 42:DQ:12:GLN:HA | 1.51 | 0.75 |
| 47:DV:2:PHE:HB2 | 47:DV:42:GLY:CA | 2.17 | 0.75 |
| 47:DV:64:HIS:O | 47:DV:64:HIS:CG | 2.38 | 0.75 |
| 48:DW:86:LEU:HD12 | 48:DW:87:PRO:HD2 | 1.68 | 0.75 |
| 28:B6:10:LEU:HD12 | 30:B8:35:GLN:NE2 | 2.02 | 0.75 |
| 31:BA:1495:A:N3 | 31:BA:1496:A:C2 | 2.54 | 0.75 |
| 32:BB:82:G:H2' | 32:BB:83:G:H5' | 1.68 | 0.75 |
| 20:CT:50:GLU:HB3 | 20:CT:100:ILE:CG1 | 2.16 | 0.75 |
| 23:D1:10:LYS:HB2 | 23:D1:14:VAL:N | 2.02 | 0.75 |
| 31:DA:212:G:O2' | 31:DA:213:A:H5' | 1.86 | 0.75 |
| 31:DA:2818:G:O2' | 31:DA:2819:G:H5' | 1.86 | 0.75 |
| 31:DA:780:G:H21 | 31:DA:783:A:H62 | 1.32 | 0.75 |
| 39:DN:119:ARG:NH1 | 39:DN:119:ARG:HG3 | 1.96 | 0.75 |
| 2:AB:185:ILE:CG2 | 2:AB:199:TYR:HB2 | 2.15 | 0.75 |
| 28:B6:13:CYS:HB3 | 28:B6:49:HIS:HB3 | 1.69 | 0.75 |
| 30:B8:32:LEU:C | 30:B8:34:TRP:N | 2.39 | 0.75 |
| 31:BA:1019:U:O2' | 31:BA:1021:A:H2 | 1.66 | 0.75 |
| 31:BA:65:C:H2' | 31:BA:66:C:H6 | 1.50 | 0.75 |
| 40:BO:2:ILE:HD12 | 40:BO:6:THR:HG21 | 1.67 | 0.75 |
| 50:BY:44:ILE:H | 50:BY:44:ILE:HD12 | 1.50 | 0.75 |
| 13:CM:61:GLU:HA | 13:CM:66:LEU:HD11 | 1.67 | 0.75 |
| 28:D6:12:GLU:HB3 | 28:D6:23:THR:HG22 | 1.67 | 0.75 |
| 31:DA:2263:C:H6 | 31:DA:2263:C:H5' | 1.50 | 0.75 |
| 34:DE:132:HIS:CD2 | 34:DE:135:HIS:CE1 | 2.74 | 0.75 |
| 39:DN:28:THR:CG2 | 39:DN:106:MET:HE1 | 2.13 | 0.75 |
| 45:DT:31:SER:C | 45:DT:32:TYR:HD2 | 1.90 | 0.75 |
| 50:DY:17:SER:OG | 50:DY:18:GLY:N | 2.17 | 0.75 |
| 1:AA:949:A:H61 | 1:AA:1232:U:H3 | 1.34 | 0.75 |
| 1:AA:148:G:O2' | 1:AA:149:A:H5' | 1.87 | 0.75 |
| 31:BA:1405:U:H2' | 31:BA:1406:U:C6 | 2.22 | 0.75 |
| 36:BG:86:MET:HB2 | 36:BG:87:PRO:CD | 2.17 | 0.75 |
| 39:BN:19:GLU:HG3 | 39:BN:20:GLY:N | 1.99 | 0.75 |
| 44:BS:89:ARG:O | 44:BS:92:TYR:HB3 | 1.87 | 0.75 |
| 1:CA:939:G:H5'' | 7:CG:102:ARG:NH1 | 2.02 | 0.75 |
| 38:DI:102:SER:HA | 38:DI:107:VAL:O | 1.86 | 0.75 |
| 1:AA:559:A:H4' | 1:AA:560:U:H3' | 1.67 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:166:ASP:HB3 | 2:AB:169:LYS:HB2 | 1.69 | 0.75 |
| 2:AB:88:ALA:HB2 | 2:AB:219:VAL:HG13 | 1.67 | 0.75 |
| 23:B1:19:GLN:OE1 | 23:B1:44:PRO:HB3 | 1.86 | 0.75 |
| 33:BD:172:TYR:CD1 | 33:BD:186:HIS:HA | 2.21 | 0.75 |
| 51:BZ:166:SER:OG | 51:BZ:167:PRO:HA | 1.86 | 0.75 |
| 31:DA:794:G:H2' | 31:DA:795:C:C6 | 2.22 | 0.75 |
| 33:DD:137:PRO:HB2 | 33:DD:140:THR:CG2 | 2.17 | 0.75 |
| 34:DE:132:HIS:CG | 34:DE:135:HIS:NE2 | 2.54 | 0.75 |
| 38:DI:9:LEU:H | 38:DI:13:GLY:HA2 | 1.50 | 0.75 |
| 39:DN:40:PRO:HB3 | 46:DU:68:ALA:HB2 | 1.69 | 0.75 |
| 33:BD:267:SER:C | 33:BD:269:PHE:N | 2.39 | 0.75 |
| 39:BN:57:ALA:C | 39:BN:58:ASP:O | 2.17 | 0.75 |
| 12:CL:47:LYS:CB | 12:CL:48:PRO:HD3 | 2.15 | 0.75 |
| 27:D5:55:ARG:CD | 27:D5:56:LYS:H | 1.95 | 0.75 |
| 29:D7:8:ASN:HD21 | 29:D7:11:LYS:H | 1.30 | 0.75 |
| 31:DA:1794:U:H2' | 31:DA:1795:C:H6 | 1.50 | 0.75 |
| 31:DA:747:U:O2 | 31:DA:2014:A:H1' | 1.86 | 0.75 |
| 40:DO:66:LYS:H | 40:DO:82:ASN:ND2 | 1.83 | 0.75 |
| 41:DP:122:PRO:HA | 41:DP:141:ALA:O | 1.87 | 0.75 |
| 41:DP:16:ARG:HG3 | 41:DP:17:LYS:N | 2.02 | 0.75 |
| 15:AO:17:ARG:NH1 | 15:AO:17:ARG:HG3 | 2.01 | 0.75 |
| 28:B6:16:CYS:O | 28:B6:17:LYS:HB2 | 1.85 | 0.75 |
| 28:B6:12:GLU:HB3 | 28:B6:23:THR:HG22 | 1.68 | 0.75 |
| 30:B8:6:THR:CG2 | 30:B8:63:PRO:HD3 | 2.17 | 0.75 |
| 31:BA:2810:A:H2' | 34:BE:61:ARG:NH2 | 2.01 | 0.75 |
| 42:BQ:63:LYS:HG2 | 42:BQ:65:PHE:CE2 | 2.22 | 0.75 |
| 47:BV:69:LYS:HB3 | 47:BV:93:GLU:OE1 | 1.87 | 0.75 |
| 47:BV:69:LYS:HG3 | 47:BV:70:ILE:N | 2.00 | 0.75 |
| 24:D2:54:LYS:N | 24:D2:56:GLN:NE2 | 2.35 | 0.75 |
| 31:DA:286:C:H2' | 31:DA:287:C:H5' | 1.68 | 0.75 |
| 31:DA:543:C:H42 | 31:DA:551:G:H1 | 1.35 | 0.75 |
| 36:DG:47:LYS:HE2 | 36:DG:81:LYS:HB2 | 1.69 | 0.75 |
| 46:DU:91:ASP:O | 46:DU:95:LEU:HB2 | 1.86 | 0.75 |
| 1:AA:392:G:H2' | 1:AA:393:A:H8 | 1.52 | 0.74 |
| 1:AA:913:A:H4' | 1:AA:914:A:O5' | 1.87 | 0.74 |
| 6:AF:30:LEU:HB3 | 6:AF:35:ALA:HB3 | 1.69 | 0.74 |
| 31:BA:286:C:H2' | 31:BA:287:C:H5' | 1.68 | 0.74 |
| 32:BB:15:A:H5' | 32:BB:16:G:C8 | 2.22 | 0.74 |
| 38:BI:82:ARG:HG2 | 38:BI:89:TYR:CD2 | 2.21 | 0.74 |
| 31:BA:2723:C:H5'' | 43:BR:2:ARG:HD2 | 1.67 | 0.74 |
| 31:DA:1339:G:N2 | 31:DA:1603:A:H1' | 2.02 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:94:C:H5' | 31:DA:94(A):G:OP2 | 1.86 | 0.74 |
| 39:DN:58:ASP:O | 39:DN:60:ILE:N | 2.19 | 0.74 |
| 46:DU:65:ILE:HG12 | 46:DU:96:ALA:HB3 | 1.69 | 0.74 |
| 51:DZ:163:LEU:HD11 | 51:DZ:167:PRO:HB3 | 1.68 | 0.74 |
| 4:AD:31:CYS:C | 4:AD:33:MET:H | 1.88 | 0.74 |
| 13:AM:3:ARG:HA | 13:AM:9:ILE:HG13 | 1.70 | 0.74 |
| 31:BA:1639:U:H2' | 31:BA:1640:C:H5'' | 1.69 | 0.74 |
| 35:BF:164:ARG:HH11 | 35:BF:164:ARG:HG2 | 1.51 | 0.74 |
| 41:BP:146:VAL:HG22 | 41:BP:147:LEU:N | 2.01 | 0.74 |
| 2:CB:88:ALA:HB2 | 2:CB:219:VAL:HG13 | 1.68 | 0.74 |
| 27:D5:2:ALA:HA | 31:DA:2015:A:C1' | 2.16 | 0.74 |
| 28:D6:13:CYS:O | 28:D6:21:TYR:HA | 1.87 | 0.74 |
| 31:DA:1181:C:O2' | 31:DA:1182:A:H5' | 1.88 | 0.74 |
| 1:AA:518:C:H2' | 1:AA:530:G:C2 | 2.22 | 0.74 |
| 11:AK:111:ASP:HA | 18:AR:84:LYS:HG3 | 1.69 | 0.74 |
| 12:AL:47:LYS:CB | 12:AL:48:PRO:HD3 | 2.15 | 0.74 |
| 16:AP:28:ARG:HG2 | 16:AP:28:ARG:NH1 | 1.87 | 0.74 |
| 29:B7:8:ASN:C | 29:B7:8:ASN:ND2 | 2.40 | 0.74 |
| 31:BA:1158:C:O2' | 31:BA:1159:U:O5' | 2.03 | 0.74 |
| 34:BE:132:HIS:CG | 34:BE:135:HIS:NE2 | 2.55 | 0.74 |
| 37:BH:153:LYS:N | 37:BH:153:LYS:HD3 | 2.02 | 0.74 |
| 39:BN:121:LYS:HD2 | 39:BN:123:TYR:CZ | 2.22 | 0.74 |
| 41:BP:120:ALA:O | 25:D3:1:MET:HA | 1.87 | 0.74 |
| 50:BY:97:ARG:O | 50:BY:97:ARG:HG3 | 1.83 | 0.74 |
| 24:D2:26:ARG:HG2 | 49:DX:5:TYR:HB3 | 1.69 | 0.74 |
| 31:DA:370:G:H4' | 31:DA:371:A:OP2 | 1.85 | 0.74 |
| 33:DD:270:ILE:O | 33:DD:270:ILE:HD12 | 1.86 | 0.74 |
| 49:DX:59:VAL:HG23 | 49:DX:60:ARG:H | 1.52 | 0.74 |
| 4:AD:12:CYS:HA | 4:AD:19:LEU:CD1 | 2.17 | 0.74 |
| 4:AD:161:ASN:O | 4:AD:165:MET:HG2 | 1.88 | 0.74 |
| 12:AL:18:VAL:HG23 | 12:AL:19:ARG:H | 1.51 | 0.74 |
| 20:AT:13:LEU:HD12 | 20:AT:13:LEU:H | 1.52 | 0.74 |
| 30:B8:34:TRP:O | 30:B8:35:GLN:HB2 | 1.85 | 0.74 |
| 37:BH:137:ASP:CB | 37:BH:140:LYS:HB2 | 2.17 | 0.74 |
| 30:B8:25:MET:HB2 | 41:BP:62:LEU:CD2 | 2.16 | 0.74 |
| 44:BS:14:VAL:HG12 | 44:BS:15:ARG:N | 2.03 | 0.74 |
| 31:DA:157:U:H5' | 31:DA:171:G:H22 | 1.51 | 0.74 |
| 31:DA:288:C:H42 | 31:DA:353:G:H1 | 1.35 | 0.74 |
| 32:DB:82:G:H2' | 32:DB:83:G:H5' | 1.67 | 0.74 |
| 33:DD:267:SER:C | 33:DD:269:PHE:H | 1.91 | 0.74 |
| 34:DE:119:ARG:CG | 34:DE:119:ARG:HH11 | 1.94 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 37:DH:153:LYS:N | 37:DH:153:LYS:HD3 | 2.01 | 0.74 |
| 48:DW:4:LYS:HE3 | 48:DW:6:ILE:HD11 | 1.69 | 0.74 |
| 50:DY:39:VAL:HG12 | 50:DY:40:GLU:N | 2.00 | 0.74 |
| 1:AA:102:G:H2' | 1:AA:103:C:H6 | 1.53 | 0.74 |
| 20:AT:89:ARG:HB2 | 20:AT:104:LEU:HD11 | 1.68 | 0.74 |
| 31:BA:92:A:H2' | 31:BA:93:G:O4' | 1.87 | 0.74 |
| 51:BZ:5:LEU:HD13 | 51:BZ:43:GLU:HB3 | 1.69 | 0.74 |
| 4:CD:12:CYS:HA | 4:CD:19:LEU:CD1 | 2.17 | 0.74 |
| 15:CO:82:ILE:HG12 | 15:CO:87:ILE:HB | 1.67 | 0.74 |
| 31:DA:1582:C:O2' | 31:DA:1586:A:C8 | 2.40 | 0.74 |
| 31:DA:1590:U:H2' | 31:DA:1591:G:H5'' | 1.70 | 0.74 |
| 31:DA:2801(A):A:H4' | 31:DA:2802:G:H5' | 1.70 | 0.74 |
| 33:DD:31:LYS:HG2 | 33:DD:34:VAL:HG13 | 1.69 | 0.74 |
| 42:DQ:134:ARG:HH21 | 51:DZ:122:ARG:HD2 | 1.51 | 0.74 |
| 50:DY:97:ARG:O | 50:DY:97:ARG:HG3 | 1.86 | 0.74 |
| 45:BT:109:GLU:O | 45:BT:112:ARG:HG3 | 1.88 | 0.74 |
| 46:BU:88:ILE:C | 46:BU:90:VAL:N | 2.39 | 0.74 |
| 46:BU:92:ARG:HD2 | 47:BV:11:GLN:HG3 | 1.69 | 0.74 |
| 10:CJ:34:VAL:HG22 | 10:CJ:74:ILE:HG22 | 1.68 | 0.74 |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:HE2 | 1.52 | 0.74 |
| 23:D1:19:GLN:NE2 | 31:DA:379:G:H21 | 1.86 | 0.74 |
| 39:DN:78:TYR:HD1 | 39:DN:79:PRO:CD | 2.00 | 0.74 |
| 45:DT:109:GLU:O | 45:DT:112:ARG:HG3 | 1.88 | 0.74 |
| 48:DW:18:ARG:HG2 | 48:DW:18:ARG:HH11 | 1.51 | 0.74 |
| 31:DA:143(A):C:H5' | 49:DX:36:LYS:HG2 | 1.69 | 0.74 |
| 1:AA:355:C:C2' | 1:AA:356:A:H5' | 2.18 | 0.74 |
| 1:AA:409:G:H2' | 1:AA:410:G:H5' | 1.68 | 0.74 |
| 1:AA:568:G:O6 | 12:AL:5:PRO:HD3 | 1.87 | 0.74 |
| 9:AI:112:LYS:HE3 | 9:AI:116:LYS:O | 1.87 | 0.74 |
| 17:AQ:59:ILE:CG2 | 17:AQ:71:PHE:HB3 | 2.17 | 0.74 |
| 31:BA:2631:G:N2 | 34:BE:61:ARG:HH12 | 1.85 | 0.74 |
| 38:BI:133:HIS:CG | 38:BI:134:PRO:HD2 | 2.22 | 0.74 |
| 39:BN:42:TRP:CB | 46:BU:64:ARG:HH11 | 1.97 | 0.74 |
| 47:BV:66:ARG:HG2 | 47:BV:94:LEU:HG | 1.70 | 0.74 |
| 47:BV:83:ARG:HH11 | 47:BV:83:ARG:HG3 | 1.52 | 0.74 |
| 1:CA:559:A:H4' | 1:CA:560:U:H3' | 1.69 | 0.74 |
| 4:CD:119:GLN:HG3 | 4:CD:123:HIS:HD2 | 1.53 | 0.74 |
| 14:CN:29:ARG:HD3 | 14:CN:40:CYS:SG | 2.27 | 0.74 |
| 31:DA:814:C:C5 | 41:DP:27:HIS:NE2 | 2.55 | 0.74 |
| 34:DE:201:THR:HG22 | 34:DE:202:LYS:N | 2.03 | 0.74 |
| 34:DE:95:ILE:H | 34:DE:95:ILE:HD12 | 1.50 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DN:47:ALA:HB2 | 39:DN:112:LEU:CD1 | 2.18 | 0.74 |
| 47:DV:51:VAL:HG12 | 47:DV:52:VAL:H | 1.53 | 0.74 |
| 2:AB:172:ILE:HD12 | 2:AB:172:ILE:H | 1.53 | 0.74 |
| 28:B6:27:LYS:HE3 | 31:BA:2285:C:H5 | 1.52 | 0.74 |
| 33:BD:27:THR:HG23 | 33:BD:28:GLU:N | 2.03 | 0.74 |
| 44:BS:95:HIS:CG | 44:BS:96:GLY:H | 2.06 | 0.74 |
| 46:BU:100:VAL:HG12 | 46:BU:101:ARG:N | 2.03 | 0.74 |
| 46:BU:83:LEU:CG | 46:BU:88:ILE:HG12 | 2.17 | 0.74 |
| 50:BY:15:VAL:HG12 | 50:BY:17:SER:H | 1.53 | 0.74 |
| 31:DA:2572:A:C8 | 34:DE:144:ARG:HD2 | 2.23 | 0.74 |
| 31:DA:65:C:H2' | 31:DA:66:C:C6 | 2.22 | 0.74 |
| 51:DZ:166:SER:OG | 51:DZ:167:PRO:HA | 1.86 | 0.74 |
| 1:AA:1096:C:H2' | 1:AA:1097:C:H6 | 1.50 | 0.74 |
| 1:AA:186:C:H2' | 1:AA:187:C:H6 | 1.52 | 0.74 |
| 2:AB:22:LYS:HA | 2:AB:22:LYS:NZ | 2.03 | 0.74 |
| 17:AQ:67:LYS:HA | 17:AQ:70:ARG:HH12 | 1.52 | 0.74 |
| 31:BA:1836:C:O2' | 31:BA:1837:C:H5' | 1.88 | 0.74 |
| 34:BE:119:ARG:CG | 34:BE:119:ARG:HH11 | 1.95 | 0.74 |
| 35:BF:24:LEU:HB3 | 35:BF:25:PRO:CD | 2.16 | 0.74 |
| 36:BG:123:ASN:O | 36:BG:126:ASP:HB2 | 1.88 | 0.74 |
| 39:BN:119:ARG:NH1 | 39:BN:119:ARG:HG3 | 1.96 | 0.74 |
| 39:BN:67:LEU:HA | 39:BN:88:GLU:HG3 | 1.69 | 0.74 |
| 40:BO:13:ASN:HD21 | 40:BO:97:ARG:H | 1.36 | 0.74 |
| 47:BV:70:ILE:HB | 47:BV:90:PRO:HB2 | 1.69 | 0.74 |
| 47:BV:90:PRO:CG | 47:BV:91:TYR:N | 2.51 | 0.74 |
| 49:BX:38:GLU:N | 49:BX:38:GLU:OE1 | 2.21 | 0.74 |
| 1:CA:102:G:C5 | 1:CA:103:C:C5 | 2.76 | 0.74 |
| 1:CA:148:G:O2' | 1:CA:149:A:H5' | 1.87 | 0.74 |
| 23:D1:14:VAL:O | 23:D1:46:LEU:HD23 | 1.88 | 0.74 |
| 30:D8:34:TRP:O | 30:D8:35:GLN:HB2 | 1.85 | 0.74 |
| 31:DA:2094:G:C2' | 31:DA:2095:C:H5' | 2.17 | 0.74 |
| 41:DP:120:ALA:CB | 41:DP:138:LEU:HB3 | 2.18 | 0.74 |
| 50:DY:71:LYS:HB2 | 50:DY:71:LYS:HZ2 | 1.53 | 0.74 |
| 1:AA:472:A:H4' | 16:AP:82:GLN:HE22 | 1.51 | 0.74 |
| 31:BA:1652:A:C2' | 31:BA:1653:G:H5' | 2.18 | 0.74 |
| 31:BA:1794:U:H2' | 31:BA:1795:C:H6 | 1.50 | 0.74 |
| 31:BA:661:C:H4' | 41:BP:16:ARG:NH1 | 2.03 | 0.74 |
| 42:BQ:20:ALA:HB2 | 42:BQ:99:PRO:HD2 | 1.69 | 0.74 |
| 27:D5:40:LYS:NZ | 27:D5:49:CYS:SG | 2.61 | 0.74 |
| 31:DA:8:A:H2' | 31:DA:9:U:C5 | 2.22 | 0.74 |
| 51:DZ:5:LEU:HD13 | 51:DZ:43:GLU:HB3 | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:859:A:H2' | 1:AA:860:A:O4' | 1.87 | 0.73 |
| 1:AA:390:C:O3' | 16:AP:28:ARG:NH2 | 2.21 | 0.73 |
| 24:B2:30:ARG:HG3 | 24:B2:30:ARG:HH11 | 1.52 | 0.73 |
| 31:BA:83:G:N2 | 31:BA:102:G:O2' | 2.21 | 0.73 |
| 31:BA:2656:U:H3 | 31:BA:2665:A:H2 | 1.32 | 0.73 |
| 39:BN:62:VAL:CG2 | 39:BN:66:LYS:HD2 | 2.18 | 0.73 |
| 34:BE:111:ARG:HA | 43:BR:2:ARG:HG3 | 1.69 | 0.73 |
| 43:BR:4:LEU:O | 43:BR:4:LEU:CD1 | 2.35 | 0.73 |
| 1:CA:163:C:H2' | 1:CA:164:U:H6 | 1.52 | 0.73 |
| 1:CA:594:G:H1 | 1:CA:645:C:H42 | 1.34 | 0.73 |
| 6:CF:20:ALA:HA | 6:CF:23:LYS:HB2 | 1.70 | 0.73 |
| 31:DA:1047:G:H21 | 31:DA:1111:A:H62 | 1.34 | 0.73 |
| 31:DA:2492:U:H2' | 31:DA:2493:U:H6 | 1.53 | 0.73 |
| 33:DD:35:LYS:CD | 33:DD:63:ARG:HB3 | 2.17 | 0.73 |
| 47:DV:1:MET:HE3 | 47:DV:44:LYS:HB3 | 1.70 | 0.73 |
| 47:DV:83:ARG:HH11 | 47:DV:83:ARG:HG3 | 1.52 | 0.73 |
| 1:AA:192:U:O4' | 20:AT:103:GLY:HA2 | 1.88 | 0.73 |
| 4:AD:119:GLN:HG3 | 4:AD:123:HIS:HD2 | 1.53 | 0.73 |
| 24:B2:41:ILE:HG21 | 31:BA:95:G:H21 | 1.52 | 0.73 |
| 32:BB:87:G:H8 | 32:BB:87:G:OP2 | 1.71 | 0.73 |
| 33:BD:25:THR:HG22 | 33:BD:82:ILE:O | 1.88 | 0.73 |
| 41:BP:71:VAL:HG12 | 41:BP:72:PRO:HD3 | 1.71 | 0.73 |
| 50:BY:96:ILE:HG21 | 50:BY:99:CYS:HB3 | 1.68 | 0.73 |
| 51:BZ:163:LEU:HD11 | 51:BZ:167:PRO:HB3 | 1.68 | 0.73 |
| 1:CA:954:G:N2 | 1:CA:1227:A:H62 | 1.85 | 0.73 |
| 5:CE:110:LEU:O | 5:CE:115:VAL:HG23 | 1.89 | 0.73 |
| 19:CS:36:ARG:HH12 | 19:CS:75:ALA:HB3 | 1.53 | 0.73 |
| 31:DA:1288:U:C2 | 31:DA:1327:C:O2 | 2.41 | 0.73 |
| 32:DB:20:C:H2' | 32:DB:21:G:C5' | 2.18 | 0.73 |
| 50:DY:81:LYS:HG2 | 50:DY:96:ILE:HG22 | 1.69 | 0.73 |
| 1:AA:939:G:H5'' | 7:AG:102:ARG:NH1 | 2.03 | 0.73 |
| 31:BA:1047:G:N2 | 31:BA:1111:A:H62 | 1.86 | 0.73 |
| 31:BA:1022:G:N2 | 31:BA:1142(A):A:C2 | 2.56 | 0.73 |
| 39:BN:119:ARG:CG | 39:BN:119:ARG:HH11 | 1.99 | 0.73 |
| 51:BZ:149:SER:HB2 | 51:BZ:172:ALA:O | 1.86 | 0.73 |
| 1:CA:1123:A:O2' | 10:CJ:38:ILE:HG22 | 1.89 | 0.73 |
| 2:CB:166:ASP:HB3 | 2:CB:169:LYS:HB2 | 1.71 | 0.73 |
| 17:CQ:59:ILE:CG2 | 17:CQ:71:PHE:HB3 | 2.19 | 0.73 |
| 31:DA:2262:U:O2' | 31:DA:2263:C:H5'' | 1.87 | 0.73 |
| 31:DA:330:A:H2 | 31:DA:1210:A:C2' | 2.01 | 0.73 |
| 39:DN:57:ALA:C | 39:DN:58:ASP:O | 2.24 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:DA:139(A):G:N2 | 49:DX:44:GLU:OE1 | 2.20 | 0.73 |
| 1:AA:954:G:N2 | 1:AA:1227:A:H62 | 1.86 | 0.73 |
| 31:BA:142:A:H5' | 31:BA:142(A):C:OP2 | 1.88 | 0.73 |
| 31:BA:2801(A):A:H4' | 31:BA:2802:G:H5' | 1.70 | 0.73 |
| 31:BA:2801(A):A:H4' | 31:BA:2802:G:H2' | 1.70 | 0.73 |
| 31:BA:309:G:O3' | 50:BY:18:GLY:HA2 | 1.88 | 0.73 |
| 31:BA:259:G:H21 | 31:BA:621:A:H8 | 1.36 | 0.73 |
| 39:BN:68:GLU:HA | 39:BN:86:PRO:HB3 | 1.70 | 0.73 |
| 30:B8:59:LYS:HD3 | 41:BP:50:ARG:HB3 | 1.69 | 0.73 |
| 45:BT:31:SER:C | 45:BT:32:TYR:HD2 | 1.91 | 0.73 |
| 1:CA:428:G:H4' | 1:CA:429:U:O5' | 1.88 | 0.73 |
| 1:CA:859:A:H2' | 1:CA:860:A:O4' | 1.88 | 0.73 |
| 1:CA:913:A:H4' | 1:CA:914:A:O5' | 1.87 | 0.73 |
| 10:CJ:63:PHE:HB3 | 14:CN:57:ARG:O | 1.87 | 0.73 |
| 30:D8:43:GLN:C | 30:D8:44:LYS:HD2 | 2.09 | 0.73 |
| 31:DA:1678:G:H21 | 31:DA:1989:G:H22 | 1.36 | 0.73 |
| 33:DD:130:ALA:C | 33:DD:131:LEU:HD12 | 2.09 | 0.73 |
| 33:DD:25:THR:HG22 | 33:DD:82:ILE:O | 1.87 | 0.73 |
| 13:CM:3:ARG:NH2 | 36:DG:139:LEU:HD13 | 2.01 | 0.73 |
| 30:D8:27:THR:HA | 41:DP:62:LEU:HD11 | 1.70 | 0.73 |
| 1:AA:1128:C:H5' | 9:AI:16:ARG:NH1 | 2.03 | 0.73 |
| 1:AA:376:G:OP2 | 16:AP:67:THR:HG21 | 1.88 | 0.73 |
| 9:AI:103:THR:HG22 | 9:AI:105:ASP:H | 1.54 | 0.73 |
| 9:AI:124:GLN:O | 9:AI:125:TYR:HB2 | 1.88 | 0.73 |
| 20:AT:50:GLU:HB3 | 20:AT:100:ILE:CG1 | 2.18 | 0.73 |
| 23:B1:10:LYS:HB2 | 23:B1:14:VAL:N | 2.03 | 0.73 |
| 31:BA:128:C:H5'' | 31:BA:128:C:H6 | 1.54 | 0.73 |
| 31:BA:543:C:H42 | 31:BA:551:G:H1 | 1.36 | 0.73 |
| 31:BA:995:C:C2 | 39:BN:4:TYR:OH | 2.36 | 0.73 |
| 32:BB:32:C:C2 | 32:BB:51:G:N2 | 2.57 | 0.73 |
| 33:BD:77:ALA:HB2 | 33:BD:97:TYR:CD2 | 2.23 | 0.73 |
| 35:BF:5:ALA:HB2 | 35:BF:24:LEU:HD11 | 1.69 | 0.73 |
| 46:BU:92:ARG:NH2 | 47:BV:10:LYS:HA | 2.04 | 0.73 |
| 49:BX:26:TYR:OH | 49:BX:89:ILE:HG21 | 1.86 | 0.73 |
| 13:CM:3:ARG:HA | 13:CM:9:ILE:HG13 | 1.70 | 0.73 |
| 31:DA:271(F):C:H2' | 31:DA:271(G):C:H6 | 1.53 | 0.73 |
| 35:DF:57:VAL:HG13 | 35:DF:58:ALA:N | 2.02 | 0.73 |
| 37:DH:13:LYS:HA | 37:DH:13:LYS:HE2 | 1.68 | 0.73 |
| 1:AA:163:C:H2' | 1:AA:164:U:H6 | 1.52 | 0.73 |
| 3:AC:34:LEU:O | 3:AC:38:ARG:HG2 | 1.89 | 0.73 |
| 3:AC:52:LEU:HD23 | 3:AC:52:LEU:H | 1.52 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:B2:26:ARG:HG2 | 49:BX:5:TYR:HB3 | 1.70 | 0.73 |
| 31:BA:1403:C:H5'' | 31:BA:1471:A:H1' | 1.69 | 0.73 |
| 31:BA:271(K):U:H3' | 31:BA:271(L):U:H5' | 1.69 | 0.73 |
| 31:BA:8:A:H2' | 31:BA:9:U:C5 | 2.22 | 0.73 |
| 35:BF:3:GLU:O | 35:BF:19:GLU:HA | 1.88 | 0.73 |
| 1:CA:1502:A:C2 | 1:CA:1505:G:N1 | 2.54 | 0.73 |
| 17:CQ:67:LYS:HA | 17:CQ:70:ARG:HH12 | 1.52 | 0.73 |
| 31:DA:1188:U:C2' | 31:DA:1189:A:H5' | 2.19 | 0.73 |
| 31:DA:142:A:H5' | 31:DA:142(A):C:OP2 | 1.88 | 0.73 |
| 31:DA:528:A:H2 | 31:DA:2043:C:H5' | 1.54 | 0.73 |
| 31:DA:2305:A:H5'' | 36:DG:134:GLY:HA3 | 1.71 | 0.73 |
| 28:B6:12:GLU:HA | 28:B6:23:THR:HA | 1.70 | 0.73 |
| 31:BA:141:A:H8 | 31:BA:1408:C:O2' | 1.69 | 0.73 |
| 31:BA:1484:G:H22 | 31:BA:1505:C:H5 | 1.36 | 0.73 |
| 36:BG:18:GLU:O | 36:BG:22:ARG:HB2 | 1.87 | 0.73 |
| 45:BT:32:TYR:HB3 | 45:BT:81:PRO:HB3 | 1.71 | 0.73 |
| 49:BX:23:GLU:CG | 49:BX:24:GLY:H | 2.01 | 0.73 |
| 1:CA:353:A:H5' | 1:CA:353:A:C8 | 2.22 | 0.73 |
| 31:DA:142:A:C8 | 31:DA:1595:G:N2 | 2.54 | 0.73 |
| 33:DD:25:THR:HG23 | 33:DD:27:THR:HB | 1.70 | 0.73 |
| 33:DD:35:LYS:HD3 | 33:DD:63:ARG:CB | 2.19 | 0.73 |
| 36:DG:86:MET:HB2 | 36:DG:87:PRO:CD | 2.18 | 0.73 |
| 37:DH:137:ASP:CB | 37:DH:140:LYS:HB2 | 2.19 | 0.73 |
| 37:DH:157:TYR:HE1 | 37:DH:171:LEU:N | 1.86 | 0.73 |
| 37:DH:17:VAL:HG21 | 37:DH:50:VAL:HG21 | 1.70 | 0.73 |
| 41:DP:47:ASP:HB3 | 41:DP:48:PRO:CA | 2.18 | 0.73 |
| 25:B3:19:GLN:NE2 | 25:B3:52:HIS:HE1 | 1.86 | 0.73 |
| 31:BA:2029:G:H2' | 31:BA:2031:A:OP2 | 1.88 | 0.73 |
| 31:BA:925:C:H2' | 31:BA:926:A:H5'' | 1.71 | 0.73 |
| 41:BP:47:ASP:HB3 | 41:BP:48:PRO:CA | 2.18 | 0.73 |
| 1:CA:224:C:H2' | 1:CA:225:C:H6 | 1.53 | 0.73 |
| 2:CB:172:ILE:H | 2:CB:172:ILE:HD12 | 1.54 | 0.73 |
| 6:CF:30:LEU:HB3 | 6:CF:35:ALA:HB3 | 1.69 | 0.73 |
| 31:DA:1899:G:N2 | 31:DA:1902:C:H5 | 1.85 | 0.73 |
| 31:DA:2660:A:C5' | 31:DA:2661:G:H21 | 2.01 | 0.73 |
| 1:AA:66:G:H4' | 1:AA:173:U:C5 | 2.23 | 0.73 |
| 10:AJ:34:VAL:HG22 | 10:AJ:74:ILE:HG22 | 1.69 | 0.73 |
| 33:BD:35:LYS:HE3 | 33:BD:65:ILE:N | 2.02 | 0.73 |
| 42:BQ:29:PHE:O | 42:BQ:30:GLY:O | 2.05 | 0.73 |
| 1:CA:240:C:H2' | 1:CA:241:C:C6 | 2.22 | 0.73 |
| 1:CA:355:C:C2' | 1:CA:356:A:H5' | 2.18 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 24:D2:30:ARG:H | 24:D2:30:ARG:HD2 | 1.53 | 0.73 |
| 31:DA:1509(A):A:H2' | 31:DA:1509(B):A:H8 | 1.53 | 0.73 |
| 31:DA:92:A:H2' | 31:DA:93:G:O4' | 1.89 | 0.73 |
| 33:DD:255:LYS:HZ1 | 33:DD:255:LYS:N | 1.86 | 0.73 |
| 36:DG:18:GLU:O | 36:DG:22:ARG:HB2 | 1.87 | 0.73 |
| 39:DN:56:ASN:H | 39:DN:125:GLY:HA3 | 1.54 | 0.73 |
| 39:DN:18:ALA:HB3 | 39:DN:26:LEU:CD2 | 2.15 | 0.73 |
| 47:DV:19:LYS:CG | 47:DV:20:LEU:N | 2.46 | 0.73 |
| 32:BB:20:C:H2' | 32:BB:21:G:C5' | 2.18 | 0.73 |
| 32:BB:87:G:C3' | 32:BB:88:C:H5' | 2.19 | 0.73 |
| 34:BE:38:THR:HG22 | 34:BE:40:GLU:N | 2.02 | 0.73 |
| 12:CL:26:ALA:O | 12:CL:27:LEU:HB2 | 1.88 | 0.73 |
| 16:CP:45:THR:HG22 | 16:CP:47:ASP:H | 1.54 | 0.73 |
| 28:D6:36:LEU:HD13 | 28:D6:50:ARG:CZ | 2.19 | 0.73 |
| 30:D8:30:ARG:O | 30:D8:31:HIS:C | 2.26 | 0.73 |
| 31:DA:2206:G:C2 | 31:DA:2207:G:H5' | 2.24 | 0.73 |
| 41:DP:85:LEU:CD2 | 41:DP:85:LEU:H | 2.01 | 0.73 |
| 49:DX:60:ARG:HG2 | 49:DX:71:GLY:HA3 | 1.70 | 0.73 |
| 16:AP:72:ARG:HH21 | 16:AP:73:LEU:HD21 | 1.52 | 0.72 |
| 20:AT:16:HIS:O | 20:AT:19:SER:HB3 | 1.88 | 0.72 |
| 23:B1:12:PRO:HD2 | 23:B1:62:VAL:HG23 | 1.69 | 0.72 |
| 31:BA:1771:C:O2' | 31:BA:1786:A:H8 | 1.67 | 0.72 |
| 31:BA:2360:A:O2' | 31:BA:2361:A:P | 2.47 | 0.72 |
| 33:BD:270:ILE:HD12 | 33:BD:270:ILE:O | 1.89 | 0.72 |
| 39:BN:56:ASN:H | 39:BN:125:GLY:HA3 | 1.53 | 0.72 |
| 1:CA:186:C:H2' | 1:CA:187:C:H6 | 1.54 | 0.72 |
| 2:CB:217:ARG:HA | 2:CB:220:ASP:HB2 | 1.69 | 0.72 |
| 5:CE:42:GLY:HA3 | 5:CE:66:MET:HG2 | 1.69 | 0.72 |
| 29:D7:9:ARG:NH1 | 31:DA:1310:G:OP2 | 2.21 | 0.72 |
| 31:DA:2801:A:O2' | 31:DA:2895:U:H4' | 1.89 | 0.72 |
| 46:DU:88:ILE:C | 46:DU:90:VAL:H | 1.89 | 0.72 |
| 47:DV:90:PRO:HG2 | 47:DV:91:TYR:N | 1.99 | 0.72 |
| 1:AA:1502:A:C2 | 1:AA:1505:G:N1 | 2.56 | 0.72 |
| 1:AA:240:C:H2' | 1:AA:241:C:C6 | 2.23 | 0.72 |
| 15:AO:39:LEU:CD1 | 15:AO:56:LEU:HB2 | 2.19 | 0.72 |
| 31:BA:2263:C:H6 | 31:BA:2263:C:H5' | 1.53 | 0.72 |
| 31:BA:2598:A:P | 33:BD:236:GLY:HA3 | 2.29 | 0.72 |
| 36:BG:55:LYS:HG2 | 36:BG:58:GLN:HE21 | 1.54 | 0.72 |
| 41:BP:140:ALA:O | 25:D3:1:MET:SD | 2.47 | 0.72 |
| 1:CA:667:G:H4' | 15:CO:51:HIS:CE1 | 2.23 | 0.72 |
| 20:CT:71:THR:HG22 | 20:CT:72:LEU:N | 2.04 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:271(R):G:O2' | 31:DA:271(S):G:H5' | 1.88 | 0.72 |
| 35:DF:3:GLU:O | 35:DF:19:GLU:HA | 1.89 | 0.72 |
| 35:DF:67:GLN:O | 35:DF:67:GLN:HG3 | 1.89 | 0.72 |
| 51:DZ:7:ALA:HB3 | 51:DZ:61:LEU:CD2 | 2.19 | 0.72 |
| 1:AA:622:A:C8 | 1:AA:623:C:C6 | 2.77 | 0.72 |
| 1:AA:627:G:H2' | 1:AA:628:G:C8 | 2.23 | 0.72 |
| 31:BA:330:A:C2 | 31:BA:1210:A:H2' | 2.22 | 0.72 |
| 31:BA:1639:U:C2' | 31:BA:1640:C:H5'' | 2.19 | 0.72 |
| 31:BA:271(F):C:H2' | 31:BA:271(G):C:H6 | 1.52 | 0.72 |
| 32:BB:87:G:C8 | 32:BB:87:G:OP2 | 2.42 | 0.72 |
| 40:BO:13:ASN:HD21 | 40:BO:96:THR:H | 1.37 | 0.72 |
| 41:BP:71:VAL:CG1 | 41:BP:72:PRO:HD3 | 2.19 | 0.72 |
| 1:CA:568:G:O6 | 12:CL:5:PRO:HD3 | 1.89 | 0.72 |
| 3:CC:34:LEU:O | 3:CC:38:ARG:HG2 | 1.90 | 0.72 |
| 31:DA:1484:G:N2 | 31:DA:1505:C:H41 | 1.86 | 0.72 |
| 31:DA:1821:A:H2' | 31:DA:1822:G:C5' | 2.19 | 0.72 |
| 33:DD:27:THR:O | 33:DD:29:PRO:HD2 | 1.90 | 0.72 |
| 39:DN:119:ARG:CG | 39:DN:119:ARG:HH11 | 1.99 | 0.72 |
| 43:DR:67:LEU:CD1 | 43:DR:76:VAL:HG21 | 2.19 | 0.72 |
| 46:DU:100:VAL:HG12 | 46:DU:101:ARG:N | 2.04 | 0.72 |
| 31:DA:518:G:H4' | 48:DW:18:ARG:NH1 | 2.04 | 0.72 |
| 4:AD:128:VAL:HG13 | 4:AD:129:ASN:ND2 | 2.02 | 0.72 |
| 1:AA:552:U:H4' | 12:AL:86:ARG:HG2 | 1.71 | 0.72 |
| 31:BA:271(R):G:O2' | 31:BA:271(S):G:H5' | 1.89 | 0.72 |
| 42:BQ:8:LYS:HG3 | 42:BQ:9:TYR:N | 2.02 | 0.72 |
| 43:BR:87:TYR:O | 43:BR:89:ASP:N | 2.21 | 0.72 |
| 1:CA:1117:G:H4' | 9:CI:104:ARG:NH2 | 2.04 | 0.72 |
| 11:CK:125:PHE:HD1 | 11:CK:125:PHE:N | 1.88 | 0.72 |
| 1:CA:552:U:H4' | 12:CL:86:ARG:HG2 | 1.71 | 0.72 |
| 12:CL:91:LYS:HG3 | 12:CL:91:LYS:O | 1.88 | 0.72 |
| 27:D5:46:CYS:SG | 27:D5:47:PRO:CD | 2.78 | 0.72 |
| 31:DA:1822:G:H5' | 31:DA:1822:G:C8 | 2.21 | 0.72 |
| 31:DA:2660:A:H5' | 31:DA:2661:G:H21 | 1.55 | 0.72 |
| 35:DF:28:ILE:HG21 | 35:DF:116:ASP:HB2 | 1.70 | 0.72 |
| 42:DQ:6:ARG:O | 42:DQ:7:MET:HG2 | 1.90 | 0.72 |
| 44:DS:28:VAL:O | 44:DS:89:ARG:HD2 | 1.89 | 0.72 |
| 44:DS:92:TYR:HD1 | 44:DS:93:LYS:N | 1.79 | 0.72 |
| 45:DT:128:GLU:O | 45:DT:130:ALA:N | 2.23 | 0.72 |
| 42:DQ:140:ALA:HA | 51:DZ:99:TYR:CD2 | 2.24 | 0.72 |
| 27:B5:2:ALA:HA | 31:BA:2015:A:C1' | 2.16 | 0.72 |
| 38:BI:133:HIS:HB2 | 38:BI:134:PRO:HD2 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 47:BV:24:LYS:HB2 | 47:BV:92:THR:OG1 | 1.89 | 0.72 |
| 1:CA:390:C:O3' | 16:CP:28:ARG:NH2 | 2.23 | 0.72 |
| 17:CQ:5:VAL:O | 17:CQ:6:LEU:HD23 | 1.90 | 0.72 |
| 24:D2:14:ARG:O | 24:D2:18:PRO:HD3 | 1.88 | 0.72 |
| 27:D5:54:GLY:O | 27:D5:56:LYS:NZ | 2.19 | 0.72 |
| 31:DA:2029:G:H2' | 31:DA:2031:A:OP2 | 1.89 | 0.72 |
| 31:DA:2418:A:H2' | 31:DA:2419:U:C6 | 2.24 | 0.72 |
| 31:DA:2801(A):A:H4' | 31:DA:2802:G:H2' | 1.70 | 0.72 |
| 32:DB:32:C:C2 | 32:DB:51:G:N2 | 2.58 | 0.72 |
| 34:DE:48:GLN:NE2 | 34:DE:78:LEU:HD13 | 2.05 | 0.72 |
| 35:DF:5:ALA:HB2 | 35:DF:24:LEU:HD11 | 1.71 | 0.72 |
| 49:DX:23:GLU:CG | 49:DX:24:GLY:H | 2.02 | 0.72 |
| 5:AE:33:VAL:HG11 | 5:AE:109:ILE:HA | 1.70 | 0.72 |
| 19:AS:36:ARG:HH12 | 19:AS:75:ALA:HB3 | 1.53 | 0.72 |
| 31:BA:607:U:N3 | 31:BA:621:A:C2 | 2.54 | 0.72 |
| 37:BH:157:TYR:HE1 | 37:BH:171:LEU:N | 1.85 | 0.72 |
| 50:BY:45:VAL:HG11 | 50:BY:60:PHE:O | 1.89 | 0.72 |
| 2:CB:185:ILE:CG2 | 2:CB:199:TYR:HB2 | 2.17 | 0.72 |
| 9:CI:53:VAL:HG12 | 9:CI:95:LYS:HG2 | 1.72 | 0.72 |
| 1:CA:247:G:OP2 | 17:CQ:100:LYS:HG2 | 1.89 | 0.72 |
| 23:D1:16:ASN:HB3 | 23:D1:46:LEU:HD12 | 1.71 | 0.72 |
| 31:DA:2523:G:H2' | 31:DA:2524:G:C5' | 2.19 | 0.72 |
| 31:DA:247:G:H4' | 31:DA:386:G:C5 | 2.25 | 0.72 |
| 39:DN:112:LEU:O | 39:DN:112:LEU:HD12 | 1.90 | 0.72 |
| 39:DN:67:LEU:HA | 39:DN:88:GLU:HG3 | 1.69 | 0.72 |
| 42:DQ:63:LYS:HG2 | 42:DQ:65:PHE:CE2 | 2.23 | 0.72 |
| 45:DT:55:ASN:H | 45:DT:59:THR:HB | 1.54 | 0.72 |
| 15:AO:82:ILE:HG12 | 15:AO:87:ILE:HB | 1.70 | 0.72 |
| 28:B6:15:GLU:HG2 | 28:B6:18:ARG:NE | 2.02 | 0.72 |
| 31:BA:1181:C:O2' | 31:BA:1182:A:H5' | 1.89 | 0.72 |
| 31:BA:528:A:H2 | 31:BA:2043:C:H5' | 1.55 | 0.72 |
| 33:BD:25:THR:O | 33:BD:27:THR:N | 2.22 | 0.72 |
| 34:BE:201:THR:HG22 | 34:BE:202:LYS:N | 2.03 | 0.72 |
| 37:BH:13:LYS:HA | 37:BH:13:LYS:HE2 | 1.71 | 0.72 |
| 47:BV:72:VAL:HG12 | 47:BV:73:SER:N | 2.04 | 0.72 |
| 48:BW:86:LEU:HD12 | 48:BW:87:PRO:HD2 | 1.71 | 0.72 |
| 1:CA:950:U:H3' | 13:CM:102:ARG:HH12 | 1.54 | 0.72 |
| 31:DA:2723:C:H5'' | 43:DR:2:ARG:HD2 | 1.70 | 0.72 |
| 31:DA:467:G:C2' | 31:DA:468:G:H5' | 2.20 | 0.72 |
| 33:DD:35:LYS:HA | 33:DD:64:ILE:HG22 | 1.72 | 0.72 |
| 36:DG:55:LYS:HG2 | 36:DG:58:GLN:HE21 | 1.54 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:DS:26:LEU:HD22 | 44:DS:87:PHE:CE1 | 2.25 | 0.72 |
| 44:DS:89:ARG:O | 44:DS:92:TYR:HB3 | 1.90 | 0.72 |
| 11:AK:125:PHE:N | 11:AK:125:PHE:HD1 | 1.88 | 0.72 |
| 47:BV:2:PHE:HE1 | 47:BV:13:ARG:NH2 | 1.88 | 0.72 |
| 30:D8:4:MET:SD | 30:D8:61:LEU:HD12 | 2.29 | 0.72 |
| 31:DA:1484:G:H21 | 31:DA:1505:C:H41 | 1.38 | 0.72 |
| 31:DA:83:G:N2 | 31:DA:102:G:O2' | 2.22 | 0.72 |
| 32:DB:44:G:H1' | 32:DB:47:C:N4 | 2.05 | 0.72 |
| 33:DD:25:THR:O | 33:DD:25:THR:HG23 | 1.88 | 0.72 |
| 37:DH:19:VAL:HB | 37:DH:44:VAL:HG13 | 1.71 | 0.72 |
| 31:DA:626:U:C2 | 41:DP:105:LEU:HG | 2.25 | 0.72 |
| 31:DA:598:G:H5' | 41:DP:15:ARG:HD2 | 1.70 | 0.72 |
| 39:DN:42:TRP:CB | 46:DU:64:ARG:HH11 | 1.98 | 0.72 |
| 1:AA:1004:A:H2' | 1:AA:1038:C:O2 | 1.90 | 0.72 |
| 13:AM:15:VAL:O | 13:AM:19:LEU:HD23 | 1.89 | 0.72 |
| 20:AT:82:SER:O | 20:AT:86:ARG:HB2 | 1.89 | 0.72 |
| 27:B5:40:LYS:HD3 | 27:B5:46:CYS:CB | 2.20 | 0.72 |
| 31:BA:1464:C:O2' | 31:BA:1528:A:H8 | 1.69 | 0.72 |
| 31:BA:1654:A:OP1 | 43:BR:3:HIS:CB | 2.35 | 0.72 |
| 23:B1:37:ILE:HG21 | 31:BA:2080:G:OP1 | 1.90 | 0.72 |
| 31:BA:370:G:H4' | 31:BA:371:A:OP2 | 1.87 | 0.72 |
| 31:BA:2415:G:H4' | 41:BP:67:MET:H | 1.53 | 0.72 |
| 2:CB:22:LYS:NZ | 2:CB:22:LYS:HA | 2.04 | 0.72 |
| 18:CR:62:GLU:HA | 18:CR:65:ILE:HD11 | 1.72 | 0.72 |
| 23:D1:37:ILE:HD12 | 31:DA:2079:U:O2' | 1.89 | 0.72 |
| 31:DA:1497:U:C5' | 31:DA:1498:C:H5 | 2.02 | 0.72 |
| 23:D1:37:ILE:HG21 | 31:DA:2080:G:OP1 | 1.90 | 0.72 |
| 24:D2:53:LEU:HD12 | 31:DA:77:C:OP1 | 1.90 | 0.72 |
| 35:DF:158:THR:HG23 | 35:DF:160:ASN:N | 2.04 | 0.72 |
| 41:DP:51:PHE:HB3 | 41:DP:52:GLU:OE2 | 1.90 | 0.72 |
| 34:DE:111:ARG:HA | 43:DR:2:ARG:HG3 | 1.72 | 0.72 |
| 11:AK:21:ILE:HG13 | 11:AK:30:VAL:HG12 | 1.72 | 0.72 |
| 18:AR:62:GLU:HA | 18:AR:65:ILE:HD11 | 1.71 | 0.72 |
| 31:BA:527:C:OP2 | 31:BA:2779:U:H5 | 1.71 | 0.72 |
| 39:BN:19:GLU:HG3 | 39:BN:20:GLY:H | 1.55 | 0.72 |
| 41:BP:112:LEU:HD22 | 41:BP:113:LYS:N | 2.05 | 0.72 |
| 41:BP:120:ALA:O | 25:D3:1:MET:HG2 | 1.88 | 0.72 |
| 1:CA:1004:A:H2' | 1:CA:1038:C:O2 | 1.90 | 0.72 |
| 1:CA:737:A:H2' | 1:CA:738:C:C6 | 2.25 | 0.72 |
| 12:CL:18:VAL:HG23 | 12:CL:19:ARG:H | 1.52 | 0.72 |
| 16:CP:76:GLN:HG2 | 16:CP:76:GLN:O | 1.89 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:D5:40:LYS:HD3 | 27:D5:46:CYS:CB | 2.20 | 0.72 |
| 34:DE:38:THR:HG22 | 34:DE:40:GLU:N | 2.04 | 0.72 |
| 45:DT:32:TYR:HB3 | 45:DT:81:PRO:HB3 | 1.71 | 0.72 |
| 1:AA:559:A:H5'' | 1:AA:560:U:H3' | 1.70 | 0.71 |
| 1:AA:662:G:H2' | 1:AA:663:A:H8 | 1.53 | 0.71 |
| 10:AJ:63:PHE:HB3 | 14:AN:57:ARG:O | 1.90 | 0.71 |
| 25:B3:6:VAL:CG1 | 25:B3:54:VAL:HG11 | 2.19 | 0.71 |
| 31:BA:1210:A:C8 | 31:BA:1210:A:H5' | 2.15 | 0.71 |
| 31:BA:1419:A:O2' | 31:BA:1420:U:H5'' | 1.88 | 0.71 |
| 31:BA:1822:G:H5' | 31:BA:1822:G:C8 | 2.19 | 0.71 |
| 31:BA:2781:A:H5'' | 31:BA:2782:G:H5' | 1.71 | 0.71 |
| 42:BQ:141:GLN:HG2 | 51:BZ:71:VAL:O | 1.90 | 0.71 |
| 2:CB:233:SER:HB2 | 2:CB:234:PRO:HD2 | 1.71 | 0.71 |
| 28:D6:44:ARG:O | 28:D6:45:LYS:HG2 | 1.90 | 0.71 |
| 29:D7:8:ASN:ND2 | 29:D7:8:ASN:C | 2.41 | 0.71 |
| 36:DG:123:ASN:O | 36:DG:126:ASP:HB2 | 1.89 | 0.71 |
| 38:DI:133:HIS:HB2 | 38:DI:134:PRO:HD2 | 1.72 | 0.71 |
| 48:DW:4:LYS:HB2 | 48:DW:106:ILE:CG2 | 2.19 | 0.71 |
| 49:DX:38:GLU:OE1 | 49:DX:38:GLU:N | 2.22 | 0.71 |
| 50:DY:44:ILE:HD12 | 50:DY:44:ILE:H | 1.54 | 0.71 |
| 18:AR:50:ILE:HD11 | 18:AR:70:ILE:HG21 | 1.71 | 0.71 |
| 31:BA:1484:G:N2 | 31:BA:1505:C:H41 | 1.89 | 0.71 |
| 31:BA:2206:G:C2 | 31:BA:2207:G:H5' | 2.24 | 0.71 |
| 38:BI:2:LYS:HB2 | 38:BI:39:ALA:HB3 | 1.70 | 0.71 |
| 47:BV:90:PRO:HG2 | 47:BV:91:TYR:N | 1.99 | 0.71 |
| 31:BA:143(A):C:H5' | 49:BX:36:LYS:HG2 | 1.71 | 0.71 |
| 1:CA:22:G:H2' | 1:CA:23:C:C6 | 2.25 | 0.71 |
| 4:CD:161:ASN:O | 4:CD:165:MET:HG2 | 1.89 | 0.71 |
| 23:D1:26:ARG:CG | 23:D1:34:THR:HB | 2.20 | 0.71 |
| 31:DA:1332:G:N2 | 31:DA:1610:A:C8 | 2.58 | 0.71 |
| 31:DA:1434:A:H61 | 31:DA:1558:A:N6 | 1.89 | 0.71 |
| 31:DA:951:C:O2' | 31:DA:952:G:H5' | 1.89 | 0.71 |
| 32:DB:62:C:H2' | 32:DB:63:G:H5'' | 1.72 | 0.71 |
| 33:DD:63:ARG:HG3 | 33:DD:63:ARG:HH11 | 1.54 | 0.71 |
| 37:DH:41:MET:HA | 37:DH:41:MET:HE2 | 1.70 | 0.71 |
| 39:DN:3:THR:HA | 39:DN:4:TYR:CD1 | 2.24 | 0.71 |
| 46:DU:92:ARG:NH2 | 47:DV:10:LYS:HA | 2.05 | 0.71 |
| 30:B8:40:GLU:OE1 | 30:B8:44:LYS:HE3 | 1.90 | 0.71 |
| 30:B8:43:GLN:C | 30:B8:44:LYS:HD2 | 2.10 | 0.71 |
| 36:BG:47:LYS:HE2 | 36:BG:81:LYS:HB2 | 1.70 | 0.71 |
| 41:BP:6:LEU:HG | 41:BP:8:PRO:O | 1.89 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:BY:81:LYS:HG2 | 50:BY:96:ILE:HG22 | 1.71 | 0.71 |
| 4:CD:189:PRO:HB3 | 4:CD:194:LEU:HD21 | 1.72 | 0.71 |
| 31:DA:2223:G:C2' | 31:DA:2224:G:H5' | 2.18 | 0.71 |
| 31:DA:527:C:OP2 | 31:DA:2779:U:H5 | 1.72 | 0.71 |
| 31:DA:993:G:H1' | 47:DV:91:TYR:CD1 | 2.25 | 0.71 |
| 31:DA:2598:A:P | 33:DD:236:GLY:HA3 | 2.30 | 0.71 |
| 34:DE:61:ARG:H | 34:DE:62:PRO:HD2 | 1.55 | 0.71 |
| 34:DE:47:VAL:HG22 | 34:DE:84:PHE:O | 1.88 | 0.71 |
| 41:DP:17:LYS:O | 41:DP:19:VAL:N | 2.22 | 0.71 |
| 44:DS:14:VAL:HG12 | 44:DS:15:ARG:N | 2.05 | 0.71 |
| 1:AA:1123:A:O2' | 10:AJ:38:ILE:HG22 | 1.91 | 0.71 |
| 12:AL:46:LYS:HG2 | 12:AL:47:LYS:H | 1.56 | 0.71 |
| 28:B6:13:CYS:O | 28:B6:21:TYR:HA | 1.91 | 0.71 |
| 31:BA:1332:G:N2 | 31:BA:1610:A:H8 | 1.88 | 0.71 |
| 31:BA:2206:G:N2 | 31:BA:2207:G:C5' | 2.48 | 0.71 |
| 31:BA:2327:A:H2' | 31:BA:2328:A:C8 | 2.25 | 0.71 |
| 31:BA:671:C:C6 | 31:BA:671:C:H5' | 2.25 | 0.71 |
| 38:BI:102:SER:HA | 38:BI:107:VAL:O | 1.90 | 0.71 |
| 1:CA:1446:U:H4' | 1:CA:1447:A:N7 | 2.06 | 0.71 |
| 1:CA:673:G:H2' | 1:CA:674:G:C8 | 2.24 | 0.71 |
| 18:CR:25:THR:HG22 | 18:CR:42:ARG:HH11 | 1.55 | 0.71 |
| 31:DA:2360:A:O2' | 31:DA:2361:A:P | 2.48 | 0.71 |
| 39:DN:18:ALA:CB | 39:DN:26:LEU:HD22 | 2.17 | 0.71 |
| 47:DV:25:LEU:HB2 | 47:DV:94:LEU:HD13 | 1.72 | 0.71 |
| 1:AA:386:C:O2' | 1:AA:387:U:H5' | 1.91 | 0.71 |
| 31:BA:1434:A:O2' | 31:BA:1435:G:H5' | 1.90 | 0.71 |
| 31:BA:1582:C:O2' | 31:BA:1586:A:C8 | 2.43 | 0.71 |
| 31:BA:2660:A:H5' | 31:BA:2661:G:H21 | 1.55 | 0.71 |
| 31:BA:2801:A:O2' | 31:BA:2895:U:H4' | 1.90 | 0.71 |
| 31:BA:322:A:H5' | 31:BA:340:A:H1' | 1.71 | 0.71 |
| 47:BV:82:ARG:CG | 47:BV:82:ARG:NH1 | 2.39 | 0.71 |
| 1:CA:687:A:N3 | 1:CA:688:G:H1' | 2.04 | 0.71 |
| 3:CC:73:PRO:O | 3:CC:76:VAL:HG22 | 1.90 | 0.71 |
| 1:CA:1128:C:H5' | 9:CI:16:ARG:NH1 | 2.05 | 0.71 |
| 12:CL:82:VAL:HG12 | 12:CL:83:VAL:N | 2.05 | 0.71 |
| 30:D8:34:TRP:HZ3 | 30:D8:41:ILE:HG23 | 1.53 | 0.71 |
| 31:DA:298:G:H5' | 31:DA:299:A:OP1 | 1.90 | 0.71 |
| 38:DI:1:MET:HB2 | 38:DI:21:VAL:O | 1.89 | 0.71 |
| 47:DV:1:MET:HE3 | 47:DV:44:LYS:CB | 2.20 | 0.71 |
| 50:DY:96:ILE:HG22 | 50:DY:97:ARG:H | 1.54 | 0.71 |
| 1:AA:1446:U:H4' | 1:AA:1447:A:N7 | 2.06 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1697:G:C5' | 31:BA:1697:G:C8 | 2.71 | 0.71 |
| 31:BA:2523:G:H2' | 31:BA:2524:G:C5' | 2.19 | 0.71 |
| 31:BA:2565:A:H5'' | 31:BA:2566:A:OP2 | 1.91 | 0.71 |
| 31:BA:510:C:C2' | 31:BA:511:U:H5' | 2.21 | 0.71 |
| 31:BA:916:G:C2' | 31:BA:917:A:H5'' | 2.21 | 0.71 |
| 37:BH:103:LEU:HD21 | 37:BH:105:LEU:HD11 | 1.72 | 0.71 |
| 40:BO:13:ASN:ND2 | 40:BO:97:ARG:H | 1.89 | 0.71 |
| 49:BX:24:GLY:HA3 | 49:BX:80:ILE:HG13 | 1.72 | 0.71 |
| 42:BQ:140:ALA:HB1 | 51:BZ:99:TYR:HB2 | 1.71 | 0.71 |
| 1:CA:108:G:H5'' | 1:CA:109:A:H5'' | 1.72 | 0.71 |
| 1:CA:392:G:H2' | 1:CA:393:A:H8 | 1.55 | 0.71 |
| 16:CP:22:THR:HA | 16:CP:33:ILE:HG12 | 1.73 | 0.71 |
| 20:CT:13:LEU:H | 20:CT:13:LEU:HD12 | 1.54 | 0.71 |
| 31:DA:794:G:H2' | 31:DA:795:C:H6 | 1.55 | 0.71 |
| 31:DA:996:A:H4' | 46:DU:92:ARG:NE | 2.06 | 0.71 |
| 33:DD:77:ALA:HB2 | 33:DD:97:TYR:CD2 | 2.25 | 0.71 |
| 31:DA:661:C:H4' | 41:DP:18:ARG:HG2 | 1.70 | 0.71 |
| 45:DT:61:PHE:CE2 | 45:DT:76:PHE:HB2 | 2.25 | 0.71 |
| 47:DV:38:LEU:HG | 47:DV:39:LEU:N | 2.04 | 0.71 |
| 50:DY:8:LYS:NZ | 50:DY:74:PRO:HD3 | 2.04 | 0.71 |
| 51:DZ:4:ARG:HG2 | 51:DZ:58:VAL:HB | 1.73 | 0.71 |
| 1:AA:1418:A:N3 | 31:BA:1959:G:H1' | 2.05 | 0.71 |
| 1:AA:382:A:H2' | 1:AA:383:A:C8 | 2.25 | 0.71 |
| 1:AA:827:U:H2' | 1:AA:859:A:H61 | 1.55 | 0.71 |
| 31:BA:910:A:H62 | 42:BQ:12:GLN:HA | 1.55 | 0.71 |
| 39:BN:65:LYS:CE | 39:BN:65:LYS:HA | 2.11 | 0.71 |
| 47:BV:1:MET:HE3 | 47:BV:44:LYS:HB3 | 1.72 | 0.71 |
| 50:BY:17:SER:CB | 50:BY:71:LYS:HD2 | 2.21 | 0.71 |
| 50:BY:96:ILE:CD1 | 50:BY:99:CYS:SG | 2.78 | 0.71 |
| 1:CA:321:A:H62 | 1:CA:328:C:H1' | 1.55 | 0.71 |
| 5:CE:33:VAL:HG11 | 5:CE:109:ILE:HA | 1.71 | 0.71 |
| 25:D3:19:GLN:NE2 | 25:D3:52:HIS:CE1 | 2.58 | 0.71 |
| 31:DA:271(K):U:H3' | 31:DA:271(L):U:H5' | 1.70 | 0.71 |
| 35:DF:34:TRP:HB2 | 41:DP:10:PRO:O | 1.90 | 0.71 |
| 42:DQ:29:PHE:O | 42:DQ:30:GLY:O | 2.08 | 0.71 |
| 49:DX:40:LYS:HG3 | 49:DX:51:VAL:HB | 1.71 | 0.71 |
| 1:AA:1418:A:H2 | 31:BA:1948:G:N3 | 1.89 | 0.71 |
| 6:AF:20:ALA:HA | 6:AF:23:LYS:HB2 | 1.72 | 0.71 |
| 23:B1:26:ARG:CG | 23:B1:34:THR:HB | 2.21 | 0.71 |
| 31:BA:1607:C:H4' | 31:BA:1608:A:O5' | 1.89 | 0.71 |
| 31:BA:2713:A:H3' | 31:BA:2714:G:C5' | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:49:A:H4' | 31:BA:50:U:H5' | 1.73 | 0.71 |
| 37:BH:149:ARG:HA | 37:BH:162:ILE:HG13 | 1.71 | 0.71 |
| 45:BT:51:ARG:HG3 | 45:BT:98:LYS:HE2 | 1.72 | 0.71 |
| 50:BY:2:ARG:O | 50:BY:4:LYS:N | 2.24 | 0.71 |
| 1:CA:1090:U:H2' | 1:CA:1091:U:C6 | 2.19 | 0.71 |
| 1:CA:353:A:C5' | 1:CA:353:A:H8 | 2.03 | 0.71 |
| 1:CA:441:A:H3' | 1:CA:442:C:H6 | 1.56 | 0.71 |
| 1:CA:622:A:C8 | 1:CA:623:C:C6 | 2.79 | 0.71 |
| 2:CB:22:LYS:HZ3 | 2:CB:22:LYS:HA | 1.55 | 0.71 |
| 9:CI:18:PHE:HB3 | 9:CI:20:ARG:HH11 | 1.56 | 0.71 |
| 10:CJ:39:PRO:HB3 | 10:CJ:70:ARG:HH12 | 1.56 | 0.71 |
| 31:DA:286:C:N4 | 31:DA:355:G:H1 | 1.89 | 0.71 |
| 39:DN:66:LYS:HA | 39:DN:69:GLN:HB2 | 1.73 | 0.71 |
| 42:DQ:78:PRO:O | 42:DQ:79:LEU:HG | 1.90 | 0.71 |
| 45:DT:31:SER:C | 45:DT:32:TYR:CD2 | 2.64 | 0.71 |
| 49:DX:24:GLY:HA3 | 49:DX:80:ILE:CG1 | 2.21 | 0.71 |
| 51:DZ:152:ALA:HB2 | 51:DZ:168:GLU:HA | 1.73 | 0.71 |
| 3:AC:73:PRO:O | 3:AC:76:VAL:HG22 | 1.91 | 0.71 |
| 11:AK:13:GLN:HB3 | 11:AK:75:TYR:O | 1.91 | 0.71 |
| 31:BA:2223:G:C2' | 31:BA:2224:G:H5' | 2.21 | 0.71 |
| 31:BA:2580:U:C5' | 34:BE:131:ALA:H | 2.04 | 0.71 |
| 31:BA:467:G:C2' | 31:BA:468:G:H5' | 2.20 | 0.71 |
| 33:BD:172:TYR:CE1 | 33:BD:186:HIS:HB2 | 2.24 | 0.71 |
| 33:BD:35:LYS:HD2 | 33:BD:104:TYR:CE1 | 2.25 | 0.71 |
| 34:BE:132:HIS:CD2 | 34:BE:135:HIS:CE1 | 2.79 | 0.71 |
| 35:BF:28:ILE:HG21 | 35:BF:116:ASP:HB2 | 1.72 | 0.71 |
| 37:BH:19:VAL:HB | 37:BH:44:VAL:HG13 | 1.72 | 0.71 |
| 39:BN:18:ALA:CB | 39:BN:21:LYS:HB2 | 2.16 | 0.71 |
| 45:BT:128:GLU:O | 45:BT:130:ALA:N | 2.24 | 0.71 |
| 45:BT:23:ARG:O | 45:BT:25:GLY:N | 2.23 | 0.71 |
| 46:BU:90:VAL:O | 46:BU:92:ARG:N | 2.23 | 0.71 |
| 47:BV:19:LYS:HG3 | 47:BV:20:LEU:O | 1.91 | 0.71 |
| 47:BV:52:VAL:O | 47:BV:53:GLU:HB3 | 1.91 | 0.71 |
| 1:CA:627:G:H2' | 1:CA:628:G:C8 | 2.24 | 0.71 |
| 3:CC:105:GLU:HG2 | 3:CC:106:VAL:H | 1.55 | 0.71 |
| 30:D8:6:THR:CG2 | 30:D8:63:PRO:HD3 | 2.21 | 0.71 |
| 31:DA:1019:U:H3 | 31:DA:1142(A):A:N6 | 1.85 | 0.71 |
| 31:DA:1348:G:H2' | 31:DA:1349:A:H5' | 1.73 | 0.71 |
| 31:DA:1836:C:O2' | 31:DA:1837:C:H5' | 1.90 | 0.71 |
| 40:DO:18:LYS:HB2 | 40:DO:45:GLU:HG2 | 1.73 | 0.71 |
| 40:DO:4:PRO:O | 40:DO:5:GLN:HB2 | 1.91 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:18:ARG:HH21 | 5:AE:25:ARG:HG2 | 1.56 | 0.71 |
| 5:AE:42:GLY:HA3 | 5:AE:66:MET:HG2 | 1.72 | 0.71 |
| 31:BA:1430:C:H2' | 31:BA:1431:U:H6 | 1.52 | 0.71 |
| 31:BA:1484:G:H21 | 31:BA:1505:C:H41 | 1.39 | 0.71 |
| 31:BA:1510:G:C2' | 31:BA:1511:C:H5' | 2.21 | 0.71 |
| 31:BA:2223:G:H2' | 31:BA:2224:G:H5' | 1.73 | 0.71 |
| 31:BA:2492:U:H2' | 31:BA:2493:U:H6 | 1.54 | 0.71 |
| 32:BB:44:G:H1' | 32:BB:47:C:N4 | 2.06 | 0.71 |
| 31:BA:2787:C:C1' | 34:BE:61:ARG:HB2 | 2.21 | 0.71 |
| 35:BF:183:VAL:O | 35:BF:187:VAL:HG23 | 1.91 | 0.71 |
| 37:BH:89:ILE:HD11 | 37:BH:129:THR:HB | 1.73 | 0.71 |
| 31:BA:626:U:C2 | 41:BP:105:LEU:HG | 2.26 | 0.71 |
| 41:BP:30:THR:CG2 | 41:BP:31:ALA:H | 2.03 | 0.71 |
| 49:BX:35:THR:O | 49:BX:36:LYS:O | 2.08 | 0.71 |
| 1:CA:163:C:H2' | 1:CA:164:U:C6 | 2.25 | 0.71 |
| 1:CA:224:C:H2' | 1:CA:225:C:C6 | 2.26 | 0.71 |
| 1:CA:80:G:H1 | 1:CA:89:C:H41 | 1.38 | 0.71 |
| 4:CD:68:TYR:CE2 | 4:CD:97:LEU:HB3 | 2.25 | 0.71 |
| 20:CT:82:SER:O | 20:CT:86:ARG:HB2 | 1.89 | 0.71 |
| 33:DD:25:THR:O | 33:DD:27:THR:N | 2.24 | 0.71 |
| 44:DS:95:HIS:CG | 44:DS:96:GLY:H | 2.08 | 0.71 |
| 49:DX:53:LYS:H | 49:DX:80:ILE:HG22 | 1.56 | 0.71 |
| 50:DY:96:ILE:CD1 | 50:DY:99:CYS:SG | 2.79 | 0.71 |
| 1:AA:108:G:H5'' | 1:AA:109:A:H5'' | 1.72 | 0.70 |
| 1:AA:163:C:H2' | 1:AA:164:U:C6 | 2.26 | 0.70 |
| 1:AA:262:A:H2' | 1:AA:263:A:C8 | 2.26 | 0.70 |
| 1:AA:877:C:H5'' | 8:AH:88:LYS:HD3 | 1.72 | 0.70 |
| 1:AA:950:U:H3' | 13:AM:102:ARG:HH12 | 1.54 | 0.70 |
| 4:AD:119:GLN:HG3 | 4:AD:123:HIS:CD2 | 2.26 | 0.70 |
| 5:AE:68:GLU:O | 5:AE:68:GLU:HG3 | 1.91 | 0.70 |
| 23:B1:9:GLY:O | 23:B1:10:LYS:HE2 | 1.89 | 0.70 |
| 31:BA:1019:U:H3 | 31:BA:1142(A):A:N6 | 1.86 | 0.70 |
| 33:BD:58:HIS:HD2 | 33:BD:59:LYS:O | 1.73 | 0.70 |
| 36:BG:124:SER:HB2 | 36:BG:131:TYR:CE1 | 2.26 | 0.70 |
| 36:BG:64:THR:HG23 | 36:BG:66:GLN:H | 1.56 | 0.70 |
| 41:BP:122:PRO:HA | 41:BP:141:ALA:O | 1.90 | 0.70 |
| 1:CA:475:G:H2' | 1:CA:476:G:H8 | 1.54 | 0.70 |
| 31:DA:1833:U:H2' | 31:DA:1834:U:H6 | 1.55 | 0.70 |
| 31:DA:184:C:H2' | 31:DA:185:U:C6 | 2.26 | 0.70 |
| 31:DA:2537:U:H2' | 31:DA:2538:C:C6 | 2.26 | 0.70 |
| 37:DH:103:LEU:HD21 | 37:DH:105:LEU:HD11 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:HE2 | 1.56 | 0.70 |
| 16:AP:45:THR:HG22 | 16:AP:47:ASP:H | 1.56 | 0.70 |
| 41:BP:75:ILE:N | 41:BP:75:ILE:HD13 | 2.06 | 0.70 |
| 42:BQ:30:GLY:HA2 | 42:BQ:107:ALA:HB2 | 1.73 | 0.70 |
| 1:CA:194:C:C2' | 1:CA:195:A:H5'' | 2.21 | 0.70 |
| 1:CA:518:C:H2' | 1:CA:530:G:C2 | 2.25 | 0.70 |
| 8:CH:120:THR:H | 8:CH:123:GLU:HB2 | 1.56 | 0.70 |
| 29:D7:5:TRP:CD1 | 29:D7:7:PRO:HG3 | 2.26 | 0.70 |
| 31:DA:1429:G:H2' | 31:DA:1430:C:C6 | 2.26 | 0.70 |
| 31:DA:1510:G:C2' | 31:DA:1511:C:H5' | 2.21 | 0.70 |
| 39:DN:62:VAL:CG2 | 39:DN:66:LYS:HD2 | 2.21 | 0.70 |
| 42:DQ:16:ARG:HB2 | 42:DQ:16:ARG:HH11 | 1.55 | 0.70 |
| 49:DX:70:LEU:HG | 49:DX:71:GLY:H | 1.56 | 0.70 |
| 1:AA:600:C:H2' | 1:AA:601:C:H6 | 1.56 | 0.70 |
| 5:AE:101:ILE:CD1 | 5:AE:119:LEU:HD23 | 2.19 | 0.70 |
| 9:AI:18:PHE:HB3 | 9:AI:20:ARG:HH11 | 1.56 | 0.70 |
| 12:AL:26:ALA:O | 12:AL:27:LEU:HB2 | 1.89 | 0.70 |
| 23:B1:16:ASN:HB3 | 23:B1:46:LEU:HD12 | 1.73 | 0.70 |
| 31:BA:2190:G:H2' | 31:BA:2191:G:H5' | 1.72 | 0.70 |
| 49:BX:40:LYS:HG3 | 49:BX:51:VAL:HB | 1.71 | 0.70 |
| 31:DA:1697:G:C5' | 31:DA:1697:G:C8 | 2.72 | 0.70 |
| 31:DA:2849:U:OP2 | 45:DT:95:ARG:NH1 | 2.25 | 0.70 |
| 31:DA:464:U:O2' | 31:DA:465:G:H5' | 1.91 | 0.70 |
| 31:DA:259:G:H21 | 31:DA:621:A:H8 | 1.39 | 0.70 |
| 31:DA:830:G:H4' | 31:DA:831:G:OP2 | 1.91 | 0.70 |
| 33:DD:260:ARG:HH22 | 33:DD:266:SER:HB2 | 1.54 | 0.70 |
| 39:DN:89:LYS:O | 39:DN:93:THR:HG22 | 1.91 | 0.70 |
| 44:DS:33:LYS:HB3 | 44:DS:34:HIS:HD2 | 1.55 | 0.70 |
| 48:DW:2:GLU:HA | 48:DW:64:MET:HE1 | 1.71 | 0.70 |
| 1:AA:1337:G:H5'' | 1:AA:1338:G:OP1 | 1.91 | 0.70 |
| 1:AA:194:C:C2' | 1:AA:195:A:H5'' | 2.20 | 0.70 |
| 27:B5:57:VAL:O | 27:B5:58:LEU:HG | 1.91 | 0.70 |
| 30:B8:32:LEU:HB2 | 30:B8:35:GLN:N | 2.06 | 0.70 |
| 31:BA:1332:G:N2 | 31:BA:1610:A:C8 | 2.60 | 0.70 |
| 31:BA:1348:G:H2' | 31:BA:1349:A:H5' | 1.73 | 0.70 |
| 31:BA:2036:C:H5' | 31:BA:2036:C:C6 | 2.26 | 0.70 |
| 31:BA:308:G:O2' | 50:BY:19:LYS:HE3 | 1.92 | 0.70 |
| 31:BA:598:G:H5' | 41:BP:15:ARG:HD2 | 1.72 | 0.70 |
| 33:BD:35:LYS:CD | 33:BD:63:ARG:HB3 | 2.20 | 0.70 |
| 34:BE:4:ILE:HD13 | 34:BE:91:VAL:HG12 | 1.73 | 0.70 |
| 39:BN:42:TRP:CA | 39:BN:48:MET:HE1 | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:BA:806:C:OP2 | 41:BP:39:LYS:CD | 2.40 | 0.70 |
| 45:BT:38:ASN:HD22 | 45:BT:40:THR:H | 1.38 | 0.70 |
| 1:CA:66:G:H4' | 1:CA:173:U:C5 | 2.26 | 0.70 |
| 31:DA:819:A:C4 | 31:DA:1189:A:C2 | 2.80 | 0.70 |
| 31:DA:1406:U:H2' | 31:DA:1407:C:C6 | 2.27 | 0.70 |
| 31:DA:2335:A:O2' | 31:DA:2336:A:H5'' | 1.91 | 0.70 |
| 35:DF:46:ARG:HG2 | 35:DF:46:ARG:NH1 | 2.00 | 0.70 |
| 44:DS:36:TYR:N | 44:DS:36:TYR:CD1 | 2.55 | 0.70 |
| 45:DT:23:ARG:O | 45:DT:25:GLY:N | 2.24 | 0.70 |
| 46:DU:88:ILE:C | 46:DU:90:VAL:N | 2.41 | 0.70 |
| 47:DV:72:VAL:HG12 | 47:DV:73:SER:N | 2.05 | 0.70 |
| 1:AA:102:G:C5 | 1:AA:103:C:C5 | 2.80 | 0.70 |
| 1:AA:475:G:H2' | 1:AA:476:G:H8 | 1.55 | 0.70 |
| 1:AA:80:G:H1 | 1:AA:89:C:H41 | 1.39 | 0.70 |
| 1:AA:1117:G:H4' | 9:AI:104:ARG:NH2 | 2.04 | 0.70 |
| 18:AR:25:THR:HG22 | 18:AR:42:ARG:HH11 | 1.56 | 0.70 |
| 24:B2:41:ILE:HG22 | 24:B2:42:GLY:N | 2.06 | 0.70 |
| 35:BF:89:VAL:HG12 | 35:BF:90:PHE:N | 2.06 | 0.70 |
| 39:BN:3:THR:HA | 39:BN:4:TYR:CD1 | 2.26 | 0.70 |
| 42:BQ:8:LYS:CG | 42:BQ:9:TYR:N | 2.55 | 0.70 |
| 3:CC:157:ILE:HD11 | 3:CC:166:GLU:HB2 | 1.73 | 0.70 |
| 31:DA:2661:G:O2' | 31:DA:2662:A:OP1 | 2.09 | 0.70 |
| 37:DH:43:VAL:HG23 | 37:DH:43:VAL:O | 1.90 | 0.70 |
| 49:DX:34:ALA:O | 49:DX:36:LYS:HG3 | 1.90 | 0.70 |
| 1:AA:1423:G:C5' | 40:BO:49:ARG:NH2 | 2.54 | 0.70 |
| 1:AA:1152:A:H5'' | 10:AJ:13:HIS:CD2 | 2.27 | 0.70 |
| 31:BA:542:C:H2' | 31:BA:543:C:OP1 | 1.92 | 0.70 |
| 31:BA:825:C:H2' | 31:BA:826:U:O5' | 1.92 | 0.70 |
| 31:BA:662:G:OP1 | 41:BP:18:ARG:HD2 | 1.91 | 0.70 |
| 42:BQ:78:PRO:O | 42:BQ:79:LEU:HG | 1.91 | 0.70 |
| 47:BV:2:PHE:HB2 | 47:BV:42:GLY:CA | 2.22 | 0.70 |
| 47:BV:25:LEU:HB2 | 47:BV:94:LEU:HD13 | 1.73 | 0.70 |
| 1:CA:376:G:OP2 | 16:CP:67:THR:HG21 | 1.92 | 0.70 |
| 4:CD:119:GLN:HG3 | 4:CD:123:HIS:CD2 | 2.26 | 0.70 |
| 13:CM:66:LEU:HD12 | 13:CM:66:LEU:H | 1.56 | 0.70 |
| 31:DA:542:C:N4 | 31:DA:543:C:H41 | 1.89 | 0.70 |
| 33:DD:58:HIS:HD2 | 33:DD:59:LYS:O | 1.74 | 0.70 |
| 33:DD:35:LYS:HE3 | 33:DD:65:ILE:N | 2.06 | 0.70 |
| 45:DT:28:VAL:O | 45:DT:28:VAL:HG12 | 1.91 | 0.70 |
| 1:AA:509:A:H2' | 1:AA:510:A:C8 | 2.26 | 0.70 |
| 2:AB:101:MET:HA | 2:AB:108:ILE:HG13 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 18:AR:43:PHE:C | 18:AR:44:LEU:HD12 | 2.12 | 0.70 |
| 31:BA:1678:G:H21 | 31:BA:1989:G:H22 | 1.38 | 0.70 |
| 31:BA:2317:C:C3' | 31:BA:2318:G:H5' | 2.21 | 0.70 |
| 33:BD:27:THR:O | 33:BD:29:PRO:HD2 | 1.91 | 0.70 |
| 33:BD:35:LYS:HD3 | 33:BD:63:ARG:CB | 2.22 | 0.70 |
| 39:BN:89:LYS:O | 39:BN:93:THR:HG22 | 1.92 | 0.70 |
| 48:BW:2:GLU:HA | 48:BW:64:MET:HE1 | 1.74 | 0.70 |
| 49:BX:53:LYS:HE3 | 49:BX:55:ASN:HD21 | 1.56 | 0.70 |
| 1:CA:853:G:H2' | 1:CA:854:G:H8 | 1.56 | 0.70 |
| 1:CA:939:G:H5'' | 7:CG:102:ARG:HH12 | 1.57 | 0.70 |
| 6:CF:62:TRP:CH2 | 6:CF:64:GLN:HB2 | 2.26 | 0.70 |
| 1:CA:877:C:H5'' | 8:CH:88:LYS:HD3 | 1.72 | 0.70 |
| 31:DA:1171:G:C8 | 31:DA:1173:G:H1' | 2.27 | 0.70 |
| 31:DA:2307:G:H21 | 31:DA:2308:G:H5' | 1.52 | 0.70 |
| 32:DB:37:C:C5 | 32:DB:38:C:C4 | 2.80 | 0.70 |
| 37:DH:90:LYS:HB2 | 37:DH:159:GLU:O | 1.91 | 0.70 |
| 40:DO:2:ILE:HD12 | 40:DO:6:THR:HG21 | 1.72 | 0.70 |
| 43:DR:87:TYR:O | 43:DR:89:ASP:N | 2.23 | 0.70 |
| 46:DU:83:LEU:CG | 46:DU:88:ILE:HG12 | 2.18 | 0.70 |
| 47:DV:70:ILE:HB | 47:DV:90:PRO:HB2 | 1.73 | 0.70 |
| 47:DV:24:LYS:HB2 | 47:DV:92:THR:OG1 | 1.91 | 0.70 |
| 8:AH:120:THR:H | 8:AH:123:GLU:HB2 | 1.55 | 0.70 |
| 27:B5:46:CYS:SG | 27:B5:47:PRO:CD | 2.80 | 0.70 |
| 31:BA:1171:G:C8 | 31:BA:1173:G:H1' | 2.27 | 0.70 |
| 31:BA:1188:U:C2' | 31:BA:1189:A:H5' | 2.22 | 0.70 |
| 31:BA:1509(A):A:H2' | 31:BA:1509(B):A:H8 | 1.55 | 0.70 |
| 31:BA:1719:G:C2' | 31:BA:1720:U:H5' | 2.21 | 0.70 |
| 27:B5:2:ALA:CA | 31:BA:2015:A:H1' | 2.18 | 0.70 |
| 33:BD:31:LYS:HG2 | 33:BD:34:VAL:HG13 | 1.72 | 0.70 |
| 41:BP:120:ALA:CB | 41:BP:138:LEU:HB3 | 2.21 | 0.70 |
| 49:BX:70:LEU:HG | 49:BX:71:GLY:H | 1.56 | 0.70 |
| 1:CA:827:U:H2' | 1:CA:859:A:H61 | 1.55 | 0.70 |
| 9:CI:103:THR:HG22 | 9:CI:105:ASP:H | 1.56 | 0.70 |
| 9:CI:124:GLN:O | 9:CI:125:TYR:HB2 | 1.90 | 0.70 |
| 39:DN:19:GLU:HG3 | 39:DN:20:GLY:N | 2.05 | 0.70 |
| 1:AA:955:U:H1' | 1:AA:1227:A:N6 | 2.06 | 0.70 |
| 7:AG:15:ASP:HB3 | 7:AG:19:GLY:H | 1.56 | 0.70 |
| 31:BA:286:C:N4 | 31:BA:355:G:H1 | 1.89 | 0.70 |
| 30:B8:58:ILE:HG22 | 41:BP:49:ARG:HD2 | 1.72 | 0.70 |
| 49:BX:34:ALA:O | 49:BX:36:LYS:HG3 | 1.91 | 0.70 |
| 1:CA:828:A:H2' | 1:CA:829:G:O4' | 1.92 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:CG:15:ASP:HB3 | 7:CG:19:GLY:H | 1.55 | 0.70 |
| 25:D3:11:SER:OG | 25:D3:13:ILE:HG12 | 1.92 | 0.70 |
| 25:D3:43:ILE:O | 25:D3:47:VAL:HG23 | 1.91 | 0.70 |
| 31:DA:1947:C:H2' | 31:DA:1948:G:H5' | 1.74 | 0.70 |
| 31:DA:542:C:H2' | 31:DA:543:C:OP1 | 1.91 | 0.70 |
| 50:DY:2:ARG:O | 50:DY:4:LYS:N | 2.25 | 0.70 |
| 1:AA:632:A:C8 | 1:AA:633:G:C8 | 2.80 | 0.70 |
| 20:AT:71:THR:HG22 | 20:AT:72:LEU:N | 2.07 | 0.70 |
| 22:B0:20:ARG:NH1 | 31:BA:2357:U:OP1 | 2.25 | 0.70 |
| 29:B7:9:ARG:NH1 | 31:BA:1310:G:OP2 | 2.19 | 0.70 |
| 30:B8:32:LEU:HD23 | 30:B8:35:GLN:CA | 2.20 | 0.70 |
| 31:BA:1722:A:C6 | 31:BA:1741:A:N1 | 2.59 | 0.70 |
| 31:BA:34:C:C2' | 31:BA:35:G:OP1 | 2.40 | 0.70 |
| 31:BA:588:U:H2' | 31:BA:589:C:C6 | 2.26 | 0.70 |
| 43:BR:11:ASN:CG | 43:BR:12:ARG:H | 1.94 | 0.70 |
| 39:BN:40:PRO:HB3 | 46:BU:68:ALA:HB2 | 1.73 | 0.70 |
| 49:BX:60:ARG:HG2 | 49:BX:71:GLY:HA3 | 1.72 | 0.70 |
| 50:BY:96:ILE:HG21 | 50:BY:99:CYS:CB | 2.21 | 0.70 |
| 1:CA:1239:A:H62 | 1:CA:1299:A:H62 | 1.40 | 0.70 |
| 31:DA:639:U:H2' | 31:DA:640:C:C6 | 2.26 | 0.70 |
| 32:DB:87:G:C3' | 32:DB:88:C:H5'' | 2.20 | 0.70 |
| 46:DU:92:ARG:HD2 | 47:DV:11:GLN:HG3 | 1.74 | 0.70 |
| 1:AA:1409:C:H42 | 1:AA:1491:G:H1 | 1.39 | 0.69 |
| 1:AA:735:C:H2' | 1:AA:736:C:C6 | 2.27 | 0.69 |
| 6:AF:62:TRP:CH2 | 6:AF:64:GLN:HB2 | 2.26 | 0.69 |
| 24:B2:30:ARG:H | 24:B2:30:ARG:HD2 | 1.55 | 0.69 |
| 28:B6:27:LYS:HE3 | 31:BA:2285:C:C5 | 2.26 | 0.69 |
| 42:BQ:81:VAL:C | 42:BQ:82:ARG:HD2 | 2.13 | 0.69 |
| 1:CA:559:A:H5'' | 1:CA:560:U:H3' | 1.73 | 0.69 |
| 1:CA:632:A:C8 | 1:CA:633:G:C8 | 2.80 | 0.69 |
| 1:CA:650:G:O2' | 1:CA:651:C:H5' | 1.92 | 0.69 |
| 1:CA:878:G:H5' | 8:CH:89:PRO:HG2 | 1.74 | 0.69 |
| 2:CB:187:LEU:HA | 2:CB:201:ILE:HB | 1.73 | 0.69 |
| 16:CP:20:VAL:HG21 | 16:CP:32:TYR:CG | 2.27 | 0.69 |
| 22:D0:43:THR:HG22 | 31:DA:2331:G:O2' | 1.92 | 0.69 |
| 25:D3:6:VAL:HG13 | 25:D3:54:VAL:HG11 | 1.72 | 0.69 |
| 30:D8:32:LEU:HB2 | 30:D8:35:GLN:N | 2.06 | 0.69 |
| 31:DA:1720:U:H2' | 31:DA:1721:G:O4' | 1.92 | 0.69 |
| 31:DA:1973:G:H2' | 31:DA:1974:C:C6 | 2.27 | 0.69 |
| 31:DA:2199:A:H3' | 31:DA:2200:C:C6 | 2.26 | 0.69 |
| 35:DF:160:ASN:HD22 | 35:DF:162:LEU:H | 1.40 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:DY:28:LYS:CB | 50:DY:37:VAL:HB | 2.15 | 0.69 |
| 3:AC:157:ILE:HD11 | 3:AC:166:GLU:HB2 | 1.74 | 0.69 |
| 9:AI:53:VAL:HG12 | 9:AI:95:LYS:HG2 | 1.73 | 0.69 |
| 39:BN:95:PRO:O | 39:BN:97:ARG:N | 2.23 | 0.69 |
| 42:BQ:16:ARG:HH11 | 42:BQ:16:ARG:HB2 | 1.57 | 0.69 |
| 46:BU:74:LEU:HD12 | 46:BU:74:LEU:N | 2.07 | 0.69 |
| 1:CA:437:U:H5'' | 4:CD:155:LEU:HD13 | 1.73 | 0.69 |
| 4:CD:57:ARG:HH22 | 5:CE:107:ARG:HD3 | 1.57 | 0.69 |
| 22:D0:2:ALA:H | 31:DA:2602:A:N6 | 1.89 | 0.69 |
| 27:D5:57:VAL:HG23 | 27:D5:58:LEU:N | 2.06 | 0.69 |
| 31:DA:1291:C:H2' | 31:DA:1292:U:H6 | 1.57 | 0.69 |
| 31:DA:1688:U:H1' | 31:DA:1701:A:C6 | 2.26 | 0.69 |
| 31:DA:2208:A:H1' | 31:DA:2219:G:C4 | 2.27 | 0.69 |
| 31:DA:2317:C:C3' | 31:DA:2318:G:H5' | 2.22 | 0.69 |
| 34:DE:76:ARG:HG3 | 34:DE:195:LEU:HD22 | 1.74 | 0.69 |
| 34:DE:8:LYS:HD2 | 34:DE:188:VAL:HG13 | 1.74 | 0.69 |
| 39:DN:15:LEU:HD21 | 39:DN:55:VAL:HG22 | 1.73 | 0.69 |
| 39:DN:68:GLU:HA | 39:DN:86:PRO:HB3 | 1.72 | 0.69 |
| 47:DV:52:VAL:O | 47:DV:53:GLU:HB3 | 1.92 | 0.69 |
| 31:DA:1162:G:H1' | 47:DV:91:TYR:OH | 1.92 | 0.69 |
| 49:DX:60:ARG:HE | 49:DX:74:PRO:CG | 2.05 | 0.69 |
| 49:DX:77:LYS:CG | 49:DX:78:LYS:HG3 | 2.22 | 0.69 |
| 1:AA:428:G:H4' | 1:AA:429:U:O5' | 1.92 | 0.69 |
| 4:AD:189:PRO:HB3 | 4:AD:194:LEU:HD21 | 1.73 | 0.69 |
| 15:AO:33:THR:HG21 | 15:AO:85:LEU:HD22 | 1.75 | 0.69 |
| 25:B3:54:VAL:HG12 | 25:B3:55:ARG:N | 2.07 | 0.69 |
| 33:BD:260:ARG:HH22 | 33:BD:266:SER:HB2 | 1.56 | 0.69 |
| 35:BF:160:ASN:HD22 | 35:BF:160:ASN:C | 1.95 | 0.69 |
| 41:BP:17:LYS:HG3 | 41:BP:19:VAL:HG23 | 1.73 | 0.69 |
| 45:BT:29:ARG:HB3 | 45:BT:85:LYS:HA | 1.73 | 0.69 |
| 47:BV:69:LYS:CG | 47:BV:70:ILE:H | 2.04 | 0.69 |
| 1:CA:659:U:C2' | 1:CA:660:G:H5' | 2.22 | 0.69 |
| 2:CB:204:ASN:ND2 | 2:CB:206:ASP:H | 1.90 | 0.69 |
| 23:D1:64:ALA:HA | 23:D1:67:ILE:HG13 | 1.74 | 0.69 |
| 35:DF:63:LYS:CE | 35:DF:67:GLN:HB2 | 2.22 | 0.69 |
| 38:DI:82:ARG:O | 38:DI:89:TYR:HB2 | 1.92 | 0.69 |
| 46:DU:69:CYS:HB3 | 46:DU:106:PHE:CZ | 2.28 | 0.69 |
| 2:AB:187:LEU:HA | 2:AB:201:ILE:HB | 1.75 | 0.69 |
| 2:AB:204:ASN:ND2 | 2:AB:206:ASP:H | 1.90 | 0.69 |
| 12:AL:27:LEU:O | 12:AL:29:GLY:N | 2.26 | 0.69 |
| 13:AM:66:LEU:HD12 | 13:AM:66:LEU:H | 1.58 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:B0:43:THR:H | 31:BA:2331:G:H4' | 1.57 | 0.69 |
| 31:BA:184:C:H2' | 31:BA:185:U:C6 | 2.26 | 0.69 |
| 31:BA:2310:A:O2' | 31:BA:2311:A:H5'' | 1.93 | 0.69 |
| 33:BD:130:ALA:C | 33:BD:131:LEU:HD12 | 2.12 | 0.69 |
| 45:BT:31:SER:C | 45:BT:32:TYR:CD2 | 2.64 | 0.69 |
| 1:CA:922:G:H4' | 5:CE:20:GLN:HA | 1.74 | 0.69 |
| 23:D1:9:GLY:O | 23:D1:10:LYS:HB3 | 1.93 | 0.69 |
| 30:D8:58:ILE:HG22 | 41:DP:49:ARG:HD2 | 1.72 | 0.69 |
| 31:DA:1790:C:H5'' | 31:DA:1791:A:OP1 | 1.92 | 0.69 |
| 39:DN:77:GLY:O | 39:DN:78:TYR:HB3 | 1.91 | 0.69 |
| 39:DN:95:PRO:O | 39:DN:97:ARG:N | 2.26 | 0.69 |
| 42:DQ:30:GLY:HA2 | 42:DQ:107:ALA:HB2 | 1.73 | 0.69 |
| 1:AA:192:U:H2' | 1:AA:193:C:H6 | 1.56 | 0.69 |
| 1:AA:328:C:O2 | 1:AA:328:C:H2' | 1.91 | 0.69 |
| 23:B1:41:ARG:CG | 23:B1:41:ARG:HH11 | 1.86 | 0.69 |
| 31:BA:2701:C:H3' | 31:BA:2702:U:H5'' | 1.73 | 0.69 |
| 33:BD:255:LYS:H | 33:BD:255:LYS:NZ | 1.90 | 0.69 |
| 33:BD:25:THR:HG21 | 33:BD:81:ALA:CB | 2.18 | 0.69 |
| 33:BD:25:THR:HG23 | 33:BD:25:THR:O | 1.92 | 0.69 |
| 40:BO:104:ARG:CZ | 45:BT:33:LYS:HD2 | 2.22 | 0.69 |
| 44:BS:28:VAL:HB | 44:BS:89:ARG:HB2 | 1.74 | 0.69 |
| 47:BV:64:HIS:CD2 | 47:BV:64:HIS:O | 2.46 | 0.69 |
| 49:BX:77:LYS:CG | 49:BX:78:LYS:HG3 | 2.18 | 0.69 |
| 50:BY:35:TYR:CE2 | 50:BY:69:ALA:HB3 | 2.27 | 0.69 |
| 1:CA:509:A:H2' | 1:CA:510:A:C8 | 2.27 | 0.69 |
| 1:CA:545:C:O2' | 1:CA:546:G:H5' | 1.93 | 0.69 |
| 3:CC:14:ILE:HG12 | 3:CC:15:THR:H | 1.58 | 0.69 |
| 13:CM:15:VAL:O | 13:CM:19:LEU:HD23 | 1.92 | 0.69 |
| 31:DA:1722:A:C6 | 31:DA:1741:A:N1 | 2.60 | 0.69 |
| 31:DA:2652:C:C2' | 31:DA:2653:U:H5' | 2.22 | 0.69 |
| 31:DA:484:C:H2' | 31:DA:485:C:C6 | 2.26 | 0.69 |
| 33:DD:137:PRO:O | 33:DD:140:THR:HG23 | 1.93 | 0.69 |
| 33:DD:228:PRO:HD3 | 33:DD:235:GLY:CA | 2.22 | 0.69 |
| 1:AA:616:G:C2 | 1:AA:617:G:C8 | 2.81 | 0.69 |
| 2:AB:233:SER:HB2 | 2:AB:234:PRO:HD2 | 1.74 | 0.69 |
| 1:AA:437:U:H5'' | 4:AD:155:LEU:HD13 | 1.73 | 0.69 |
| 24:B2:54:LYS:N | 24:B2:56:GLN:NE2 | 2.39 | 0.69 |
| 27:B5:16:ARG:NH1 | 27:B5:17:ASP:OD1 | 2.25 | 0.69 |
| 28:B6:15:GLU:OE1 | 28:B6:43:CYS:SG | 2.51 | 0.69 |
| 31:BA:1022:G:H22 | 31:BA:1142(A):A:H2 | 1.35 | 0.69 |
| 31:BA:1162:G:H1' | 47:BV:91:TYR:OH | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:2859:G:C8 | 31:BA:2859:G:H3' | 2.28 | 0.69 |
| 31:BA:71:A:H5' | 31:BA:71:A:H8 | 1.56 | 0.69 |
| 1:CA:382:A:H2' | 1:CA:383:A:C8 | 2.26 | 0.69 |
| 31:DA:1116:C:C2' | 31:DA:1117:G:H5' | 2.21 | 0.69 |
| 31:DA:1652:A:C2' | 31:DA:1653:G:H5' | 2.21 | 0.69 |
| 31:DA:2106:G:H1' | 31:DA:2184:G:N2 | 2.08 | 0.69 |
| 32:DB:87:G:OP2 | 32:DB:87:G:H8 | 1.74 | 0.69 |
| 34:DE:92:THR:H | 34:DE:95:ILE:HD11 | 1.58 | 0.69 |
| 41:DP:17:LYS:C | 41:DP:19:VAL:H | 1.95 | 0.69 |
| 45:DT:29:ARG:HB3 | 45:DT:85:LYS:HA | 1.74 | 0.69 |
| 20:AT:37:SER:O | 20:AT:41:ILE:HG12 | 1.93 | 0.69 |
| 31:BA:1794:U:H2' | 31:BA:1795:C:C6 | 2.28 | 0.69 |
| 31:BA:2208:A:H1' | 31:BA:2219:G:C4 | 2.27 | 0.69 |
| 33:BD:17:THR:CG2 | 33:BD:205:VAL:H | 1.86 | 0.69 |
| 38:BI:9:LEU:H | 38:BI:13:GLY:HA2 | 1.56 | 0.69 |
| 39:BN:66:LYS:HA | 39:BN:69:GLN:HB2 | 1.75 | 0.69 |
| 30:B8:27:THR:HA | 41:BP:62:LEU:HD11 | 1.75 | 0.69 |
| 45:BT:106:SER:O | 45:BT:107:ASP:OD1 | 2.11 | 0.69 |
| 1:CA:1154:G:H2' | 1:CA:1155:G:H8 | 1.58 | 0.69 |
| 31:DA:1047:G:N2 | 31:DA:1111:A:H62 | 1.91 | 0.69 |
| 31:DA:916:G:C2' | 31:DA:917:A:H5'' | 2.23 | 0.69 |
| 32:DB:87:G:OP2 | 32:DB:87:G:C8 | 2.45 | 0.69 |
| 34:DE:9:VAL:HG13 | 34:DE:25:VAL:O | 1.93 | 0.69 |
| 34:DE:93:VAL:H | 34:DE:95:ILE:CD1 | 2.06 | 0.69 |
| 39:DN:42:TRP:CA | 39:DN:48:MET:HE1 | 2.23 | 0.69 |
| 45:DT:24:PRO:HA | 45:DT:49:VAL:HG13 | 1.74 | 0.69 |
| 47:DV:5:VAL:CG2 | 47:DV:36:PRO:HB2 | 2.22 | 0.69 |
| 51:DZ:39:VAL:HG21 | 51:DZ:44:PHE:HB2 | 1.75 | 0.69 |
| 1:AA:224:C:H2' | 1:AA:225:C:H6 | 1.56 | 0.69 |
| 3:AC:150:LYS:HB3 | 3:AC:201:TYR:HB2 | 1.73 | 0.69 |
| 23:B1:26:ARG:HB2 | 23:B1:34:THR:HA | 1.75 | 0.69 |
| 31:BA:747:U:O2 | 31:BA:2014:A:H1' | 1.91 | 0.69 |
| 33:BD:35:LYS:HA | 33:BD:64:ILE:HG22 | 1.74 | 0.69 |
| 37:BH:141:VAL:HG12 | 37:BH:142:GLY:N | 2.07 | 0.69 |
| 37:BH:32:GLU:O | 37:BH:33:LEU:HD23 | 1.92 | 0.69 |
| 39:BN:18:ALA:HB3 | 39:BN:26:LEU:CD2 | 2.20 | 0.69 |
| 44:BS:28:VAL:O | 44:BS:89:ARG:HD2 | 1.92 | 0.69 |
| 42:BQ:141:GLN:HG3 | 51:BZ:72:ARG:HH11 | 1.58 | 0.69 |
| 1:CA:1422:G:O2' | 1:CA:1423:G:H5' | 1.92 | 0.69 |
| 1:CA:616:G:C2 | 1:CA:617:G:C8 | 2.80 | 0.69 |
| 1:CA:662:G:H2' | 1:CA:663:A:H8 | 1.58 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:18:ARG:HH21 | 5:CE:25:ARG:HG2 | 1.57 | 0.69 |
| 31:DA:1157:G:C6 | 31:DA:1158:C:N4 | 2.60 | 0.69 |
| 31:DA:1169:G:H1 | 31:DA:1180:C:N4 | 1.89 | 0.69 |
| 44:DS:28:VAL:HB | 44:DS:89:ARG:HB2 | 1.75 | 0.69 |
| 1:AA:659:U:C2' | 1:AA:660:G:H5' | 2.22 | 0.69 |
| 1:AA:1057:G:H5'' | 3:AC:154:SER:HB2 | 1.75 | 0.69 |
| 12:AL:91:LYS:O | 12:AL:91:LYS:HG3 | 1.91 | 0.69 |
| 1:CA:417:C:O2' | 1:CA:418:C:H5' | 1.92 | 0.69 |
| 2:CB:17:PHE:CD1 | 2:CB:44:LEU:HD11 | 2.28 | 0.69 |
| 5:CE:55:VAL:O | 5:CE:58:ALA:HB3 | 1.93 | 0.69 |
| 1:CA:192:U:O4' | 20:CT:103:GLY:HA2 | 1.92 | 0.69 |
| 31:DA:107:C:H2' | 31:DA:108:U:H6 | 1.57 | 0.69 |
| 31:DA:2023:G:H5' | 31:DA:2617:C:H4' | 1.75 | 0.69 |
| 36:DG:64:THR:HG23 | 36:DG:66:GLN:H | 1.57 | 0.69 |
| 36:DG:7:LEU:HB2 | 36:DG:104:GLU:OE2 | 1.93 | 0.69 |
| 42:DQ:141:GLN:HG3 | 51:DZ:72:ARG:HH11 | 1.58 | 0.69 |
| 47:DV:19:LYS:CE | 47:DV:20:LEU:H | 2.06 | 0.69 |
| 49:DX:35:THR:O | 49:DX:36:LYS:O | 2.11 | 0.69 |
| 1:AA:321:A:H62 | 1:AA:328:C:H1' | 1.56 | 0.69 |
| 31:BA:1339:G:N2 | 31:BA:1603:A:H1' | 2.08 | 0.69 |
| 35:BF:22:ALA:HB1 | 35:BF:26:ALA:CB | 2.23 | 0.69 |
| 40:BO:18:LYS:HB2 | 40:BO:45:GLU:HG2 | 1.75 | 0.69 |
| 43:BR:53:HIS:HD2 | 43:BR:94:TYR:OH | 1.76 | 0.69 |
| 44:BS:36:TYR:N | 44:BS:36:TYR:CD1 | 2.55 | 0.69 |
| 44:BS:89:ARG:HA | 44:BS:89:ARG:NE | 2.08 | 0.69 |
| 31:BA:2849:U:O4 | 45:BT:23:ARG:NH2 | 2.26 | 0.69 |
| 42:BQ:141:GLN:HE21 | 51:BZ:72:ARG:N | 1.91 | 0.69 |
| 1:CA:600:C:H2' | 1:CA:601:C:H6 | 1.58 | 0.69 |
| 28:D6:12:GLU:HA | 28:D6:23:THR:HA | 1.75 | 0.69 |
| 31:DA:1719:G:C2' | 31:DA:1720:U:H5' | 2.22 | 0.69 |
| 31:DA:588:U:C6 | 31:DA:588:U:OP2 | 2.44 | 0.69 |
| 35:DF:110:LEU:HD21 | 35:DF:181:LEU:HD23 | 1.75 | 0.69 |
| 40:DO:2:ILE:HG13 | 40:DO:8:LEU:HD11 | 1.75 | 0.69 |
| 48:DW:86:LEU:HD12 | 48:DW:87:PRO:CD | 2.23 | 0.69 |
| 50:DY:35:TYR:CE2 | 50:DY:69:ALA:HB3 | 2.27 | 0.69 |
| 1:AA:1154:G:H2' | 1:AA:1155:G:H8 | 1.58 | 0.69 |
| 1:AA:673:G:H2' | 1:AA:674:G:C8 | 2.27 | 0.69 |
| 5:AE:110:LEU:O | 5:AE:115:VAL:HG23 | 1.92 | 0.69 |
| 31:BA:1429:G:H2' | 31:BA:1430:C:C6 | 2.28 | 0.69 |
| 31:BA:1472:A:C2' | 31:BA:1473:G:H5' | 2.23 | 0.69 |
| 31:BA:1688:U:H1' | 31:BA:1701:A:C6 | 2.28 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:896:A:C2 | 31:BA:898:C:H5'' | 2.28 | 0.69 |
| 32:BB:75:G:H5' | 32:BB:75:G:H8 | 1.58 | 0.69 |
| 32:BB:87:G:P | 32:BB:87:G:H8 | 2.16 | 0.69 |
| 33:BD:133:LEU:HA | 33:BD:136:ILE:HD13 | 1.73 | 0.69 |
| 34:BE:47:VAL:HG22 | 34:BE:84:PHE:O | 1.92 | 0.69 |
| 49:BX:60:ARG:HE | 49:BX:74:PRO:CG | 2.05 | 0.69 |
| 27:D5:2:ALA:CA | 31:DA:2015:A:H1' | 2.20 | 0.69 |
| 34:DE:4:ILE:HD13 | 34:DE:91:VAL:HG12 | 1.74 | 0.69 |
| 35:DF:160:ASN:ND2 | 35:DF:162:LEU:H | 1.90 | 0.69 |
| 38:DI:61:ARG:O | 38:DI:133:HIS:HE1 | 1.76 | 0.69 |
| 31:DA:661:C:H4' | 41:DP:16:ARG:HH12 | 1.57 | 0.69 |
| 2:AB:17:PHE:CD1 | 2:AB:44:LEU:HD11 | 2.28 | 0.68 |
| 22:B0:2:ALA:H | 31:BA:2602:A:N6 | 1.91 | 0.68 |
| 27:B5:50:GLY:O | 27:B5:51:TYR:HD1 | 1.76 | 0.68 |
| 35:BF:160:ASN:ND2 | 35:BF:162:LEU:H | 1.91 | 0.68 |
| 44:BS:95:HIS:ND1 | 44:BS:96:GLY:N | 2.41 | 0.68 |
| 50:BY:38:ILE:HG22 | 50:BY:39:VAL:N | 2.07 | 0.68 |
| 1:CA:736:C:H2' | 1:CA:737:A:C8 | 2.28 | 0.68 |
| 24:D2:41:ILE:HG22 | 24:D2:42:GLY:N | 2.07 | 0.68 |
| 24:D2:54:LYS:H | 24:D2:56:GLN:NE2 | 1.90 | 0.68 |
| 31:DA:1592:C:H2' | 31:DA:1593:G:C5' | 2.21 | 0.68 |
| 31:DA:2190:G:H2' | 31:DA:2191:G:H5' | 1.74 | 0.68 |
| 47:DV:47:VAL:HG13 | 47:DV:48:GLY:N | 2.07 | 0.68 |
| 27:D5:25:LEU:HD12 | 48:DW:19:LEU:O | 1.93 | 0.68 |
| 3:AC:105:GLU:HG2 | 3:AC:106:VAL:H | 1.56 | 0.68 |
| 24:B2:14:ARG:NH1 | 24:B2:57:ILE:HG22 | 2.08 | 0.68 |
| 31:BA:1116:C:C2' | 31:BA:1117:G:H5' | 2.22 | 0.68 |
| 31:BA:2464:C:O2' | 31:BA:2465:C:O5' | 2.10 | 0.68 |
| 31:BA:2610:C:H4' | 31:BA:2611:U:OP2 | 1.94 | 0.68 |
| 31:BA:288:C:H42 | 31:BA:353:G:H1 | 1.40 | 0.68 |
| 45:BT:54:ARG:HA | 45:BT:59:THR:HB | 1.74 | 0.68 |
| 1:CA:1097:C:H1' | 1:CA:1170:A:H1' | 1.75 | 0.68 |
| 1:CA:1337:G:H5'' | 1:CA:1338:G:OP1 | 1.94 | 0.68 |
| 3:CC:125:GLU:HA | 3:CC:191:THR:HG22 | 1.75 | 0.68 |
| 4:CD:138:TYR:C | 4:CD:138:TYR:HD2 | 1.96 | 0.68 |
| 11:CK:13:GLN:HB3 | 11:CK:75:TYR:O | 1.94 | 0.68 |
| 27:D5:16:ARG:NH1 | 27:D5:16:ARG:HG2 | 1.95 | 0.68 |
| 31:DA:896:A:C2 | 31:DA:898:C:H5'' | 2.28 | 0.68 |
| 33:DD:35:LYS:HD3 | 33:DD:63:ARG:CA | 2.23 | 0.68 |
| 34:DE:93:VAL:H | 34:DE:95:ILE:HD13 | 1.58 | 0.68 |
| 39:DN:65:LYS:HA | 39:DN:65:LYS:CE | 2.11 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 42:DQ:140:ALA:HB1 | 51:DZ:99:TYR:HB2 | 1.75 | 0.68 |
| 51:DZ:61:LEU:HB2 | 51:DZ:65:GLN:HB2 | 1.75 | 0.68 |
| 1:AA:1158:C:O2' | 2:AB:132:LYS:HD3 | 1.94 | 0.68 |
| 1:AA:1242:C:P | 21:AU:10:ARG:HH22 | 2.16 | 0.68 |
| 1:AA:266:G:H5'' | 1:AA:268:C:N4 | 2.08 | 0.68 |
| 31:BA:1658:C:OP1 | 34:BE:132:HIS:ND1 | 2.25 | 0.68 |
| 31:BA:1721:G:C2 | 31:BA:1739:U:OP2 | 2.46 | 0.68 |
| 31:BA:2652:C:C2' | 31:BA:2653:U:H5' | 2.23 | 0.68 |
| 31:BA:296:C:O2' | 31:BA:297:C:H5' | 1.93 | 0.68 |
| 31:BA:542:C:N4 | 31:BA:543:C:H41 | 1.91 | 0.68 |
| 40:BO:10:VAL:HG23 | 40:BO:10:VAL:O | 1.93 | 0.68 |
| 50:BY:8:LYS:NZ | 50:BY:74:PRO:HD3 | 2.08 | 0.68 |
| 1:CA:1184:G:H2' | 1:CA:1185:G:H8 | 1.58 | 0.68 |
| 1:CA:559:A:C5' | 1:CA:560:U:H3' | 2.24 | 0.68 |
| 1:CA:949:A:H1' | 1:CA:1364:U:N3 | 2.09 | 0.68 |
| 29:D7:43:THR:HG23 | 29:D7:44:PRO:HD2 | 1.75 | 0.68 |
| 30:D8:32:LEU:C | 30:D8:34:TRP:N | 2.43 | 0.68 |
| 30:D8:61:LEU:HB3 | 31:DA:593:G:H4' | 1.75 | 0.68 |
| 33:DD:255:LYS:NZ | 33:DD:255:LYS:H | 1.91 | 0.68 |
| 35:DF:160:ASN:HD21 | 35:DF:162:LEU:HB2 | 1.59 | 0.68 |
| 39:DN:128:HIS:CD2 | 39:DN:131:GLN:HB2 | 2.28 | 0.68 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:H62 | 1.41 | 0.68 |
| 1:AA:176:C:H2' | 1:AA:177:C:C6 | 2.28 | 0.68 |
| 1:AA:192:U:C4' | 20:AT:103:GLY:HA2 | 2.24 | 0.68 |
| 1:AA:22:G:H2' | 1:AA:23:C:C6 | 2.27 | 0.68 |
| 4:AD:68:TYR:CE2 | 4:AD:97:LEU:HB3 | 2.29 | 0.68 |
| 22:B0:71:ASP:C | 22:B0:72:ARG:HG2 | 2.12 | 0.68 |
| 23:B1:8:SER:N | 23:B1:46:LEU:HD13 | 2.08 | 0.68 |
| 27:B5:16:ARG:HG2 | 27:B5:16:ARG:NH1 | 1.98 | 0.68 |
| 27:B5:48:GLU:O | 27:B5:50:GLY:N | 2.26 | 0.68 |
| 31:BA:1109:C:H5 | 31:BA:1110:G:C5 | 2.11 | 0.68 |
| 31:BA:2801(A):A:O3' | 31:BA:2802:G:H3' | 1.92 | 0.68 |
| 31:BA:307:G:H22 | 31:BA:310:A:C5' | 2.06 | 0.68 |
| 31:BA:71:A:H5' | 31:BA:71:A:C8 | 2.29 | 0.68 |
| 22:B0:23:VAL:HG21 | 31:BA:857:C:H4' | 1.76 | 0.68 |
| 39:BN:58:ASP:O | 39:BN:60:ILE:N | 2.25 | 0.68 |
| 50:BY:96:ILE:HG22 | 50:BY:97:ARG:H | 1.57 | 0.68 |
| 51:BZ:11:GLU:H | 51:BZ:11:GLU:CD | 1.96 | 0.68 |
| 1:CA:1228:C:H2' | 1:CA:1229:A:H8 | 1.56 | 0.68 |
| 4:CD:128:VAL:CG1 | 4:CD:129:ASN:HD22 | 2.01 | 0.68 |
| 22:D0:23:VAL:HG21 | 31:DA:857:C:H4' | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:DA:2300:G:N2 | 31:DA:2317:C:C2 | 2.62 | 0.68 |
| 31:DA:310:A:P | 50:DY:18:GLY:HA2 | 2.34 | 0.68 |
| 31:DA:34:C:C2' | 31:DA:35:G:OP1 | 2.41 | 0.68 |
| 31:DA:607:U:N3 | 31:DA:621:A:C2 | 2.57 | 0.68 |
| 33:DD:35:LYS:HD2 | 33:DD:104:TYR:CE1 | 2.27 | 0.68 |
| 38:DI:56:LYS:HA | 38:DI:59:ALA:HB3 | 1.75 | 0.68 |
| 41:DP:85:LEU:HD23 | 41:DP:85:LEU:N | 2.01 | 0.68 |
| 45:DT:106:SER:O | 45:DT:107:ASP:OD1 | 2.10 | 0.68 |
| 49:DX:56:THR:C | 49:DX:57:LEU:HD12 | 2.14 | 0.68 |
| 1:AA:1128:C:H5' | 9:AI:16:ARG:HH12 | 1.59 | 0.68 |
| 35:BF:34:TRP:HB2 | 41:BP:10:PRO:O | 1.93 | 0.68 |
| 45:BT:12:SER:O | 45:BT:13:ARG:HG2 | 1.93 | 0.68 |
| 51:BZ:7:ALA:HB3 | 51:BZ:61:LEU:CD2 | 2.23 | 0.68 |
| 1:CA:1239:A:H62 | 1:CA:1299:A:N6 | 1.92 | 0.68 |
| 31:DA:1205:U:H4' | 31:DA:1206:G:OP2 | 1.94 | 0.68 |
| 31:DA:2469:A:H2 | 31:DA:2481:G:N2 | 1.88 | 0.68 |
| 31:DA:2787:C:C1' | 34:DE:61:ARG:HB2 | 2.20 | 0.68 |
| 1:AA:191:G:C4 | 20:AT:105:SER:HB3 | 2.29 | 0.68 |
| 3:AC:125:GLU:HA | 3:AC:191:THR:HG22 | 1.76 | 0.68 |
| 12:AL:82:VAL:HG12 | 12:AL:83:VAL:N | 2.08 | 0.68 |
| 31:BA:212:G:O2' | 31:BA:213:A:H5' | 1.92 | 0.68 |
| 37:BH:19:VAL:HG21 | 37:BH:44:VAL:HA | 1.76 | 0.68 |
| 37:BH:17:VAL:HG21 | 37:BH:50:VAL:HG21 | 1.75 | 0.68 |
| 41:BP:62:LEU:CD2 | 41:BP:62:LEU:H | 1.92 | 0.68 |
| 48:BW:4:LYS:HE3 | 48:BW:6:ILE:HD11 | 1.76 | 0.68 |
| 15:CO:33:THR:HG21 | 15:CO:85:LEU:HD22 | 1.74 | 0.68 |
| 18:CR:53:ARG:HH21 | 18:CR:60:ALA:N | 1.91 | 0.68 |
| 31:DA:1639:U:C2' | 31:DA:1640:C:H5'' | 2.23 | 0.68 |
| 31:DA:2068:U:N3 | 31:DA:2430:A:C2 | 2.51 | 0.68 |
| 31:DA:2801(A):A:O3' | 31:DA:2802:G:H3' | 1.93 | 0.68 |
| 31:DA:919:G:H5' | 32:DB:81:G:H1' | 1.75 | 0.68 |
| 33:DD:25:THR:HG21 | 33:DD:81:ALA:CB | 2.21 | 0.68 |
| 33:DD:30:GLU:HG3 | 33:DD:63:ARG:NE | 2.07 | 0.68 |
| 35:DF:24:LEU:HB3 | 35:DF:25:PRO:CD | 2.17 | 0.68 |
| 42:DQ:14:ARG:HG2 | 42:DQ:41:TRP:HH2 | 1.59 | 0.68 |
| 42:DQ:24:GLY:HA3 | 51:DZ:78:LYS:CB | 2.23 | 0.68 |
| 42:DQ:52:VAL:HA | 42:DQ:55:VAL:HG13 | 1.75 | 0.68 |
| 44:DS:89:ARG:HA | 44:DS:89:ARG:NE | 2.09 | 0.68 |
| 51:DZ:74:VAL:HG22 | 51:DZ:86:VAL:HG13 | 1.74 | 0.68 |
| 31:BA:2208:A:H1' | 31:BA:2219:G:C5 | 2.29 | 0.68 |
| 31:BA:272:G:H4' | 31:BA:272(B):G:OP1 | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BD:70:TRP:CH2 | 33:BD:150:LYS:HA | 2.29 | 0.68 |
| 34:BE:8:LYS:HD2 | 34:BE:188:VAL:HG13 | 1.75 | 0.68 |
| 34:BE:92:THR:H | 34:BE:95:ILE:HD11 | 1.58 | 0.68 |
| 35:BF:22:ALA:C | 35:BF:26:ALA:HB2 | 2.13 | 0.68 |
| 36:BG:7:LEU:HB2 | 36:BG:104:GLU:OE2 | 1.94 | 0.68 |
| 1:CA:102:G:C4 | 1:CA:103:C:C5 | 2.82 | 0.68 |
| 23:D1:9:GLY:O | 23:D1:10:LYS:HE2 | 1.92 | 0.68 |
| 24:D2:47:ASN:C | 24:D2:49:LYS:H | 1.97 | 0.68 |
| 24:D2:54:LYS:N | 24:D2:56:GLN:HE22 | 1.91 | 0.68 |
| 31:DA:1794:U:H2' | 31:DA:1795:C:C6 | 2.27 | 0.68 |
| 31:DA:2418:A:H2' | 31:DA:2419:U:H6 | 1.58 | 0.68 |
| 31:DA:719:C:H2' | 31:DA:720:C:C6 | 2.27 | 0.68 |
| 34:DE:52:LEU:O | 34:DE:74:PRO:HA | 1.93 | 0.68 |
| 31:DA:1006:C:H1' | 39:DN:106:MET:CE | 2.24 | 0.68 |
| 1:AA:425:G:C2' | 1:AA:426:G:H5' | 2.23 | 0.68 |
| 1:AA:828:A:H2' | 1:AA:829:G:O4' | 1.92 | 0.68 |
| 1:AA:914:A:O2' | 1:AA:915:A:H5' | 1.93 | 0.68 |
| 3:AC:14:ILE:HG12 | 3:AC:15:THR:H | 1.57 | 0.68 |
| 14:AN:25:VAL:HG23 | 14:AN:38:GLY:O | 1.94 | 0.68 |
| 18:AR:53:ARG:HH21 | 18:AR:60:ALA:N | 1.91 | 0.68 |
| 31:BA:1434:A:H61 | 31:BA:1558:A:N6 | 1.90 | 0.68 |
| 31:BA:1821:A:H2' | 31:BA:1822:G:C5' | 2.24 | 0.68 |
| 31:BA:467:G:O2' | 31:BA:468:G:H5' | 1.94 | 0.68 |
| 36:BG:16:ARG:HH11 | 36:BG:31:VAL:HG11 | 1.58 | 0.68 |
| 39:BN:28:THR:CG2 | 39:BN:106:MET:HE1 | 2.14 | 0.68 |
| 39:BN:4:TYR:N | 39:BN:4:TYR:CD1 | 2.61 | 0.68 |
| 41:BP:17:LYS:C | 41:BP:19:VAL:H | 1.95 | 0.68 |
| 41:BP:62:LEU:N | 41:BP:62:LEU:CD2 | 2.53 | 0.68 |
| 1:CA:266:G:H5'' | 1:CA:268:C:N4 | 2.08 | 0.68 |
| 1:CA:9:G:OP1 | 5:CE:122:GLU:HB2 | 1.93 | 0.68 |
| 4:CD:68:TYR:HE2 | 4:CD:97:LEU:HB3 | 1.58 | 0.68 |
| 8:CH:53:VAL:O | 8:CH:54:ASP:HB2 | 1.94 | 0.68 |
| 23:D1:73:LEU:HB3 | 23:D1:90:ILE:HG23 | 1.76 | 0.68 |
| 31:DA:1721:G:C2 | 31:DA:1739:U:OP2 | 2.47 | 0.68 |
| 31:DA:2787:C:H1' | 34:DE:61:ARG:CB | 2.22 | 0.68 |
| 35:DF:34:TRP:CZ2 | 41:DP:12:ALA:HB2 | 2.29 | 0.68 |
| 39:DN:19:GLU:HG3 | 39:DN:20:GLY:H | 1.57 | 0.68 |
| 47:DV:69:LYS:HB3 | 47:DV:93:GLU:OE1 | 1.93 | 0.68 |
| 42:DQ:141:GLN:HA | 51:DZ:53:ILE:HB | 1.76 | 0.68 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:C6 | 2.20 | 0.68 |
| 1:AA:1184:G:H2' | 1:AA:1185:G:H8 | 1.59 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1239:A:H62 | 1:AA:1299:A:N6 | 1.92 | 0.68 |
| 1:AA:441:A:H3' | 1:AA:442:C:H6 | 1.59 | 0.68 |
| 2:AB:19:HIS:CD2 | 2:AB:20:GLU:HG2 | 2.27 | 0.68 |
| 5:AE:12:LEU:O | 5:AE:13:ILE:HD12 | 1.94 | 0.68 |
| 31:BA:2199:A:OP2 | 31:BA:2200:C:H5 | 1.77 | 0.68 |
| 28:B6:27:LYS:HD3 | 31:BA:2285:C:OP2 | 1.94 | 0.68 |
| 38:BI:129:THR:HA | 38:BI:137:PRO:HA | 1.75 | 0.68 |
| 39:BN:128:HIS:CD2 | 39:BN:131:GLN:HB2 | 2.28 | 0.68 |
| 47:BV:72:VAL:HG12 | 47:BV:73:SER:H | 1.58 | 0.68 |
| 2:CB:19:HIS:CD2 | 2:CB:20:GLU:HG2 | 2.28 | 0.68 |
| 14:CN:25:VAL:HG23 | 14:CN:38:GLY:O | 1.94 | 0.68 |
| 22:D0:20:ARG:NH1 | 31:DA:2357:U:OP1 | 2.26 | 0.68 |
| 31:DA:1403:C:C5' | 31:DA:1471:A:H1' | 2.24 | 0.68 |
| 31:DA:1689:A:H62 | 31:DA:1698:A:H2 | 1.42 | 0.68 |
| 31:DA:2524:G:C8 | 31:DA:2524:G:H5' | 2.25 | 0.68 |
| 31:DA:2859:G:C8 | 31:DA:2859:G:H3' | 2.28 | 0.68 |
| 31:DA:943:U:OP2 | 41:DP:38:GLN:CD | 2.32 | 0.68 |
| 50:DY:38:ILE:HG22 | 50:DY:39:VAL:H | 1.58 | 0.68 |
| 50:DY:17:SER:CB | 50:DY:71:LYS:HD2 | 2.24 | 0.68 |
| 1:AA:186:C:H2' | 1:AA:187:C:C6 | 2.29 | 0.68 |
| 1:AA:55:A:C5 | 1:AA:56:U:C5 | 2.82 | 0.68 |
| 2:AB:185:ILE:HG22 | 2:AB:199:TYR:CB | 2.20 | 0.68 |
| 11:AK:41:THR:HG22 | 11:AK:42:TRP:N | 2.09 | 0.68 |
| 23:B1:64:ALA:HA | 23:B1:67:ILE:HG13 | 1.75 | 0.68 |
| 31:BA:2199:A:H3' | 31:BA:2200:C:C6 | 2.28 | 0.68 |
| 31:BA:1902:C:O2' | 33:BD:244:ARG:HB2 | 1.93 | 0.68 |
| 35:BF:28:ILE:HA | 35:BF:112:MET:HG2 | 1.74 | 0.68 |
| 35:BF:63:LYS:CE | 35:BF:67:GLN:HB2 | 2.24 | 0.68 |
| 1:CA:1073:U:H2' | 1:CA:1074:G:H8 | 1.58 | 0.68 |
| 23:D1:26:ARG:HB2 | 23:D1:34:THR:HA | 1.74 | 0.68 |
| 27:D5:57:VAL:O | 27:D5:58:LEU:HG | 1.94 | 0.68 |
| 31:DA:620:G:H4' | 31:DA:621:A:C5' | 2.24 | 0.68 |
| 36:DG:124:SER:HB2 | 36:DG:131:TYR:CE1 | 2.28 | 0.68 |
| 39:DN:121:LYS:HD2 | 39:DN:123:TYR:CZ | 2.29 | 0.68 |
| 41:DP:146:VAL:HG22 | 41:DP:147:LEU:N | 2.08 | 0.68 |
| 4:AD:57:ARG:HH22 | 5:AE:107:ARG:HD3 | 1.58 | 0.67 |
| 1:AA:134:A:H61 | 16:AP:25:ARG:HH12 | 1.40 | 0.67 |
| 28:B6:15:GLU:CG | 28:B6:18:ARG:HE | 2.02 | 0.67 |
| 31:BA:708:C:H5' | 31:BA:709:U:OP2 | 1.94 | 0.67 |
| 34:BE:117:MET:O | 34:BE:118:LYS:HB2 | 1.93 | 0.67 |
| 31:BA:2849:U:OP2 | 45:BT:95:ARG:NH1 | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:BV:19:LYS:CE | 47:BV:20:LEU:H | 2.08 | 0.67 |
| 50:BY:37:VAL:HG13 | 50:BY:69:ALA:HA | 1.74 | 0.67 |
| 1:CA:1152:A:H5'' | 10:CJ:13:HIS:CD2 | 2.28 | 0.67 |
| 1:CA:386:C:O2' | 1:CA:387:U:H5' | 1.94 | 0.67 |
| 1:CA:955:U:H1' | 1:CA:1227:A:N6 | 2.09 | 0.67 |
| 31:DA:141:A:H8 | 31:DA:1408:C:O2' | 1.73 | 0.67 |
| 31:DA:1963:U:H4' | 31:DA:1964:G:OP1 | 1.94 | 0.67 |
| 31:DA:2713:A:H3' | 31:DA:2714:G:C5' | 2.23 | 0.67 |
| 31:DA:272:G:H4' | 31:DA:272(B):G:OP1 | 1.93 | 0.67 |
| 31:DA:528:A:C2 | 31:DA:2043:C:H4' | 2.28 | 0.67 |
| 31:DA:2599:G:OP2 | 33:DD:236:GLY:N | 2.27 | 0.67 |
| 33:DD:27:THR:HG23 | 33:DD:28:GLU:N | 2.09 | 0.67 |
| 38:DI:133:HIS:CB | 38:DI:134:PRO:HD2 | 2.23 | 0.67 |
| 41:DP:112:LEU:H | 41:DP:128:HIS:HD2 | 1.42 | 0.67 |
| 47:DV:19:LYS:HG2 | 47:DV:96:ILE:HB | 1.75 | 0.67 |
| 49:DX:65:ARG:CZ | 49:DX:66:LEU:N | 2.58 | 0.67 |
| 1:AA:1497:G:H2' | 1:AA:1498:U:H5' | 1.76 | 0.67 |
| 1:AA:600:C:H2' | 1:AA:601:C:C6 | 2.29 | 0.67 |
| 3:AC:20:SER:HB2 | 3:AC:40:ARG:NH2 | 2.08 | 0.67 |
| 1:AA:939:G:H5'' | 7:AG:102:ARG:HH12 | 1.58 | 0.67 |
| 11:AK:125:PHE:N | 11:AK:125:PHE:CD1 | 2.61 | 0.67 |
| 1:AA:254:G:OP1 | 17:AQ:67:LYS:O | 2.11 | 0.67 |
| 25:B3:43:ILE:O | 25:B3:47:VAL:HG23 | 1.95 | 0.67 |
| 31:BA:827:U:O2' | 31:BA:2068:U:C2 | 2.42 | 0.67 |
| 31:BA:2655:G:H2' | 31:BA:2655:G:N3 | 2.09 | 0.67 |
| 31:BA:271(Q):G:O2' | 31:BA:271(R):G:OP2 | 2.12 | 0.67 |
| 33:BD:71:ASP:HB3 | 33:BD:103:ARG:NH2 | 2.09 | 0.67 |
| 39:BN:3:THR:HG22 | 39:BN:4:TYR:N | 2.07 | 0.67 |
| 42:BQ:141:GLN:CG | 51:BZ:72:ARG:HA | 2.25 | 0.67 |
| 49:BX:31:HIS:HD2 | 49:BX:33:LYS:H | 1.42 | 0.67 |
| 1:CA:254:G:OP1 | 17:CQ:67:LYS:O | 2.12 | 0.67 |
| 1:CA:448:A:OP2 | 1:CA:485:G:N2 | 2.23 | 0.67 |
| 2:CB:167:PRO:HG3 | 2:CB:188:ALA:HB2 | 1.76 | 0.67 |
| 8:CH:36:LEU:HA | 8:CH:39:LEU:HD23 | 1.77 | 0.67 |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:CE2 | 2.30 | 0.67 |
| 24:D2:49:LYS:O | 24:D2:52:ASP:HB3 | 1.94 | 0.67 |
| 30:D8:52:LYS:N | 30:D8:54:GLU:HG2 | 2.08 | 0.67 |
| 31:DA:1713:U:O2' | 31:DA:1714:G:H5' | 1.94 | 0.67 |
| 33:DD:31:LYS:HG2 | 33:DD:34:VAL:CG1 | 2.24 | 0.67 |
| 40:DO:104:ARG:CZ | 45:DT:33:LYS:HD2 | 2.25 | 0.67 |
| 50:DY:96:ILE:HG21 | 50:DY:99:CYS:HB3 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:114:ARG:HD3 | 2:AB:114:ARG:O | 1.95 | 0.67 |
| 4:AD:94:LEU:HA | 4:AD:97:LEU:HB2 | 1.75 | 0.67 |
| 38:BI:133:HIS:CB | 38:BI:134:PRO:HD2 | 2.25 | 0.67 |
| 47:BV:5:VAL:CG2 | 47:BV:36:PRO:HB2 | 2.23 | 0.67 |
| 47:BV:72:VAL:O | 47:BV:73:SER:OG | 2.12 | 0.67 |
| 50:BY:68:HIS:H | 50:BY:71:LYS:HZ1 | 1.42 | 0.67 |
| 50:BY:96:ILE:CG2 | 50:BY:99:CYS:HB3 | 2.24 | 0.67 |
| 1:CA:501:C:H2' | 1:CA:502:G:H8 | 1.59 | 0.67 |
| 1:CA:914:A:O2' | 1:CA:915:A:H5' | 1.95 | 0.67 |
| 24:D2:14:ARG:NH1 | 24:D2:57:ILE:HG22 | 2.09 | 0.67 |
| 26:D4:19:GLY:C | 26:D4:21:VAL:H | 1.97 | 0.67 |
| 30:D8:32:LEU:O | 30:D8:33:ASN:CB | 2.41 | 0.67 |
| 31:DA:1309:G:C2' | 31:DA:1310:G:H5' | 2.24 | 0.67 |
| 31:DA:2208:A:H1' | 31:DA:2219:G:C5 | 2.29 | 0.67 |
| 33:DD:70:TRP:CH2 | 33:DD:150:LYS:HA | 2.29 | 0.67 |
| 34:DE:117:MET:O | 34:DE:118:LYS:HB2 | 1.94 | 0.67 |
| 34:DE:60:ASN:N | 34:DE:60:ASN:ND2 | 2.43 | 0.67 |
| 35:DF:89:VAL:HG12 | 35:DF:90:PHE:H | 1.58 | 0.67 |
| 42:DQ:81:VAL:C | 42:DQ:82:ARG:HD2 | 2.15 | 0.67 |
| 47:DV:25:LEU:H | 47:DV:94:LEU:CD1 | 2.07 | 0.67 |
| 47:DV:25:LEU:H | 47:DV:94:LEU:HD13 | 1.60 | 0.67 |
| 51:DZ:11:GLU:H | 51:DZ:11:GLU:CD | 1.95 | 0.67 |
| 1:AA:1228:C:H2' | 1:AA:1229:A:H8 | 1.58 | 0.67 |
| 1:AA:949:A:H1' | 1:AA:1364:U:N3 | 2.09 | 0.67 |
| 1:AA:524:G:H2' | 1:AA:525:C:C6 | 2.30 | 0.67 |
| 31:BA:107:C:H2' | 31:BA:108:U:H6 | 1.58 | 0.67 |
| 31:BA:1434:A:H61 | 31:BA:1558:A:H62 | 1.42 | 0.67 |
| 31:BA:2287:A:N6 | 31:BA:2344:U:N3 | 2.37 | 0.67 |
| 31:BA:2658:C:H3' | 31:BA:2659:G:H5'' | 1.76 | 0.67 |
| 31:BA:2787:C:H1' | 34:BE:61:ARG:CB | 2.23 | 0.67 |
| 31:BA:2818:G:O2' | 31:BA:2819:G:H5' | 1.95 | 0.67 |
| 31:BA:9:U:C4 | 31:BA:2629:A:N6 | 2.62 | 0.67 |
| 35:BF:83:PHE:O | 35:BF:84:VAL:HB | 1.94 | 0.67 |
| 47:BV:72:VAL:HA | 47:BV:88:ARG:NH1 | 2.09 | 0.67 |
| 51:BZ:4:ARG:HG2 | 51:BZ:58:VAL:HB | 1.75 | 0.67 |
| 1:CA:1003:G:H2' | 1:CA:1004:A:C4' | 2.24 | 0.67 |
| 16:CP:34:GLU:OE2 | 16:CP:55:ARG:HD3 | 1.95 | 0.67 |
| 1:CA:192:U:C4' | 20:CT:103:GLY:HA2 | 2.25 | 0.67 |
| 28:D6:12:GLU:OE1 | 28:D6:23:THR:HG22 | 1.94 | 0.67 |
| 31:DA:1419:A:O2' | 31:DA:1420:U:H5'' | 1.94 | 0.67 |
| 33:DD:35:LYS:HG2 | 33:DD:64:ILE:HG23 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:2580:U:H5' | 34:DE:131:ALA:HB3 | 1.75 | 0.67 |
| 39:DN:128:HIS:O | 39:DN:130:HIS:N | 2.27 | 0.67 |
| 41:DP:17:LYS:HG3 | 41:DP:19:VAL:HG23 | 1.76 | 0.67 |
| 42:DQ:23:GLY:HA3 | 42:DQ:99:PRO:O | 1.94 | 0.67 |
| 46:DU:65:ILE:HG12 | 46:DU:96:ALA:CB | 2.24 | 0.67 |
| 1:AA:1003:G:H2' | 1:AA:1004:A:C4' | 2.23 | 0.67 |
| 2:AB:187:LEU:HD13 | 2:AB:187:LEU:O | 1.95 | 0.67 |
| 4:AD:112:VAL:HG12 | 4:AD:116:GLN:OE1 | 1.95 | 0.67 |
| 10:AJ:39:PRO:HB3 | 10:AJ:70:ARG:HH12 | 1.59 | 0.67 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CG | 2.29 | 0.67 |
| 23:B1:37:ILE:HD12 | 31:BA:2079:U:O2' | 1.94 | 0.67 |
| 31:BA:1418:G:OP1 | 31:BA:1588:C:O2' | 2.11 | 0.67 |
| 31:BA:1488:G:C6 | 31:BA:1489:U:N3 | 2.63 | 0.67 |
| 31:BA:1528(A):A:N7 | 31:BA:1529:G:C8 | 2.63 | 0.67 |
| 35:BF:46:ARG:NH1 | 35:BF:46:ARG:HG2 | 1.99 | 0.67 |
| 41:BP:144:GLU:N | 41:BP:145:PRO:HD3 | 2.10 | 0.67 |
| 47:BV:38:LEU:HG | 47:BV:39:LEU:N | 2.08 | 0.67 |
| 49:BX:33:LYS:C | 49:BX:35:THR:N | 2.48 | 0.67 |
| 5:CE:68:GLU:O | 5:CE:68:GLU:HG3 | 1.94 | 0.67 |
| 31:DA:2701:C:H3' | 31:DA:2702:U:H5'' | 1.76 | 0.67 |
| 49:DX:53:LYS:HE3 | 49:DX:55:ASN:HD21 | 1.58 | 0.67 |
| 1:AA:224:C:H2' | 1:AA:225:C:C6 | 2.29 | 0.67 |
| 1:AA:663:A:O2' | 1:AA:664:G:H5' | 1.95 | 0.67 |
| 4:AD:68:TYR:N | 4:AD:68:TYR:HD1 | 1.93 | 0.67 |
| 10:AJ:51:ARG:NE | 10:AJ:61:GLU:HB2 | 2.09 | 0.67 |
| 23:B1:13:ILE:O | 23:B1:14:VAL:HB | 1.95 | 0.67 |
| 23:B1:75:GLU:O | 23:B1:76:ARG:HD3 | 1.95 | 0.67 |
| 31:BA:1292:U:H2' | 31:BA:1293:C:C6 | 2.29 | 0.67 |
| 31:BA:1598:C:H5' | 49:BX:37:THR:HB | 1.76 | 0.67 |
| 31:BA:1713:U:O2' | 31:BA:1714:G:H5' | 1.94 | 0.67 |
| 32:BB:62:C:H2' | 32:BB:63:G:H5'' | 1.76 | 0.67 |
| 35:BF:9:ILE:HG23 | 35:BF:13:SER:O | 1.94 | 0.67 |
| 42:BQ:75:THR:CA | 42:BQ:88:GLY:HA2 | 2.24 | 0.67 |
| 42:BQ:60:ARG:HA | 51:BZ:179:ASP:N | 2.08 | 0.67 |
| 1:CA:55:A:C5 | 1:CA:56:U:C5 | 2.81 | 0.67 |
| 1:CA:600:C:H2' | 1:CA:601:C:C6 | 2.29 | 0.67 |
| 1:CA:659:U:H2' | 1:CA:660:G:H5' | 1.76 | 0.67 |
| 30:D8:43:GLN:O | 30:D8:44:LYS:HD2 | 1.95 | 0.67 |
| 31:DA:1528(A):A:N7 | 31:DA:1529:G:C8 | 2.62 | 0.67 |
| 32:DB:21:G:O6 | 32:DB:63:G:C5 | 2.47 | 0.67 |
| 41:DP:149:GLU:O | 41:DP:149:GLU:HG3 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:DP:65:ARG:O | 41:DP:68:GLN:HB3 | 1.95 | 0.67 |
| 50:DY:38:ILE:HG22 | 50:DY:39:VAL:N | 2.08 | 0.67 |
| 50:DY:81:LYS:HG2 | 50:DY:96:ILE:CG2 | 2.24 | 0.67 |
| 1:AA:650:G:O2' | 1:AA:651:C:H5' | 1.94 | 0.67 |
| 1:AA:687:A:N3 | 1:AA:688:G:H1' | 2.08 | 0.67 |
| 9:AI:17:VAL:HG11 | 9:AI:81:ILE:HD13 | 1.77 | 0.67 |
| 23:B1:19:GLN:HE21 | 31:BA:379:G:N2 | 1.85 | 0.67 |
| 23:B1:25:LYS:O | 23:B1:26:ARG:CB | 2.41 | 0.67 |
| 41:BP:149:GLU:HG3 | 41:BP:149:GLU:O | 1.94 | 0.67 |
| 42:BQ:141:GLN:HA | 51:BZ:53:ILE:HB | 1.75 | 0.67 |
| 51:BZ:69:THR:HG22 | 51:BZ:90:VAL:HA | 1.77 | 0.67 |
| 51:BZ:74:VAL:HG22 | 51:BZ:86:VAL:HG13 | 1.77 | 0.67 |
| 1:CA:1227:A:OP2 | 13:CM:111:LYS:HE2 | 1.94 | 0.67 |
| 1:CA:16:A:O2' | 1:CA:17:U:H5' | 1.94 | 0.67 |
| 1:CA:22:G:H2' | 1:CA:23:C:H6 | 1.60 | 0.67 |
| 1:CA:735:C:H2' | 1:CA:736:C:C6 | 2.25 | 0.67 |
| 2:CB:101:MET:HA | 2:CB:108:ILE:HG13 | 1.75 | 0.67 |
| 2:CB:124:SER:OG | 2:CB:125:PRO:HD2 | 1.94 | 0.67 |
| 7:CG:26:PHE:O | 7:CG:30:ILE:HG12 | 1.94 | 0.67 |
| 1:CA:191:G:C4 | 20:CT:105:SER:HB3 | 2.30 | 0.67 |
| 20:CT:75:ASN:HA | 20:CT:78:ALA:HB3 | 1.77 | 0.67 |
| 31:DA:1434:A:H61 | 31:DA:1558:A:H62 | 1.43 | 0.67 |
| 31:DA:2036:C:C6 | 31:DA:2036:C:H5' | 2.29 | 0.67 |
| 31:DA:467:G:O2' | 31:DA:468:G:H5' | 1.93 | 0.67 |
| 31:DA:531:C:H4' | 31:DA:532:A:H5'' | 1.77 | 0.67 |
| 31:DA:542:C:N3 | 31:DA:543:C:N4 | 2.42 | 0.67 |
| 31:DA:867:C:C5 | 31:DA:868:U:C5 | 2.83 | 0.67 |
| 42:DQ:141:GLN:HG2 | 51:DZ:71:VAL:O | 1.95 | 0.67 |
| 42:DQ:75:THR:CA | 42:DQ:88:GLY:HA2 | 2.24 | 0.67 |
| 1:AA:853:G:H2' | 1:AA:854:G:H8 | 1.60 | 0.67 |
| 24:B2:34:GLU:O | 24:B2:36:ARG:N | 2.28 | 0.67 |
| 31:BA:1171:G:OP2 | 31:BA:1171:G:H8 | 1.77 | 0.67 |
| 31:BA:2524:G:C8 | 31:BA:2524:G:H5' | 2.25 | 0.67 |
| 31:BA:464:U:O2' | 31:BA:465:G:H5' | 1.95 | 0.67 |
| 33:BD:35:LYS:HD3 | 33:BD:63:ARG:CA | 2.24 | 0.67 |
| 38:BI:82:ARG:O | 38:BI:89:TYR:HB2 | 1.94 | 0.67 |
| 39:BN:112:LEU:HD12 | 39:BN:112:LEU:O | 1.95 | 0.67 |
| 31:BA:494:G:H21 | 48:BW:57:ASN:HD21 | 1.42 | 0.67 |
| 1:CA:1409:C:H42 | 1:CA:1491:G:H1 | 1.41 | 0.67 |
| 1:CA:963:G:H21 | 10:CJ:55:LYS:HE2 | 1.60 | 0.67 |
| 23:D1:23:LYS:HB2 | 23:D1:37:ILE:HG22 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 23:D1:48:LYS:O | 23:D1:49:VAL:HB | 1.94 | 0.67 |
| 31:DA:1021:A:C8 | 31:DA:1021:A:H3' | 2.30 | 0.67 |
| 31:DA:1405:U:H2' | 31:DA:1406:U:H6 | 1.58 | 0.67 |
| 31:DA:2584:U:O2 | 31:DA:2584:U:O4' | 2.11 | 0.67 |
| 31:DA:2801(A):A:C4' | 31:DA:2802:G:H5' | 2.25 | 0.67 |
| 32:DB:30:C:OP2 | 44:DS:32:LEU:HD11 | 1.94 | 0.67 |
| 37:DH:89:ILE:HD11 | 37:DH:129:THR:HB | 1.76 | 0.67 |
| 39:DN:4:TYR:CD1 | 39:DN:4:TYR:N | 2.61 | 0.67 |
| 40:DO:10:VAL:HG23 | 40:DO:10:VAL:O | 1.93 | 0.67 |
| 44:DS:95:HIS:ND1 | 44:DS:96:GLY:N | 2.43 | 0.67 |
| 49:DX:89:ILE:HA | 49:DX:92:LEU:HD12 | 1.76 | 0.67 |
| 8:AH:1:MET:H3 | 8:AH:1:MET:HE2 | 1.58 | 0.67 |
| 9:AI:18:PHE:HB3 | 9:AI:20:ARG:NH1 | 2.09 | 0.67 |
| 1:AA:963:G:H21 | 10:AJ:55:LYS:HE2 | 1.60 | 0.67 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CD1 | 2.30 | 0.67 |
| 23:B1:10:LYS:O | 23:B1:13:ILE:HG23 | 1.95 | 0.67 |
| 31:BA:1899:G:H21 | 31:BA:1902:C:H5 | 1.40 | 0.67 |
| 31:BA:2106:G:H1' | 31:BA:2184:G:N2 | 2.09 | 0.67 |
| 31:BA:2475:C:H6 | 31:BA:2475:C:H5'' | 1.60 | 0.67 |
| 31:BA:2567:G:H2' | 31:BA:2568:C:C6 | 2.30 | 0.67 |
| 31:BA:794:G:H2' | 31:BA:795:C:C6 | 2.30 | 0.67 |
| 35:BF:160:ASN:HD22 | 35:BF:162:LEU:H | 1.42 | 0.67 |
| 37:BH:43:VAL:HG21 | 37:BH:52:VAL:HG22 | 1.75 | 0.67 |
| 46:BU:95:LEU:HD22 | 47:BV:4:ILE:HD13 | 1.76 | 0.67 |
| 49:BX:24:GLY:HA3 | 49:BX:80:ILE:CG1 | 2.25 | 0.67 |
| 50:BY:95:LYS:HD3 | 50:BY:100:ALA:CB | 2.14 | 0.67 |
| 1:CA:1238:A:H62 | 1:CA:1299:A:H62 | 1.43 | 0.67 |
| 4:CD:112:VAL:HG12 | 4:CD:116:GLN:OE1 | 1.95 | 0.67 |
| 6:CF:18:GLN:HA | 6:CF:21:LEU:CD2 | 2.19 | 0.67 |
| 22:D0:24:LYS:O | 22:D0:25:ARG:HD2 | 1.94 | 0.67 |
| 23:D1:46:LEU:N | 23:D1:46:LEU:HD12 | 2.05 | 0.67 |
| 23:D1:75:GLU:O | 23:D1:76:ARG:HD3 | 1.95 | 0.67 |
| 24:D2:46:GLN:HE21 | 24:D2:47:ASN:CA | 2.08 | 0.67 |
| 30:D8:6:THR:HG21 | 31:DA:243:U:OP1 | 1.94 | 0.67 |
| 35:DF:160:ASN:C | 35:DF:160:ASN:HD22 | 1.97 | 0.67 |
| 47:DV:64:HIS:CD2 | 47:DV:64:HIS:O | 2.48 | 0.67 |
| 51:DZ:5:LEU:CD1 | 51:DZ:43:GLU:HB3 | 2.25 | 0.67 |
| 2:AB:187:LEU:HD23 | 2:AB:201:ILE:HG22 | 1.77 | 0.67 |
| 9:AI:97:LYS:HB3 | 9:AI:98:PRO:HD3 | 1.77 | 0.67 |
| 15:AO:3:ILE:H | 15:AO:3:ILE:HD13 | 1.60 | 0.67 |
| 16:AP:22:THR:HA | 16:AP:33:ILE:HG12 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:B2:49:LYS:O | 24:B2:52:ASP:HB3 | 1.95 | 0.67 |
| 25:B3:19:GLN:HE22 | 25:B3:52:HIS:HE1 | 1.41 | 0.67 |
| 27:B5:40:LYS:CD | 27:B5:46:CYS:HB3 | 2.25 | 0.67 |
| 31:BA:1021:A:C8 | 31:BA:1021:A:H3' | 2.29 | 0.67 |
| 31:BA:1592:C:O2' | 31:BA:1593:G:H5'' | 1.95 | 0.67 |
| 31:BA:614(A):U:H4' | 31:BA:614(B):G:H5'' | 1.77 | 0.67 |
| 31:BA:631:A:O2' | 41:BP:67:MET:HB3 | 1.95 | 0.67 |
| 33:BD:35:LYS:HG2 | 33:BD:64:ILE:N | 2.09 | 0.67 |
| 34:BE:52:LEU:O | 34:BE:74:PRO:HA | 1.95 | 0.67 |
| 35:BF:18:ARG:CG | 35:BF:19:GLU:H | 2.06 | 0.67 |
| 37:BH:137:ASP:O | 37:BH:138:LYS:CB | 2.42 | 0.67 |
| 37:BH:40:GLU:O | 37:BH:41:MET:SD | 2.53 | 0.67 |
| 38:BI:12:LEU:HG | 38:BI:12:LEU:O | 1.94 | 0.67 |
| 42:BQ:54:MET:HG3 | 42:BQ:117:ALA:HB1 | 1.77 | 0.67 |
| 47:BV:46:VAL:O | 47:BV:47:VAL:HB | 1.94 | 0.67 |
| 1:CA:192:U:H2' | 1:CA:193:C:H6 | 1.59 | 0.67 |
| 1:CA:425:G:C2' | 1:CA:426:G:H5' | 2.24 | 0.67 |
| 2:CB:130:ARG:HE | 2:CB:130:ARG:HA | 1.60 | 0.67 |
| 16:CP:20:VAL:HG21 | 16:CP:32:TYR:CD1 | 2.30 | 0.67 |
| 1:CA:1242:C:P | 21:CU:10:ARG:HH22 | 2.17 | 0.67 |
| 25:D3:54:VAL:HG12 | 25:D3:55:ARG:N | 2.10 | 0.67 |
| 31:DA:1598:C:H5' | 49:DX:37:THR:HB | 1.76 | 0.67 |
| 31:DA:354:G:H8 | 31:DA:354:G:O5' | 1.78 | 0.67 |
| 31:DA:953:A:O2' | 31:DA:954:G:H5' | 1.95 | 0.67 |
| 47:DV:51:VAL:CG1 | 47:DV:52:VAL:H | 2.08 | 0.67 |
| 50:DY:15:VAL:O | 50:DY:22:GLY:HA2 | 1.94 | 0.67 |
| 1:AA:1422:G:O2' | 1:AA:1423:G:H5' | 1.95 | 0.66 |
| 2:AB:124:SER:OG | 2:AB:125:PRO:HD2 | 1.95 | 0.66 |
| 4:AD:138:TYR:HD2 | 4:AD:138:TYR:C | 1.98 | 0.66 |
| 1:AA:1291:G:H4' | 9:AI:38:GLN:O | 1.94 | 0.66 |
| 29:B7:16:HIS:CB | 29:B7:44:PRO:HG2 | 2.24 | 0.66 |
| 31:BA:1448:G:H1' | 31:BA:1528:A:H62 | 1.58 | 0.66 |
| 31:BA:1720:U:H2' | 31:BA:1721:G:O4' | 1.95 | 0.66 |
| 31:BA:588:U:OP2 | 31:BA:588:U:C6 | 2.48 | 0.66 |
| 37:BH:90:LYS:HB2 | 37:BH:159:GLU:O | 1.94 | 0.66 |
| 45:BT:24:PRO:HA | 45:BT:49:VAL:HG13 | 1.76 | 0.66 |
| 46:BU:92:ARG:CZ | 47:BV:11:GLN:H | 2.08 | 0.66 |
| 46:BU:91:ASP:O | 46:BU:95:LEU:HB2 | 1.95 | 0.66 |
| 49:BX:83:VAL:O | 49:BX:84:ALA:HB3 | 1.94 | 0.66 |
| 50:BY:28:LYS:HA | 50:BY:39:VAL:H | 1.60 | 0.66 |
| 1:CA:1289:A:H3' | 1:CA:1290:G:H8 | 1.60 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1342:C:H1' | 9:CI:124:GLN:HE22 | 1.60 | 0.66 |
| 2:CB:97:TRP:CH2 | 2:CB:173:ALA:HA | 2.30 | 0.66 |
| 4:CD:68:TYR:HD1 | 4:CD:68:TYR:N | 1.92 | 0.66 |
| 9:CI:18:PHE:HB3 | 9:CI:20:ARG:NH1 | 2.09 | 0.66 |
| 10:CJ:32:ALA:CB | 10:CJ:76:ASN:HB3 | 2.25 | 0.66 |
| 12:CL:46:LYS:HG2 | 12:CL:47:LYS:H | 1.59 | 0.66 |
| 31:DA:1109:C:H5 | 31:DA:1110:G:C5 | 2.12 | 0.66 |
| 31:DA:1448:G:H1' | 31:DA:1528:A:H62 | 1.60 | 0.66 |
| 31:DA:2292:C:O2' | 31:DA:2293:C:H5' | 1.95 | 0.66 |
| 39:DN:40:PRO:CA | 46:DU:64:ARG:HH22 | 2.07 | 0.66 |
| 41:DP:144:GLU:N | 41:DP:145:PRO:HD3 | 2.09 | 0.66 |
| 1:AA:373:A:H2' | 1:AA:374:A:H8 | 1.60 | 0.66 |
| 1:AA:501:C:H2' | 1:AA:502:G:H8 | 1.60 | 0.66 |
| 13:AM:12:ASN:OD1 | 13:AM:46:LYS:HE2 | 1.96 | 0.66 |
| 23:B1:9:GLY:O | 23:B1:10:LYS:HB3 | 1.94 | 0.66 |
| 27:B5:57:VAL:HG23 | 27:B5:58:LEU:N | 2.09 | 0.66 |
| 31:BA:1205:U:H4' | 31:BA:1206:G:OP2 | 1.94 | 0.66 |
| 31:BA:1948:G:H8 | 31:BA:1948:G:H5' | 1.59 | 0.66 |
| 41:BP:48:PRO:HG2 | 41:BP:49:ARG:H | 1.59 | 0.66 |
| 47:BV:47:VAL:HG13 | 47:BV:48:GLY:N | 2.10 | 0.66 |
| 49:BX:76:ARG:HH11 | 49:BX:76:ARG:CG | 2.06 | 0.66 |
| 49:BX:89:ILE:HD12 | 49:BX:92:LEU:HD12 | 1.76 | 0.66 |
| 50:BY:42:VAL:HB | 50:BY:65:ALA:HB3 | 1.76 | 0.66 |
| 3:CC:86:VAL:O | 3:CC:90:GLU:HG2 | 1.94 | 0.66 |
| 4:CD:94:LEU:HA | 4:CD:97:LEU:HB2 | 1.76 | 0.66 |
| 5:CE:101:ILE:CD1 | 5:CE:119:LEU:HD23 | 2.21 | 0.66 |
| 7:CG:73:MET:HA | 7:CG:91:VAL:HG23 | 1.77 | 0.66 |
| 13:CM:46:LYS:HG3 | 13:CM:47:ASP:N | 2.10 | 0.66 |
| 25:D3:19:GLN:HE22 | 25:D3:52:HIS:CE1 | 2.10 | 0.66 |
| 31:DA:1171:G:H8 | 31:DA:1171:G:OP2 | 1.78 | 0.66 |
| 31:DA:767:U:O2' | 31:DA:768:G:H5' | 1.96 | 0.66 |
| 35:DF:103:LYS:HA | 35:DF:106:ARG:HG3 | 1.76 | 0.66 |
| 37:DH:43:VAL:HG21 | 37:DH:52:VAL:HG22 | 1.77 | 0.66 |
| 45:DT:78:LEU:O | 45:DT:78:LEU:HD23 | 1.95 | 0.66 |
| 1:AA:814:A:N7 | 1:AA:816:A:C4 | 2.63 | 0.66 |
| 28:B6:12:GLU:OE1 | 28:B6:23:THR:HG22 | 1.95 | 0.66 |
| 29:B7:43:THR:HG23 | 29:B7:44:PRO:HD2 | 1.78 | 0.66 |
| 31:BA:943:U:OP2 | 41:BP:38:GLN:CD | 2.33 | 0.66 |
| 32:BB:87:G:H3' | 32:BB:88:C:H5'' | 1.75 | 0.66 |
| 33:BD:35:LYS:HG2 | 33:BD:64:ILE:HG23 | 1.76 | 0.66 |
| 49:BX:72:LYS:CG | 49:BX:74:PRO:HD3 | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:186:C:H2' | 1:CA:187:C:C6 | 2.31 | 0.66 |
| 1:CA:1057:G:H5'' | 3:CC:154:SER:HB2 | 1.76 | 0.66 |
| 11:CK:21:ILE:HG13 | 11:CK:30:VAL:HG12 | 1.77 | 0.66 |
| 24:D2:30:ARG:N | 24:D2:30:ARG:HD2 | 2.10 | 0.66 |
| 31:DA:1418:G:OP1 | 31:DA:1588:C:O2' | 2.12 | 0.66 |
| 31:DA:1472:A:O2' | 31:DA:1473:G:H5' | 1.96 | 0.66 |
| 31:DA:1497:U:H2' | 31:DA:1497:U:O2 | 1.96 | 0.66 |
| 31:DA:1719:G:H2' | 31:DA:1720:U:H5' | 1.77 | 0.66 |
| 33:DD:253:GLN:HB3 | 33:DD:255:LYS:CE | 2.25 | 0.66 |
| 34:DE:27:LEU:HD22 | 45:DT:1:MET:CE | 2.26 | 0.66 |
| 35:DF:16:GLY:O | 35:DF:17:ARG:HG3 | 1.95 | 0.66 |
| 41:DP:30:THR:CG2 | 41:DP:31:ALA:H | 2.08 | 0.66 |
| 45:DT:12:SER:O | 45:DT:13:ARG:HG2 | 1.95 | 0.66 |
| 47:DV:2:PHE:HE1 | 47:DV:13:ARG:NH2 | 1.93 | 0.66 |
| 1:AA:417:C:O2' | 1:AA:418:C:H5' | 1.94 | 0.66 |
| 1:AA:833:U:H2' | 1:AA:834:C:H6 | 1.61 | 0.66 |
| 1:AA:1190:G:H3' | 3:AC:3:ASN:ND2 | 2.10 | 0.66 |
| 1:AA:625:G:H4' | 16:AP:16:HIS:CD2 | 2.30 | 0.66 |
| 20:AT:75:ASN:HA | 20:AT:78:ALA:HB3 | 1.77 | 0.66 |
| 24:B2:32:LEU:O | 24:B2:33:MET:C | 2.33 | 0.66 |
| 31:BA:1109:C:H5 | 31:BA:1110:G:C4 | 2.13 | 0.66 |
| 31:BA:2335:A:O2' | 31:BA:2336:A:H5'' | 1.94 | 0.66 |
| 31:BA:639:U:H2' | 31:BA:640:C:C6 | 2.30 | 0.66 |
| 39:BN:40:PRO:CA | 46:BU:64:ARG:HH22 | 2.09 | 0.66 |
| 9:CI:46:ALA:HB2 | 9:CI:74:ILE:HG23 | 1.77 | 0.66 |
| 31:DA:271(Q):G:O2' | 31:DA:271(R):G:OP2 | 2.13 | 0.66 |
| 31:DA:587:C:C4' | 31:DA:588:U:OP2 | 2.42 | 0.66 |
| 33:DD:10:THR:OG1 | 33:DD:13:ARG:HB2 | 1.96 | 0.66 |
| 37:DH:105:LEU:HD22 | 37:DH:105:LEU:H | 1.61 | 0.66 |
| 39:DN:68:GLU:HA | 39:DN:86:PRO:CB | 2.25 | 0.66 |
| 41:DP:51:PHE:O | 41:DP:52:GLU:HB2 | 1.92 | 0.66 |
| 1:CA:346:G:H5'' | 45:DT:41:ARG:CZ | 2.24 | 0.66 |
| 1:AA:1225:A:N3 | 1:AA:1225:A:H2' | 2.11 | 0.66 |
| 1:AA:561:U:O2' | 1:AA:562:C:P | 2.53 | 0.66 |
| 6:AF:60:PHE:C | 6:AF:61:LEU:HD12 | 2.16 | 0.66 |
| 7:AG:73:MET:HA | 7:AG:91:VAL:HG23 | 1.76 | 0.66 |
| 31:BA:1472:A:O2' | 31:BA:1473:G:H5' | 1.96 | 0.66 |
| 31:BA:910:A:C5 | 42:BQ:13:GLN:OE1 | 2.48 | 0.66 |
| 35:BF:57:VAL:HG13 | 35:BF:58:ALA:N | 2.11 | 0.66 |
| 41:BP:25:SER:O | 41:BP:30:THR:HG23 | 1.95 | 0.66 |
| 42:BQ:23:GLY:O | 42:BQ:100:GLY:CA | 2.44 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:BY:81:LYS:HG2 | 50:BY:97:ARG:H | 1.60 | 0.66 |
| 51:BZ:150:LEU:HD23 | 51:BZ:171:ILE:HD11 | 1.78 | 0.66 |
| 1:CA:1238:A:H62 | 1:CA:1299:A:N6 | 1.93 | 0.66 |
| 7:CG:108:ALA:O | 7:CG:119:ARG:HD2 | 1.96 | 0.66 |
| 8:CH:6:ILE:H | 8:CH:6:ILE:HD12 | 1.59 | 0.66 |
| 30:D8:4:MET:HE1 | 31:DA:593:G:H1' | 1.75 | 0.66 |
| 32:DB:66:A:N6 | 32:DB:108:U:H2' | 2.10 | 0.66 |
| 36:DG:61:ALA:HA | 36:DG:64:THR:HG22 | 1.77 | 0.66 |
| 42:DQ:81:VAL:O | 42:DQ:82:ARG:CD | 2.30 | 0.66 |
| 45:DT:27:THR:O | 45:DT:28:VAL:HG23 | 1.96 | 0.66 |
| 8:AH:53:VAL:O | 8:AH:54:ASP:HB2 | 1.96 | 0.66 |
| 13:AM:46:LYS:HG3 | 13:AM:47:ASP:N | 2.10 | 0.66 |
| 24:B2:37:PHE:HZ | 24:B2:43:GLN:HB2 | 1.60 | 0.66 |
| 33:BD:145:VAL:HG12 | 33:BD:146:GLU:O | 1.96 | 0.66 |
| 37:BH:99:VAL:O | 37:BH:99:VAL:HG12 | 1.96 | 0.66 |
| 41:BP:10:PRO:CD | 41:BP:11:GLY:H | 2.08 | 0.66 |
| 41:BP:112:LEU:H | 41:BP:128:HIS:HD2 | 1.42 | 0.66 |
| 50:BY:39:VAL:HG12 | 50:BY:40:GLU:H | 1.61 | 0.66 |
| 51:BZ:64:GLY:O | 51:BZ:65:GLN:O | 2.12 | 0.66 |
| 24:D2:37:PHE:HZ | 24:D2:43:GLN:HB2 | 1.60 | 0.66 |
| 31:DA:1472:A:C2' | 31:DA:1473:G:H5' | 2.25 | 0.66 |
| 28:D6:27:LYS:HD3 | 31:DA:2285:C:OP2 | 1.95 | 0.66 |
| 31:DA:2536:G:C6 | 31:DA:2537:U:C4 | 2.84 | 0.66 |
| 31:DA:626:U:N3 | 41:DP:105:LEU:HG | 2.11 | 0.66 |
| 37:DH:19:VAL:HG21 | 37:DH:44:VAL:HA | 1.78 | 0.66 |
| 50:DY:96:ILE:HG22 | 50:DY:97:ARG:N | 2.10 | 0.66 |
| 1:AA:1238:A:H62 | 1:AA:1299:A:H62 | 1.43 | 0.66 |
| 2:AB:97:TRP:CH2 | 2:AB:173:ALA:HA | 2.30 | 0.66 |
| 2:AB:87:ARG:NE | 2:AB:233:SER:HB3 | 2.09 | 0.66 |
| 10:AJ:32:ALA:CB | 10:AJ:76:ASN:HB3 | 2.24 | 0.66 |
| 11:AK:29:ILE:HB | 11:AK:44:SER:HB3 | 1.76 | 0.66 |
| 17:AQ:5:VAL:O | 17:AQ:6:LEU:HD23 | 1.96 | 0.66 |
| 22:B0:24:LYS:O | 22:B0:25:ARG:HD2 | 1.95 | 0.66 |
| 31:BA:1790:C:H5'' | 31:BA:1791:A:OP1 | 1.95 | 0.66 |
| 39:BN:15:LEU:HD21 | 39:BN:55:VAL:HG22 | 1.78 | 0.66 |
| 39:BN:25:ARG:HH11 | 39:BN:25:ARG:HG3 | 1.60 | 0.66 |
| 31:BA:661:C:H4' | 41:BP:16:ARG:HH12 | 1.61 | 0.66 |
| 47:BV:25:LEU:H | 47:BV:94:LEU:HD13 | 1.60 | 0.66 |
| 51:BZ:105:VAL:HG12 | 51:BZ:139:VAL:O | 1.96 | 0.66 |
| 1:CA:355:C:H2' | 1:CA:356:A:H5' | 1.78 | 0.66 |
| 1:CA:950:U:H2' | 1:CA:951:G:H8 | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:CA:972:C:H4' | 10:CJ:57:LYS:HG3 | 1.78 | 0.66 |
| 15:CO:39:LEU:CD1 | 15:CO:56:LEU:HB2 | 2.24 | 0.66 |
| 28:D6:10:LEU:H | 28:D6:10:LEU:CD2 | 2.09 | 0.66 |
| 28:D6:15:GLU:CG | 28:D6:18:ARG:HE | 2.04 | 0.66 |
| 31:DA:1528(A):A:C5 | 31:DA:1529:G:H8 | 2.14 | 0.66 |
| 31:DA:2789:C:H4' | 31:DA:2789:C:OP1 | 1.95 | 0.66 |
| 32:DB:87:G:P | 32:DB:87:G:H8 | 2.19 | 0.66 |
| 33:DD:106:ILE:O | 33:DD:106:ILE:HD13 | 1.95 | 0.66 |
| 33:DD:65:ILE:HD11 | 33:DD:67:PHE:CD1 | 2.30 | 0.66 |
| 43:DR:4:LEU:O | 43:DR:6:SER:N | 2.27 | 0.66 |
| 45:DT:83:ILE:HG13 | 45:DT:84:GLN:N | 2.06 | 0.66 |
| 49:DX:89:ILE:HA | 49:DX:92:LEU:HB2 | 1.78 | 0.66 |
| 1:AA:1288:A:H2 | 1:AA:1352:C:O2 | 1.79 | 0.66 |
| 1:AA:189:G:C6 | 1:AA:189(L):G:C6 | 2.84 | 0.66 |
| 8:AH:51:VAL:HG11 | 8:AH:60:ARG:HG3 | 1.77 | 0.66 |
| 24:B2:46:GLN:HE21 | 24:B2:47:ASN:CA | 2.08 | 0.66 |
| 31:BA:2404:C:H2' | 31:BA:2405:G:H5' | 1.78 | 0.66 |
| 31:BA:2801(A):A:C4' | 31:BA:2802:G:H5' | 2.25 | 0.66 |
| 31:BA:912:C:C2 | 31:BA:913:U:C5 | 2.84 | 0.66 |
| 36:BG:76:SER:CB | 36:BG:83:ARG:HB3 | 2.26 | 0.66 |
| 37:BH:30:LYS:HZ3 | 37:BH:81:GLU:HA | 1.61 | 0.66 |
| 39:BN:95:PRO:C | 39:BN:97:ARG:H | 1.98 | 0.66 |
| 31:BA:196:A:O4' | 41:BP:46:LYS:HE2 | 1.96 | 0.66 |
| 49:BX:60:ARG:HB2 | 49:BX:74:PRO:HD2 | 1.78 | 0.66 |
| 1:CA:1003:G:C2 | 1:CA:1004:A:H1' | 2.30 | 0.66 |
| 2:CB:114:ARG:HD3 | 2:CB:114:ARG:O | 1.96 | 0.66 |
| 2:CB:19:HIS:CE1 | 2:CB:206:ASP:HB2 | 2.31 | 0.66 |
| 2:CB:77:ALA:HB2 | 2:CB:211:ILE:HD13 | 1.76 | 0.66 |
| 5:CE:76:ILE:HG12 | 5:CE:77:PRO:HD2 | 1.76 | 0.66 |
| 10:CJ:26:ALA:HB1 | 10:CJ:29:ARG:HH21 | 1.60 | 0.66 |
| 11:CK:29:ILE:HB | 11:CK:44:SER:HB3 | 1.77 | 0.66 |
| 20:CT:37:SER:O | 20:CT:41:ILE:HG12 | 1.96 | 0.66 |
| 31:DA:1592:C:O2' | 31:DA:1593:G:H5'' | 1.95 | 0.66 |
| 31:DA:322:A:H5' | 31:DA:340:A:C1' | 2.26 | 0.66 |
| 34:DE:51:PHE:O | 34:DE:74:PRO:HB3 | 1.95 | 0.66 |
| 35:DF:28:ILE:HA | 35:DF:112:MET:HG2 | 1.77 | 0.66 |
| 36:DG:139:LEU:HA | 36:DG:144:ILE:HG23 | 1.78 | 0.66 |
| 41:DP:48:PRO:O | 41:DP:50:ARG:N | 2.29 | 0.66 |
| 42:DQ:37:LEU:HB2 | 42:DQ:128:LYS:O | 1.96 | 0.66 |
| 43:DR:33:ARG:CG | 43:DR:115:GLU:HG3 | 2.20 | 0.66 |
| 43:DR:11:ASN:CG | 43:DR:12:ARG:H | 1.99 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:DS:66:ALA:HA | 44:DS:69:VAL:CG1 | 2.26 | 0.66 |
| 31:DA:2849:U:O4 | 45:DT:23:ARG:NH2 | 2.28 | 0.66 |
| 47:DV:72:VAL:HG12 | 47:DV:73:SER:H | 1.61 | 0.66 |
| 47:DV:90:PRO:CG | 47:DV:91:TYR:N | 2.50 | 0.66 |
| 1:AA:1097:C:H1' | 1:AA:1170:A:H1' | 1.76 | 0.66 |
| 1:AA:1333:A:H2' | 1:AA:1334:G:O4' | 1.96 | 0.66 |
| 1:AA:1442:G:C8 | 1:AA:1442(B):A:C2 | 2.84 | 0.66 |
| 1:AA:349:A:O2' | 1:AA:350:G:H5' | 1.95 | 0.66 |
| 2:AB:19:HIS:CE1 | 2:AB:206:ASP:HB2 | 2.31 | 0.66 |
| 30:B8:34:TRP:HZ3 | 30:B8:41:ILE:HG23 | 1.60 | 0.66 |
| 31:BA:1528(A):A:C5 | 31:BA:1529:G:H8 | 2.13 | 0.66 |
| 31:BA:953:A:O2' | 31:BA:954:G:H5' | 1.96 | 0.66 |
| 33:BD:65:ILE:HD11 | 33:BD:67:PHE:CD1 | 2.29 | 0.66 |
| 39:BN:128:HIS:O | 39:BN:130:HIS:N | 2.28 | 0.66 |
| 45:BT:57:PHE:O | 45:BT:59:THR:N | 2.28 | 0.66 |
| 2:CB:201:ILE:HG21 | 2:CB:214:ILE:HG21 | 1.78 | 0.66 |
| 8:CH:51:VAL:HG11 | 8:CH:60:ARG:HG3 | 1.76 | 0.66 |
| 1:CA:1291:G:H4' | 9:CI:38:GLN:O | 1.95 | 0.66 |
| 24:D2:51:ARG:HD3 | 24:D2:51:ARG:O | 1.94 | 0.66 |
| 28:D6:15:GLU:OE2 | 28:D6:41:PRO:CG | 2.44 | 0.66 |
| 30:D8:26:LYS:HE2 | 30:D8:47:LYS:HZ2 | 1.60 | 0.66 |
| 31:DA:2314:C:O2' | 31:DA:2315:G:H5' | 1.95 | 0.66 |
| 31:DA:52:A:O2' | 31:DA:53:A:H5' | 1.96 | 0.66 |
| 35:DF:9:ILE:HG23 | 35:DF:13:SER:O | 1.96 | 0.66 |
| 44:DS:66:ALA:O | 44:DS:67:ARG:CB | 2.43 | 0.66 |
| 45:DT:82:LEU:N | 45:DT:82:LEU:HD12 | 2.11 | 0.66 |
| 1:AA:1321:C:C5' | 1:AA:1322:C:H5'' | 2.25 | 0.66 |
| 3:AC:86:VAL:O | 3:AC:90:GLU:HG2 | 1.96 | 0.66 |
| 10:AJ:26:ALA:HB1 | 10:AJ:29:ARG:HH21 | 1.61 | 0.66 |
| 31:BA:146:G:H5' | 31:BA:146:G:C8 | 2.27 | 0.66 |
| 37:BH:155:SER:O | 37:BH:157:TYR:N | 2.29 | 0.66 |
| 41:BP:13:ASN:HD22 | 41:BP:13:ASN:C | 1.99 | 0.66 |
| 47:BV:1:MET:HA | 47:BV:1:MET:HE2 | 1.78 | 0.66 |
| 50:BY:95:LYS:HE2 | 50:BY:101:LYS:HA | 1.77 | 0.66 |
| 1:CA:134:A:H61 | 16:CP:25:ARG:HH12 | 1.42 | 0.66 |
| 1:CA:441:A:H3' | 1:CA:442:C:C6 | 2.30 | 0.66 |
| 1:CA:949:A:H1' | 1:CA:1364:U:H3 | 1.61 | 0.66 |
| 9:CI:97:LYS:HB3 | 9:CI:98:PRO:HD3 | 1.78 | 0.66 |
| 6:CF:99:ALA:HB1 | 18:CR:23:LYS:HZ2 | 1.61 | 0.66 |
| 31:DA:1028:A:N6 | 31:DA:1125:G:H2' | 2.11 | 0.66 |
| 31:DA:2591:C:P | 33:DD:239:ARG:HG3 | 2.36 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:614(A):U:H4' | 31:DA:614(B):G:H5' | 1.78 | 0.66 |
| 31:DA:631:A:O2' | 41:DP:67:MET:HB3 | 1.94 | 0.66 |
| 32:DB:87:G:H3' | 32:DB:88:C:H5' | 1.76 | 0.66 |
| 33:DD:173:VAL:HG23 | 33:DD:174:ILE:N | 2.11 | 0.66 |
| 35:DF:18:ARG:HG2 | 35:DF:19:GLU:N | 2.08 | 0.66 |
| 39:DN:95:PRO:C | 39:DN:97:ARG:H | 1.97 | 0.66 |
| 1:AA:552:U:C2' | 1:AA:553:A:H5' | 2.26 | 0.65 |
| 8:AH:10:LEU:HD23 | 8:AH:10:LEU:N | 2.10 | 0.65 |
| 27:B5:25:LEU:HD12 | 48:BW:19:LEU:O | 1.96 | 0.65 |
| 31:BA:1531:C:H3' | 31:BA:1532:C:C5' | 2.26 | 0.65 |
| 31:BA:2301:C:H2' | 31:BA:2302:G:O4' | 1.96 | 0.65 |
| 31:BA:2789:C:OP1 | 31:BA:2789:C:H4' | 1.96 | 0.65 |
| 32:BB:21:G:O2' | 32:BB:22:U:P | 2.53 | 0.65 |
| 39:BN:68:GLU:HA | 39:BN:86:PRO:CB | 2.27 | 0.65 |
| 42:BQ:58:PHE:O | 42:BQ:58:PHE:HD1 | 1.79 | 0.65 |
| 46:BU:88:ILE:HD13 | 46:BU:88:ILE:O | 1.96 | 0.65 |
| 49:BX:24:GLY:O | 49:BX:25:LYS:O | 2.12 | 0.65 |
| 1:CA:625:G:H4' | 16:CP:16:HIS:CD2 | 2.32 | 0.65 |
| 15:CO:3:ILE:H | 15:CO:3:ILE:HD13 | 1.61 | 0.65 |
| 27:D5:50:GLY:O | 27:D5:51:TYR:HD1 | 1.79 | 0.65 |
| 31:DA:1022:G:N2 | 31:DA:1142(A):A:H2 | 1.89 | 0.65 |
| 31:DA:1109:C:H5 | 31:DA:1110:G:C4 | 2.14 | 0.65 |
| 22:D0:8:GLY:HA3 | 31:DA:2255:G:H21 | 1.61 | 0.65 |
| 42:DQ:20:ALA:HB2 | 42:DQ:99:PRO:CD | 2.25 | 0.65 |
| 47:DV:46:VAL:O | 47:DV:47:VAL:HB | 1.96 | 0.65 |
| 47:DV:72:VAL:HA | 47:DV:88:ARG:NH1 | 2.09 | 0.65 |
| 1:AA:335:C:O2' | 1:AA:336:C:H5' | 1.95 | 0.65 |
| 1:AA:559:A:C5' | 1:AA:560:U:H3' | 2.25 | 0.65 |
| 1:AA:659:U:H2' | 1:AA:660:G:H5' | 1.77 | 0.65 |
| 2:AB:201:ILE:HG21 | 2:AB:214:ILE:HG21 | 1.79 | 0.65 |
| 1:AA:972:C:H4' | 10:AJ:57:LYS:HG3 | 1.78 | 0.65 |
| 23:B1:73:LEU:HB3 | 23:B1:90:ILE:HG23 | 1.79 | 0.65 |
| 30:B8:13:ARG:NH2 | 31:BA:250:G:OP2 | 2.29 | 0.65 |
| 31:BA:2870:C:C2' | 31:BA:2871:C:H5' | 2.25 | 0.65 |
| 31:BA:807:U:H2' | 31:BA:808:G:O5' | 1.96 | 0.65 |
| 31:BA:951:C:O2' | 31:BA:952:G:H5' | 1.96 | 0.65 |
| 36:BG:106:LEU:O | 36:BG:111:LEU:HG | 1.96 | 0.65 |
| 47:BV:25:LEU:H | 47:BV:94:LEU:CD1 | 2.09 | 0.65 |
| 50:BY:99:CYS:SG | 50:BY:99:CYS:O | 2.55 | 0.65 |
| 51:BZ:5:LEU:CD1 | 51:BZ:43:GLU:HB3 | 2.24 | 0.65 |
| 1:CA:1169:A:H2' | 1:CA:1170:A:H8 | 1.61 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:922:G:O2' | 1:CA:1398:A:N1 | 2.29 | 0.65 |
| 1:CA:1530:G:OP1 | 1:CA:1530:G:H4' | 1.96 | 0.65 |
| 2:CB:22:LYS:NZ | 2:CB:40:HIS:HE1 | 1.94 | 0.65 |
| 3:CC:20:SER:HB2 | 3:CC:40:ARG:NH2 | 2.09 | 0.65 |
| 1:CA:1128:C:H5' | 9:CI:16:ARG:HH12 | 1.61 | 0.65 |
| 16:CP:22:THR:CG2 | 16:CP:32:TYR:HA | 2.26 | 0.65 |
| 31:DA:2206:G:N2 | 31:DA:2207:G:C5' | 2.48 | 0.65 |
| 31:DA:2564:A:C2 | 31:DA:2647:U:H4' | 2.29 | 0.65 |
| 31:DA:2022:U:O2' | 31:DA:2617:C:H5' | 1.96 | 0.65 |
| 31:DA:287:C:C2 | 31:DA:288:C:C6 | 2.84 | 0.65 |
| 38:DI:129:THR:HA | 38:DI:137:PRO:HA | 1.78 | 0.65 |
| 47:DV:19:LYS:HG3 | 47:DV:20:LEU:O | 1.95 | 0.65 |
| 31:DA:26:G:OP1 | 48:DW:80:PRO:HB3 | 1.96 | 0.65 |
| 49:DX:33:LYS:C | 49:DX:35:THR:N | 2.50 | 0.65 |
| 1:AA:949:A:H1' | 1:AA:1364:U:H3 | 1.62 | 0.65 |
| 19:AS:19:VAL:HG11 | 19:AS:44:MET:HG3 | 1.77 | 0.65 |
| 31:BA:1509:C:OP1 | 31:BA:1509:C:H4' | 1.95 | 0.65 |
| 22:B0:41:ARG:HB2 | 31:BA:2330:G:O2' | 1.96 | 0.65 |
| 31:BA:2580:U:H5' | 34:BE:131:ALA:H | 1.61 | 0.65 |
| 31:BA:2564:A:C2 | 31:BA:2647:U:H4' | 2.30 | 0.65 |
| 31:BA:340:A:H2' | 31:BA:341:G:H5' | 1.79 | 0.65 |
| 36:BG:61:ALA:HA | 36:BG:64:THR:HG22 | 1.77 | 0.65 |
| 37:BH:89:ILE:O | 37:BH:90:LYS:CG | 2.44 | 0.65 |
| 41:BP:17:LYS:CG | 41:BP:17:LYS:O | 2.43 | 0.65 |
| 44:BS:33:LYS:HB3 | 44:BS:34:HIS:HD2 | 1.57 | 0.65 |
| 44:BS:66:ALA:O | 44:BS:67:ARG:CB | 2.45 | 0.65 |
| 46:BU:16:LYS:O | 46:BU:20:LEU:HD23 | 1.97 | 0.65 |
| 39:BN:40:PRO:O | 46:BU:64:ARG:NH2 | 2.30 | 0.65 |
| 4:CD:117:ALA:O | 4:CD:121:VAL:HG23 | 1.96 | 0.65 |
| 4:CD:105:VAL:HG21 | 4:CD:126:ILE:HG21 | 1.78 | 0.65 |
| 24:D2:55:ARG:H | 24:D2:56:GLN:NE2 | 1.93 | 0.65 |
| 31:DA:1478:G:O2' | 31:DA:1479:G:H5' | 1.97 | 0.65 |
| 31:DA:958:U:O2' | 31:DA:959:A:P | 2.55 | 0.65 |
| 34:DE:36:ARG:HH11 | 34:DE:85:ASN:HD21 | 1.43 | 0.65 |
| 42:DQ:141:GLN:HE21 | 51:DZ:72:ARG:N | 1.95 | 0.65 |
| 1:AA:1289:A:H3' | 1:AA:1290:G:H8 | 1.61 | 0.65 |
| 1:AA:448:A:H62 | 1:AA:486:U:H3 | 1.45 | 0.65 |
| 1:AA:706:A:N7 | 1:AA:707:C:H5 | 1.95 | 0.65 |
| 2:AB:130:ARG:HA | 2:AB:130:ARG:HE | 1.61 | 0.65 |
| 10:AJ:6:ILE:HG13 | 10:AJ:72:VAL:O | 1.97 | 0.65 |
| 13:AM:10:PRO:CB | 13:AM:18:ALA:HB1 | 2.25 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AN:23:ARG:NH1 | 14:AN:30:ALA:HB2 | 2.11 | 0.65 |
| 24:B2:15:LYS:O | 24:B2:16:LEU:CB | 2.44 | 0.65 |
| 31:BA:1169:G:H1 | 31:BA:1180:C:N4 | 1.89 | 0.65 |
| 33:BD:137:PRO:O | 33:BD:140:THR:HG23 | 1.97 | 0.65 |
| 1:CA:1333:A:H2' | 1:CA:1334:G:O4' | 1.96 | 0.65 |
| 1:CA:503:C:H2' | 1:CA:504:C:H6 | 1.61 | 0.65 |
| 3:CC:71:ALA:HA | 3:CC:106:VAL:HB | 1.79 | 0.65 |
| 6:CF:5:GLU:HG3 | 6:CF:93:SER:OG | 1.96 | 0.65 |
| 31:DA:1464:C:O2' | 31:DA:1528:A:C8 | 2.44 | 0.65 |
| 31:DA:49:A:H4' | 31:DA:50:U:H5' | 1.78 | 0.65 |
| 37:DH:30:LYS:HG2 | 37:DH:79:VAL:O | 1.96 | 0.65 |
| 39:DN:125:GLY:HA2 | 39:DN:126:PRO:O | 1.97 | 0.65 |
| 42:DQ:141:GLN:CG | 51:DZ:72:ARG:HA | 2.26 | 0.65 |
| 51:DZ:151:HIS:HD2 | 51:DZ:151:HIS:N | 1.94 | 0.65 |
| 1:AA:333:G:H4' | 20:AT:16:HIS:CE1 | 2.32 | 0.65 |
| 1:AA:663:A:C2' | 1:AA:664:G:H5' | 2.26 | 0.65 |
| 1:AA:736:C:H2' | 1:AA:737:A:C8 | 2.31 | 0.65 |
| 1:AA:818:G:HO2' | 1:AA:820:U:H6 | 1.44 | 0.65 |
| 35:BF:158:THR:HG23 | 35:BF:160:ASN:N | 2.10 | 0.65 |
| 49:BX:57:LEU:HD11 | 49:BX:77:LYS:HD2 | 1.78 | 0.65 |
| 1:CA:539:A:H2' | 1:CA:540:G:C8 | 2.32 | 0.65 |
| 1:CA:1190:G:H3' | 3:CC:3:ASN:ND2 | 2.11 | 0.65 |
| 4:CD:9:CYS:SG | 4:CD:22:LYS:HD2 | 2.36 | 0.65 |
| 14:CN:23:ARG:NH1 | 14:CN:30:ALA:HB2 | 2.11 | 0.65 |
| 23:D1:19:GLN:HG3 | 23:D1:44:PRO:HG3 | 1.77 | 0.65 |
| 31:DA:1531:C:H3' | 31:DA:1532:C:C5' | 2.26 | 0.65 |
| 31:DA:2328:A:H2' | 31:DA:2329:G:C8 | 2.31 | 0.65 |
| 31:DA:307:G:H22 | 31:DA:310:A:C5' | 2.08 | 0.65 |
| 31:DA:579:G:H2' | 31:DA:580:C:C6 | 2.31 | 0.65 |
| 50:DY:39:VAL:HG12 | 50:DY:40:GLU:H | 1.62 | 0.65 |
| 50:DY:86:ARG:HG2 | 50:DY:87:LYS:H | 1.62 | 0.65 |
| 1:AA:113:G:H2' | 1:AA:114:U:C6 | 2.32 | 0.65 |
| 1:AA:1301:U:H3' | 1:AA:1302:U:H5'' | 1.79 | 0.65 |
| 1:AA:707:C:O2' | 1:AA:708:C:H5' | 1.97 | 0.65 |
| 18:AR:45:SER:H | 18:AR:51:LEU:HD11 | 1.62 | 0.65 |
| 26:B4:25:TYR:C | 26:B4:27:THR:H | 2.00 | 0.65 |
| 28:B6:20:ASN:O | 28:B6:21:TYR:CG | 2.48 | 0.65 |
| 30:B8:32:LEU:CB | 30:B8:34:TRP:H | 2.10 | 0.65 |
| 31:BA:620:G:H4' | 31:BA:621:A:C5' | 2.24 | 0.65 |
| 31:BA:830:G:H4' | 31:BA:831:G:OP2 | 1.96 | 0.65 |
| 33:BD:27:THR:CG2 | 33:BD:28:GLU:N | 2.60 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BT:28:VAL:HG13 | 45:BT:46:GLU:HB2 | 1.78 | 0.65 |
| 45:BT:28:VAL:CG2 | 45:BT:46:GLU:HG3 | 2.27 | 0.65 |
| 48:BW:86:LEU:HD12 | 48:BW:87:PRO:CD | 2.26 | 0.65 |
| 49:BX:89:ILE:HA | 49:BX:92:LEU:HD12 | 1.79 | 0.65 |
| 51:BZ:152:ALA:HB2 | 51:BZ:168:GLU:HA | 1.77 | 0.65 |
| 8:CH:86:ILE:HB | 8:CH:133:LEU:HD22 | 1.79 | 0.65 |
| 14:CN:23:ARG:HH11 | 14:CN:30:ALA:HB2 | 1.61 | 0.65 |
| 24:D2:30:ARG:HH11 | 24:D2:30:ARG:CG | 2.09 | 0.65 |
| 31:DA:1204:A:C2 | 31:DA:1241:A:C2 | 2.85 | 0.65 |
| 31:DA:1945:G:H2' | 31:DA:1946:U:C6 | 2.31 | 0.65 |
| 36:DG:52:ILE:HG22 | 36:DG:54:GLU:HG2 | 1.78 | 0.65 |
| 40:DO:13:ASN:HD21 | 40:DO:97:ARG:H | 1.45 | 0.65 |
| 47:DV:51:VAL:HG12 | 47:DV:52:VAL:N | 2.11 | 0.65 |
| 50:DY:96:ILE:HG21 | 50:DY:99:CYS:CB | 2.27 | 0.65 |
| 51:DZ:152:ALA:HB2 | 51:DZ:168:GLU:CA | 2.26 | 0.65 |
| 1:AA:1530:G:H4' | 1:AA:1530:G:OP1 | 1.94 | 0.65 |
| 1:AA:410:G:H1' | 1:AA:432:A:N6 | 2.12 | 0.65 |
| 6:AF:97:PHE:O | 18:AR:31:LEU:HD23 | 1.97 | 0.65 |
| 30:B8:32:LEU:HG | 30:B8:34:TRP:HE3 | 1.62 | 0.65 |
| 31:BA:151:C:O2' | 31:BA:152:G:H5' | 1.97 | 0.65 |
| 31:BA:1580:A:H8 | 31:BA:1580:A:OP2 | 1.80 | 0.65 |
| 34:BE:76:ARG:HG3 | 34:BE:195:LEU:HD22 | 1.79 | 0.65 |
| 37:BH:41:MET:CE | 37:BH:55:PRO:HD3 | 2.26 | 0.65 |
| 31:BA:814:C:H5 | 41:BP:27:HIS:NE2 | 1.93 | 0.65 |
| 1:CA:176:C:H2' | 1:CA:177:C:C6 | 2.32 | 0.65 |
| 1:CA:706:A:N7 | 1:CA:707:C:H5 | 1.94 | 0.65 |
| 5:CE:12:LEU:O | 5:CE:13:ILE:HD12 | 1.97 | 0.65 |
| 11:CK:125:PHE:CD1 | 11:CK:125:PHE:N | 2.61 | 0.65 |
| 30:D8:13:ARG:NH2 | 31:DA:250:G:OP2 | 2.29 | 0.65 |
| 31:DA:1509:C:OP1 | 31:DA:1509:C:H4' | 1.95 | 0.65 |
| 31:DA:1899:G:H21 | 31:DA:1902:C:H5 | 1.43 | 0.65 |
| 31:DA:2309:A:N3 | 31:DA:2310:A:H2 | 1.95 | 0.65 |
| 31:DA:823:G:O2' | 31:DA:824:A:H5' | 1.95 | 0.65 |
| 32:DB:44:G:H1' | 32:DB:47:C:H42 | 1.62 | 0.65 |
| 33:DD:173:VAL:HG23 | 33:DD:174:ILE:H | 1.62 | 0.65 |
| 33:DD:71:ASP:HB3 | 33:DD:103:ARG:NH2 | 2.12 | 0.65 |
| 50:DY:95:LYS:HE2 | 50:DY:101:LYS:HA | 1.79 | 0.65 |
| 51:DZ:51:ALA:O | 51:DZ:52:SER:HB3 | 1.97 | 0.65 |
| 51:DZ:64:GLY:O | 51:DZ:65:GLN:O | 2.13 | 0.65 |
| 1:AA:1003:G:C2 | 1:AA:1004:A:H1' | 2.32 | 0.65 |
| 1:AA:1169:A:H2' | 1:AA:1170:A:H8 | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:950:U:H2' | 1:AA:951:G:H8 | 1.60 | 0.65 |
| 18:AR:32:ARG:HA | 18:AR:69:THR:HG21 | 1.78 | 0.65 |
| 30:B8:61:LEU:HD13 | 31:BA:593:G:O2' | 1.97 | 0.65 |
| 31:BA:244:A:C2 | 31:BA:255:A:C4 | 2.84 | 0.65 |
| 31:BA:2836:U:H2' | 31:BA:2837:G:C8 | 2.32 | 0.65 |
| 31:BA:34:C:O2' | 31:BA:35:G:OP1 | 2.13 | 0.65 |
| 33:BD:31:LYS:HG2 | 33:BD:34:VAL:CG1 | 2.26 | 0.65 |
| 45:BT:50:ILE:HA | 45:BT:99:LEU:HD11 | 1.78 | 0.65 |
| 50:BY:46:LYS:C | 50:BY:47:LYS:HD2 | 2.17 | 0.65 |
| 51:BZ:61:LEU:HB2 | 51:BZ:65:GLN:HB2 | 1.78 | 0.65 |
| 1:CA:1497:G:H2' | 1:CA:1498:U:H5' | 1.79 | 0.65 |
| 1:CA:677:U:H3 | 1:CA:713:G:H22 | 1.45 | 0.65 |
| 2:CB:211:ILE:O | 2:CB:215:LEU:HB2 | 1.97 | 0.65 |
| 4:CD:164:ALA:HB1 | 4:CD:168:ARG:NH1 | 2.11 | 0.65 |
| 5:CE:51:VAL:O | 5:CE:55:VAL:HG23 | 1.97 | 0.65 |
| 9:CI:17:VAL:HG11 | 9:CI:81:ILE:HD13 | 1.78 | 0.65 |
| 18:CR:67:ALA:HA | 18:CR:70:ILE:HG13 | 1.76 | 0.65 |
| 23:D1:67:ILE:N | 23:D1:68:PRO:HD2 | 2.11 | 0.65 |
| 24:D2:15:LYS:O | 24:D2:16:LEU:CB | 2.45 | 0.65 |
| 30:D8:32:LEU:HD23 | 30:D8:35:GLN:CA | 2.27 | 0.65 |
| 31:DA:1884:A:C2' | 31:DA:1885:A:C5' | 2.74 | 0.65 |
| 31:DA:9:U:C4 | 31:DA:2629:A:N6 | 2.65 | 0.65 |
| 35:DF:22:ALA:HB1 | 35:DF:26:ALA:HB1 | 1.79 | 0.65 |
| 36:DG:106:LEU:O | 36:DG:111:LEU:HG | 1.96 | 0.65 |
| 36:DG:16:ARG:HH11 | 36:DG:31:VAL:HG11 | 1.61 | 0.65 |
| 37:DH:97:ARG:O | 37:DH:99:VAL:HG23 | 1.97 | 0.65 |
| 47:DV:18:LEU:HD13 | 47:DV:98:GLU:OE1 | 1.97 | 0.65 |
| 49:DX:24:GLY:O | 49:DX:25:LYS:O | 2.14 | 0.65 |
| 31:BA:1288:U:C2 | 31:BA:1327:C:O2 | 2.50 | 0.65 |
| 31:BA:1884:A:C2' | 31:BA:1885:A:C5' | 2.75 | 0.65 |
| 31:BA:2584:U:O4' | 31:BA:2584:U:O2 | 2.11 | 0.65 |
| 30:B8:61:LEU:HB3 | 31:BA:593:G:H4' | 1.78 | 0.65 |
| 31:BA:719:C:H2' | 31:BA:720:C:C6 | 2.32 | 0.65 |
| 31:BA:919:G:H5' | 32:BB:81:G:H1' | 1.78 | 0.65 |
| 26:B4:12:ALA:O | 36:BG:101:ILE:HD11 | 1.96 | 0.65 |
| 45:BT:17:THR:O | 45:BT:18:ASP:CB | 2.44 | 0.65 |
| 45:BT:42:ILE:HD13 | 45:BT:83:ILE:HD11 | 1.79 | 0.65 |
| 50:BY:96:ILE:HG22 | 50:BY:97:ARG:N | 2.11 | 0.65 |
| 1:CA:1321:C:C5' | 1:CA:1322:C:H5'' | 2.26 | 0.65 |
| 1:CA:499:A:H4' | 1:CA:500:G:OP1 | 1.96 | 0.65 |
| 1:CA:814:A:N7 | 1:CA:816:A:C4 | 2.65 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:983:A:H2 | 1:CA:984:C:C6 | 2.15 | 0.65 |
| 6:CF:60:PHE:C | 6:CF:61:LEU:HD12 | 2.16 | 0.65 |
| 8:CH:112:LEU:O | 8:CH:112:LEU:HD12 | 1.97 | 0.65 |
| 16:CP:45:THR:HG23 | 16:CP:46:PRO:HD2 | 1.78 | 0.65 |
| 24:D2:34:GLU:O | 24:D2:36:ARG:N | 2.29 | 0.65 |
| 31:DA:146:G:H5' | 31:DA:146:G:C8 | 2.26 | 0.65 |
| 31:DA:2464:C:O2' | 31:DA:2465:C:O5' | 2.13 | 0.65 |
| 31:DA:779:U:OP1 | 33:DD:49:ILE:HG13 | 1.97 | 0.65 |
| 31:DA:912:C:C2 | 31:DA:913:U:C5 | 2.85 | 0.65 |
| 31:DA:1844:C:OP1 | 33:DD:257:LEU:HD23 | 1.97 | 0.65 |
| 33:DD:83:GLU:HB2 | 33:DD:92:ILE:CD1 | 2.25 | 0.65 |
| 37:DH:32:GLU:O | 37:DH:33:LEU:HD23 | 1.97 | 0.65 |
| 38:DI:117:GLU:HG3 | 38:DI:118:LYS:H | 1.62 | 0.65 |
| 50:DY:10:GLY:O | 50:DY:27:VAL:HG22 | 1.97 | 0.65 |
| 1:AA:1172:C:H2' | 1:AA:1173:G:C8 | 2.32 | 0.65 |
| 8:AH:6:ILE:H | 8:AH:6:ILE:HD12 | 1.62 | 0.65 |
| 10:AJ:78:ASN:HB2 | 10:AJ:81:THR:HG23 | 1.78 | 0.65 |
| 14:AN:23:ARG:HH11 | 14:AN:30:ALA:HB2 | 1.61 | 0.65 |
| 28:B6:11:LEU:CD1 | 28:B6:51:GLU:HB2 | 2.27 | 0.65 |
| 31:BA:1693:U:OP2 | 31:BA:1694:C:H5 | 1.80 | 0.65 |
| 31:BA:2314:C:O2' | 31:BA:2315:G:H5' | 1.96 | 0.65 |
| 35:BF:117:ARG:HG2 | 35:BF:192:LEU:HB2 | 1.79 | 0.65 |
| 36:BG:115:ARG:NH1 | 36:BG:136:ARG:HG3 | 2.12 | 0.65 |
| 41:BP:120:ALA:O | 25:D3:1:MET:CA | 2.45 | 0.65 |
| 35:BF:34:TRP:CZ2 | 41:BP:12:ALA:HB2 | 2.32 | 0.65 |
| 41:BP:62:LEU:HD13 | 41:BP:62:LEU:H | 1.62 | 0.65 |
| 46:BU:88:ILE:O | 46:BU:88:ILE:CD1 | 2.44 | 0.65 |
| 47:BV:51:VAL:HG12 | 47:BV:52:VAL:H | 1.62 | 0.65 |
| 50:BY:86:ARG:HG2 | 50:BY:87:LYS:H | 1.62 | 0.65 |
| 50:BY:81:LYS:HG2 | 50:BY:96:ILE:CG2 | 2.26 | 0.65 |
| 1:CA:1159:U:H4' | 1:CA:1160:G:OP1 | 1.96 | 0.65 |
| 1:CA:1057:G:C5 | 1:CA:1204:A:C2 | 2.85 | 0.65 |
| 1:CA:1301:U:H3' | 1:CA:1302:U:H5'' | 1.79 | 0.65 |
| 6:CF:50:TYR:HE2 | 6:CF:52:ILE:HD11 | 1.62 | 0.65 |
| 8:CH:14:ARG:O | 8:CH:18:ARG:HD3 | 1.97 | 0.65 |
| 31:DA:1292:U:H2' | 31:DA:1293:C:C6 | 2.31 | 0.65 |
| 31:DA:2199:A:OP2 | 31:DA:2200:C:H5 | 1.80 | 0.65 |
| 31:DA:286:C:O2' | 31:DA:287:C:H5' | 1.97 | 0.65 |
| 31:DA:910:A:C5 | 42:DQ:13:GLN:OE1 | 2.50 | 0.65 |
| 33:DD:140:THR:O | 33:DD:165:ILE:HG12 | 1.97 | 0.65 |
| 33:DD:224:ALA:HB2 | 33:DD:233:HIS:HB3 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:DW:66:GLU:HA | 48:DW:69:LEU:HD11 | 1.77 | 0.65 |
| 1:AA:102:G:C4 | 1:AA:103:C:C5 | 2.85 | 0.64 |
| 1:AA:22:G:H2' | 1:AA:23:C:H6 | 1.62 | 0.64 |
| 1:AA:878:G:H5' | 8:AH:89:PRO:HG2 | 1.77 | 0.64 |
| 26:B4:19:GLY:C | 26:B4:21:VAL:H | 1.97 | 0.64 |
| 29:B7:11:LYS:HE2 | 31:BA:686:G:H5'' | 1.78 | 0.64 |
| 22:B0:55:ARG:HG3 | 31:BA:2365:G:OP1 | 1.97 | 0.64 |
| 33:BD:30:GLU:HG3 | 33:BD:63:ARG:NE | 2.12 | 0.64 |
| 34:BE:3:GLY:HA3 | 34:BE:81:ILE:HG13 | 1.78 | 0.64 |
| 37:BH:43:VAL:HG11 | 37:BH:53:GLU:H | 1.62 | 0.64 |
| 45:BT:28:VAL:O | 45:BT:28:VAL:HG12 | 1.96 | 0.64 |
| 1:CA:1288:A:H2 | 1:CA:1352:C:O2 | 1.80 | 0.64 |
| 1:CA:417:C:C2' | 1:CA:418:C:H5' | 2.25 | 0.64 |
| 1:CA:1371:G:O3' | 9:CI:69:GLY:HA3 | 1.98 | 0.64 |
| 20:CT:97:ALA:O | 20:CT:99:LEU:N | 2.29 | 0.64 |
| 31:DA:128:C:C6 | 31:DA:128:C:H3' | 2.33 | 0.64 |
| 38:DI:77:LEU:HD11 | 38:DI:101:LEU:HD22 | 1.79 | 0.64 |
| 41:DP:23:PRO:O | 41:DP:33:ARG:NE | 2.29 | 0.64 |
| 42:DQ:58:PHE:HD1 | 42:DQ:58:PHE:O | 1.80 | 0.64 |
| 48:DW:51:LEU:HD23 | 48:DW:105:VAL:HG11 | 1.80 | 0.64 |
| 1:AA:1238:A:H62 | 1:AA:1299:A:N6 | 1.94 | 0.64 |
| 1:AA:1501:C:H5'' | 1:AA:1502:A:OP2 | 1.97 | 0.64 |
| 1:AA:175:C:H2' | 1:AA:176:C:H6 | 1.61 | 0.64 |
| 1:AA:60:A:P | 1:AA:60:A:H8 | 2.20 | 0.64 |
| 2:AB:167:PRO:HG3 | 2:AB:188:ALA:HB2 | 1.77 | 0.64 |
| 1:AA:9:G:OP1 | 5:AE:122:GLU:HB2 | 1.97 | 0.64 |
| 7:AG:108:ALA:O | 7:AG:119:ARG:HD2 | 1.97 | 0.64 |
| 11:AK:125:PHE:H | 11:AK:125:PHE:HD1 | 1.45 | 0.64 |
| 16:AP:22:THR:CG2 | 16:AP:32:TYR:HA | 2.27 | 0.64 |
| 20:AT:97:ALA:O | 20:AT:99:LEU:N | 2.30 | 0.64 |
| 30:B8:32:LEU:HG | 30:B8:34:TRP:CE3 | 2.32 | 0.64 |
| 31:BA:1021:A:N6 | 31:BA:1141:U:H3 | 1.93 | 0.64 |
| 31:BA:1719:G:H2' | 31:BA:1720:U:H5' | 1.78 | 0.64 |
| 31:BA:174:C:C3' | 31:BA:175:G:H5'' | 2.27 | 0.64 |
| 31:BA:528:A:C2 | 31:BA:2043:C:H4' | 2.32 | 0.64 |
| 31:BA:2286:A:O2' | 31:BA:2286:A:C8 | 2.50 | 0.64 |
| 31:BA:2713:A:H3' | 31:BA:2714:G:H5' | 1.79 | 0.64 |
| 31:BA:65:C:H2' | 31:BA:66:C:C6 | 2.30 | 0.64 |
| 34:BE:101:ARG:HB3 | 34:BE:169:ASN:HD22 | 1.61 | 0.64 |
| 34:BE:73:GLU:HG3 | 34:BE:74:PRO:CD | 2.17 | 0.64 |
| 37:BH:158:HIS:CE1 | 37:BH:168:PRO:HB2 | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:BT:61:PHE:CE2 | 45:BT:76:PHE:HB2 | 2.32 | 0.64 |
| 31:BA:996:A:H4' | 46:BU:92:ARG:NE | 2.10 | 0.64 |
| 47:BV:2:PHE:HE1 | 47:BV:13:ARG:CZ | 2.10 | 0.64 |
| 47:BV:66:ARG:CD | 47:BV:67:GLY:N | 2.60 | 0.64 |
| 49:BX:65:ARG:CZ | 49:BX:66:LEU:N | 2.60 | 0.64 |
| 51:BZ:151:HIS:N | 51:BZ:151:HIS:HD2 | 1.93 | 0.64 |
| 1:CA:1346:A:H5'' | 9:CI:120:ARG:HH12 | 1.61 | 0.64 |
| 1:CA:663:A:C2' | 1:CA:664:G:H5' | 2.27 | 0.64 |
| 6:CF:48:LEU:HD13 | 6:CF:52:ILE:HG12 | 1.79 | 0.64 |
| 9:CI:114:TYR:CD2 | 9:CI:114:TYR:N | 2.65 | 0.64 |
| 27:D5:40:LYS:CD | 27:D5:46:CYS:HB3 | 2.26 | 0.64 |
| 31:DA:1291:C:H2' | 31:DA:1292:U:C6 | 2.32 | 0.64 |
| 31:DA:1694:C:O2' | 31:DA:1695:G:C2 | 2.48 | 0.64 |
| 31:DA:1833:U:H2' | 31:DA:1834:U:C6 | 2.31 | 0.64 |
| 31:DA:1839:G:C8 | 31:DA:1839:G:H5' | 2.31 | 0.64 |
| 33:DD:35:LYS:HG2 | 33:DD:64:ILE:N | 2.12 | 0.64 |
| 35:DF:18:ARG:CG | 35:DF:19:GLU:H | 2.06 | 0.64 |
| 49:DX:89:ILE:HD12 | 49:DX:92:LEU:HD12 | 1.77 | 0.64 |
| 1:AA:448:A:H2' | 1:AA:449:C:C6 | 2.32 | 0.64 |
| 2:AB:77:ALA:HB2 | 2:AB:211:ILE:HD13 | 1.79 | 0.64 |
| 3:AC:108:ASN:HB3 | 3:AC:111:LEU:HB2 | 1.79 | 0.64 |
| 30:B8:26:LYS:HE2 | 30:B8:47:LYS:HZ2 | 1.63 | 0.64 |
| 31:BA:1833:U:H2' | 31:BA:1834:U:H6 | 1.62 | 0.64 |
| 31:BA:2309:A:N3 | 31:BA:2310:A:H2 | 1.96 | 0.64 |
| 31:BA:847:U:H5 | 31:BA:933:A:H62 | 1.42 | 0.64 |
| 33:BD:118:VAL:HG22 | 33:BD:119:ALA:N | 2.13 | 0.64 |
| 1:CA:542:G:H2' | 1:CA:543:C:H6 | 1.61 | 0.64 |
| 1:CA:818:G:O2' | 1:CA:819:A:H5' | 1.97 | 0.64 |
| 2:CB:187:LEU:HD23 | 2:CB:201:ILE:HG22 | 1.78 | 0.64 |
| 4:CD:68:TYR:N | 4:CD:68:TYR:CD1 | 2.65 | 0.64 |
| 6:CF:23:LYS:O | 6:CF:27:GLN:HG2 | 1.96 | 0.64 |
| 23:D1:94:LEU:HD22 | 23:D1:95:LEU:N | 2.13 | 0.64 |
| 31:DA:2262:U:H2' | 31:DA:2263:C:C5' | 2.26 | 0.64 |
| 31:DA:2836:U:H2' | 31:DA:2837:G:C8 | 2.32 | 0.64 |
| 45:DT:129:ARG:NH1 | 45:DT:131:ALA:HB3 | 2.12 | 0.64 |
| 47:DV:73:SER:OG | 47:DV:75:PHE:CE1 | 2.50 | 0.64 |
| 1:AA:1159:U:H4' | 1:AA:1160:G:OP1 | 1.96 | 0.64 |
| 1:AA:1287:A:C2 | 1:AA:1353:G:H1' | 2.33 | 0.64 |
| 1:AA:977:A:H2' | 1:AA:978:A:H5' | 1.79 | 0.64 |
| 11:AK:24:SER:HB3 | 11:AK:27:ASN:O | 1.97 | 0.64 |
| 15:AO:8:LYS:O | 15:AO:12:ILE:HG13 | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AT:11:SER:HA | 20:AT:13:LEU:HD13 | 1.80 | 0.64 |
| 31:BA:195:A:H4' | 31:BA:251:A:O2' | 1.97 | 0.64 |
| 32:BB:44:G:H1' | 32:BB:47:C:H42 | 1.62 | 0.64 |
| 33:BD:10:THR:OG1 | 33:BD:13:ARG:HB2 | 1.97 | 0.64 |
| 33:BD:266:SER:O | 33:BD:267:SER:CB | 2.44 | 0.64 |
| 38:BI:61:ARG:O | 38:BI:133:HIS:HE1 | 1.80 | 0.64 |
| 41:BP:10:PRO:HD2 | 41:BP:11:GLY:H | 1.62 | 0.64 |
| 43:BR:33:ARG:CG | 43:BR:115:GLU:HG3 | 2.21 | 0.64 |
| 48:BW:18:ARG:CG | 48:BW:18:ARG:HH11 | 2.10 | 0.64 |
| 50:BY:8:LYS:HD2 | 50:BY:8:LYS:N | 2.12 | 0.64 |
| 22:D0:72:ARG:HH21 | 22:D0:75:LEU:CD1 | 2.10 | 0.64 |
| 25:D3:49:LYS:HE2 | 31:DA:850:C:O3' | 1.98 | 0.64 |
| 31:DA:142:A:H8 | 31:DA:1595:G:N2 | 1.93 | 0.64 |
| 31:DA:2404:C:H2' | 31:DA:2405:G:H5' | 1.80 | 0.64 |
| 33:DD:249:PRO:HD2 | 33:DD:250:TRP:CE3 | 2.32 | 0.64 |
| 37:DH:35:VAL:O | 37:DH:37:VAL:HG23 | 1.97 | 0.64 |
| 41:DP:25:SER:O | 41:DP:30:THR:HG23 | 1.98 | 0.64 |
| 42:DQ:8:LYS:HG3 | 42:DQ:9:TYR:N | 2.10 | 0.64 |
| 45:DT:32:TYR:CD2 | 45:DT:32:TYR:N | 2.64 | 0.64 |
| 47:DV:69:LYS:HB3 | 47:DV:93:GLU:CD | 2.18 | 0.64 |
| 1:AA:874:G:O2' | 1:AA:875:C:H5' | 1.97 | 0.64 |
| 1:AA:983:A:H2 | 1:AA:984:C:C6 | 2.16 | 0.64 |
| 2:AB:162:ILE:O | 2:AB:185:ILE:HG12 | 1.98 | 0.64 |
| 2:AB:211:ILE:O | 2:AB:215:LEU:HB2 | 1.96 | 0.64 |
| 4:AD:68:TYR:HE2 | 4:AD:97:LEU:HB3 | 1.62 | 0.64 |
| 24:B2:54:LYS:H | 24:B2:56:GLN:NE2 | 1.96 | 0.64 |
| 31:BA:1973:G:H2' | 31:BA:1974:C:C6 | 2.32 | 0.64 |
| 33:BD:106:ILE:O | 33:BD:106:ILE:HD13 | 1.98 | 0.64 |
| 1:AA:1442(A):G:H8 | 45:BT:118:ARG:HH11 | 1.40 | 0.64 |
| 46:BU:40:PHE:HB3 | 47:BV:78:LYS:HD2 | 1.79 | 0.64 |
| 47:BV:1:MET:HE3 | 47:BV:44:LYS:CB | 2.27 | 0.64 |
| 18:CR:45:SER:HB3 | 18:CR:51:LEU:HD21 | 1.80 | 0.64 |
| 22:D0:55:ARG:HG3 | 31:DA:2365:G:OP1 | 1.98 | 0.64 |
| 31:DA:1531:C:H5'' | 31:DA:1532:C:H6 | 1.63 | 0.64 |
| 31:DA:2655:G:H2' | 31:DA:2655:G:N3 | 2.12 | 0.64 |
| 45:DT:54:ARG:HA | 45:DT:59:THR:HB | 1.80 | 0.64 |
| 48:DW:4:LYS:CB | 48:DW:106:ILE:HG22 | 2.20 | 0.64 |
| 31:BA:2422:A:H4' | 31:BA:2423:U:OP1 | 1.97 | 0.64 |
| 39:BN:125:GLY:HA2 | 39:BN:126:PRO:O | 1.96 | 0.64 |
| 45:BT:30:VAL:HG23 | 45:BT:31:SER:N | 2.13 | 0.64 |
| 47:BV:18:LEU:HD13 | 47:BV:98:GLU:OE1 | 1.96 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:BX:56:THR:C | 49:BX:57:LEU:HD12 | 2.18 | 0.64 |
| 1:CA:833:U:H2' | 1:CA:834:C:H6 | 1.62 | 0.64 |
| 2:CB:187:LEU:HD13 | 2:CB:187:LEU:O | 1.98 | 0.64 |
| 1:CA:921:U:O2 | 5:CE:19:MET:HB2 | 1.96 | 0.64 |
| 18:CR:45:SER:H | 18:CR:51:LEU:HD11 | 1.62 | 0.64 |
| 30:D8:14:VAL:HG13 | 30:D8:22:VAL:HG13 | 1.80 | 0.64 |
| 31:DA:1204:A:C2 | 31:DA:1241:A:N1 | 2.66 | 0.64 |
| 23:D1:47:GLN:CG | 31:DA:2230:G:H1' | 2.20 | 0.64 |
| 31:DA:2310:A:O2' | 31:DA:2311:A:H5'' | 1.98 | 0.64 |
| 31:DA:234:C:H2' | 31:DA:235:U:C6 | 2.33 | 0.64 |
| 23:D1:32:LYS:HG2 | 31:DA:2396:G:O2' | 1.98 | 0.64 |
| 31:DA:244:A:C2 | 31:DA:255:A:C4 | 2.85 | 0.64 |
| 31:DA:708:C:H5' | 31:DA:709:U:OP2 | 1.97 | 0.64 |
| 41:DP:16:ARG:CZ | 41:DP:16:ARG:HB2 | 2.27 | 0.64 |
| 41:DP:80:TYR:CD1 | 41:DP:111:ARG:HB3 | 2.32 | 0.64 |
| 45:DT:38:ASN:HD22 | 45:DT:40:THR:H | 1.43 | 0.64 |
| 45:DT:57:PHE:O | 45:DT:59:THR:N | 2.30 | 0.64 |
| 46:DU:90:VAL:O | 46:DU:92:ARG:N | 2.30 | 0.64 |
| 47:DV:72:VAL:O | 47:DV:73:SER:OG | 2.14 | 0.64 |
| 7:AG:26:PHE:O | 7:AG:30:ILE:HG12 | 1.96 | 0.64 |
| 17:AQ:40:LYS:HG2 | 17:AQ:41:LYS:N | 2.13 | 0.64 |
| 18:AR:67:ALA:HA | 18:AR:70:ILE:HG13 | 1.80 | 0.64 |
| 24:B2:51:ARG:HD3 | 24:B2:51:ARG:O | 1.97 | 0.64 |
| 30:B8:32:LEU:HB3 | 30:B8:34:TRP:CB | 2.23 | 0.64 |
| 31:BA:1405:U:H2' | 31:BA:1406:U:H6 | 1.59 | 0.64 |
| 35:BF:16:GLY:O | 35:BF:17:ARG:HG3 | 1.97 | 0.64 |
| 46:BU:31:SER:C | 46:BU:33:ARG:H | 2.01 | 0.64 |
| 46:BU:87:GLY:O | 47:BV:52:VAL:HA | 1.98 | 0.64 |
| 47:BV:54:GLY:O | 47:BV:56:SER:N | 2.30 | 0.64 |
| 50:BY:15:VAL:O | 50:BY:22:GLY:HA2 | 1.98 | 0.64 |
| 1:CA:1501:C:H5'' | 1:CA:1502:A:OP2 | 1.98 | 0.64 |
| 1:CA:355:C:C4 | 1:CA:356:A:N7 | 2.66 | 0.64 |
| 1:CA:863:U:H2' | 1:CA:865:A:OP2 | 1.98 | 0.64 |
| 10:CJ:51:ARG:NE | 10:CJ:61:GLU:HB2 | 2.10 | 0.64 |
| 18:CR:32:ARG:HA | 18:CR:69:THR:HG21 | 1.79 | 0.64 |
| 22:D0:43:THR:O | 22:D0:45:PHE:N | 2.30 | 0.64 |
| 23:D1:47:GLN:HG2 | 31:DA:2230:G:C1' | 2.18 | 0.64 |
| 31:DA:1173:G:H3' | 31:DA:1174:A:C5' | 2.28 | 0.64 |
| 31:DA:2610:C:H4' | 31:DA:2611:U:OP2 | 1.97 | 0.64 |
| 24:D2:48:HIS:NE2 | 31:DA:75:G:H4' | 2.13 | 0.64 |
| 31:DA:760:G:H2' | 31:DA:761:A:O4' | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:DH:43:VAL:HG11 | 37:DH:53:GLU:H | 1.62 | 0.64 |
| 31:DA:1187:G:H5'' | 47:DV:82:ARG:NH1 | 2.13 | 0.64 |
| 1:AA:166:G:H2' | 1:AA:167:G:H8 | 1.63 | 0.64 |
| 1:AA:16:A:O2' | 1:AA:17:U:H5' | 1.98 | 0.64 |
| 1:AA:447:G:H2' | 1:AA:485:G:N2 | 2.13 | 0.64 |
| 6:AF:23:LYS:O | 6:AF:27:GLN:HG2 | 1.97 | 0.64 |
| 7:AG:91:VAL:HG13 | 7:AG:95:ARG:HD3 | 1.80 | 0.64 |
| 24:B2:54:LYS:N | 24:B2:56:GLN:HE22 | 1.96 | 0.64 |
| 25:B3:11:SER:OG | 25:B3:13:ILE:HG12 | 1.97 | 0.64 |
| 31:BA:1884:A:H2' | 31:BA:1885:A:H5' | 1.77 | 0.64 |
| 30:B8:4:MET:HE1 | 31:BA:593:G:C1' | 2.27 | 0.64 |
| 32:BB:37:C:C5 | 32:BB:38:C:C4 | 2.85 | 0.64 |
| 34:BE:128:SER:O | 34:BE:130:GLY:N | 2.31 | 0.64 |
| 34:BE:60:ASN:ND2 | 34:BE:60:ASN:N | 2.46 | 0.64 |
| 37:BH:97:ARG:O | 37:BH:98:LEU:C | 2.36 | 0.64 |
| 38:BI:56:LYS:HA | 38:BI:59:ALA:HB3 | 1.80 | 0.64 |
| 51:BZ:152:ALA:HB2 | 51:BZ:168:GLU:N | 2.12 | 0.64 |
| 1:CA:1152:A:O2' | 1:CA:1153:C:H5' | 1.98 | 0.64 |
| 1:CA:524:G:H2' | 1:CA:525:C:C6 | 2.33 | 0.64 |
| 6:CF:91:VAL:HG11 | 18:CR:72:ARG:NH1 | 2.12 | 0.64 |
| 10:CJ:78:ASN:HB2 | 10:CJ:81:THR:HG23 | 1.79 | 0.64 |
| 19:CS:19:VAL:HG11 | 19:CS:44:MET:HG3 | 1.79 | 0.64 |
| 30:D8:40:GLU:OE1 | 30:D8:44:LYS:HE3 | 1.98 | 0.64 |
| 31:DA:542:C:H42 | 31:DA:543:C:N4 | 1.94 | 0.64 |
| 31:DA:828:U:H3' | 31:DA:828:U:O2 | 1.96 | 0.64 |
| 32:DB:47:C:O2' | 44:DS:93:LYS:HG2 | 1.98 | 0.64 |
| 33:DD:158:ALA:O | 33:DD:159:ALA:CB | 2.46 | 0.64 |
| 33:DD:44:ASN:HB3 | 33:DD:49:ILE:CA | 2.28 | 0.64 |
| 34:DE:37:ARG:HD3 | 34:DE:44:TYR:OH | 1.98 | 0.64 |
| 39:DN:25:ARG:HG3 | 39:DN:25:ARG:HH11 | 1.63 | 0.64 |
| 46:DU:87:GLY:O | 47:DV:52:VAL:HA | 1.97 | 0.64 |
| 47:DV:69:LYS:CG | 47:DV:70:ILE:H | 2.02 | 0.64 |
| 50:DY:28:LYS:HA | 50:DY:39:VAL:H | 1.62 | 0.64 |
| 1:AA:448:A:OP2 | 1:AA:485:G:N2 | 2.25 | 0.64 |
| 1:AA:504:C:H1' | 1:AA:510:A:C4 | 2.33 | 0.64 |
| 3:AC:155:GLY:O | 3:AC:156:ARG:HB2 | 1.98 | 0.64 |
| 1:AA:134:A:H61 | 16:AP:25:ARG:NH1 | 1.96 | 0.64 |
| 24:B2:47:ASN:C | 24:B2:49:LYS:H | 2.01 | 0.64 |
| 31:BA:1478:G:O2' | 31:BA:1479:G:H5' | 1.97 | 0.64 |
| 31:BA:1784:A:H4' | 31:BA:1785:A:O5' | 1.96 | 0.64 |
| 31:BA:2689:U:H4' | 31:BA:2690:C:OP2 | 1.95 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BD:210:GLY:O | 33:BD:211:ARG:HB3 | 1.95 | 0.64 |
| 33:BD:25:THR:O | 33:BD:27:THR:HB | 1.98 | 0.64 |
| 31:BA:1568:G:H21 | 33:BD:58:HIS:CE1 | 2.14 | 0.64 |
| 33:BD:35:LYS:HE3 | 33:BD:65:ILE:CA | 2.28 | 0.64 |
| 36:BG:139:LEU:HA | 36:BG:144:ILE:HG23 | 1.79 | 0.64 |
| 36:BG:55:LYS:HG2 | 36:BG:58:GLN:NE2 | 2.11 | 0.64 |
| 39:BN:56:ASN:H | 39:BN:125:GLY:CA | 2.11 | 0.64 |
| 41:BP:85:LEU:HD23 | 41:BP:85:LEU:N | 2.09 | 0.64 |
| 44:BS:26:LEU:O | 44:BS:88:ASP:HB3 | 1.98 | 0.64 |
| 46:BU:90:VAL:HG13 | 47:BV:39:LEU:HG | 1.79 | 0.64 |
| 47:BV:69:LYS:HB3 | 47:BV:93:GLU:CD | 2.18 | 0.64 |
| 49:BX:82:GLN:C | 49:BX:85:PRO:HD2 | 2.17 | 0.64 |
| 1:CA:1287:A:C2 | 1:CA:1353:G:H1' | 2.33 | 0.64 |
| 3:CC:36:ASP:HB3 | 3:CC:40:ARG:NH1 | 2.13 | 0.64 |
| 18:CR:43:PHE:C | 18:CR:44:LEU:HD12 | 2.17 | 0.64 |
| 41:BP:140:ALA:CB | 25:D3:38:GLU:HG2 | 2.23 | 0.64 |
| 31:DA:1916:A:H2' | 31:DA:1917:U:O4' | 1.98 | 0.64 |
| 31:DA:827:U:O2' | 31:DA:2068:U:C2 | 2.45 | 0.64 |
| 37:DH:30:LYS:HZ3 | 37:DH:81:GLU:HA | 1.61 | 0.64 |
| 1:AA:417:C:C2' | 1:AA:418:C:H5' | 2.27 | 0.64 |
| 2:AB:141:GLU:O | 2:AB:145:LEU:HB2 | 1.97 | 0.64 |
| 4:AD:105:VAL:HG21 | 4:AD:126:ILE:HG21 | 1.79 | 0.64 |
| 22:B0:68:GLU:HG3 | 22:B0:80:HIS:HB2 | 1.79 | 0.64 |
| 31:BA:1497:U:C5' | 31:BA:1498:C:H5 | 2.08 | 0.64 |
| 31:BA:2205:C:O2 | 31:BA:2220:G:C2 | 2.51 | 0.64 |
| 31:BA:272(J):C:H42 | 31:BA:363(A):A:N6 | 1.95 | 0.64 |
| 31:BA:767:U:O2' | 31:BA:768:G:H5' | 1.98 | 0.64 |
| 31:BA:993:G:H1' | 47:BV:91:TYR:CD1 | 2.32 | 0.64 |
| 40:BO:85:VAL:HG11 | 40:BO:114:ILE:CD1 | 2.28 | 0.64 |
| 44:BS:66:ALA:HA | 44:BS:69:VAL:CG1 | 2.29 | 0.64 |
| 44:BS:77:ALA:O | 44:BS:80:LEU:HD12 | 1.97 | 0.64 |
| 45:BT:91:ARG:CB | 45:BT:116:ALA:HA | 2.28 | 0.64 |
| 46:BU:65:ILE:HG12 | 46:BU:96:ALA:HB3 | 1.80 | 0.64 |
| 4:CD:64:LEU:HD12 | 4:CD:64:LEU:C | 2.17 | 0.64 |
| 31:DA:1278:A:OP1 | 43:DR:36:THR:CG2 | 2.45 | 0.64 |
| 31:DA:1763:G:OP1 | 31:DA:1763:G:H4' | 1.98 | 0.64 |
| 31:DA:2475:C:H6 | 31:DA:2475:C:H5'' | 1.63 | 0.64 |
| 34:DE:87:GLU:O | 34:DE:89:ASP:N | 2.31 | 0.64 |
| 36:DG:76:SER:CB | 36:DG:83:ARG:HB3 | 2.27 | 0.64 |
| 39:DN:3:THR:CA | 39:DN:4:TYR:CD1 | 2.81 | 0.64 |
| 39:DN:67:LEU:O | 39:DN:69:GLN:N | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 44:DS:77:ALA:O | 44:DS:80:LEU:HD12 | 1.98 | 0.64 |
| 48:DW:59:VAL:HG12 | 48:DW:60:ASN:N | 2.13 | 0.64 |
| 50:DY:2:ARG:C | 50:DY:4:LYS:H | 2.01 | 0.64 |
| 1:AA:355:C:H2' | 1:AA:356:A:H5' | 1.80 | 0.63 |
| 1:AA:539:A:H2' | 1:AA:540:G:C8 | 2.32 | 0.63 |
| 1:AA:677:U:H3 | 1:AA:713:G:H22 | 1.45 | 0.63 |
| 5:AE:51:VAL:O | 5:AE:55:VAL:HG23 | 1.98 | 0.63 |
| 8:AH:20:TYR:HA | 8:AH:65:TYR:CZ | 2.33 | 0.63 |
| 24:B2:26:ARG:HA | 24:B2:29:LYS:HE3 | 1.79 | 0.63 |
| 31:BA:1980:G:O2' | 31:BA:1982:C:OP2 | 2.16 | 0.63 |
| 31:BA:2307:G:H3' | 31:BA:2307:G:N3 | 2.13 | 0.63 |
| 31:BA:2712:U:O2' | 31:BA:2712(A):A:OP2 | 2.13 | 0.63 |
| 31:BA:443:A:H1' | 31:BA:1201:C:O4' | 1.98 | 0.63 |
| 35:BF:18:ARG:HG2 | 35:BF:19:GLU:N | 2.08 | 0.63 |
| 38:BI:29:TYR:HD2 | 38:BI:30:LEU:HD23 | 1.64 | 0.63 |
| 47:BV:72:VAL:O | 47:BV:73:SER:CB | 2.46 | 0.63 |
| 5:CE:144:THR:O | 5:CE:148:VAL:HG23 | 1.97 | 0.63 |
| 17:CQ:40:LYS:HD2 | 17:CQ:42:TYR:CZ | 2.33 | 0.63 |
| 31:DA:1884:A:H2' | 31:DA:1885:A:H5' | 1.79 | 0.63 |
| 31:DA:2475:C:C5' | 31:DA:2476:A:OP2 | 2.43 | 0.63 |
| 31:DA:358:U:H3' | 31:DA:358:U:H6 | 1.63 | 0.63 |
| 32:DB:37:C:C5 | 32:DB:38:C:C5 | 2.86 | 0.63 |
| 38:DI:9:LEU:H | 38:DI:13:GLY:CA | 2.10 | 0.63 |
| 45:DT:28:VAL:CG2 | 45:DT:46:GLU:HG3 | 2.27 | 0.63 |
| 49:DX:83:VAL:O | 49:DX:84:ALA:HB3 | 1.98 | 0.63 |
| 1:AA:1446:U:O2' | 1:AA:1447:A:C8 | 2.50 | 0.63 |
| 1:AA:830:G:H2' | 1:AA:831:U:H6 | 1.63 | 0.63 |
| 2:AB:22:LYS:NZ | 2:AB:40:HIS:HE1 | 1.95 | 0.63 |
| 23:B1:67:ILE:N | 23:B1:68:PRO:HD2 | 2.13 | 0.63 |
| 23:B1:85:LEU:CA | 23:B1:87:PRO:HD3 | 2.28 | 0.63 |
| 27:B5:57:VAL:HB | 27:B5:58:LEU:HD12 | 1.80 | 0.63 |
| 31:BA:2328:A:H2' | 31:BA:2329:G:C8 | 2.33 | 0.63 |
| 31:BA:530:G:O4' | 31:BA:530:G:N3 | 2.31 | 0.63 |
| 33:BD:253:GLN:HB3 | 33:BD:255:LYS:CE | 2.28 | 0.63 |
| 35:BF:10:PRO:HG2 | 35:BF:13:SER:OG | 1.98 | 0.63 |
| 40:BO:4:PRO:O | 40:BO:5:GLN:CB | 2.46 | 0.63 |
| 31:BA:626:U:N3 | 41:BP:105:LEU:HG | 2.13 | 0.63 |
| 45:BT:50:ILE:HD13 | 45:BT:64:ARG:HB3 | 1.79 | 0.63 |
| 42:BQ:24:GLY:HA3 | 51:BZ:78:LYS:CB | 2.25 | 0.63 |
| 1:CA:1392:G:C2' | 1:CA:1393:U:H5' | 2.29 | 0.63 |
| 1:CA:793:U:O2 | 1:CA:1516:G:H4' | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:977:A:H2' | 1:CA:978:A:H5' | 1.79 | 0.63 |
| 2:CB:71:VAL:HB | 2:CB:164:VAL:CG2 | 2.28 | 0.63 |
| 2:CB:188:ALA:HB1 | 2:CB:192:SER:HB2 | 1.81 | 0.63 |
| 3:CC:91:LEU:HB3 | 3:CC:99:VAL:HG21 | 1.79 | 0.63 |
| 16:CP:17:TYR:HE1 | 16:CP:41:PRO:HG3 | 1.63 | 0.63 |
| 31:DA:1499:C:C2' | 31:DA:1500:G:H5' | 2.28 | 0.63 |
| 31:DA:150:C:H2' | 31:DA:151:C:H6 | 1.63 | 0.63 |
| 32:DB:21:G:O2' | 32:DB:22:U:P | 2.55 | 0.63 |
| 33:DD:267:SER:C | 33:DD:269:PHE:N | 2.48 | 0.63 |
| 33:DD:71:ASP:CB | 33:DD:103:ARG:NH2 | 2.61 | 0.63 |
| 39:DN:62:VAL:HG21 | 39:DN:66:LYS:HD2 | 1.80 | 0.63 |
| 41:DP:95:VAL:HG22 | 41:DP:125:VAL:HB | 1.80 | 0.63 |
| 3:AC:71:ALA:HA | 3:AC:106:VAL:HB | 1.78 | 0.63 |
| 4:AD:138:TYR:CD2 | 4:AD:138:TYR:C | 2.70 | 0.63 |
| 16:AP:17:TYR:HE1 | 16:AP:41:PRO:HG3 | 1.63 | 0.63 |
| 31:BA:1593:G:H8 | 31:BA:1593:G:H5' | 1.63 | 0.63 |
| 33:BD:255:LYS:H | 33:BD:255:LYS:HZ1 | 1.44 | 0.63 |
| 34:BE:37:ARG:HD3 | 34:BE:44:TYR:OH | 1.98 | 0.63 |
| 34:BE:51:PHE:O | 34:BE:74:PRO:HB3 | 1.98 | 0.63 |
| 41:BP:107:LYS:C | 41:BP:109:GLY:H | 1.98 | 0.63 |
| 46:BU:83:LEU:HG | 46:BU:88:ILE:CG1 | 2.23 | 0.63 |
| 31:BA:518:G:H4' | 48:BW:18:ARG:NH1 | 2.13 | 0.63 |
| 1:CA:373:A:H2' | 1:CA:374:A:H8 | 1.64 | 0.63 |
| 2:CB:111:ARG:HH11 | 2:CB:111:ARG:CG | 1.92 | 0.63 |
| 2:CB:87:ARG:NE | 2:CB:233:SER:HB3 | 2.10 | 0.63 |
| 15:CO:17:ARG:HG3 | 15:CO:17:ARG:NH1 | 1.99 | 0.63 |
| 31:DA:1434:A:H2' | 31:DA:1435:G:C8 | 2.33 | 0.63 |
| 31:DA:2327:A:H2' | 31:DA:2328:A:H8 | 1.62 | 0.63 |
| 31:DA:2335:A:C8 | 31:DA:2337:G:C5 | 2.86 | 0.63 |
| 31:DA:2364:C:H2' | 31:DA:2365:G:O4' | 1.99 | 0.63 |
| 31:DA:2580:U:H5' | 34:DE:131:ALA:H | 1.62 | 0.63 |
| 31:DA:2637:U:O2' | 31:DA:2638:G:H5' | 1.98 | 0.63 |
| 31:DA:340:A:H2' | 31:DA:341:G:H5' | 1.79 | 0.63 |
| 35:DF:117:ARG:HG2 | 35:DF:192:LEU:HB2 | 1.80 | 0.63 |
| 48:DW:73:ALA:HB3 | 48:DW:106:ILE:HD11 | 1.80 | 0.63 |
| 1:AA:499:A:H4' | 1:AA:500:G:OP1 | 1.97 | 0.63 |
| 2:AB:21:ARG:HB3 | 2:AB:39:ILE:HA | 1.80 | 0.63 |
| 4:AD:9:CYS:SG | 4:AD:22:LYS:HD2 | 2.38 | 0.63 |
| 5:AE:78:HIS:CE1 | 5:AE:142:LEU:HD23 | 2.34 | 0.63 |
| 25:B3:19:GLN:NE2 | 25:B3:52:HIS:CE1 | 2.66 | 0.63 |
| 28:B6:16:CYS:O | 28:B6:18:ARG:NH2 | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1503:U:C4 | 31:BA:1504:C:N4 | 2.67 | 0.63 |
| 31:BA:466:A:H5'' | 31:BA:467:G:OP2 | 1.99 | 0.63 |
| 36:BG:52:ILE:HG22 | 36:BG:54:GLU:HG2 | 1.78 | 0.63 |
| 44:BS:26:LEU:HD22 | 44:BS:87:PHE:CE1 | 2.34 | 0.63 |
| 45:BT:32:TYR:CG | 45:BT:81:PRO:HB2 | 2.34 | 0.63 |
| 46:BU:64:ARG:NH2 | 46:BU:64:ARG:CA | 2.60 | 0.63 |
| 1:CA:1172:C:H2' | 1:CA:1173:G:C8 | 2.33 | 0.63 |
| 6:CF:76:ALA:HB1 | 6:CF:80:ARG:HH21 | 1.64 | 0.63 |
| 16:CP:53:VAL:O | 16:CP:57:ARG:HG2 | 1.98 | 0.63 |
| 31:DA:2238:G:H4' | 31:DA:2239:G:OP1 | 1.98 | 0.63 |
| 31:DA:676:A:H2 | 31:DA:802:A:H61 | 1.42 | 0.63 |
| 34:DE:167:VAL:HG23 | 34:DE:170:LEU:HD11 | 1.80 | 0.63 |
| 34:DE:73:GLU:HG3 | 34:DE:74:PRO:CD | 2.20 | 0.63 |
| 34:DE:95:ILE:N | 34:DE:95:ILE:HD12 | 2.14 | 0.63 |
| 26:D4:12:ALA:O | 36:DG:101:ILE:HD11 | 1.99 | 0.63 |
| 36:DG:55:LYS:HG2 | 36:DG:58:GLN:NE2 | 2.13 | 0.63 |
| 39:DN:67:LEU:C | 39:DN:69:GLN:H | 2.02 | 0.63 |
| 40:DO:13:ASN:ND2 | 40:DO:97:ARG:H | 1.96 | 0.63 |
| 4:AD:61:LYS:HD3 | 4:AD:62:GLN:N | 2.14 | 0.63 |
| 1:AA:1080:A:H5' | 5:AE:14:ARG:NH2 | 2.12 | 0.63 |
| 6:AF:18:GLN:HA | 6:AF:21:LEU:CD2 | 2.19 | 0.63 |
| 7:AG:13:GLN:O | 7:AG:24:THR:HG21 | 1.98 | 0.63 |
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:CE2 | 2.34 | 0.63 |
| 16:AP:34:GLU:OE2 | 16:AP:55:ARG:HD3 | 1.98 | 0.63 |
| 23:B1:25:LYS:O | 23:B1:26:ARG:HB3 | 1.96 | 0.63 |
| 23:B1:87:PRO:CD | 23:B1:88:LYS:H | 2.12 | 0.63 |
| 30:B8:52:LYS:N | 30:B8:54:GLU:HG2 | 2.11 | 0.63 |
| 31:BA:1157:G:C6 | 31:BA:1158:C:N4 | 2.66 | 0.63 |
| 31:BA:1210:A:C8 | 31:BA:1210:A:C5' | 2.79 | 0.63 |
| 23:B1:32:LYS:HG2 | 31:BA:2396:G:O2' | 1.98 | 0.63 |
| 33:BD:224:ALA:HB2 | 33:BD:233:HIS:HB3 | 1.79 | 0.63 |
| 35:BF:103:LYS:HA | 35:BF:106:ARG:HG3 | 1.80 | 0.63 |
| 38:BI:133:HIS:CB | 38:BI:134:PRO:CD | 2.77 | 0.63 |
| 41:BP:95:VAL:HG22 | 41:BP:125:VAL:HB | 1.80 | 0.63 |
| 30:B8:46:ARG:NH2 | 41:BP:65:ARG:NH2 | 2.40 | 0.63 |
| 45:BT:129:ARG:NH1 | 45:BT:131:ALA:HB3 | 2.13 | 0.63 |
| 49:BX:57:LEU:CD1 | 49:BX:77:LYS:HD2 | 2.28 | 0.63 |
| 49:BX:89:ILE:HA | 49:BX:92:LEU:HB2 | 1.81 | 0.63 |
| 1:CA:175:C:H2' | 1:CA:176:C:H6 | 1.63 | 0.63 |
| 1:CA:335:C:O2' | 1:CA:336:C:H5' | 1.98 | 0.63 |
| 4:CD:138:TYR:CD2 | 4:CD:138:TYR:C | 2.69 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 12:CL:51:ALA:O | 12:CL:52:LEU:HD23 | 1.98 | 0.63 |
| 13:CM:10:PRO:CB | 13:CM:18:ALA:HB1 | 2.24 | 0.63 |
| 31:DA:1882:C:H2' | 31:DA:1882:C:O2 | 1.98 | 0.63 |
| 22:D0:41:ARG:HB2 | 31:DA:2330:G:O2' | 1.99 | 0.63 |
| 31:DA:2712(A):A:H5'' | 31:DA:2713:A:OP2 | 1.98 | 0.63 |
| 31:DA:296:C:O2' | 31:DA:297:C:H5' | 1.98 | 0.63 |
| 33:DD:28:GLU:HB2 | 33:DD:29:PRO:HD3 | 1.80 | 0.63 |
| 31:DA:1670:C:O2 | 34:DE:129:HIS:HE1 | 1.81 | 0.63 |
| 35:DF:20:LEU:HD22 | 35:DF:203:GLN:NE2 | 2.12 | 0.63 |
| 40:DO:85:VAL:HG11 | 40:DO:114:ILE:CD1 | 2.29 | 0.63 |
| 42:DQ:20:ALA:O | 42:DQ:22:LYS:N | 2.31 | 0.63 |
| 31:DA:911:A:C2' | 42:DQ:9:TYR:OH | 2.43 | 0.63 |
| 45:DT:32:TYR:CG | 45:DT:81:PRO:HB2 | 2.33 | 0.63 |
| 50:DY:17:SER:HA | 50:DY:71:LYS:HG2 | 1.80 | 0.63 |
| 1:AA:1371:G:O3' | 9:AI:69:GLY:HA3 | 1.99 | 0.63 |
| 1:AA:952:U:H4' | 1:AA:964:A:H61 | 1.63 | 0.63 |
| 12:AL:86:ARG:HB2 | 12:AL:101:VAL:HG22 | 1.81 | 0.63 |
| 12:AL:51:ALA:O | 12:AL:52:LEU:HD23 | 1.97 | 0.63 |
| 23:B1:94:LEU:HD22 | 23:B1:95:LEU:N | 2.14 | 0.63 |
| 31:BA:1504:C:O2' | 31:BA:1505:C:O5' | 2.16 | 0.63 |
| 31:BA:542:C:H42 | 31:BA:543:C:H42 | 1.46 | 0.63 |
| 32:BB:86:G:C3' | 32:BB:87:G:C8 | 2.81 | 0.63 |
| 35:BF:3:GLU:HA | 35:BF:24:LEU:CB | 2.29 | 0.63 |
| 41:BP:65:ARG:O | 41:BP:68:GLN:HB3 | 1.98 | 0.63 |
| 46:BU:69:CYS:HB3 | 46:BU:106:PHE:CZ | 2.33 | 0.63 |
| 47:BV:36:PRO:HG2 | 47:BV:62:LEU:HD11 | 1.81 | 0.63 |
| 1:CA:113:G:H2' | 1:CA:114:U:C6 | 2.34 | 0.63 |
| 1:CA:262:A:H2' | 1:CA:263:A:C8 | 2.34 | 0.63 |
| 1:CA:539:A:OP2 | 12:CL:115:LYS:HE3 | 1.99 | 0.63 |
| 1:CA:604:G:C5 | 1:CA:605:U:C5 | 2.87 | 0.63 |
| 1:CA:693:G:H1' | 7:CG:82:GLY:HA3 | 1.79 | 0.63 |
| 8:CH:88:LYS:HB3 | 8:CH:89:PRO:HD2 | 1.81 | 0.63 |
| 23:D1:87:PRO:CD | 23:D1:88:LYS:H | 2.12 | 0.63 |
| 23:D1:85:LEU:CA | 23:D1:87:PRO:HD3 | 2.28 | 0.63 |
| 31:DA:1339:G:H21 | 31:DA:1603:A:H1' | 1.64 | 0.63 |
| 31:DA:1694:C:O2' | 31:DA:1695:G:C4 | 2.51 | 0.63 |
| 31:DA:1947:C:H2' | 31:DA:1948:G:C5' | 2.29 | 0.63 |
| 31:DA:2262:U:C2' | 31:DA:2263:C:C5' | 2.77 | 0.63 |
| 31:DA:2360:A:O2' | 31:DA:2361:A:C5' | 2.47 | 0.63 |
| 31:DA:2478:A:H2' | 31:DA:2479:G:H5' | 1.79 | 0.63 |
| 29:D7:11:LYS:HE2 | 31:DA:686:G:H5'' | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DD:210:GLY:O | 33:DD:211:ARG:HB3 | 1.97 | 0.63 |
| 33:DD:25:THR:O | 33:DD:27:THR:HB | 1.99 | 0.63 |
| 34:DE:14:ILE:HG12 | 34:DE:21:VAL:HG22 | 1.80 | 0.63 |
| 34:DE:120:TRP:CE3 | 34:DE:155:LYS:HD3 | 2.33 | 0.63 |
| 39:DN:45:ASN:HD22 | 39:DN:45:ASN:N | 1.91 | 0.63 |
| 41:DP:17:LYS:O | 41:DP:17:LYS:CG | 2.45 | 0.63 |
| 39:DN:40:PRO:HA | 46:DU:64:ARG:NH2 | 2.14 | 0.63 |
| 1:AA:255:G:H1' | 17:AQ:16:GLN:NE2 | 2.14 | 0.63 |
| 9:AI:45:ALA:O | 9:AI:48:GLU:HB2 | 1.98 | 0.63 |
| 12:AL:87:GLY:HA2 | 12:AL:98:TYR:HA | 1.80 | 0.63 |
| 23:B1:14:VAL:O | 23:B1:46:LEU:HD23 | 1.99 | 0.63 |
| 31:BA:1173:G:H3' | 31:BA:1174:A:C5' | 2.28 | 0.63 |
| 31:BA:2023:G:H5' | 31:BA:2617:C:H4' | 1.80 | 0.63 |
| 31:BA:8:A:H2' | 31:BA:9:U:C6 | 2.34 | 0.63 |
| 33:BD:35:LYS:CE | 33:BD:104:TYR:HD1 | 2.11 | 0.63 |
| 31:BA:322:A:OP2 | 35:BF:169:ASN:HB2 | 1.98 | 0.63 |
| 39:BN:62:VAL:HG21 | 39:BN:66:LYS:HD2 | 1.79 | 0.63 |
| 44:BS:53:SER:OG | 44:BS:54:LEU:N | 2.30 | 0.63 |
| 44:BS:66:ALA:O | 44:BS:67:ARG:HB2 | 1.99 | 0.63 |
| 31:BA:17:G:H4' | 46:BU:25:TRP:CH2 | 2.32 | 0.63 |
| 1:CA:693:G:O2' | 7:CG:82:GLY:HA3 | 1.98 | 0.63 |
| 27:D5:48:GLU:O | 27:D5:50:GLY:N | 2.32 | 0.63 |
| 31:DA:2307:G:N3 | 31:DA:2307:G:H3' | 2.13 | 0.63 |
| 31:DA:2591:C:OP2 | 33:DD:239:ARG:HB2 | 1.99 | 0.63 |
| 31:DA:662:G:P | 41:DP:18:ARG:HD2 | 2.38 | 0.63 |
| 38:DI:6:LEU:O | 38:DI:15:VAL:HB | 1.98 | 0.63 |
| 42:DQ:8:LYS:CG | 42:DQ:9:TYR:N | 2.62 | 0.63 |
| 49:DX:70:LEU:HG | 49:DX:71:GLY:N | 2.13 | 0.63 |
| 42:DQ:60:ARG:HA | 51:DZ:179:ASP:N | 2.13 | 0.63 |
| 2:AB:71:VAL:HB | 2:AB:164:VAL:CG2 | 2.29 | 0.63 |
| 4:AD:68:TYR:N | 4:AD:68:TYR:CD1 | 2.66 | 0.63 |
| 31:BA:1204:A:C2 | 31:BA:1241:A:C2 | 2.86 | 0.63 |
| 31:BA:1744:C:C2' | 31:BA:1745:C:H5' | 2.28 | 0.63 |
| 31:BA:2360:A:O2' | 31:BA:2361:A:C5' | 2.47 | 0.63 |
| 31:BA:2364:C:H2' | 31:BA:2365:G:O4' | 1.99 | 0.63 |
| 31:BA:676:A:H8 | 31:BA:2069:G:N2 | 1.86 | 0.63 |
| 31:BA:760:G:H2' | 31:BA:761:A:O4' | 1.99 | 0.63 |
| 33:BD:27:THR:CG2 | 33:BD:28:GLU:H | 2.11 | 0.63 |
| 38:BI:117:GLU:HG3 | 38:BI:118:LYS:H | 1.64 | 0.63 |
| 41:BP:48:PRO:O | 41:BP:50:ARG:N | 2.32 | 0.63 |
| 31:BA:2496:C:OP1 | 42:BQ:82:ARG:HD3 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BT:32:TYR:CD2 | 45:BT:81:PRO:O | 2.52 | 0.63 |
| 51:BZ:152:ALA:HB2 | 51:BZ:168:GLU:CA | 2.29 | 0.63 |
| 1:CA:1072:G:H2' | 1:CA:1073:U:C6 | 2.34 | 0.63 |
| 12:CL:110:VAL:HG21 | 12:CL:120:TYR:HB3 | 1.80 | 0.63 |
| 23:D1:26:ARG:CB | 23:D1:34:THR:HA | 2.29 | 0.63 |
| 31:DA:2286:A:O2' | 31:DA:2286:A:C8 | 2.48 | 0.63 |
| 31:DA:2301:C:H2' | 31:DA:2302:G:O4' | 1.98 | 0.63 |
| 31:DA:195:A:H4' | 31:DA:251:A:O2' | 1.97 | 0.63 |
| 31:DA:34:C:O2' | 31:DA:35:G:OP1 | 2.15 | 0.63 |
| 33:DD:35:LYS:CE | 33:DD:104:TYR:HD1 | 2.11 | 0.63 |
| 33:DD:35:LYS:NZ | 33:DD:64:ILE:O | 2.30 | 0.63 |
| 49:DX:72:LYS:CG | 49:DX:74:PRO:HD3 | 2.29 | 0.63 |
| 1:AA:1057:G:C5 | 1:AA:1204:A:C2 | 2.87 | 0.63 |
| 16:AP:45:THR:HG23 | 16:AP:46:PRO:HD2 | 1.80 | 0.63 |
| 18:AR:43:PHE:O | 18:AR:44:LEU:HD12 | 1.99 | 0.63 |
| 24:B2:31:GLU:HG2 | 24:B2:37:PHE:HD1 | 1.64 | 0.63 |
| 30:B8:6:THR:HG21 | 31:BA:243:U:OP1 | 1.99 | 0.63 |
| 31:BA:354:G:O5' | 31:BA:354:G:H8 | 1.81 | 0.63 |
| 33:BD:63:ARG:NH1 | 33:BD:63:ARG:HG3 | 2.04 | 0.63 |
| 31:BA:1030:G:OP2 | 42:BQ:128:LYS:HE2 | 1.99 | 0.63 |
| 50:BY:10:GLY:O | 50:BY:27:VAL:HG22 | 1.98 | 0.63 |
| 4:CD:61:LYS:HD3 | 4:CD:62:GLN:N | 2.14 | 0.63 |
| 8:CH:20:TYR:HA | 8:CH:65:TYR:CZ | 2.34 | 0.63 |
| 10:CJ:6:ILE:HG13 | 10:CJ:72:VAL:O | 1.98 | 0.63 |
| 12:CL:86:ARG:HB2 | 12:CL:101:VAL:HG22 | 1.80 | 0.63 |
| 24:D2:56:GLN:CD | 24:D2:56:GLN:H | 2.01 | 0.63 |
| 31:DA:314:A:O2' | 31:DA:315:G:H5' | 1.99 | 0.63 |
| 31:DA:1658:C:OP1 | 34:DE:132:HIS:ND1 | 2.30 | 0.63 |
| 39:DN:67:LEU:HB3 | 39:DN:88:GLU:OE2 | 1.99 | 0.63 |
| 49:DX:57:LEU:HD11 | 49:DX:77:LYS:HD2 | 1.80 | 0.63 |
| 1:AA:793:U:O2 | 1:AA:1516:G:H4' | 1.99 | 0.62 |
| 3:AC:50:ALA:HB1 | 3:AC:70:VAL:HG11 | 1.81 | 0.62 |
| 16:AP:53:VAL:O | 16:AP:57:ARG:HG2 | 1.99 | 0.62 |
| 30:B8:61:LEU:HD22 | 31:BA:593:G:O3' | 1.99 | 0.62 |
| 31:BA:2317:C:C2' | 31:BA:2318:G:C5' | 2.65 | 0.62 |
| 33:BD:35:LYS:NZ | 33:BD:64:ILE:O | 2.32 | 0.62 |
| 34:BE:46:ALA:HA | 34:BE:82:ARG:O | 1.98 | 0.62 |
| 41:BP:80:TYR:CD1 | 41:BP:111:ARG:HB3 | 2.34 | 0.62 |
| 49:BX:70:LEU:HG | 49:BX:71:GLY:N | 2.14 | 0.62 |
| 1:CA:1073:U:H2' | 1:CA:1074:G:C8 | 2.34 | 0.62 |
| 1:CA:1225:A:H2' | 1:CA:1225:A:N3 | 2.13 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 12:CL:27:LEU:O | 12:CL:29:GLY:N | 2.29 | 0.62 |
| 23:D1:25:LYS:O | 23:D1:26:ARG:CB | 2.46 | 0.62 |
| 23:D1:92:LYS:C | 23:D1:94:LEU:N | 2.52 | 0.62 |
| 31:DA:2058:A:H5'' | 31:DA:2059:A:OP2 | 2.00 | 0.62 |
| 31:DA:2192:G:H2' | 31:DA:2193:G:H5' | 1.81 | 0.62 |
| 31:DA:2565:A:H5'' | 31:DA:2566:A:OP2 | 1.99 | 0.62 |
| 31:DA:8:A:H2' | 31:DA:9:U:C6 | 2.33 | 0.62 |
| 33:DD:133:LEU:HB3 | 33:DD:173:VAL:HG11 | 1.80 | 0.62 |
| 45:DT:91:ARG:CB | 45:DT:116:ALA:HA | 2.30 | 0.62 |
| 1:AA:543:C:C2 | 1:AA:544:G:C8 | 2.87 | 0.62 |
| 2:AB:188:ALA:HB1 | 2:AB:192:SER:HB2 | 1.81 | 0.62 |
| 23:B1:23:LYS:HB2 | 23:B1:37:ILE:HG22 | 1.79 | 0.62 |
| 27:B5:51:TYR:CD2 | 27:B5:52:TYR:CZ | 2.87 | 0.62 |
| 31:BA:184:C:H2' | 31:BA:185:U:H6 | 1.63 | 0.62 |
| 31:BA:2537:U:H2' | 31:BA:2538:C:C6 | 2.34 | 0.62 |
| 31:BA:2712(A):A:H5'' | 31:BA:2713:A:OP2 | 1.98 | 0.62 |
| 33:BD:143:HIS:HD2 | 33:BD:144:ALA:CB | 2.12 | 0.62 |
| 36:BG:10:LYS:O | 36:BG:15:VAL:HG23 | 2.00 | 0.62 |
| 42:BQ:52:VAL:HA | 42:BQ:55:VAL:HG13 | 1.81 | 0.62 |
| 1:CA:166:G:H2' | 1:CA:167:G:H8 | 1.64 | 0.62 |
| 1:CA:344:A:O2' | 1:CA:346:G:N7 | 2.32 | 0.62 |
| 1:CA:797:C:OP1 | 11:CK:124:LYS:HE2 | 1.99 | 0.62 |
| 2:CB:114:ARG:HD2 | 2:CB:141:GLU:OE1 | 1.99 | 0.62 |
| 8:CH:17:THR:HB | 8:CH:78:GLN:OE1 | 1.99 | 0.62 |
| 17:CQ:40:LYS:HG2 | 17:CQ:41:LYS:N | 2.14 | 0.62 |
| 22:D0:68:GLU:HG3 | 22:D0:80:HIS:HB2 | 1.81 | 0.62 |
| 26:D4:25:TYR:C | 26:D4:27:THR:H | 2.01 | 0.62 |
| 31:DA:1839:G:H8 | 31:DA:1839:G:H5' | 1.64 | 0.62 |
| 31:DA:2681:C:C5 | 31:DA:2725:A:N6 | 2.48 | 0.62 |
| 31:DA:2897:U:H2' | 31:DA:2897:U:O2 | 1.99 | 0.62 |
| 31:DA:530:G:N3 | 31:DA:530:G:O4' | 2.32 | 0.62 |
| 38:DI:117:GLU:HG3 | 38:DI:118:LYS:N | 2.13 | 0.62 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:H8 | 1.64 | 0.62 |
| 1:AA:1199:U:H4' | 10:AJ:54:PHE:CZ | 2.34 | 0.62 |
| 1:AA:355:C:C4 | 1:AA:356:A:N7 | 2.67 | 0.62 |
| 1:AA:503:C:H2' | 1:AA:504:C:H6 | 1.64 | 0.62 |
| 1:AA:542:G:H2' | 1:AA:543:C:H6 | 1.63 | 0.62 |
| 6:AF:5:GLU:HG3 | 6:AF:93:SER:OG | 1.99 | 0.62 |
| 1:AA:1227:A:OP2 | 13:AM:111:LYS:HE2 | 1.98 | 0.62 |
| 27:B5:51:TYR:CD2 | 27:B5:52:TYR:CE2 | 2.87 | 0.62 |
| 31:BA:1478:G:C2' | 31:BA:1479:G:H5' | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1694:C:O2' | 31:BA:1695:G:C4 | 2.52 | 0.62 |
| 31:BA:1916:A:H2' | 31:BA:1917:U:O4' | 1.99 | 0.62 |
| 31:BA:2262:U:H2' | 31:BA:2263:C:C5' | 2.29 | 0.62 |
| 31:BA:2307:G:C2 | 31:BA:2308:G:H5' | 2.35 | 0.62 |
| 33:BD:158:ALA:O | 33:BD:159:ALA:CB | 2.47 | 0.62 |
| 33:BD:247:ALA:HA | 33:BD:254:THR:HG22 | 1.80 | 0.62 |
| 33:BD:35:LYS:CG | 33:BD:64:ILE:N | 2.62 | 0.62 |
| 33:BD:83:GLU:HB2 | 33:BD:92:ILE:CD1 | 2.28 | 0.62 |
| 34:BE:39:PRO:HA | 34:BE:43:GLY:HA2 | 1.79 | 0.62 |
| 37:BH:30:LYS:HG2 | 37:BH:79:VAL:O | 1.99 | 0.62 |
| 50:BY:38:ILE:HG22 | 50:BY:39:VAL:H | 1.64 | 0.62 |
| 1:CA:448:A:H62 | 1:CA:486:U:H3 | 1.46 | 0.62 |
| 1:CA:684:A:H2' | 1:CA:685:G:C8 | 2.34 | 0.62 |
| 2:CB:162:ILE:O | 2:CB:185:ILE:HG12 | 1.99 | 0.62 |
| 3:CC:108:ASN:HB3 | 3:CC:111:LEU:HB2 | 1.81 | 0.62 |
| 6:CF:99:ALA:HB1 | 18:CR:23:LYS:NZ | 2.13 | 0.62 |
| 8:CH:1:MET:HE2 | 8:CH:1:MET:H3 | 1.64 | 0.62 |
| 1:CA:1199:U:H4' | 10:CJ:54:PHE:CZ | 2.34 | 0.62 |
| 23:D1:8:SER:N | 23:D1:46:LEU:HD13 | 2.14 | 0.62 |
| 31:DA:1332:G:C8 | 31:DA:1332:G:H5' | 2.35 | 0.62 |
| 31:DA:1796:U:H2' | 31:DA:1797:C:C6 | 2.34 | 0.62 |
| 31:DA:195:A:C8 | 31:DA:197:A:OP1 | 2.53 | 0.62 |
| 31:DA:71:A:C8 | 31:DA:71:A:H5' | 2.35 | 0.62 |
| 33:DD:13:ARG:HD2 | 33:DD:16:MET:HE3 | 1.82 | 0.62 |
| 37:DH:149:ARG:HD3 | 37:DH:164:TYR:HE1 | 1.65 | 0.62 |
| 38:DI:12:LEU:O | 38:DI:12:LEU:HG | 1.99 | 0.62 |
| 43:DR:53:HIS:HD2 | 43:DR:94:TYR:OH | 1.82 | 0.62 |
| 44:DS:87:PHE:HB2 | 44:DS:106:ARG:HD3 | 1.81 | 0.62 |
| 46:DU:102:GLU:HG3 | 47:DV:2:PHE:HZ | 1.64 | 0.62 |
| 1:AA:1392:G:O2' | 1:AA:1393:U:H5' | 2.00 | 0.62 |
| 1:AA:684:A:H2' | 1:AA:685:G:C8 | 2.34 | 0.62 |
| 12:AL:41:ARG:CG | 12:AL:42:THR:H | 2.12 | 0.62 |
| 16:AP:19:ILE:HG22 | 16:AP:36:ILE:HG13 | 1.82 | 0.62 |
| 23:B1:19:GLN:HG3 | 23:B1:44:PRO:HG3 | 1.80 | 0.62 |
| 24:B2:48:HIS:NE2 | 31:BA:75:G:H4' | 2.14 | 0.62 |
| 31:BA:1265:A:OP1 | 31:BA:1265:A:H8 | 1.82 | 0.62 |
| 31:BA:1531:C:H5'' | 31:BA:1532:C:H6 | 1.64 | 0.62 |
| 31:BA:2101:G:C6 | 31:BA:2102:U:C5 | 2.88 | 0.62 |
| 31:BA:2392:A:H2 | 31:BA:2424:C:H42 | 1.46 | 0.62 |
| 33:BD:71:ASP:CB | 33:BD:103:ARG:NH2 | 2.61 | 0.62 |
| 34:BE:167:VAL:HG23 | 34:BE:170:LEU:HD11 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BG:64:THR:HG23 | 36:BG:65:GLY:N | 2.14 | 0.62 |
| 37:BH:41:MET:HE1 | 37:BH:54:ARG:HA | 1.82 | 0.62 |
| 37:BH:85:LYS:HZ2 | 37:BH:133:VAL:HB | 1.64 | 0.62 |
| 45:BT:82:LEU:N | 45:BT:82:LEU:HD12 | 2.15 | 0.62 |
| 49:BX:85:PRO:O | 49:BX:86:GLY:C | 2.37 | 0.62 |
| 50:BY:10:GLY:CA | 50:BY:27:VAL:HG13 | 2.14 | 0.62 |
| 7:CG:116:ALA:O | 7:CG:120:ILE:HG12 | 2.00 | 0.62 |
| 28:D6:9:LEU:HD13 | 28:D6:9:LEU:C | 2.19 | 0.62 |
| 31:DA:528:A:C2 | 31:DA:2043:C:H5' | 2.35 | 0.62 |
| 44:DS:74:ALA:O | 44:DS:77:ALA:HB3 | 1.99 | 0.62 |
| 47:DV:2:PHE:HE1 | 47:DV:13:ARG:CZ | 2.13 | 0.62 |
| 49:DX:57:LEU:CD1 | 49:DX:77:LYS:HD2 | 2.29 | 0.62 |
| 50:DY:81:LYS:HG2 | 50:DY:97:ARG:H | 1.64 | 0.62 |
| 1:AA:1096:C:O2' | 1:AA:1097:C:H5' | 2.00 | 0.62 |
| 2:AB:22:LYS:HZ3 | 2:AB:22:LYS:HA | 1.62 | 0.62 |
| 3:AC:138:VAL:HG22 | 3:AC:151:VAL:HG23 | 1.80 | 0.62 |
| 4:AD:64:LEU:HD12 | 4:AD:64:LEU:C | 2.20 | 0.62 |
| 5:AE:144:THR:O | 5:AE:148:VAL:HG23 | 2.00 | 0.62 |
| 23:B1:48:LYS:O | 23:B1:49:VAL:HB | 2.00 | 0.62 |
| 24:B2:15:LYS:HA | 24:B2:18:PRO:HD2 | 1.80 | 0.62 |
| 31:BA:1497:U:H2' | 31:BA:1497:U:O2 | 2.00 | 0.62 |
| 31:BA:195:A:C8 | 31:BA:197:A:OP1 | 2.53 | 0.62 |
| 31:BA:2287:A:H61 | 31:BA:2344:U:H3 | 1.45 | 0.62 |
| 31:BA:389:G:H1 | 41:BP:71:VAL:H | 1.48 | 0.62 |
| 34:BE:87:GLU:O | 34:BE:89:ASP:N | 2.32 | 0.62 |
| 44:BS:97:ARG:C | 44:BS:97:ARG:HD2 | 2.20 | 0.62 |
| 50:BY:79:CYS:O | 50:BY:80:GLY:C | 2.37 | 0.62 |
| 1:CA:1321:C:C3' | 1:CA:1322:C:H5'' | 2.30 | 0.62 |
| 1:CA:1446:U:O2' | 1:CA:1447:A:C8 | 2.51 | 0.62 |
| 1:CA:333:G:H4' | 20:CT:16:HIS:CE1 | 2.35 | 0.62 |
| 1:CA:626:U:C2 | 1:CA:627:G:N7 | 2.67 | 0.62 |
| 11:CK:41:THR:HG22 | 11:CK:42:TRP:N | 2.14 | 0.62 |
| 6:CF:97:PHE:O | 18:CR:31:LEU:HD23 | 2.00 | 0.62 |
| 31:DA:196:A:O4' | 41:DP:46:LYS:HE2 | 1.99 | 0.62 |
| 35:DF:3:GLU:HA | 35:DF:24:LEU:CB | 2.30 | 0.62 |
| 37:DH:85:LYS:HZ2 | 37:DH:133:VAL:HB | 1.65 | 0.62 |
| 31:DA:494:G:H21 | 48:DW:57:ASN:HD21 | 1.45 | 0.62 |
| 1:AA:1064:G:H5' | 1:AA:1066:C:H1' | 1.82 | 0.62 |
| 1:AA:1281:U:H5' | 1:AA:1282:C:C5 | 2.31 | 0.62 |
| 4:AD:107:ARG:HD2 | 4:AD:173:TRP:HZ2 | 1.65 | 0.62 |
| 10:AJ:34:VAL:CG2 | 10:AJ:74:ILE:HG22 | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:16:ASP:HB3 | 13:AM:41:PRO:HB3 | 1.82 | 0.62 |
| 10:AJ:49:VAL:HG13 | 14:AN:41:ARG:HB2 | 1.80 | 0.62 |
| 31:BA:1481:U:H5' | 31:BA:1482:G:OP2 | 2.00 | 0.62 |
| 31:BA:2661:G:O2' | 31:BA:2662:A:OP1 | 2.12 | 0.62 |
| 31:BA:828:U:O2 | 31:BA:828:U:H3' | 1.98 | 0.62 |
| 33:BD:35:LYS:CE | 33:BD:104:TYR:CD1 | 2.82 | 0.62 |
| 51:BZ:125:LEU:HD23 | 51:BZ:126:VAL:N | 2.15 | 0.62 |
| 1:CA:410:G:H1' | 1:CA:432:A:N6 | 2.14 | 0.62 |
| 1:CA:561:U:O2' | 1:CA:562:C:P | 2.57 | 0.62 |
| 27:D5:36:CYS:C | 27:D5:38:ALA:H | 2.02 | 0.62 |
| 31:DA:2074:U:H2' | 31:DA:2075:U:C6 | 2.34 | 0.62 |
| 32:DB:28:C:C2 | 32:DB:29:A:C8 | 2.87 | 0.62 |
| 33:DD:35:LYS:HE3 | 33:DD:65:ILE:CA | 2.30 | 0.62 |
| 35:DF:10:PRO:HG2 | 35:DF:13:SER:OG | 2.00 | 0.62 |
| 38:DI:133:HIS:CB | 38:DI:134:PRO:CD | 2.76 | 0.62 |
| 45:DT:32:TYR:CD2 | 45:DT:81:PRO:O | 2.53 | 0.62 |
| 46:DU:92:ARG:CZ | 47:DV:11:GLN:H | 2.13 | 0.62 |
| 49:DX:54:VAL:C | 49:DX:55:ASN:HD22 | 2.02 | 0.62 |
| 1:AA:441:A:H3' | 1:AA:442:C:C6 | 2.34 | 0.62 |
| 2:AB:213:LEU:HD23 | 2:AB:213:LEU:O | 2.00 | 0.62 |
| 16:AP:20:VAL:HG22 | 16:AP:34:GLU:O | 1.98 | 0.62 |
| 27:B5:2:ALA:N | 31:BA:747:U:N3 | 2.48 | 0.62 |
| 31:BA:102:G:C8 | 31:BA:102:G:C5' | 2.69 | 0.62 |
| 31:BA:528:A:N1 | 31:BA:2042:A:H2' | 2.15 | 0.62 |
| 31:BA:287:C:C2 | 31:BA:288:C:C6 | 2.88 | 0.62 |
| 31:BA:587:C:C4' | 31:BA:588:U:OP2 | 2.48 | 0.62 |
| 34:BE:101:ARG:HB3 | 34:BE:169:ASN:ND2 | 2.15 | 0.62 |
| 35:BF:160:ASN:HD21 | 35:BF:162:LEU:HB2 | 1.62 | 0.62 |
| 36:BG:46:ALA:H | 36:BG:82:LEU:HD11 | 1.63 | 0.62 |
| 38:BI:77:LEU:HD11 | 38:BI:101:LEU:HD22 | 1.80 | 0.62 |
| 41:BP:23:PRO:O | 41:BP:33:ARG:NE | 2.32 | 0.62 |
| 45:BT:33:LYS:NZ | 45:BT:33:LYS:N | 2.47 | 0.62 |
| 47:BV:52:VAL:O | 47:BV:53:GLU:CB | 2.47 | 0.62 |
| 50:BY:17:SER:HA | 50:BY:71:LYS:HG2 | 1.80 | 0.62 |
| 1:CA:1442:G:C8 | 1:CA:1442(B):A:C2 | 2.87 | 0.62 |
| 1:CA:1477:C:H2' | 1:CA:1478:C:C6 | 2.35 | 0.62 |
| 2:CB:141:GLU:O | 2:CB:145:LEU:HB2 | 1.99 | 0.62 |
| 2:CB:21:ARG:HB3 | 2:CB:39:ILE:HA | 1.81 | 0.62 |
| 3:CC:43:LEU:O | 3:CC:47:LEU:HB3 | 1.99 | 0.62 |
| 4:CD:133:VAL:HG12 | 4:CD:135:LEU:H | 1.63 | 0.62 |
| 28:D6:11:LEU:CD1 | 28:D6:51:GLU:HB2 | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:DA:1385:G:H4' | 31:DA:1386:C:OP1 | 1.99 | 0.62 |
| 31:DA:2032:G:H21 | 34:DE:146:THR:HG23 | 1.64 | 0.62 |
| 31:DA:68:G:H2' | 31:DA:69:C:H6 | 1.64 | 0.62 |
| 31:DA:1568:G:H21 | 33:DD:58:HIS:CE1 | 2.18 | 0.62 |
| 31:DA:2749:A:H4' | 37:DH:62:LYS:HB3 | 1.81 | 0.62 |
| 48:DW:6:ILE:HA | 48:DW:103:ILE:O | 1.99 | 0.62 |
| 3:AC:130:VAL:O | 3:AC:134:ILE:HG12 | 1.99 | 0.62 |
| 9:AI:46:ALA:HB2 | 9:AI:74:ILE:HG23 | 1.80 | 0.62 |
| 11:AK:57:THR:HG22 | 11:AK:59:TYR:H | 1.65 | 0.62 |
| 24:B2:55:ARG:H | 24:B2:56:GLN:NE2 | 1.98 | 0.62 |
| 31:BA:27:G:N2 | 31:BA:512:G:H1' | 2.15 | 0.62 |
| 31:BA:542:C:N3 | 31:BA:543:C:N4 | 2.47 | 0.62 |
| 44:BS:92:TYR:HD1 | 44:BS:93:LYS:N | 1.82 | 0.62 |
| 50:BY:46:LYS:HG2 | 50:BY:47:LYS:HD2 | 1.82 | 0.62 |
| 1:CA:1392:G:O2' | 1:CA:1393:U:H5' | 2.00 | 0.62 |
| 1:CA:1442(A):G:C3' | 1:CA:1442(B):A:H5'' | 2.30 | 0.62 |
| 1:CA:685:G:N2 | 1:CA:686:U:C4 | 2.68 | 0.62 |
| 1:CA:687:A:H1' | 1:CA:688:G:OP2 | 1.99 | 0.62 |
| 5:CE:98:THR:HG22 | 5:CE:99:GLY:N | 2.13 | 0.62 |
| 20:CT:23:ARG:HA | 20:CT:26:ASN:HD21 | 1.65 | 0.62 |
| 23:D1:21:ARG:NH1 | 31:DA:380:U:OP1 | 2.33 | 0.62 |
| 24:D2:15:LYS:HA | 24:D2:18:PRO:HD2 | 1.80 | 0.62 |
| 31:DA:1488:G:C6 | 31:DA:1489:U:N3 | 2.68 | 0.62 |
| 31:DA:2252:G:H2' | 31:DA:2253:G:H8 | 1.64 | 0.62 |
| 31:DA:71:A:H5' | 31:DA:71:A:H8 | 1.64 | 0.62 |
| 31:DA:794:G:O2' | 31:DA:795:C:H5' | 2.00 | 0.62 |
| 32:DB:10:C:C4 | 32:DB:11:C:C5 | 2.88 | 0.62 |
| 32:DB:75:G:C5' | 32:DB:75:G:H8 | 2.12 | 0.62 |
| 45:DT:28:VAL:HG13 | 45:DT:46:GLU:HB2 | 1.82 | 0.62 |
| 1:AA:1442(A):G:C3' | 1:AA:1442(B):A:H5'' | 2.30 | 0.62 |
| 1:AA:322:C:H5 | 1:AA:328:C:C5 | 2.16 | 0.62 |
| 5:AE:55:VAL:O | 5:AE:58:ALA:HB3 | 2.00 | 0.62 |
| 1:AA:1366:C:OP1 | 9:AI:117:HIS:HE1 | 1.82 | 0.62 |
| 1:AA:1342:C:H4' | 9:AI:125:TYR:HB3 | 1.82 | 0.62 |
| 31:BA:9:U:N3 | 31:BA:2629:A:N6 | 2.48 | 0.62 |
| 31:BA:635:C:O2' | 31:BA:639:U:OP1 | 2.18 | 0.62 |
| 34:BE:27:LEU:HD22 | 45:BT:1:MET:CE | 2.30 | 0.62 |
| 37:BH:97:ARG:O | 37:BH:99:VAL:HG23 | 1.98 | 0.62 |
| 42:BQ:23:GLY:HA3 | 42:BQ:99:PRO:O | 1.99 | 0.62 |
| 31:BA:911:A:C2' | 42:BQ:9:TYR:OH | 2.46 | 0.62 |
| 50:BY:28:LYS:CD | 50:BY:37:VAL:HG12 | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:BZ:39:VAL:HG21 | 51:BZ:44:PHE:HB2 | 1.81 | 0.62 |
| 1:CA:1306:A:H1' | 1:CA:1332:A:C2 | 2.34 | 0.62 |
| 1:CA:1342:C:H4' | 9:CI:125:TYR:HB3 | 1.82 | 0.62 |
| 1:CA:134:A:H61 | 16:CP:25:ARG:NH1 | 1.98 | 0.62 |
| 1:CA:180:U:H2' | 1:CA:181:G:H5' | 1.82 | 0.62 |
| 1:CA:410:G:H1' | 1:CA:432:A:H61 | 1.65 | 0.62 |
| 3:CC:182:ILE:HG12 | 3:CC:203:PHE:HA | 1.82 | 0.62 |
| 9:CI:112:LYS:HA | 9:CI:119:ALA:HB2 | 1.81 | 0.62 |
| 10:CJ:63:PHE:HD1 | 14:CN:58:LYS:HA | 1.64 | 0.62 |
| 10:CJ:34:VAL:CG2 | 10:CJ:74:ILE:HG22 | 2.29 | 0.62 |
| 23:D1:10:LYS:O | 23:D1:13:ILE:HG23 | 2.00 | 0.62 |
| 31:DA:1499:C:O2' | 31:DA:1500:G:H5' | 2.00 | 0.62 |
| 31:DA:1515:G:H2' | 31:DA:1516:C:H6 | 1.65 | 0.62 |
| 31:DA:2192:G:C2' | 31:DA:2193:G:H5' | 2.30 | 0.62 |
| 31:DA:2582:G:C2 | 31:DA:2583:G:C8 | 2.87 | 0.62 |
| 31:DA:2713:A:H3' | 31:DA:2714:G:H5' | 1.82 | 0.62 |
| 31:DA:671:C:H5' | 31:DA:671:C:C6 | 2.33 | 0.62 |
| 31:DA:754:C:H2' | 31:DA:755:C:H6 | 1.64 | 0.62 |
| 36:DG:10:LYS:O | 36:DG:15:VAL:HG23 | 1.99 | 0.62 |
| 41:DP:56:SER:O | 41:DP:58:THR:N | 2.33 | 0.62 |
| 44:DS:53:SER:OG | 44:DS:54:LEU:N | 2.33 | 0.62 |
| 47:DV:43:GLU:H | 47:DV:48:GLY:HA2 | 1.65 | 0.62 |
| 1:AA:1116:C:H3' | 1:AA:1117:G:H5'' | 1.82 | 0.62 |
| 1:AA:1306:A:H1' | 1:AA:1332:A:C2 | 2.34 | 0.62 |
| 3:AC:91:LEU:HB3 | 3:AC:99:VAL:HG21 | 1.80 | 0.62 |
| 10:AJ:63:PHE:HD1 | 14:AN:58:LYS:HA | 1.65 | 0.62 |
| 31:BA:2094:G:H2' | 31:BA:2095:C:H5' | 1.81 | 0.62 |
| 31:BA:2897:U:O2 | 31:BA:2897:U:H2' | 1.99 | 0.62 |
| 31:BA:958:U:HO2' | 31:BA:959:A:P | 2.23 | 0.62 |
| 35:BF:83:PHE:O | 35:BF:84:VAL:CB | 2.48 | 0.62 |
| 47:BV:19:LYS:HG2 | 47:BV:96:ILE:HB | 1.82 | 0.62 |
| 51:BZ:165:VAL:HG12 | 51:BZ:166:SER:OG | 2.00 | 0.62 |
| 1:CA:1096:C:O2' | 1:CA:1097:C:H5' | 2.00 | 0.62 |
| 1:CA:1117:G:H4' | 9:CI:104:ARG:CZ | 2.30 | 0.62 |
| 1:CA:1477:C:H2' | 1:CA:1478:C:H6 | 1.65 | 0.62 |
| 1:CA:322:C:H5 | 1:CA:328:C:C5 | 2.14 | 0.62 |
| 1:CA:1366:C:OP1 | 9:CI:117:HIS:HE1 | 1.82 | 0.62 |
| 9:CI:45:ALA:O | 9:CI:48:GLU:HB2 | 2.00 | 0.62 |
| 31:DA:1503:U:C4 | 31:DA:1504:C:N4 | 2.67 | 0.62 |
| 31:DA:1268:A:C2 | 31:DA:2013:A:C4 | 2.88 | 0.62 |
| 31:DA:2392:A:H2 | 31:DA:2424:C:H42 | 1.48 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:2790:A:H2' | 31:DA:2791:C:C5' | 2.30 | 0.62 |
| 32:DB:13:A:H2' | 32:DB:70:C:O2' | 2.00 | 0.62 |
| 33:DD:43:ARG:HH11 | 33:DD:44:ASN:CG | 2.03 | 0.62 |
| 34:DE:39:PRO:HA | 34:DE:43:GLY:HA2 | 1.82 | 0.62 |
| 31:DA:322:A:OP2 | 35:DF:169:ASN:HB2 | 1.99 | 0.62 |
| 37:DH:158:HIS:CE1 | 37:DH:168:PRO:HB2 | 2.35 | 0.62 |
| 49:DX:24:GLY:HA3 | 49:DX:80:ILE:HG12 | 1.81 | 0.62 |
| 1:AA:604:G:C5 | 1:AA:605:U:C5 | 2.88 | 0.61 |
| 5:AE:76:ILE:HG12 | 5:AE:77:PRO:HD2 | 1.82 | 0.61 |
| 9:AI:96:LEU:HG | 9:AI:102:LEU:HB2 | 1.81 | 0.61 |
| 1:AA:1342:C:H1' | 9:AI:124:GLN:HE22 | 1.64 | 0.61 |
| 13:AM:46:LYS:HG3 | 13:AM:47:ASP:H | 1.64 | 0.61 |
| 28:B6:15:GLU:OE2 | 28:B6:41:PRO:CG | 2.46 | 0.61 |
| 31:BA:1309:G:C2' | 31:BA:1310:G:H5' | 2.30 | 0.61 |
| 31:BA:2475:C:C5' | 31:BA:2476:A:OP2 | 2.44 | 0.61 |
| 31:BA:794:G:H2' | 31:BA:795:C:H6 | 1.65 | 0.61 |
| 36:BG:71:THR:HG22 | 36:BG:72:ARG:N | 2.14 | 0.61 |
| 45:BT:32:TYR:CD2 | 45:BT:32:TYR:N | 2.68 | 0.61 |
| 48:BW:66:GLU:HA | 48:BW:69:LEU:HD11 | 1.80 | 0.61 |
| 51:BZ:151:HIS:HB3 | 51:BZ:170:THR:HA | 1.82 | 0.61 |
| 1:CA:857:C:H2' | 1:CA:858:G:O4' | 1.99 | 0.61 |
| 1:CA:874:G:O2' | 1:CA:875:C:H5' | 1.99 | 0.61 |
| 3:CC:138:VAL:HG22 | 3:CC:151:VAL:HG23 | 1.81 | 0.61 |
| 31:DA:1486:A:O2' | 31:DA:1487:G:H5' | 2.00 | 0.61 |
| 31:DA:1744:C:C2' | 31:DA:1745:C:H5' | 2.30 | 0.61 |
| 35:DF:80:ALA:O | 35:DF:83:PHE:HB2 | 2.00 | 0.61 |
| 36:DG:46:ALA:H | 36:DG:82:LEU:HD11 | 1.65 | 0.61 |
| 37:DH:89:ILE:O | 37:DH:90:LYS:CG | 2.48 | 0.61 |
| 41:DP:26:GLY:HA2 | 41:DP:30:THR:HG21 | 1.80 | 0.61 |
| 46:DU:31:SER:C | 46:DU:33:ARG:H | 2.03 | 0.61 |
| 51:DZ:152:ALA:HB2 | 51:DZ:168:GLU:N | 2.15 | 0.61 |
| 1:AA:166:G:O2' | 1:AA:167:G:H5' | 2.00 | 0.61 |
| 1:AA:376:G:OP1 | 16:AP:5:ARG:HB2 | 2.00 | 0.61 |
| 1:AA:687:A:H1' | 1:AA:688:G:OP2 | 2.00 | 0.61 |
| 7:AG:62:PHE:HA | 7:AG:124:LEU:HD22 | 1.82 | 0.61 |
| 18:AR:45:SER:HB3 | 18:AR:51:LEU:HD21 | 1.81 | 0.61 |
| 23:B1:30:VAL:O | 23:B1:30:VAL:HG12 | 1.98 | 0.61 |
| 31:BA:1021:A:H8 | 31:BA:1021:A:H3' | 1.63 | 0.61 |
| 22:B0:43:THR:HG22 | 31:BA:2331:G:O2' | 2.00 | 0.61 |
| 31:BA:494:G:H8 | 31:BA:494:G:H5'' | 1.63 | 0.61 |
| 33:BD:44:ASN:N | 33:BD:44:ASN:OD1 | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BE:16:ARG:O | 34:BE:18:ASP:N | 2.34 | 0.61 |
| 41:BP:16:ARG:CZ | 41:BP:16:ARG:HB2 | 2.29 | 0.61 |
| 49:BX:54:VAL:C | 49:BX:55:ASN:HD22 | 2.03 | 0.61 |
| 49:BX:60:ARG:CB | 49:BX:72:LYS:H | 2.13 | 0.61 |
| 50:BY:28:LYS:HD2 | 50:BY:37:VAL:HG12 | 1.80 | 0.61 |
| 51:BZ:130:PRO:HA | 51:BZ:133:ILE:HD11 | 1.82 | 0.61 |
| 1:CA:37:U:O2' | 1:CA:38:G:H5' | 2.00 | 0.61 |
| 1:CA:93:G:H2' | 1:CA:96:U:H5' | 1.82 | 0.61 |
| 13:CM:12:ASN:OD1 | 13:CM:46:LYS:HE2 | 1.99 | 0.61 |
| 23:D1:27:GLU:OE2 | 23:D1:32:LYS:HB2 | 1.99 | 0.61 |
| 24:D2:31:GLU:HG2 | 24:D2:37:PHE:HD1 | 1.64 | 0.61 |
| 31:DA:174:C:C3' | 31:DA:175:G:H5'' | 2.28 | 0.61 |
| 31:DA:2252:G:H2' | 31:DA:2253:G:C8 | 2.34 | 0.61 |
| 31:DA:2492:U:H2' | 31:DA:2493:U:C6 | 2.34 | 0.61 |
| 32:DB:60:C:C2 | 32:DB:61:G:C8 | 2.88 | 0.61 |
| 33:DD:125:ILE:HG21 | 33:DD:137:PRO:HG2 | 1.82 | 0.61 |
| 33:DD:166:GLN:HB3 | 33:DD:174:ILE:HG22 | 1.82 | 0.61 |
| 33:DD:167:GLY:O | 33:DD:168:ARG:HG2 | 2.00 | 0.61 |
| 35:DF:128:ALA:O | 35:DF:142:TRP:NE1 | 2.33 | 0.61 |
| 35:DF:178:PRO:HB2 | 35:DF:201:VAL:CG1 | 2.26 | 0.61 |
| 31:DA:1030:G:OP2 | 42:DQ:128:LYS:HE2 | 1.99 | 0.61 |
| 45:DT:31:SER:HA | 45:DT:32:TYR:CD2 | 2.35 | 0.61 |
| 49:DX:65:ARG:CZ | 49:DX:66:LEU:H | 2.13 | 0.61 |
| 49:DX:82:GLN:C | 49:DX:85:PRO:HD2 | 2.20 | 0.61 |
| 50:DY:96:ILE:CG2 | 50:DY:99:CYS:HB3 | 2.30 | 0.61 |
| 1:AA:1162:C:H2' | 1:AA:1163:C:C6 | 2.35 | 0.61 |
| 1:AA:1418:A:C2 | 31:BA:1948:G:N3 | 2.68 | 0.61 |
| 1:AA:152:A:N6 | 1:AA:170:U:C2 | 2.69 | 0.61 |
| 5:AE:101:ILE:O | 5:AE:101:ILE:HG12 | 2.01 | 0.61 |
| 8:AH:36:LEU:HA | 8:AH:39:LEU:HD23 | 1.82 | 0.61 |
| 27:B5:40:LYS:NZ | 27:B5:49:CYS:SG | 2.69 | 0.61 |
| 31:BA:1204:A:C2 | 31:BA:1241:A:N1 | 2.66 | 0.61 |
| 31:BA:2894:G:H2' | 31:BA:2894:G:N3 | 2.15 | 0.61 |
| 41:BP:121:LYS:HB3 | 41:BP:123:LEU:HD23 | 1.82 | 0.61 |
| 50:BY:44:ILE:HG22 | 50:BY:45:VAL:H | 1.65 | 0.61 |
| 1:CA:327:A:C4 | 1:CA:329:A:C8 | 2.88 | 0.61 |
| 1:CA:341:C:O2' | 1:CA:342:C:H5' | 2.01 | 0.61 |
| 1:CA:60:A:P | 1:CA:60:A:H8 | 2.23 | 0.61 |
| 4:CD:104:VAL:O | 4:CD:108:LEU:HB2 | 2.01 | 0.61 |
| 1:CA:923:A:H5' | 5:CE:21:ALA:HB2 | 1.82 | 0.61 |
| 7:CG:91:VAL:HG13 | 7:CG:95:ARG:HD3 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CP:4:ILE:HB | 16:CP:66:PRO:HB3 | 1.83 | 0.61 |
| 17:CQ:40:LYS:HG2 | 17:CQ:41:LYS:H | 1.65 | 0.61 |
| 31:DA:1279:G:H5' | 43:DR:34:ILE:HD11 | 1.81 | 0.61 |
| 31:DA:1484:G:N2 | 31:DA:1505:C:H5 | 1.97 | 0.61 |
| 31:DA:1580:A:OP2 | 31:DA:1580:A:H8 | 1.83 | 0.61 |
| 31:DA:2657:A:H2 | 31:DA:2664:G:H21 | 1.45 | 0.61 |
| 31:DA:2870:C:H5'' | 43:DR:65:LEU:HD21 | 1.81 | 0.61 |
| 31:DA:671:C:C5' | 31:DA:671:C:H6 | 2.13 | 0.61 |
| 31:DA:864:G:C6 | 31:DA:865:C:N4 | 2.68 | 0.61 |
| 31:DA:901:A:H5' | 31:DA:902:C:OP2 | 2.00 | 0.61 |
| 33:DD:143:HIS:HD2 | 33:DD:144:ALA:CB | 2.13 | 0.61 |
| 33:DD:35:LYS:CE | 33:DD:104:TYR:CD1 | 2.84 | 0.61 |
| 36:DG:64:THR:HG23 | 36:DG:65:GLY:N | 2.16 | 0.61 |
| 38:DI:85:GLU:O | 38:DI:123:LEU:HD12 | 2.00 | 0.61 |
| 44:DS:66:ALA:O | 44:DS:67:ARG:HB2 | 2.01 | 0.61 |
| 49:DX:76:ARG:CG | 49:DX:76:ARG:HH11 | 2.02 | 0.61 |
| 50:DY:44:ILE:HG22 | 50:DY:45:VAL:H | 1.65 | 0.61 |
| 51:DZ:102:LEU:HD11 | 51:DZ:124:ILE:HG22 | 1.82 | 0.61 |
| 1:AA:1152:A:O2' | 1:AA:1153:C:H5' | 1.99 | 0.61 |
| 6:AF:67:MET:HB2 | 6:AF:68:PRO:HD2 | 1.81 | 0.61 |
| 22:B0:53:MET:HB2 | 22:B0:59:LEU:HD23 | 1.82 | 0.61 |
| 28:B6:32:ASN:O | 28:B6:33:LYS:HB2 | 2.00 | 0.61 |
| 31:BA:1301:A:C8 | 31:BA:1303:G:C8 | 2.88 | 0.61 |
| 31:BA:1486:A:O2' | 31:BA:1487:G:H5' | 1.99 | 0.61 |
| 31:BA:2870:C:H2' | 31:BA:2871:C:H5' | 1.83 | 0.61 |
| 31:BA:2580:U:H5' | 34:BE:131:ALA:HB3 | 1.82 | 0.61 |
| 34:BE:95:ILE:N | 34:BE:95:ILE:HD12 | 2.14 | 0.61 |
| 35:BF:8:GLN:HB3 | 35:BF:126:VAL:HA | 1.82 | 0.61 |
| 31:BA:1006:C:H1' | 39:BN:106:MET:CE | 2.31 | 0.61 |
| 1:CA:504:C:H1' | 1:CA:510:A:C4 | 2.34 | 0.61 |
| 5:CE:78:HIS:CE1 | 5:CE:142:LEU:HD23 | 2.36 | 0.61 |
| 9:CI:96:LEU:HG | 9:CI:102:LEU:HB2 | 1.80 | 0.61 |
| 11:CK:24:SER:HB3 | 11:CK:27:ASN:O | 2.00 | 0.61 |
| 28:D6:10:LEU:HD22 | 28:D6:10:LEU:H | 1.65 | 0.61 |
| 31:DA:1945:G:H2' | 31:DA:1946:U:H6 | 1.64 | 0.61 |
| 31:DA:2317:C:C2' | 31:DA:2318:G:C5' | 2.67 | 0.61 |
| 31:DA:236:C:H2' | 31:DA:237:C:C6 | 2.34 | 0.61 |
| 31:DA:825:C:H2' | 31:DA:826:U:O5' | 2.00 | 0.61 |
| 36:DG:115:ARG:NH1 | 36:DG:136:ARG:HG3 | 2.15 | 0.61 |
| 37:DH:40:GLU:O | 37:DH:41:MET:SD | 2.59 | 0.61 |
| 41:DP:88:LEU:HD11 | 41:DP:95:VAL:HG21 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:DW:83:LYS:O | 48:DW:84:ARG:HD3 | 2.01 | 0.61 |
| 49:DX:73:ARG:O | 49:DX:74:PRO:C | 2.39 | 0.61 |
| 1:AA:1109:C:P | 3:AC:176:HIS:HD1 | 2.24 | 0.61 |
| 1:AA:1264:C:H2' | 1:AA:1265:G:H8 | 1.65 | 0.61 |
| 1:AA:327:A:C4 | 1:AA:329:A:C8 | 2.89 | 0.61 |
| 2:AB:194:PRO:O | 2:AB:196:LEU:N | 2.33 | 0.61 |
| 3:AC:182:ILE:HG12 | 3:AC:203:PHE:HA | 1.82 | 0.61 |
| 5:AE:32:VAL:HB | 5:AE:58:ALA:HB1 | 1.82 | 0.61 |
| 30:B8:30:ARG:O | 30:B8:31:HIS:O | 2.18 | 0.61 |
| 31:BA:1844:C:OP1 | 33:BD:257:LEU:HD23 | 2.00 | 0.61 |
| 31:BA:1882:C:O2 | 31:BA:1882:C:H2' | 1.99 | 0.61 |
| 22:B0:16:SER:HB3 | 31:BA:2262:U:OP2 | 2.00 | 0.61 |
| 31:BA:2492:U:H2' | 31:BA:2493:U:C6 | 2.34 | 0.61 |
| 31:BA:286:C:O2' | 31:BA:287:C:H5' | 2.00 | 0.61 |
| 31:BA:536:A:H2' | 31:BA:537:C:C6 | 2.36 | 0.61 |
| 31:BA:814:C:C5 | 41:BP:27:HIS:CE1 | 2.89 | 0.61 |
| 31:BA:867:C:C5 | 31:BA:868:U:C5 | 2.88 | 0.61 |
| 37:BH:88:LEU:O | 37:BH:89:ILE:HG23 | 2.00 | 0.61 |
| 38:BI:9:LEU:H | 38:BI:13:GLY:CA | 2.13 | 0.61 |
| 45:BT:31:SER:HA | 45:BT:32:TYR:CD2 | 2.36 | 0.61 |
| 45:BT:78:LEU:O | 45:BT:78:LEU:HD23 | 2.00 | 0.61 |
| 1:CA:552:U:C2' | 1:CA:553:A:H5' | 2.30 | 0.61 |
| 1:CA:663:A:O2' | 1:CA:664:G:H5' | 2.00 | 0.61 |
| 6:CF:45:LEU:HD11 | 6:CF:57:GLN:OE1 | 2.00 | 0.61 |
| 6:CF:5:GLU:HB3 | 6:CF:62:TRP:HE1 | 1.64 | 0.61 |
| 24:D2:57:ILE:HG21 | 24:D2:59:ARG:HH11 | 1.66 | 0.61 |
| 27:D5:57:VAL:CG2 | 27:D5:58:LEU:H | 2.12 | 0.61 |
| 37:DH:41:MET:CE | 37:DH:55:PRO:HD3 | 2.30 | 0.61 |
| 42:DQ:54:MET:HG3 | 42:DQ:117:ALA:HB1 | 1.81 | 0.61 |
| 44:DS:30:ARG:NH2 | 44:DS:62:LYS:HD2 | 2.08 | 0.61 |
| 46:DU:64:ARG:NH2 | 46:DU:64:ARG:CA | 2.62 | 0.61 |
| 51:DZ:151:HIS:HB3 | 51:DZ:170:THR:HA | 1.82 | 0.61 |
| 51:DZ:71:VAL:HG22 | 51:DZ:88:PHE:CE2 | 2.34 | 0.61 |
| 1:AA:760:G:H2' | 1:AA:761:G:H5' | 1.82 | 0.61 |
| 4:AD:112:VAL:HG13 | 4:AD:113:SER:H | 1.66 | 0.61 |
| 4:AD:117:ALA:O | 4:AD:121:VAL:HG23 | 1.98 | 0.61 |
| 4:AD:19:LEU:HB2 | 4:AD:21:LEU:CD2 | 2.29 | 0.61 |
| 4:AD:19:LEU:HB2 | 4:AD:21:LEU:HD21 | 1.82 | 0.61 |
| 9:AI:112:LYS:HA | 9:AI:119:ALA:HB2 | 1.81 | 0.61 |
| 1:AA:1346:A:H5'' | 9:AI:120:ARG:HH12 | 1.64 | 0.61 |
| 24:B2:30:ARG:HD2 | 24:B2:30:ARG:N | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:B2:56:GLN:H | 24:B2:56:GLN:CD | 2.04 | 0.61 |
| 31:BA:128:C:C6 | 31:BA:128:C:H3' | 2.35 | 0.61 |
| 31:BA:1527:G:H5'' | 31:BA:1528:A:OP1 | 2.01 | 0.61 |
| 31:BA:2292:C:O2' | 31:BA:2293:C:H5' | 1.99 | 0.61 |
| 31:BA:484:C:H2' | 31:BA:485:C:C6 | 2.35 | 0.61 |
| 31:BA:715:G:O2' | 31:BA:716:A:H5' | 2.01 | 0.61 |
| 38:BI:88:ILE:HD11 | 38:BI:123:LEU:HD23 | 1.82 | 0.61 |
| 42:BQ:43:THR:HG22 | 42:BQ:94:VAL:HG12 | 1.81 | 0.61 |
| 43:BR:116:LEU:O | 43:BR:117:VAL:HB | 1.99 | 0.61 |
| 44:BS:42:ASP:C | 44:BS:44:LYS:H | 2.04 | 0.61 |
| 44:BS:95:HIS:O | 44:BS:98:VAL:HG23 | 2.01 | 0.61 |
| 45:BT:100:TYR:HD2 | 45:BT:103:ARG:HH21 | 1.46 | 0.61 |
| 48:BW:51:LEU:HD23 | 48:BW:105:VAL:HG11 | 1.83 | 0.61 |
| 1:CA:447:G:H2' | 1:CA:485:G:N2 | 2.15 | 0.61 |
| 4:CD:79:PHE:CZ | 4:CD:204:ILE:HD13 | 2.36 | 0.61 |
| 8:CH:5:PRO:O | 8:CH:8:ASP:HB3 | 2.01 | 0.61 |
| 13:CM:15:VAL:HG12 | 13:CM:45:VAL:HG22 | 1.81 | 0.61 |
| 41:BP:122:PRO:HB3 | 25:D3:1:MET:CE | 2.30 | 0.61 |
| 31:DA:1946:U:H2' | 31:DA:1947:C:C6 | 2.35 | 0.61 |
| 31:DA:528:A:C2 | 31:DA:2043:C:C5' | 2.84 | 0.61 |
| 33:DD:266:SER:O | 33:DD:267:SER:CB | 2.49 | 0.61 |
| 37:DH:141:VAL:HG12 | 37:DH:142:GLY:N | 2.13 | 0.61 |
| 37:DH:155:SER:OG | 37:DH:155:SER:O | 2.18 | 0.61 |
| 39:DN:18:ALA:CB | 39:DN:21:LYS:HB2 | 2.21 | 0.61 |
| 39:DN:3:THR:HG22 | 39:DN:4:TYR:N | 2.12 | 0.61 |
| 40:DO:35:VAL:HG11 | 40:DO:103:ALA:HB3 | 1.82 | 0.61 |
| 30:D8:27:THR:HA | 41:DP:62:LEU:CD1 | 2.31 | 0.61 |
| 49:DX:55:ASN:HD22 | 49:DX:55:ASN:N | 1.99 | 0.61 |
| 1:AA:836:G:C6 | 1:AA:851:G:C6 | 2.88 | 0.61 |
| 5:AE:98:THR:HG22 | 5:AE:99:GLY:N | 2.14 | 0.61 |
| 6:AF:100:ASN:O | 18:AR:28:GLU:HG2 | 2.00 | 0.61 |
| 6:AF:50:TYR:HE2 | 6:AF:52:ILE:HD11 | 1.66 | 0.61 |
| 6:AF:82:ARG:HH11 | 6:AF:82:ARG:HA | 1.66 | 0.61 |
| 29:B7:5:TRP:CD1 | 29:B7:7:PRO:HG3 | 2.36 | 0.61 |
| 31:BA:1427:A:H4' | 31:BA:1428:C:O5' | 2.01 | 0.61 |
| 31:BA:1528:A:O2' | 31:BA:1528(A):A:O5' | 2.18 | 0.61 |
| 31:BA:2190:G:C2' | 31:BA:2191:G:H5' | 2.31 | 0.61 |
| 31:BA:2192:G:C2' | 31:BA:2193:G:H5' | 2.29 | 0.61 |
| 31:BA:2192:G:H2' | 31:BA:2193:G:H5' | 1.81 | 0.61 |
| 31:BA:234:C:H2' | 31:BA:235:U:C6 | 2.36 | 0.61 |
| 31:BA:542:C:H42 | 31:BA:543:C:N4 | 1.94 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BG:131:TYR:HB3 | 36:BG:159:VAL:CG1 | 2.31 | 0.61 |
| 39:BN:3:THR:CA | 39:BN:4:TYR:CD1 | 2.82 | 0.61 |
| 41:BP:107:LYS:O | 41:BP:109:GLY:N | 2.34 | 0.61 |
| 41:BP:146:VAL:HG22 | 41:BP:147:LEU:H | 1.65 | 0.61 |
| 31:BA:833:U:O2 | 41:BP:55:ARG:NH1 | 2.33 | 0.61 |
| 45:BT:83:ILE:HG13 | 45:BT:84:GLN:N | 2.07 | 0.61 |
| 42:BQ:141:GLN:CG | 51:BZ:72:ARG:HH11 | 2.14 | 0.61 |
| 1:CA:1109:C:H2' | 1:CA:1110:A:O4' | 2.00 | 0.61 |
| 1:CA:1321:C:H3' | 1:CA:1322:C:H5'' | 1.82 | 0.61 |
| 1:CA:1399:C:C2 | 1:CA:1502:A:N6 | 2.69 | 0.61 |
| 1:CA:318:G:H1 | 1:CA:335:C:H42 | 1.49 | 0.61 |
| 1:CA:819:A:H4' | 1:CA:820:U:OP2 | 2.01 | 0.61 |
| 1:CA:952:U:H4' | 1:CA:964:A:H61 | 1.65 | 0.61 |
| 7:CG:13:GLN:O | 7:CG:24:THR:HG21 | 1.99 | 0.61 |
| 27:D5:16:ARG:NH1 | 27:D5:17:ASP:OD1 | 2.34 | 0.61 |
| 30:D8:4:MET:HE1 | 31:DA:593:G:C1' | 2.31 | 0.61 |
| 31:DA:1693:U:H4' | 31:DA:1694:C:OP2 | 2.00 | 0.61 |
| 31:DA:2544:G:H8 | 31:DA:2544:G:O5' | 1.84 | 0.61 |
| 31:DA:2699:C:H2' | 31:DA:2700:C:O4' | 2.00 | 0.61 |
| 34:DE:27:LEU:HD22 | 45:DT:1:MET:HE3 | 1.81 | 0.61 |
| 35:DF:83:PHE:O | 35:DF:84:VAL:HB | 2.01 | 0.61 |
| 39:DN:40:PRO:O | 46:DU:64:ARG:NH2 | 2.33 | 0.61 |
| 41:DP:62:LEU:N | 41:DP:62:LEU:CD2 | 2.61 | 0.61 |
| 44:DS:90:GLY:O | 44:DS:92:TYR:N | 2.33 | 0.61 |
| 45:DT:55:ASN:N | 45:DT:59:THR:HB | 2.15 | 0.61 |
| 50:DY:8:LYS:HD2 | 50:DY:8:LYS:N | 2.16 | 0.61 |
| 1:AA:192:U:H2' | 1:AA:193:C:C6 | 2.34 | 0.61 |
| 1:AA:243:A:H4' | 1:AA:244:U:O5' | 2.01 | 0.61 |
| 1:AA:977:A:C8 | 1:AA:1223:C:C4 | 2.89 | 0.61 |
| 2:AB:44:LEU:O | 2:AB:47:THR:HB | 2.01 | 0.61 |
| 8:AH:88:LYS:HB3 | 8:AH:89:PRO:HD2 | 1.83 | 0.61 |
| 31:BA:1751:C:HO2' | 31:BA:2861:G:HO2' | 1.45 | 0.61 |
| 31:BA:1887:C:H2' | 31:BA:1888:G:H5' | 1.82 | 0.61 |
| 31:BA:708:C:O2 | 31:BA:708:C:H2' | 2.00 | 0.61 |
| 31:BA:828:U:H4' | 31:BA:831:G:N1 | 2.16 | 0.61 |
| 31:BA:92:A:O2' | 31:BA:93:G:H5' | 2.01 | 0.61 |
| 31:BA:952:G:C6 | 31:BA:953:A:N7 | 2.68 | 0.61 |
| 37:BH:85:LYS:HD3 | 37:BH:133:VAL:HB | 1.82 | 0.61 |
| 41:BP:56:SER:O | 41:BP:58:THR:N | 2.33 | 0.61 |
| 43:BR:50:HIS:CE1 | 43:BR:54:LEU:HD21 | 2.36 | 0.61 |
| 44:BS:87:PHE:HB2 | 44:BS:106:ARG:HD3 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:BW:111:HIS:CD2 | 48:BW:112:GLY:N | 2.69 | 0.61 |
| 1:CA:189:G:C6 | 1:CA:189(L):G:C6 | 2.89 | 0.61 |
| 2:CB:194:PRO:O | 2:CB:196:LEU:N | 2.34 | 0.61 |
| 13:CM:16:ASP:HB3 | 13:CM:41:PRO:HB3 | 1.82 | 0.61 |
| 31:DA:1188:U:O2' | 31:DA:1189:A:H5' | 2.00 | 0.61 |
| 31:DA:1497:U:C5' | 31:DA:1498:C:C5 | 2.84 | 0.61 |
| 31:DA:184:C:H2' | 31:DA:185:U:H6 | 1.66 | 0.61 |
| 31:DA:194:G:H2' | 31:DA:195:A:O4' | 2.01 | 0.61 |
| 31:DA:236:C:H2' | 31:DA:237:C:H6 | 1.66 | 0.61 |
| 31:DA:2753:A:O2' | 31:DA:2754:U:O5' | 2.18 | 0.61 |
| 31:DA:196:A:C4 | 31:DA:805:G:C6 | 2.88 | 0.61 |
| 44:DS:74:ALA:HB1 | 44:DS:103:GLU:CB | 2.31 | 0.61 |
| 45:DT:50:ILE:HA | 45:DT:99:LEU:HD11 | 1.81 | 0.61 |
| 45:DT:42:ILE:HD13 | 45:DT:83:ILE:HD11 | 1.81 | 0.61 |
| 47:DV:1:MET:N | 47:DV:44:LYS:HD2 | 2.16 | 0.61 |
| 48:DW:70:TYR:O | 48:DW:107:LEU:HD12 | 2.00 | 0.61 |
| 1:AA:170:U:O2' | 1:AA:171:A:H5' | 2.01 | 0.61 |
| 1:AA:318:G:H1 | 1:AA:335:C:H42 | 1.48 | 0.61 |
| 2:AB:114:ARG:HD2 | 2:AB:141:GLU:OE1 | 2.00 | 0.61 |
| 4:AD:104:VAL:O | 4:AD:108:LEU:HB2 | 2.00 | 0.61 |
| 12:AL:115:LYS:O | 12:AL:117:ARG:HG3 | 2.00 | 0.61 |
| 31:BA:1418:G:H8 | 31:BA:1418:G:O5' | 1.84 | 0.61 |
| 31:BA:1839:G:C8 | 31:BA:1839:G:H5' | 2.36 | 0.61 |
| 31:BA:2030:A:H5'' | 31:BA:2031:A:P | 2.41 | 0.61 |
| 31:BA:257:A:H2' | 31:BA:258:G:H5' | 1.82 | 0.61 |
| 24:B2:53:LEU:HD12 | 31:BA:77:C:OP1 | 2.00 | 0.61 |
| 31:BA:779:U:OP1 | 33:BD:49:ILE:HG13 | 2.00 | 0.61 |
| 41:BP:122:PRO:HB3 | 25:D3:1:MET:HE1 | 1.83 | 0.61 |
| 49:BX:72:LYS:HG3 | 49:BX:74:PRO:CD | 2.29 | 0.61 |
| 50:BY:2:ARG:C | 50:BY:4:LYS:H | 2.02 | 0.61 |
| 1:CA:360:A:O2' | 1:CA:361:G:H5' | 2.00 | 0.61 |
| 1:CA:622:A:C8 | 1:CA:623:C:C5 | 2.89 | 0.61 |
| 2:CB:111:ARG:O | 2:CB:145:LEU:HD11 | 2.01 | 0.61 |
| 2:CB:213:LEU:O | 2:CB:213:LEU:HD23 | 2.00 | 0.61 |
| 3:CC:155:GLY:O | 3:CC:156:ARG:HB2 | 2.01 | 0.61 |
| 3:CC:54:ARG:HD3 | 3:CC:69:HIS:CE1 | 2.35 | 0.61 |
| 4:CD:117:ALA:O | 4:CD:120:LEU:HB2 | 2.01 | 0.61 |
| 9:CI:53:VAL:HB | 9:CI:92:TYR:CE2 | 2.36 | 0.61 |
| 15:CO:8:LYS:O | 15:CO:12:ILE:HG13 | 2.00 | 0.61 |
| 6:CF:100:ASN:O | 18:CR:28:GLU:HG2 | 2.01 | 0.61 |
| 27:D5:57:VAL:HB | 27:D5:58:LEU:HD12 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:1042:G:N3 | 31:DA:1042:G:H2' | 2.15 | 0.61 |
| 31:DA:1265:A:OP1 | 31:DA:1265:A:H8 | 1.84 | 0.61 |
| 31:DA:1348:G:C2' | 31:DA:1349:A:H5' | 2.31 | 0.61 |
| 31:DA:1803:A:H4' | 33:DD:259:THR:HG23 | 1.83 | 0.61 |
| 31:DA:2884:U:H2' | 31:DA:2885:C:H5' | 1.82 | 0.61 |
| 31:DA:769:G:O2' | 31:DA:770:G:H5' | 2.00 | 0.61 |
| 33:DD:63:ARG:HG3 | 33:DD:63:ARG:NH1 | 2.15 | 0.61 |
| 34:DE:6:GLY:O | 34:DE:195:LEU:HD12 | 2.01 | 0.61 |
| 37:DH:137:ASP:O | 37:DH:138:LYS:CB | 2.47 | 0.61 |
| 43:DR:50:HIS:CE1 | 43:DR:54:LEU:HD21 | 2.35 | 0.61 |
| 44:DS:35:ILE:C | 44:DS:36:TYR:HD1 | 2.04 | 0.61 |
| 1:AA:392:G:H2' | 1:AA:393:A:C8 | 2.34 | 0.61 |
| 8:AH:5:PRO:O | 8:AH:8:ASP:HB3 | 2.01 | 0.61 |
| 15:AO:67:LEU:HD22 | 15:AO:78:TYR:HE1 | 1.65 | 0.61 |
| 23:B1:47:GLN:HG2 | 31:BA:2230:G:C1' | 2.26 | 0.61 |
| 31:BA:819:A:C4 | 31:BA:1189:A:C2 | 2.88 | 0.61 |
| 31:BA:1763:G:H4' | 31:BA:1763:G:OP1 | 2.01 | 0.61 |
| 31:BA:2418:A:H2' | 31:BA:2419:U:C6 | 2.36 | 0.61 |
| 31:BA:901:A:H5' | 31:BA:902:C:OP2 | 2.00 | 0.61 |
| 31:BA:568:U:H5' | 31:BA:945:A:C2 | 2.36 | 0.61 |
| 39:BN:77:GLY:O | 39:BN:78:TYR:HB3 | 2.01 | 0.61 |
| 40:BO:35:VAL:HG11 | 40:BO:103:ALA:HB3 | 1.83 | 0.61 |
| 44:BS:53:SER:O | 44:BS:56:LEU:N | 2.34 | 0.61 |
| 47:BV:43:GLU:H | 47:BV:48:GLY:HA2 | 1.66 | 0.61 |
| 46:BU:50:ARG:CZ | 47:BV:75:PHE:CE2 | 2.84 | 0.61 |
| 1:CA:543:C:C2 | 1:CA:544:G:C8 | 2.89 | 0.61 |
| 1:CA:629:G:H2' | 1:CA:630:G:O4' | 2.01 | 0.61 |
| 1:CA:1109:C:P | 3:CC:176:HIS:HD1 | 2.24 | 0.61 |
| 4:CD:43:HIS:O | 4:CD:45:GLN:N | 2.34 | 0.61 |
| 5:CE:57:LYS:O | 5:CE:61:TYR:HD2 | 1.84 | 0.61 |
| 6:CF:67:MET:HB2 | 6:CF:68:PRO:HD2 | 1.83 | 0.61 |
| 24:D2:32:LEU:O | 24:D2:33:MET:C | 2.38 | 0.61 |
| 27:D5:33:CYS:SG | 27:D5:49:CYS:CB | 2.89 | 0.61 |
| 31:DA:271(Q):G:O2' | 31:DA:271(R):G:P | 2.59 | 0.61 |
| 31:DA:528:A:H2 | 31:DA:2043:C:C5' | 2.14 | 0.61 |
| 33:DD:125:ILE:HG22 | 33:DD:125:ILE:O | 1.99 | 0.61 |
| 33:DD:44:ASN:OD1 | 33:DD:44:ASN:N | 2.34 | 0.61 |
| 33:DD:30:GLU:CD | 33:DD:63:ARG:HE | 2.03 | 0.61 |
| 37:DH:66:GLY:HA2 | 37:DH:69:ARG:HB2 | 1.82 | 0.61 |
| 38:DI:52:ARG:O | 38:DI:53:ALA:C | 2.38 | 0.61 |
| 43:DR:51:LEU:HD13 | 43:DR:70:LEU:HD21 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:DT:50:ILE:HA | 45:DT:99:LEU:CD1 | 2.31 | 0.61 |
| 50:DY:45:VAL:HG13 | 50:DY:62:GLU:CB | 2.27 | 0.61 |
| 51:DZ:19:ARG:HA | 51:DZ:23:LYS:O | 2.00 | 0.61 |
| 1:AA:921:U:O2 | 5:AE:19:MET:HB2 | 2.01 | 0.60 |
| 1:AA:93:G:H2' | 1:AA:96:U:H5' | 1.82 | 0.60 |
| 3:AC:35:GLU:CD | 3:AC:59:ARG:HH22 | 2.05 | 0.60 |
| 5:AE:7:GLU:HG2 | 5:AE:112:LEU:HD22 | 1.83 | 0.60 |
| 8:AH:14:ARG:O | 8:AH:18:ARG:HD3 | 2.00 | 0.60 |
| 20:AT:23:ARG:HA | 20:AT:26:ASN:HD21 | 1.65 | 0.60 |
| 25:B3:44:ARG:O | 25:B3:48:GLU:HG2 | 2.00 | 0.60 |
| 30:B8:58:ILE:HG22 | 41:BP:49:ARG:CD | 2.31 | 0.60 |
| 31:BA:1028:A:N6 | 31:BA:1125:G:H2' | 2.16 | 0.60 |
| 31:BA:1291:C:H2' | 31:BA:1292:U:H6 | 1.66 | 0.60 |
| 31:BA:2753:A:O2' | 31:BA:2754:U:O5' | 2.19 | 0.60 |
| 31:BA:2572:A:N7 | 34:BE:144:ARG:HD2 | 2.16 | 0.60 |
| 35:BF:3:GLU:HA | 35:BF:24:LEU:HB3 | 1.81 | 0.60 |
| 37:BH:156:ALA:C | 37:BH:158:HIS:N | 2.54 | 0.60 |
| 46:BU:49:HIS:HA | 46:BU:52:ARG:HB2 | 1.83 | 0.60 |
| 50:BY:45:VAL:HG13 | 50:BY:62:GLU:CB | 2.29 | 0.60 |
| 1:CA:1116:C:H3' | 1:CA:1117:G:H5'' | 1.82 | 0.60 |
| 1:CA:342:C:O2' | 1:CA:343:U:H5' | 2.01 | 0.60 |
| 1:CA:448:A:H2' | 1:CA:449:C:C6 | 2.35 | 0.60 |
| 1:CA:509:A:O2' | 1:CA:510:A:P | 2.59 | 0.60 |
| 2:CB:76:GLN:O | 2:CB:208:ILE:HG12 | 2.01 | 0.60 |
| 5:CE:78:HIS:CE1 | 5:CE:143:ARG:H | 2.19 | 0.60 |
| 13:CM:46:LYS:HG3 | 13:CM:47:ASP:H | 1.63 | 0.60 |
| 31:DA:1484:G:N2 | 31:DA:1505:C:C5 | 2.69 | 0.60 |
| 31:DA:2360:A:HO2' | 31:DA:2361:A:H8 | 1.49 | 0.60 |
| 31:DA:298:G:C5' | 31:DA:299:A:OP1 | 2.49 | 0.60 |
| 31:DA:443:A:H1' | 31:DA:1201:C:O4' | 2.01 | 0.60 |
| 31:DA:626:U:H3 | 41:DP:105:LEU:HG | 1.66 | 0.60 |
| 31:DA:823:G:C2' | 31:DA:824:A:H5' | 2.31 | 0.60 |
| 33:DD:142:VAL:HG23 | 33:DD:193:VAL:HA | 1.83 | 0.60 |
| 38:DI:5:LEU:C | 38:DI:6:LEU:HD23 | 2.21 | 0.60 |
| 44:DS:53:SER:O | 44:DS:56:LEU:N | 2.34 | 0.60 |
| 46:DU:16:LYS:O | 46:DU:20:LEU:HD23 | 2.01 | 0.60 |
| 51:DZ:130:PRO:HA | 51:DZ:133:ILE:HD11 | 1.82 | 0.60 |
| 51:DZ:150:LEU:HD23 | 51:DZ:171:ILE:HD11 | 1.82 | 0.60 |
| 1:AA:1244:C:H2' | 1:AA:1245:A:C8 | 2.36 | 0.60 |
| 1:AA:421:U:C4 | 3:AC:127:ARG:NH1 | 2.67 | 0.60 |
| 1:AA:960:U:O2 | 1:AA:960:U:H2' | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:AE:78:HIS:CE1 | 5:AE:143:ARG:H | 2.18 | 0.60 |
| 8:AH:86:ILE:HB | 8:AH:133:LEU:HD22 | 1.82 | 0.60 |
| 9:AI:73:GLN:O | 9:AI:77:ILE:HG13 | 2.01 | 0.60 |
| 31:BA:150:C:H2' | 31:BA:151:C:H6 | 1.65 | 0.60 |
| 31:BA:157:U:H5' | 31:BA:171:G:N2 | 2.16 | 0.60 |
| 37:BH:28:GLY:HA3 | 37:BH:79:VAL:HB | 1.83 | 0.60 |
| 38:BI:5:LEU:C | 38:BI:6:LEU:HD23 | 2.21 | 0.60 |
| 44:BS:85:VAL:CG2 | 44:BS:106:ARG:HB2 | 2.23 | 0.60 |
| 45:BT:93:ARG:O | 45:BT:94:ALA:C | 2.40 | 0.60 |
| 48:BW:64:MET:O | 48:BW:65:LEU:CB | 2.39 | 0.60 |
| 1:CA:437:U:O2' | 1:CA:438:G:H5' | 2.01 | 0.60 |
| 4:CD:127:THR:OG1 | 4:CD:128:VAL:N | 2.32 | 0.60 |
| 8:CH:10:LEU:HD23 | 8:CH:10:LEU:N | 2.15 | 0.60 |
| 16:CP:19:ILE:HG22 | 16:CP:36:ILE:HG13 | 1.82 | 0.60 |
| 29:D7:16:HIS:CB | 29:D7:44:PRO:HG2 | 2.27 | 0.60 |
| 31:DA:151:C:O2' | 31:DA:152:G:H5' | 2.01 | 0.60 |
| 31:DA:2376:A:OP1 | 31:DA:2376:A:H8 | 1.84 | 0.60 |
| 31:DA:673:C:H5'' | 35:DF:81:PRO:HD2 | 1.82 | 0.60 |
| 31:DA:971:C:H2' | 31:DA:972:G:H5' | 1.82 | 0.60 |
| 44:DS:26:LEU:O | 44:DS:88:ASP:HB3 | 2.01 | 0.60 |
| 46:DU:83:LEU:HG | 46:DU:88:ILE:CG1 | 2.25 | 0.60 |
| 47:DV:1:MET:HE2 | 47:DV:1:MET:HA | 1.82 | 0.60 |
| 47:DV:72:VAL:O | 47:DV:73:SER:CB | 2.49 | 0.60 |
| 50:DY:45:VAL:HG11 | 50:DY:60:PHE:O | 2.00 | 0.60 |
| 51:DZ:165:VAL:HG12 | 51:DZ:166:SER:OG | 1.99 | 0.60 |
| 1:AA:857:C:H2' | 1:AA:858:G:O4' | 2.01 | 0.60 |
| 4:AD:133:VAL:HG12 | 4:AD:135:LEU:H | 1.66 | 0.60 |
| 6:AF:7:ASN:HD22 | 6:AF:7:ASN:N | 1.98 | 0.60 |
| 16:AP:4:ILE:HB | 16:AP:66:PRO:HB3 | 1.82 | 0.60 |
| 16:AP:74:LEU:O | 16:AP:79:VAL:HB | 2.01 | 0.60 |
| 6:AF:99:ALA:HB1 | 18:AR:23:LYS:NZ | 2.15 | 0.60 |
| 23:B1:26:ARG:CB | 23:B1:34:THR:HA | 2.31 | 0.60 |
| 31:BA:1441:G:O2' | 31:BA:1442:G:H5' | 2.01 | 0.60 |
| 31:BA:2536:G:C6 | 31:BA:2537:U:C4 | 2.89 | 0.60 |
| 31:BA:2699:C:H2' | 31:BA:2700:C:O4' | 2.01 | 0.60 |
| 31:BA:626:U:O2 | 41:BP:105:LEU:HG | 2.01 | 0.60 |
| 34:BE:48:GLN:NE2 | 34:BE:78:LEU:HD13 | 2.16 | 0.60 |
| 34:BE:9:VAL:HG13 | 34:BE:25:VAL:O | 2.01 | 0.60 |
| 1:CA:1049:U:H4' | 1:CA:1050:G:O5' | 2.00 | 0.60 |
| 1:CA:1049:U:H4' | 1:CA:1050:G:C5' | 2.31 | 0.60 |
| 1:CA:349:A:O2' | 1:CA:350:G:H5' | 2.00 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:CA:392:G:H2' | 1:CA:393:A:C8 | 2.36 | 0.60 |
| 1:CA:963:G:H21 | 10:CJ:55:LYS:CE | 2.14 | 0.60 |
| 3:CC:35:GLU:CD | 3:CC:59:ARG:HH22 | 2.04 | 0.60 |
| 3:CC:50:ALA:HB1 | 3:CC:70:VAL:HG11 | 1.83 | 0.60 |
| 6:CF:42:GLU:OE1 | 6:CF:59:TYR:HE2 | 1.84 | 0.60 |
| 16:CP:20:VAL:HG22 | 16:CP:34:GLU:O | 2.01 | 0.60 |
| 31:DA:1021:A:H3' | 31:DA:1021:A:H8 | 1.65 | 0.60 |
| 31:DA:1528:A:O2' | 31:DA:1528(A):A:O5' | 2.19 | 0.60 |
| 31:DA:2101:G:C6 | 31:DA:2102:U:C5 | 2.89 | 0.60 |
| 31:DA:2790:A:H2' | 31:DA:2791:C:H5'' | 1.83 | 0.60 |
| 33:DD:27:THR:CG2 | 33:DD:28:GLU:N | 2.64 | 0.60 |
| 35:DF:3:GLU:O | 35:DF:24:LEU:HG | 2.01 | 0.60 |
| 38:DI:63:ALA:O | 38:DI:67:ARG:HD2 | 2.00 | 0.60 |
| 41:DP:107:LYS:O | 41:DP:109:GLY:N | 2.34 | 0.60 |
| 41:DP:107:LYS:C | 41:DP:109:GLY:H | 2.01 | 0.60 |
| 50:DY:76:CYS:O | 50:DY:99:CYS:SG | 2.60 | 0.60 |
| 1:AA:1026:G:H2' | 1:AA:1026:G:N3 | 2.16 | 0.60 |
| 1:AA:1109:C:H2' | 1:AA:1110:A:O4' | 2.01 | 0.60 |
| 1:AA:1117:G:H4' | 9:AI:104:ARG:CZ | 2.31 | 0.60 |
| 1:AA:1321:C:C3' | 1:AA:1322:C:H5'' | 2.31 | 0.60 |
| 1:AA:622:A:C8 | 1:AA:623:C:C5 | 2.88 | 0.60 |
| 1:AA:967:C:H5'' | 1:AA:968:A:OP2 | 2.02 | 0.60 |
| 4:AD:127:THR:OG1 | 4:AD:128:VAL:N | 2.33 | 0.60 |
| 4:AD:138:TYR:HD2 | 4:AD:139:ARG:N | 2.00 | 0.60 |
| 4:AD:164:ALA:HB1 | 4:AD:168:ARG:NH1 | 2.16 | 0.60 |
| 4:AD:79:PHE:CZ | 4:AD:204:ILE:HD13 | 2.36 | 0.60 |
| 4:AD:43:HIS:O | 4:AD:45:GLN:N | 2.33 | 0.60 |
| 6:AF:42:GLU:OE1 | 6:AF:59:TYR:HE2 | 1.83 | 0.60 |
| 9:AI:53:VAL:HB | 9:AI:92:TYR:CE2 | 2.35 | 0.60 |
| 24:B2:41:ILE:O | 24:B2:42:GLY:O | 2.19 | 0.60 |
| 31:BA:1722:A:N6 | 31:BA:1741:A:C2 | 2.70 | 0.60 |
| 31:BA:1893:C:C5 | 31:BA:1894:C:C5 | 2.89 | 0.60 |
| 31:BA:307:G:N2 | 31:BA:310:A:H5'' | 2.16 | 0.60 |
| 31:BA:322:A:H5' | 31:BA:340:A:C1' | 2.32 | 0.60 |
| 32:BB:37:C:C5 | 32:BB:38:C:C5 | 2.89 | 0.60 |
| 32:BB:21:G:O6 | 32:BB:63:G:C5 | 2.54 | 0.60 |
| 36:BG:57:ALA:HB2 | 36:BG:90:LEU:HD21 | 1.83 | 0.60 |
| 38:BI:117:GLU:HG3 | 38:BI:118:LYS:N | 2.15 | 0.60 |
| 38:BI:83:ALA:HA | 38:BI:89:TYR:CD1 | 2.37 | 0.60 |
| 41:BP:7:ARG:O | 41:BP:10:PRO:HD3 | 2.01 | 0.60 |
| 43:BR:116:LEU:O | 43:BR:117:VAL:CB | 2.50 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BS:30:ARG:NH2 | 44:BS:62:LYS:HD2 | 2.09 | 0.60 |
| 48:BW:6:ILE:HA | 48:BW:103:ILE:O | 2.02 | 0.60 |
| 1:CA:1157:A:H4' | 1:CA:1158:C:O5' | 2.00 | 0.60 |
| 1:CA:192:U:H2' | 1:CA:193:C:C6 | 2.36 | 0.60 |
| 1:CA:343:U:C2 | 1:CA:347:G:N1 | 2.70 | 0.60 |
| 1:CA:960:U:O2 | 1:CA:960:U:H2' | 2.00 | 0.60 |
| 2:CB:121:LEU:HD23 | 2:CB:127:ILE:HD11 | 1.83 | 0.60 |
| 4:CD:107:ARG:HD2 | 4:CD:173:TRP:HZ2 | 1.66 | 0.60 |
| 18:CR:50:ILE:CD1 | 18:CR:70:ILE:HG21 | 2.32 | 0.60 |
| 31:DA:1427:A:H4' | 31:DA:1428:C:O5' | 2.01 | 0.60 |
| 31:DA:17:G:H4' | 46:DU:25:TRP:CH2 | 2.36 | 0.60 |
| 22:D0:16:SER:HB3 | 31:DA:2262:U:OP2 | 2.00 | 0.60 |
| 31:DA:310:A:OP1 | 50:DY:18:GLY:HA2 | 2.00 | 0.60 |
| 35:DF:3:GLU:HA | 35:DF:24:LEU:HB3 | 1.82 | 0.60 |
| 41:DP:121:LYS:HB3 | 41:DP:123:LEU:HD23 | 1.82 | 0.60 |
| 1:AA:1158:C:N3 | 1:AA:1181:G:N2 | 2.49 | 0.60 |
| 22:B0:8:GLY:HA3 | 31:BA:2255:G:H21 | 1.67 | 0.60 |
| 23:B1:34:THR:HG23 | 31:BA:388:G:P | 2.41 | 0.60 |
| 24:B2:45:SER:O | 24:B2:48:HIS:CB | 2.49 | 0.60 |
| 31:BA:1484:G:N2 | 31:BA:1505:C:H5 | 1.98 | 0.60 |
| 33:BD:125:ILE:HG21 | 33:BD:137:PRO:HG2 | 1.83 | 0.60 |
| 33:BD:44:ASN:HB3 | 33:BD:49:ILE:CA | 2.32 | 0.60 |
| 34:BE:51:PHE:CD1 | 34:BE:52:LEU:N | 2.69 | 0.60 |
| 35:BF:128:ALA:O | 35:BF:142:TRP:NE1 | 2.35 | 0.60 |
| 37:BH:154:PRO:O | 37:BH:156:ALA:N | 2.31 | 0.60 |
| 37:BH:155:SER:OG | 37:BH:155:SER:O | 2.11 | 0.60 |
| 40:BO:4:PRO:O | 40:BO:5:GLN:HB2 | 2.00 | 0.60 |
| 44:BS:74:ALA:HB1 | 44:BS:103:GLU:CB | 2.31 | 0.60 |
| 45:BT:30:VAL:HG21 | 45:BT:83:ILE:H | 1.66 | 0.60 |
| 48:BW:73:ALA:HB3 | 48:BW:106:ILE:HD11 | 1.83 | 0.60 |
| 31:BA:26:G:OP1 | 48:BW:80:PRO:HB3 | 2.02 | 0.60 |
| 49:BX:65:ARG:CZ | 49:BX:66:LEU:H | 2.14 | 0.60 |
| 50:BY:76:CYS:O | 50:BY:99:CYS:SG | 2.59 | 0.60 |
| 1:CA:612:C:O2' | 1:CA:613:C:H5' | 2.01 | 0.60 |
| 3:CC:130:VAL:O | 3:CC:134:ILE:HG12 | 2.01 | 0.60 |
| 8:CH:69:ARG:HD3 | 8:CH:75:ARG:O | 2.01 | 0.60 |
| 12:CL:32:PHE:HE1 | 12:CL:86:ARG:HG3 | 1.65 | 0.60 |
| 22:D0:2:ALA:H | 31:DA:2602:A:H61 | 1.49 | 0.60 |
| 23:D1:25:LYS:O | 23:D1:26:ARG:HB3 | 2.01 | 0.60 |
| 27:D5:2:ALA:N | 31:DA:747:U:N3 | 2.49 | 0.60 |
| 30:D8:62:LEU:CD1 | 31:DA:242:G:H5'' | 2.29 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:272(J):C:H42 | 31:DA:363(A):A:N6 | 2.00 | 0.60 |
| 33:DD:133:LEU:HA | 33:DD:136:ILE:HD13 | 1.82 | 0.60 |
| 37:DH:144:VAL:O | 37:DH:148:ILE:HG12 | 2.02 | 0.60 |
| 38:DI:88:ILE:HD11 | 38:DI:123:LEU:HD23 | 1.83 | 0.60 |
| 39:DN:39:ARG:CD | 39:DN:41:ASP:HB2 | 2.32 | 0.60 |
| 41:DP:45:LEU:HD22 | 41:DP:46:LYS:H | 1.65 | 0.60 |
| 43:DR:13:HIS:HE1 | 43:DR:15:SER:OG | 1.84 | 0.60 |
| 49:DX:66:LEU:O | 49:DX:66:LEU:HD23 | 2.02 | 0.60 |
| 50:DY:46:LYS:HG2 | 50:DY:47:LYS:HD2 | 1.84 | 0.60 |
| 51:DZ:69:THR:HG22 | 51:DZ:90:VAL:HA | 1.83 | 0.60 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:H6 | 1.66 | 0.60 |
| 1:AA:343:U:C2 | 1:AA:347:G:N1 | 2.69 | 0.60 |
| 1:AA:360:A:O2' | 1:AA:361:G:H5' | 2.02 | 0.60 |
| 2:AB:111:ARG:O | 2:AB:145:LEU:HD11 | 2.01 | 0.60 |
| 3:AC:43:LEU:O | 3:AC:47:LEU:HB3 | 2.02 | 0.60 |
| 10:AJ:57:LYS:HD3 | 10:AJ:60:ARG:NH2 | 2.16 | 0.60 |
| 19:AS:29:ARG:HD3 | 19:AS:48:THR:OG1 | 2.01 | 0.60 |
| 20:AT:75:ASN:O | 20:AT:79:ARG:HB2 | 2.01 | 0.60 |
| 28:B6:16:CYS:O | 28:B6:18:ARG:CZ | 2.50 | 0.60 |
| 30:B8:32:LEU:O | 30:B8:33:ASN:CB | 2.39 | 0.60 |
| 31:BA:2661:G:C8 | 31:BA:2662:A:C2 | 2.90 | 0.60 |
| 32:BB:10:C:C4 | 32:BB:11:C:C5 | 2.89 | 0.60 |
| 32:BB:47:C:O2' | 44:BS:93:LYS:HG2 | 2.01 | 0.60 |
| 33:BD:68:LYS:HB3 | 33:BD:70:TRP:CH2 | 2.37 | 0.60 |
| 34:BE:65:GLY:C | 34:BE:67:PHE:H | 2.04 | 0.60 |
| 35:BF:3:GLU:O | 35:BF:24:LEU:HG | 2.01 | 0.60 |
| 42:BQ:14:ARG:HG2 | 42:BQ:41:TRP:HH2 | 1.67 | 0.60 |
| 45:BT:55:ASN:H | 45:BT:59:THR:HB | 1.66 | 0.60 |
| 47:BV:1:MET:N | 47:BV:44:LYS:HD2 | 2.16 | 0.60 |
| 50:BY:38:ILE:CG2 | 50:BY:39:VAL:N | 2.64 | 0.60 |
| 50:BY:68:HIS:N | 50:BY:71:LYS:HZ1 | 2.00 | 0.60 |
| 1:CA:1162:C:H2' | 1:CA:1163:C:C6 | 2.36 | 0.60 |
| 2:CB:187:LEU:HD11 | 2:CB:204:ASN:O | 2.00 | 0.60 |
| 4:CD:73:ARG:HD2 | 4:CD:77:ASN:HD21 | 1.66 | 0.60 |
| 1:CA:1250:A:H4' | 9:CI:68:GLY:H | 1.66 | 0.60 |
| 13:CM:31:LYS:HA | 13:CM:34:LEU:HD12 | 1.83 | 0.60 |
| 31:DA:1434:A:H2' | 31:DA:1435:G:H8 | 1.65 | 0.60 |
| 31:DA:2658:C:H3' | 31:DA:2659:G:H5'' | 1.83 | 0.60 |
| 31:DA:863:A:C2' | 31:DA:864:G:H5' | 2.30 | 0.60 |
| 41:DP:26:GLY:HA2 | 41:DP:30:THR:CG2 | 2.32 | 0.60 |
| 31:DA:956:G:OP2 | 42:DQ:14:ARG:NH2 | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 49:DX:60:ARG:HH21 | 49:DX:74:PRO:HG2 | 1.67 | 0.60 |
| 1:AA:1065:U:C1' | 1:AA:1066:C:OP2 | 2.50 | 0.60 |
| 1:AA:1157:A:H4' | 1:AA:1158:C:O5' | 2.01 | 0.60 |
| 1:AA:1172:C:H2' | 1:AA:1173:G:H8 | 1.67 | 0.60 |
| 1:AA:709:G:H2' | 1:AA:710:G:H8 | 1.66 | 0.60 |
| 1:AA:872:A:C4 | 1:AA:874:G:N7 | 2.69 | 0.60 |
| 3:AC:73:PRO:HG3 | 3:AC:105:GLU:HG3 | 1.82 | 0.60 |
| 3:AC:83:ARG:O | 3:AC:86:VAL:HG22 | 2.02 | 0.60 |
| 27:B5:33:CYS:SG | 27:B5:49:CYS:CB | 2.89 | 0.60 |
| 31:BA:102:G:HO2' | 31:BA:103:A:P | 2.20 | 0.60 |
| 31:BA:271(Q):G:O2' | 31:BA:271(R):G:P | 2.59 | 0.60 |
| 31:BA:673:C:H5'' | 35:BF:81:PRO:HD2 | 1.83 | 0.60 |
| 49:BX:80:ILE:O | 49:BX:81:VAL:HB | 2.00 | 0.60 |
| 1:CA:1065:U:C1' | 1:CA:1066:C:OP2 | 2.50 | 0.60 |
| 2:CB:8:LYS:NZ | 2:CB:217:ARG:HH11 | 1.99 | 0.60 |
| 4:CD:62:GLN:HE22 | 4:CD:65:ARG:HE | 1.49 | 0.60 |
| 5:CE:7:GLU:HG2 | 5:CE:112:LEU:HD22 | 1.82 | 0.60 |
| 10:CJ:57:LYS:HD3 | 10:CJ:60:ARG:NH2 | 2.17 | 0.60 |
| 11:CK:125:PHE:H | 11:CK:125:PHE:HD1 | 1.49 | 0.60 |
| 23:D1:30:VAL:O | 23:D1:30:VAL:HG12 | 2.01 | 0.60 |
| 25:D3:28:LEU:HA | 25:D3:33:GLN:OE1 | 2.02 | 0.60 |
| 31:DA:1252:G:C2 | 31:DA:1253:A:C2 | 2.90 | 0.60 |
| 31:DA:1478:G:C2' | 31:DA:1479:G:H5' | 2.32 | 0.60 |
| 28:D6:27:LYS:HE3 | 31:DA:2285:C:H5 | 1.67 | 0.60 |
| 31:DA:2422:A:H4' | 31:DA:2423:U:OP1 | 2.00 | 0.60 |
| 31:DA:2881:C:H2' | 31:DA:2882:A:O4' | 2.02 | 0.60 |
| 31:DA:642:G:H21 | 31:DA:646:A:H2 | 1.50 | 0.60 |
| 31:DA:568:U:H5' | 31:DA:945:A:C2 | 2.36 | 0.60 |
| 31:DA:832:G:OP1 | 41:DP:40:SER:HB3 | 2.02 | 0.60 |
| 31:DA:833:U:O2 | 41:DP:55:ARG:NH1 | 2.34 | 0.60 |
| 41:DP:62:LEU:H | 41:DP:62:LEU:CD2 | 1.99 | 0.60 |
| 41:DP:62:LEU:H | 41:DP:62:LEU:HD13 | 1.67 | 0.60 |
| 50:DY:27:VAL:HB | 50:DY:29:GLU:OE1 | 2.01 | 0.60 |
| 1:AA:473:G:H2' | 1:AA:474:G:H8 | 1.65 | 0.60 |
| 1:AA:491:G:H2' | 1:AA:492:G:H8 | 1.65 | 0.60 |
| 25:B3:28:LEU:HA | 25:B3:33:GLN:OE1 | 2.02 | 0.60 |
| 31:BA:1188:U:H2' | 31:BA:1189:A:H5' | 1.83 | 0.60 |
| 31:BA:2656:U:H2' | 31:BA:2657:A:H5'' | 1.84 | 0.60 |
| 31:BA:2681:C:C5 | 31:BA:2725:A:N6 | 2.58 | 0.60 |
| 31:BA:288:C:O2 | 31:BA:288:C:H2' | 2.01 | 0.60 |
| 31:BA:607:U:O2 | 31:BA:621:A:N1 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:823:G:O2' | 31:BA:824:A:H5' | 2.01 | 0.60 |
| 33:BD:158:ALA:O | 33:BD:159:ALA:HB2 | 2.01 | 0.60 |
| 33:BD:228:PRO:HD3 | 33:BD:235:GLY:CA | 2.31 | 0.60 |
| 38:BI:56:LYS:C | 38:BI:56:LYS:HZ3 | 2.05 | 0.60 |
| 39:BN:67:LEU:HB3 | 39:BN:88:GLU:OE2 | 2.01 | 0.60 |
| 45:BT:27:THR:O | 45:BT:28:VAL:HG23 | 2.01 | 0.60 |
| 45:BT:33:LYS:NZ | 45:BT:33:LYS:CA | 2.65 | 0.60 |
| 47:BV:96:ILE:CG2 | 47:BV:97:LYS:N | 2.65 | 0.60 |
| 49:BX:83:VAL:O | 49:BX:84:ALA:CB | 2.49 | 0.60 |
| 1:CA:403:C:O2' | 1:CA:404:U:H5' | 2.02 | 0.60 |
| 5:CE:68:GLU:O | 5:CE:70:PRO:HD3 | 2.01 | 0.60 |
| 7:CG:69:VAL:HA | 7:CG:138:LYS:HD2 | 1.84 | 0.60 |
| 7:CG:138:LYS:HE2 | 7:CG:142:GLU:OE2 | 2.00 | 0.60 |
| 31:DA:1204:A:N1 | 31:DA:1241:A:C2 | 2.67 | 0.60 |
| 31:DA:1481:U:H5' | 31:DA:1482:G:OP2 | 2.00 | 0.60 |
| 33:DD:31:LYS:O | 33:DD:35:LYS:O | 2.20 | 0.60 |
| 37:DH:85:LYS:HD3 | 37:DH:133:VAL:HB | 1.83 | 0.60 |
| 37:DH:97:ARG:O | 37:DH:98:LEU:C | 2.40 | 0.60 |
| 49:DX:21:PHE:N | 49:DX:21:PHE:CD1 | 2.69 | 0.60 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:C6 | 2.37 | 0.60 |
| 1:AA:1090:U:C2 | 1:AA:1091:U:C5 | 2.90 | 0.60 |
| 1:AA:1250:A:H4' | 9:AI:68:GLY:H | 1.66 | 0.60 |
| 2:AB:71:VAL:O | 2:AB:164:VAL:HG22 | 2.01 | 0.60 |
| 6:AF:5:GLU:HB3 | 6:AF:62:TRP:HE1 | 1.66 | 0.60 |
| 12:AL:32:PHE:HE1 | 12:AL:86:ARG:HG3 | 1.66 | 0.60 |
| 16:AP:39:TYR:C | 16:AP:39:TYR:CD1 | 2.73 | 0.60 |
| 17:AQ:97:SER:O | 17:AQ:98:LEU:HD23 | 2.01 | 0.60 |
| 23:B1:92:LYS:C | 23:B1:94:LEU:N | 2.55 | 0.60 |
| 28:B6:11:LEU:CD2 | 28:B6:26:ASN:H | 2.15 | 0.60 |
| 31:BA:1497:U:C2' | 31:BA:1498:C:OP1 | 2.50 | 0.60 |
| 31:BA:2749:A:H4' | 37:BH:62:LYS:HB3 | 1.84 | 0.60 |
| 32:BB:66:A:N6 | 32:BB:108:U:H2' | 2.16 | 0.60 |
| 33:BD:28:GLU:HB2 | 33:BD:29:PRO:HD3 | 1.82 | 0.60 |
| 35:BF:205:ARG:C | 35:BF:206:ILE:HG13 | 2.22 | 0.60 |
| 37:BH:138:LYS:H | 37:BH:141:VAL:H | 1.50 | 0.60 |
| 37:BH:35:VAL:O | 37:BH:37:VAL:HG23 | 2.01 | 0.60 |
| 37:BH:66:GLY:HA2 | 37:BH:69:ARG:HB2 | 1.82 | 0.60 |
| 31:BA:943:U:OP2 | 41:BP:38:GLN:OE1 | 2.20 | 0.60 |
| 1:CA:594:G:H1 | 1:CA:645:C:N4 | 2.00 | 0.60 |
| 1:CA:7:G:H21 | 5:CE:121:LYS:HG2 | 1.65 | 0.60 |
| 3:CC:7:PRO:O | 3:CC:11:ARG:HG2 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1325:C:H4' | 21:CU:17:THR:HG21 | 1.84 | 0.60 |
| 31:DA:626:U:O2 | 41:DP:105:LEU:HG | 2.01 | 0.60 |
| 35:DF:22:ALA:HB1 | 35:DF:26:ALA:CB | 2.32 | 0.60 |
| 38:DI:61:ARG:O | 38:DI:133:HIS:CE1 | 2.55 | 0.60 |
| 48:DW:56:ALA:O | 48:DW:57:ASN:C | 2.38 | 0.60 |
| 49:DX:72:LYS:HG3 | 49:DX:74:PRO:CD | 2.31 | 0.60 |
| 4:AD:119:GLN:O | 4:AD:123:HIS:CD2 | 2.55 | 0.60 |
| 4:AD:62:GLN:HE22 | 4:AD:65:ARG:HE | 1.48 | 0.60 |
| 7:AG:116:ALA:O | 7:AG:120:ILE:HG12 | 2.02 | 0.60 |
| 22:B0:72:ARG:HH21 | 22:B0:75:LEU:CD1 | 2.15 | 0.60 |
| 31:BA:1348:G:C2' | 31:BA:1349:A:H5' | 2.32 | 0.60 |
| 31:BA:1378:A:H4' | 31:BA:1379:A:OP1 | 2.02 | 0.60 |
| 31:BA:1963:U:H2' | 31:BA:1963:U:O2 | 2.02 | 0.60 |
| 33:BD:255:LYS:N | 33:BD:255:LYS:HZ1 | 2.00 | 0.60 |
| 34:BE:3:GLY:CA | 34:BE:81:ILE:HG21 | 2.32 | 0.60 |
| 37:BH:149:ARG:HD3 | 37:BH:164:TYR:HE1 | 1.67 | 0.60 |
| 46:BU:50:ARG:NH2 | 47:BV:75:PHE:CD2 | 2.70 | 0.60 |
| 47:BV:51:VAL:HG12 | 47:BV:52:VAL:N | 2.17 | 0.60 |
| 31:BA:1225:G:OP1 | 47:BV:88:ARG:HD2 | 2.02 | 0.60 |
| 49:BX:35:THR:O | 49:BX:36:LYS:C | 2.41 | 0.60 |
| 49:BX:36:LYS:NZ | 49:BX:38:GLU:C | 2.56 | 0.60 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:H6 | 1.67 | 0.60 |
| 1:CA:1392:G:N2 | 1:CA:1502:A:C8 | 2.67 | 0.60 |
| 1:CA:80:G:H1 | 1:CA:89:C:N4 | 1.99 | 0.60 |
| 23:D1:13:ILE:O | 23:D1:14:VAL:HB | 2.00 | 0.60 |
| 31:DA:128:C:H2' | 31:DA:129:C:O4' | 2.01 | 0.60 |
| 31:DA:1451:C:N3 | 31:DA:1459:G:O6 | 2.35 | 0.60 |
| 31:DA:1692:U:H2' | 31:DA:1694:C:C5 | 2.37 | 0.60 |
| 31:DA:2094:G:N2 | 31:DA:2196:C:H1' | 2.17 | 0.60 |
| 31:DA:829:A:N7 | 31:DA:2248:C:H5' | 2.17 | 0.60 |
| 32:DB:15:A:H5' | 32:DB:16:G:H8 | 1.67 | 0.60 |
| 35:DF:88:VAL:HG11 | 35:DF:91:GLY:HA3 | 1.84 | 0.60 |
| 38:DI:2:LYS:HB2 | 38:DI:39:ALA:CB | 2.32 | 0.60 |
| 43:DR:74:LYS:HD2 | 43:DR:77:ARG:HH21 | 1.66 | 0.60 |
| 47:DV:52:VAL:O | 47:DV:53:GLU:CB | 2.49 | 0.60 |
| 47:DV:72:VAL:CG1 | 47:DV:88:ARG:HH22 | 2.11 | 0.60 |
| 1:AA:25:C:H2' | 1:AA:26:A:C8 | 2.37 | 0.59 |
| 1:AA:604:G:C6 | 1:AA:605:U:C4 | 2.90 | 0.59 |
| 3:AC:36:ASP:HB3 | 3:AC:40:ARG:NH1 | 2.17 | 0.59 |
| 6:AF:91:VAL:HG11 | 18:AR:72:ARG:NH1 | 2.17 | 0.59 |
| 9:AI:122:ALA:HB1 | 9:AI:123:PRO:HD2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:AJ:40:LEU:HD23 | 10:AJ:40:LEU:H | 1.66 | 0.59 |
| 23:B1:87:PRO:HD2 | 23:B1:88:LYS:H | 1.67 | 0.59 |
| 27:B5:4:HIS:HB3 | 27:B5:5:PRO:CD | 2.28 | 0.59 |
| 31:BA:1042:G:N3 | 31:BA:1042:G:H2' | 2.17 | 0.59 |
| 31:BA:1947:C:H2' | 31:BA:1948:G:C5' | 2.31 | 0.59 |
| 31:BA:2058:A:H5'' | 31:BA:2059:A:OP2 | 2.02 | 0.59 |
| 31:BA:2544:G:O5' | 31:BA:2544:G:H8 | 1.84 | 0.59 |
| 31:BA:2790:A:H2' | 31:BA:2791:C:C5' | 2.31 | 0.59 |
| 31:BA:528:A:C2 | 31:BA:2043:C:H5' | 2.36 | 0.59 |
| 31:BA:774:A:C2 | 31:BA:787:U:O2' | 2.53 | 0.59 |
| 31:BA:995:C:N3 | 39:BN:4:TYR:CE1 | 2.69 | 0.59 |
| 35:BF:20:LEU:HD22 | 35:BF:203:GLN:NE2 | 2.17 | 0.59 |
| 37:BH:121:ILE:HD11 | 37:BH:140:LYS:HB3 | 1.83 | 0.59 |
| 38:BI:99:GLU:HG3 | 38:BI:103:ARG:CZ | 2.32 | 0.59 |
| 47:BV:83:ARG:O | 47:BV:84:LYS:HD2 | 2.02 | 0.59 |
| 1:CA:255:G:H1' | 17:CQ:16:GLN:NE2 | 2.16 | 0.59 |
| 1:CA:760:G:H2' | 1:CA:761:G:H5' | 1.84 | 0.59 |
| 6:CF:49:ALA:HB2 | 18:CR:78:LEU:O | 2.02 | 0.59 |
| 11:CK:29:ILE:HB | 11:CK:44:SER:CB | 2.32 | 0.59 |
| 30:D8:35:GLN:NE2 | 30:D8:36:LYS:HZ2 | 1.99 | 0.59 |
| 31:DA:1359:A:C8 | 31:DA:1372:U:O4 | 2.55 | 0.59 |
| 31:DA:1441:G:O2' | 31:DA:1442:G:H5' | 2.01 | 0.59 |
| 31:DA:1497:U:C2' | 31:DA:1498:C:OP1 | 2.50 | 0.59 |
| 31:DA:1902:C:O2' | 33:DD:244:ARG:HB2 | 2.02 | 0.59 |
| 31:DA:2307:G:C2 | 31:DA:2308:G:H5' | 2.37 | 0.59 |
| 31:DA:2762:G:H8 | 31:DA:2762:G:C5' | 2.14 | 0.59 |
| 31:DA:796:C:H2' | 31:DA:797:C:H6 | 1.61 | 0.59 |
| 31:DA:873:G:N2 | 31:DA:905:U:C2 | 2.70 | 0.59 |
| 32:DB:15:A:H1' | 32:DB:110:G:N9 | 2.17 | 0.59 |
| 36:DG:43:LEU:CD1 | 36:DG:153:ARG:HD2 | 2.32 | 0.59 |
| 36:DG:60:LEU:O | 36:DG:64:THR:HG22 | 2.02 | 0.59 |
| 43:DR:84:ALA:HB3 | 43:DR:85:PRO:HD3 | 1.82 | 0.59 |
| 45:DT:129:ARG:CZ | 45:DT:131:ALA:HB3 | 2.32 | 0.59 |
| 50:DY:38:ILE:CG2 | 50:DY:39:VAL:N | 2.64 | 0.59 |
| 1:AA:738:C:H2' | 1:AA:739:C:H6 | 1.67 | 0.59 |
| 2:AB:204:ASN:HD21 | 2:AB:207:ALA:H | 1.48 | 0.59 |
| 16:AP:3:LYS:O | 16:AP:21:VAL:HA | 2.03 | 0.59 |
| 31:BA:1025:G:C4 | 31:BA:1135:C:H1' | 2.37 | 0.59 |
| 31:BA:1403:C:C5' | 31:BA:1471:A:H1' | 2.32 | 0.59 |
| 31:BA:1762:A:H8 | 31:BA:1762:A:O5' | 1.85 | 0.59 |
| 31:BA:2186:G:C3' | 31:BA:2187:G:H5'' | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:2308:G:H2' | 31:BA:2309:A:C8 | 2.37 | 0.59 |
| 33:BD:79:VAL:HG21 | 33:BD:111:LEU:HD11 | 1.84 | 0.59 |
| 34:BE:56:PRO:O | 34:BE:58:ARG:N | 2.34 | 0.59 |
| 34:BE:95:ILE:CD1 | 34:BE:95:ILE:H | 2.16 | 0.59 |
| 35:BF:101:LEU:CD1 | 35:BF:102:PRO:HD2 | 2.25 | 0.59 |
| 44:BS:35:ILE:C | 44:BS:36:TYR:HD1 | 2.05 | 0.59 |
| 44:BS:57:LYS:HG2 | 44:BS:58:LEU:H | 1.67 | 0.59 |
| 50:BY:27:VAL:HB | 50:BY:29:GLU:OE1 | 2.02 | 0.59 |
| 1:CA:977:A:C8 | 1:CA:1223:C:C4 | 2.90 | 0.59 |
| 1:CA:1228:C:H2' | 1:CA:1229:A:C8 | 2.36 | 0.59 |
| 1:CA:1244:C:H2' | 1:CA:1245:A:C8 | 2.37 | 0.59 |
| 1:CA:195:A:C6 | 1:CA:196:A:N1 | 2.70 | 0.59 |
| 1:CA:273:A:O2' | 1:CA:274:A:H5' | 2.02 | 0.59 |
| 1:CA:818:G:HO2' | 1:CA:820:U:H6 | 1.49 | 0.59 |
| 10:CJ:39:PRO:HB3 | 10:CJ:70:ARG:NH1 | 2.17 | 0.59 |
| 31:DA:1784:A:H4' | 31:DA:1785:A:O5' | 2.02 | 0.59 |
| 27:D5:4:HIS:O | 31:DA:2056:G:N2 | 2.35 | 0.59 |
| 31:DA:2190:G:C2' | 31:DA:2191:G:H5' | 2.32 | 0.59 |
| 31:DA:2262:U:H2' | 31:DA:2263:C:H5' | 1.84 | 0.59 |
| 22:D0:18:ALA:HB1 | 31:DA:2271:G:OP1 | 2.01 | 0.59 |
| 31:DA:389:G:H22 | 41:DP:71:VAL:HG12 | 1.67 | 0.59 |
| 32:DB:20:C:C2' | 32:DB:21:G:C5' | 2.80 | 0.59 |
| 32:DB:86:G:C3' | 32:DB:87:G:C8 | 2.84 | 0.59 |
| 34:DE:46:ALA:HA | 34:DE:82:ARG:O | 2.01 | 0.59 |
| 35:DF:132:VAL:HG22 | 35:DF:133:ASN:N | 2.16 | 0.59 |
| 39:DN:56:ASN:H | 39:DN:125:GLY:CA | 2.13 | 0.59 |
| 46:DU:69:CYS:HB3 | 46:DU:106:PHE:HZ | 1.66 | 0.59 |
| 50:DY:37:VAL:CG2 | 50:DY:67:LEU:HB3 | 2.32 | 0.59 |
| 3:AC:111:LEU:HD22 | 3:AC:204:LEU:HD21 | 1.85 | 0.59 |
| 7:AG:138:LYS:HE2 | 7:AG:142:GLU:OE2 | 2.01 | 0.59 |
| 1:AA:963:G:H21 | 10:AJ:55:LYS:CE | 2.15 | 0.59 |
| 22:B0:43:THR:O | 22:B0:45:PHE:N | 2.35 | 0.59 |
| 23:B1:25:LYS:C | 23:B1:26:ARG:HG3 | 2.23 | 0.59 |
| 27:B5:36:CYS:C | 27:B5:38:ALA:H | 2.04 | 0.59 |
| 30:B8:43:GLN:O | 30:B8:44:LYS:HD2 | 2.03 | 0.59 |
| 31:BA:2334:G:H21 | 44:BS:18:ILE:CD1 | 2.07 | 0.59 |
| 31:BA:543:C:C6 | 31:BA:547:A:N7 | 2.70 | 0.59 |
| 31:BA:953:A:C2' | 31:BA:954:G:H5' | 2.32 | 0.59 |
| 32:BB:20:C:C2' | 32:BB:21:G:C5' | 2.80 | 0.59 |
| 35:BF:132:VAL:HG22 | 35:BF:133:ASN:N | 2.16 | 0.59 |
| 36:BG:43:LEU:CD1 | 36:BG:153:ARG:HD2 | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BG:127:GLY:CA | 36:BG:166:ASP:HB3 | 2.33 | 0.59 |
| 37:BH:127:GLU:OE1 | 37:BH:127:GLU:HA | 2.02 | 0.59 |
| 41:BP:98:GLU:HG3 | 41:BP:99:LEU:N | 2.16 | 0.59 |
| 42:BQ:20:ALA:O | 42:BQ:22:LYS:N | 2.35 | 0.59 |
| 1:CA:180:U:C2' | 1:CA:181:G:H5' | 2.32 | 0.59 |
| 1:CA:604:G:C6 | 1:CA:605:U:C4 | 2.90 | 0.59 |
| 1:CA:546:G:P | 4:CD:72:GLU:HB3 | 2.42 | 0.59 |
| 9:CI:48:GLU:N | 9:CI:49:PRO:HD2 | 2.17 | 0.59 |
| 12:CL:110:VAL:CG2 | 12:CL:120:TYR:HB3 | 2.33 | 0.59 |
| 16:CP:39:TYR:CD1 | 16:CP:39:TYR:C | 2.74 | 0.59 |
| 13:CM:86:CYS:HB2 | 19:CS:73:GLU:HB3 | 1.83 | 0.59 |
| 24:D2:52:ASP:O | 24:D2:56:GLN:NE2 | 2.34 | 0.59 |
| 31:DA:2281:C:O2' | 31:DA:2282:G:H5' | 2.03 | 0.59 |
| 31:DA:1803:A:O2' | 33:DD:259:THR:HG21 | 2.02 | 0.59 |
| 46:DU:49:HIS:HA | 46:DU:52:ARG:HB2 | 1.84 | 0.59 |
| 50:DY:71:LYS:CB | 50:DY:71:LYS:NZ | 2.64 | 0.59 |
| 4:AD:28:SER:HB3 | 4:AD:30:LYS:HG2 | 1.83 | 0.59 |
| 1:AA:923:A:H5'' | 5:AE:21:ALA:HB2 | 1.83 | 0.59 |
| 8:AH:86:ILE:HG22 | 8:AH:87:SER:N | 2.17 | 0.59 |
| 31:BA:2313:C:H2' | 31:BA:2314:C:H6 | 1.67 | 0.59 |
| 31:BA:2335:A:C8 | 31:BA:2337:G:C5 | 2.90 | 0.59 |
| 31:BA:2790:A:H2' | 31:BA:2791:C:H5'' | 1.84 | 0.59 |
| 42:BQ:141:GLN:HE21 | 51:BZ:71:VAL:C | 2.05 | 0.59 |
| 1:CA:473:G:H2' | 1:CA:474:G:H8 | 1.67 | 0.59 |
| 1:CA:594:G:H2' | 1:CA:595:G:O4' | 2.01 | 0.59 |
| 23:D1:92:LYS:C | 23:D1:94:LEU:H | 2.04 | 0.59 |
| 31:DA:1504:C:O2' | 31:DA:1505:C:O5' | 2.20 | 0.59 |
| 31:DA:2030:A:H5'' | 31:DA:2031:A:P | 2.42 | 0.59 |
| 31:DA:500:G:N2 | 31:DA:502:A:H3' | 2.17 | 0.59 |
| 31:DA:971:C:C2' | 31:DA:972:G:H5' | 2.33 | 0.59 |
| 35:DF:70:THR:HG22 | 35:DF:72:ARG:H | 1.66 | 0.59 |
| 39:DN:58:ASP:OD1 | 39:DN:124:ALA:HB1 | 2.03 | 0.59 |
| 48:DW:111:HIS:CD2 | 48:DW:112:GLY:N | 2.71 | 0.59 |
| 49:DX:24:GLY:HA3 | 49:DX:80:ILE:HG13 | 1.85 | 0.59 |
| 4:AD:117:ALA:O | 4:AD:120:LEU:HB2 | 2.03 | 0.59 |
| 23:B1:27:GLU:OE2 | 23:B1:32:LYS:HB2 | 2.01 | 0.59 |
| 31:BA:676:A:H2 | 31:BA:802:A:H61 | 1.50 | 0.59 |
| 31:BA:823:G:C2' | 31:BA:824:A:H5' | 2.31 | 0.59 |
| 32:BB:86:G:H3' | 32:BB:87:G:C8 | 2.38 | 0.59 |
| 34:BE:27:LEU:HD22 | 45:BT:1:MET:HE3 | 1.83 | 0.59 |
| 39:BN:67:LEU:O | 39:BN:69:GLN:N | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:BP:85:LEU:CD2 | 41:BP:85:LEU:H | 2.07 | 0.59 |
| 45:BT:31:SER:HB3 | 45:BT:43:GLN:O | 2.03 | 0.59 |
| 49:BX:73:ARG:O | 49:BX:74:PRO:O | 2.20 | 0.59 |
| 1:CA:1090:U:C2 | 1:CA:1091:U:C5 | 2.90 | 0.59 |
| 2:CB:20:GLU:O | 2:CB:40:HIS:HB2 | 2.03 | 0.59 |
| 4:CD:189:PRO:CB | 4:CD:194:LEU:HD21 | 2.32 | 0.59 |
| 4:CD:4:TYR:O | 4:CD:5:ILE:HB | 2.03 | 0.59 |
| 9:CI:73:GLN:O | 9:CI:77:ILE:HG13 | 2.02 | 0.59 |
| 30:D8:32:LEU:HG | 30:D8:34:TRP:HE3 | 1.68 | 0.59 |
| 31:DA:1158:C:HO2' | 31:DA:1159:U:P | 2.21 | 0.59 |
| 31:DA:1188:U:H2' | 31:DA:1189:A:H5' | 1.84 | 0.59 |
| 31:DA:212:G:C2' | 31:DA:213:A:H5' | 2.32 | 0.59 |
| 31:DA:2287:A:N6 | 31:DA:2344:U:N3 | 2.41 | 0.59 |
| 31:DA:510:C:O2' | 31:DA:511:U:H5' | 2.02 | 0.59 |
| 31:DA:587:C:H5 | 41:DP:33:ARG:HH11 | 1.51 | 0.59 |
| 31:DA:995:C:N3 | 39:DN:4:TYR:CE1 | 2.71 | 0.59 |
| 32:DB:82:G:O2' | 32:DB:83:G:H5' | 2.03 | 0.59 |
| 33:DD:132:PRO:O | 33:DD:136:ILE:HD12 | 2.03 | 0.59 |
| 34:DE:167:VAL:CG2 | 34:DE:170:LEU:HD11 | 2.32 | 0.59 |
| 34:DE:75:VAL:O | 34:DE:77:ILE:N | 2.35 | 0.59 |
| 34:DE:36:ARG:HH21 | 34:DE:88:GLY:HA2 | 1.66 | 0.59 |
| 35:DF:2:LYS:HG3 | 35:DF:25:PRO:HB2 | 1.85 | 0.59 |
| 36:DG:47:LYS:HG3 | 36:DG:82:LEU:HD11 | 1.83 | 0.59 |
| 37:DH:28:GLY:HA3 | 37:DH:79:VAL:HB | 1.83 | 0.59 |
| 38:DI:29:TYR:HD2 | 38:DI:30:LEU:HD23 | 1.67 | 0.59 |
| 40:DO:4:PRO:O | 40:DO:5:GLN:CB | 2.50 | 0.59 |
| 42:DQ:39:PRO:HA | 42:DQ:97:VAL:O | 2.03 | 0.59 |
| 1:AA:1058:G:H2' | 1:AA:1059:C:O4' | 2.03 | 0.59 |
| 2:AB:121:LEU:HD23 | 2:AB:127:ILE:HD11 | 1.85 | 0.59 |
| 4:AD:189:PRO:CB | 4:AD:194:LEU:HD21 | 2.31 | 0.59 |
| 11:AK:29:ILE:HB | 11:AK:44:SER:CB | 2.32 | 0.59 |
| 31:BA:231:C:C2' | 31:BA:232:G:H5' | 2.33 | 0.59 |
| 44:BS:59:LYS:HE3 | 44:BS:68:GLN:HE22 | 1.67 | 0.59 |
| 44:BS:74:ALA:O | 44:BS:77:ALA:HB3 | 2.02 | 0.59 |
| 50:BY:96:ILE:HG13 | 50:BY:99:CYS:C | 2.22 | 0.59 |
| 1:CA:1072:G:C6 | 1:CA:1073:U:C4 | 2.91 | 0.59 |
| 6:CF:50:TYR:CE2 | 6:CF:52:ILE:HD11 | 2.37 | 0.59 |
| 6:CF:7:ASN:HD22 | 6:CF:7:ASN:N | 2.00 | 0.59 |
| 19:CS:29:ARG:HD3 | 19:CS:48:THR:OG1 | 2.02 | 0.59 |
| 23:D1:56:GLN:OE1 | 23:D1:56:GLN:HA | 2.02 | 0.59 |
| 41:BP:141:ALA:HB3 | 25:D3:1:MET:CE | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:D6:20:ASN:O | 28:D6:21:TYR:CG | 2.55 | 0.59 |
| 31:DA:2472:G:N1 | 31:DA:2477:C:OP1 | 2.21 | 0.59 |
| 31:DA:2632:A:H1' | 34:DE:61:ARG:NH1 | 2.18 | 0.59 |
| 31:DA:310:A:OP1 | 50:DY:17:SER:O | 2.19 | 0.59 |
| 33:DD:167:GLY:C | 33:DD:168:ARG:HG2 | 2.22 | 0.59 |
| 34:DE:34:VAL:CG2 | 34:DE:48:GLN:HE21 | 2.15 | 0.59 |
| 35:DF:8:GLN:HB3 | 35:DF:126:VAL:HA | 1.84 | 0.59 |
| 36:DG:71:THR:HB | 36:DG:89:GLY:HA3 | 1.83 | 0.59 |
| 42:DQ:32:TYR:HE2 | 42:DQ:133:ARG:HG2 | 1.67 | 0.59 |
| 46:DU:93:LYS:CD | 46:DU:93:LYS:H | 2.15 | 0.59 |
| 50:DY:79:CYS:O | 50:DY:80:GLY:C | 2.39 | 0.59 |
| 1:AA:629:G:H2' | 1:AA:630:G:O4' | 2.01 | 0.59 |
| 1:AA:757:U:H2' | 1:AA:758:G:O4' | 2.02 | 0.59 |
| 1:AA:80:G:H1 | 1:AA:89:C:N4 | 2.00 | 0.59 |
| 1:AA:957:U:H4' | 19:AS:79:THR:HB | 1.84 | 0.59 |
| 2:AB:76:GLN:O | 2:AB:208:ILE:HG12 | 2.03 | 0.59 |
| 1:AA:1048:G:OP1 | 14:AN:4:LYS:HB2 | 2.03 | 0.59 |
| 20:AT:89:ARG:HH21 | 20:AT:104:LEU:HD21 | 1.68 | 0.59 |
| 31:BA:2300:G:N2 | 31:BA:2317:C:C2 | 2.71 | 0.59 |
| 31:BA:358:U:H6 | 31:BA:358:U:H3' | 1.68 | 0.59 |
| 31:BA:2599:G:OP2 | 33:BD:236:GLY:N | 2.36 | 0.59 |
| 35:BF:123:LEU:HD12 | 35:BF:124:LEU:H | 1.67 | 0.59 |
| 36:BG:47:LYS:HG3 | 36:BG:82:LEU:HD11 | 1.85 | 0.59 |
| 42:BQ:32:TYR:HE2 | 42:BQ:133:ARG:HG2 | 1.67 | 0.59 |
| 42:BQ:20:ALA:HB2 | 42:BQ:99:PRO:CD | 2.32 | 0.59 |
| 43:BR:84:ALA:HB3 | 43:BR:85:PRO:HD3 | 1.84 | 0.59 |
| 44:BS:87:PHE:CE2 | 44:BS:97:ARG:NH2 | 2.71 | 0.59 |
| 46:BU:102:GLU:HG3 | 47:BV:2:PHE:HZ | 1.67 | 0.59 |
| 48:BW:4:LYS:HB2 | 48:BW:106:ILE:CG2 | 2.30 | 0.59 |
| 1:CA:1150:U:O4 | 1:CA:1151:A:N6 | 2.36 | 0.59 |
| 2:CB:185:ILE:HG22 | 2:CB:199:TYR:CB | 2.22 | 0.59 |
| 4:CD:110:PHE:HD1 | 4:CD:110:PHE:H | 1.51 | 0.59 |
| 4:CD:33:MET:CE | 4:CD:37:PRO:HA | 2.33 | 0.59 |
| 6:CF:11:ASN:O | 6:CF:14:LEU:HB2 | 2.02 | 0.59 |
| 31:DA:1021:A:N6 | 31:DA:1141:U:H3 | 1.92 | 0.59 |
| 31:DA:2342:C:OP2 | 31:DA:2342:C:H6 | 1.86 | 0.59 |
| 31:DA:2463:C:O2' | 31:DA:2464:C:H5' | 2.03 | 0.59 |
| 31:DA:491:G:H2' | 31:DA:492:A:C8 | 2.38 | 0.59 |
| 33:DD:30:GLU:HG3 | 33:DD:63:ARG:NH2 | 2.18 | 0.59 |
| 34:DE:95:ILE:CD1 | 34:DE:95:ILE:H | 2.15 | 0.59 |
| 36:DG:127:GLY:CA | 36:DG:166:ASP:HB3 | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:2312:U:O3' | 36:DG:71:THR:HG21 | 2.02 | 0.59 |
| 39:DN:78:TYR:CE1 | 39:DN:79:PRO:HB3 | 2.38 | 0.59 |
| 43:DR:55:ALA:CB | 43:DR:79:LEU:HD13 | 2.32 | 0.59 |
| 1:AA:1049:U:H4' | 1:AA:1050:G:C5' | 2.32 | 0.59 |
| 1:AA:273:A:O2' | 1:AA:274:A:H5' | 2.03 | 0.59 |
| 1:AA:403:C:O2' | 1:AA:404:U:H5' | 2.03 | 0.59 |
| 2:AB:8:LYS:NZ | 2:AB:217:ARG:HH11 | 2.01 | 0.59 |
| 3:AC:54:ARG:HD3 | 3:AC:69:HIS:CE1 | 2.38 | 0.59 |
| 6:AF:45:LEU:HD11 | 6:AF:57:GLN:OE1 | 2.03 | 0.59 |
| 9:AI:46:ALA:O | 9:AI:49:PRO:HD2 | 2.03 | 0.59 |
| 20:AT:26:ASN:O | 20:AT:30:LYS:HB2 | 2.02 | 0.59 |
| 31:BA:1833:U:H2' | 31:BA:1834:U:C6 | 2.37 | 0.59 |
| 31:BA:528:A:C2 | 31:BA:2043:C:C5' | 2.86 | 0.59 |
| 34:BE:116:VAL:HG13 | 34:BE:122:PHE:CG | 2.38 | 0.59 |
| 34:BE:36:ARG:HH11 | 34:BE:85:ASN:HD21 | 1.50 | 0.59 |
| 34:BE:61:ARG:N | 34:BE:62:PRO:HD2 | 2.16 | 0.59 |
| 44:BS:42:ASP:O | 44:BS:43:GLU:HB2 | 2.03 | 0.59 |
| 44:BS:76:LYS:O | 44:BS:79:ALA:HB3 | 2.02 | 0.59 |
| 46:BU:92:ARG:HD2 | 47:BV:11:GLN:CG | 2.32 | 0.59 |
| 47:BV:51:VAL:CG1 | 47:BV:52:VAL:H | 2.16 | 0.59 |
| 50:BY:37:VAL:HG23 | 50:BY:38:ILE:N | 2.18 | 0.59 |
| 50:BY:71:LYS:HZ3 | 50:BY:71:LYS:HB2 | 1.68 | 0.59 |
| 1:CA:170:U:O2' | 1:CA:171:A:H5' | 2.02 | 0.59 |
| 2:CB:204:ASN:HD21 | 2:CB:207:ALA:H | 1.50 | 0.59 |
| 3:CC:23:TYR:CG | 3:CC:24:ALA:N | 2.70 | 0.59 |
| 4:CD:109:GLY:O | 4:CD:111:ALA:N | 2.36 | 0.59 |
| 8:CH:113:SER:H | 8:CH:134:ILE:HG12 | 1.66 | 0.59 |
| 22:D0:53:MET:HB2 | 22:D0:59:LEU:HD23 | 1.83 | 0.59 |
| 23:D1:26:ARG:HG2 | 23:D1:34:THR:HB | 1.84 | 0.59 |
| 31:DA:2186:G:C3' | 31:DA:2187:G:H5'' | 2.33 | 0.59 |
| 31:DA:2350:C:H2' | 31:DA:2351:G:O4' | 2.03 | 0.59 |
| 30:D8:35:GLN:HA | 31:DA:2420:C:OP2 | 2.02 | 0.59 |
| 31:DA:2536:G:C5 | 31:DA:2537:U:C5 | 2.91 | 0.59 |
| 31:DA:2894:G:N3 | 31:DA:2894:G:H2' | 2.17 | 0.59 |
| 37:DH:137:ASP:HB3 | 37:DH:140:LYS:HB2 | 1.83 | 0.59 |
| 39:DN:65:LYS:CD | 39:DN:67:LEU:HG | 2.33 | 0.59 |
| 44:DS:93:LYS:HE3 | 44:DS:93:LYS:O | 2.02 | 0.59 |
| 50:DY:99:CYS:SG | 50:DY:99:CYS:O | 2.60 | 0.59 |
| 1:AA:180:U:H2' | 1:AA:181:G:H5' | 1.84 | 0.59 |
| 1:AA:186:C:C2 | 1:AA:187:C:C5 | 2.91 | 0.59 |
| 1:AA:626:U:C2 | 1:AA:627:G:N7 | 2.71 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:797:C:OP1 | 11:AK:124:LYS:HE2 | 2.03 | 0.59 |
| 3:AC:95:THR:HG22 | 3:AC:97:LYS:H | 1.68 | 0.59 |
| 4:AD:90:GLY:O | 4:AD:94:LEU:HD12 | 2.02 | 0.59 |
| 6:AF:76:ALA:HB1 | 6:AF:80:ARG:HH21 | 1.67 | 0.59 |
| 7:AG:47:CYS:O | 7:AG:50:ILE:HB | 2.03 | 0.59 |
| 17:AQ:40:LYS:HG2 | 17:AQ:41:LYS:H | 1.64 | 0.59 |
| 31:BA:1158:C:O2' | 31:BA:1159:U:OP2 | 2.20 | 0.59 |
| 31:BA:1417:C:C2' | 31:BA:1418:G:H5' | 2.33 | 0.59 |
| 31:BA:2262:U:O2' | 31:BA:2263:C:H5'' | 2.03 | 0.59 |
| 44:BS:90:GLY:O | 44:BS:92:TYR:N | 2.36 | 0.59 |
| 46:BU:90:VAL:HG12 | 46:BU:91:ASP:H | 1.68 | 0.59 |
| 50:BY:68:HIS:ND1 | 50:BY:70:SER:HB3 | 2.18 | 0.59 |
| 1:CA:166:G:O2' | 1:CA:167:G:H5' | 2.02 | 0.59 |
| 1:CA:501:C:H2' | 1:CA:502:G:C8 | 2.38 | 0.59 |
| 3:CC:73:PRO:HG3 | 3:CC:105:GLU:HG3 | 1.84 | 0.59 |
| 5:CE:36:ASP:OD1 | 5:CE:37:ARG:N | 2.36 | 0.59 |
| 31:DA:1270:C:H5'' | 31:DA:1271:G:O5' | 2.02 | 0.59 |
| 31:DA:607:U:OP1 | 35:DF:102:PRO:HA | 2.03 | 0.59 |
| 31:DA:71:A:C2 | 49:DX:31:HIS:CE1 | 2.72 | 0.59 |
| 31:DA:848:G:H2' | 31:DA:849:A:C8 | 2.38 | 0.59 |
| 31:DA:953:A:C2 | 31:DA:954:G:C8 | 2.91 | 0.59 |
| 38:DI:99:GLU:HG3 | 38:DI:103:ARG:CZ | 2.33 | 0.59 |
| 41:DP:7:ARG:O | 41:DP:10:PRO:HD3 | 2.03 | 0.59 |
| 47:DV:96:ILE:CG2 | 47:DV:97:LYS:N | 2.65 | 0.59 |
| 50:DY:37:VAL:HG11 | 50:DY:72:VAL:CG2 | 2.33 | 0.59 |
| 1:AA:1049:U:H4' | 1:AA:1050:G:O5' | 2.01 | 0.59 |
| 1:AA:175:C:H2' | 1:AA:176:C:C6 | 2.37 | 0.59 |
| 1:AA:250:A:H1' | 1:AA:251:G:OP2 | 2.03 | 0.59 |
| 1:AA:341:C:O2' | 1:AA:342:C:H5' | 2.03 | 0.59 |
| 1:AA:594:G:H2' | 1:AA:595:G:O4' | 2.02 | 0.59 |
| 2:AB:20:GLU:O | 2:AB:40:HIS:HB2 | 2.03 | 0.59 |
| 4:AD:109:GLY:O | 4:AD:111:ALA:N | 2.36 | 0.59 |
| 6:AF:48:LEU:HD13 | 6:AF:52:ILE:HG12 | 1.84 | 0.59 |
| 23:B1:46:LEU:N | 23:B1:46:LEU:HD12 | 2.05 | 0.59 |
| 28:B6:35:GLU:HG3 | 28:B6:35:GLU:O | 2.00 | 0.59 |
| 31:BA:1497:U:H3 | 31:BA:1578:U:P | 2.26 | 0.59 |
| 31:BA:2895:U:H5 | 31:BA:2896:C:C5 | 2.20 | 0.59 |
| 31:BA:671:C:C5' | 31:BA:671:C:H6 | 2.12 | 0.59 |
| 31:BA:61:G:H1 | 31:BA:94:C:H42 | 1.50 | 0.59 |
| 33:BD:175:LEU:HD12 | 33:BD:185:VAL:HG21 | 1.85 | 0.59 |
| 36:BG:71:THR:HB | 36:BG:89:GLY:HA3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BS:67:ARG:H | 44:BS:69:VAL:HG13 | 1.68 | 0.59 |
| 45:BT:33:LYS:NZ | 45:BT:33:LYS:HA | 2.17 | 0.59 |
| 45:BT:80:SER:HB3 | 45:BT:81:PRO:HD3 | 1.85 | 0.59 |
| 47:BV:73:SER:OG | 47:BV:75:PHE:CE1 | 2.56 | 0.59 |
| 49:BX:55:ASN:HD22 | 49:BX:55:ASN:N | 1.99 | 0.59 |
| 1:CA:836:G:C6 | 1:CA:851:G:C6 | 2.91 | 0.59 |
| 4:CD:119:GLN:O | 4:CD:123:HIS:CD2 | 2.56 | 0.59 |
| 4:CD:19:LEU:HB2 | 4:CD:21:LEU:CD2 | 2.31 | 0.59 |
| 4:CD:88:VAL:O | 4:CD:92:VAL:HG23 | 2.02 | 0.59 |
| 5:CE:32:VAL:HB | 5:CE:58:ALA:HB1 | 1.85 | 0.59 |
| 7:CG:47:CYS:O | 7:CG:50:ILE:HB | 2.02 | 0.59 |
| 31:DA:954:G:C5 | 31:DA:955:C:C5 | 2.90 | 0.59 |
| 36:DG:106:LEU:O | 36:DG:110:ALA:HB3 | 2.02 | 0.59 |
| 37:DH:155:SER:O | 37:DH:157:TYR:N | 2.36 | 0.59 |
| 38:DI:98:ALA:HA | 38:DI:109:ILE:HD11 | 1.83 | 0.59 |
| 44:DS:83:LYS:CE | 44:DS:105:ALA:HB2 | 2.33 | 0.59 |
| 44:DS:42:ASP:C | 44:DS:44:LYS:H | 2.05 | 0.59 |
| 45:DT:30:VAL:HG23 | 45:DT:31:SER:N | 2.18 | 0.59 |
| 45:DT:33:LYS:N | 45:DT:33:LYS:NZ | 2.51 | 0.59 |
| 49:DX:21:PHE:N | 49:DX:21:PHE:HD1 | 2.00 | 0.59 |
| 1:AA:1054:C:O2' | 1:AA:1055:A:H5'' | 2.03 | 0.58 |
| 5:AE:11:ILE:HD11 | 5:AE:108:ALA:HB3 | 1.85 | 0.58 |
| 8:AH:113:SER:H | 8:AH:134:ILE:HG12 | 1.67 | 0.58 |
| 8:AH:6:ILE:N | 8:AH:6:ILE:HD12 | 2.18 | 0.58 |
| 13:AM:25:ILE:HD11 | 13:AM:66:LEU:HD23 | 1.85 | 0.58 |
| 25:B3:54:VAL:CG1 | 25:B3:55:ARG:N | 2.65 | 0.58 |
| 27:B5:2:ALA:N | 31:BA:747:U:C4 | 2.71 | 0.58 |
| 28:B6:30:THR:O | 28:B6:31:PRO:C | 2.40 | 0.58 |
| 31:BA:247:G:H4' | 31:BA:386:G:C5 | 2.38 | 0.58 |
| 31:BA:776:G:H4' | 31:BA:777:A:O5' | 2.02 | 0.58 |
| 33:BD:142:VAL:HG23 | 33:BD:193:VAL:HA | 1.84 | 0.58 |
| 31:BA:2591:C:P | 33:BD:239:ARG:HG3 | 2.43 | 0.58 |
| 41:BP:101:VAL:C | 41:BP:103:ALA:H | 2.07 | 0.58 |
| 45:BT:42:ILE:O | 45:BT:42:ILE:HG13 | 2.01 | 0.58 |
| 1:CA:937:A:H1' | 1:CA:1379:G:N2 | 2.18 | 0.58 |
| 4:CD:138:TYR:HD2 | 4:CD:139:ARG:N | 2.01 | 0.58 |
| 20:CT:39:LYS:O | 20:CT:43:LEU:HG | 2.03 | 0.58 |
| 25:D3:44:ARG:O | 25:D3:48:GLU:HG2 | 2.03 | 0.58 |
| 31:DA:1027:A:C6 | 31:DA:1126:A:C4 | 2.91 | 0.58 |
| 31:DA:1138:G:H21 | 39:DN:106:MET:HE3 | 1.68 | 0.58 |
| 31:DA:1406:U:H2' | 31:DA:1407:C:H6 | 1.67 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:2700:C:C2' | 31:DA:2701:C:H5' | 2.33 | 0.58 |
| 31:DA:2703:C:H2' | 31:DA:2704:C:H6 | 1.68 | 0.58 |
| 31:DA:27:G:N2 | 31:DA:512:G:H1' | 2.17 | 0.58 |
| 31:DA:547:A:H8 | 31:DA:549:G:C6 | 2.20 | 0.58 |
| 31:DA:743:G:C2' | 31:DA:744:G:H5' | 2.33 | 0.58 |
| 31:DA:754:C:H2' | 31:DA:755:C:C6 | 2.38 | 0.58 |
| 35:DF:101:LEU:CD1 | 35:DF:102:PRO:HD2 | 2.19 | 0.58 |
| 43:DR:4:LEU:CD1 | 43:DR:4:LEU:O | 2.45 | 0.58 |
| 47:DV:36:PRO:HG2 | 47:DV:62:LEU:HD11 | 1.85 | 0.58 |
| 49:DX:60:ARG:HB2 | 49:DX:74:PRO:HD2 | 1.85 | 0.58 |
| 50:DY:37:VAL:HG11 | 50:DY:72:VAL:HG21 | 1.85 | 0.58 |
| 1:AA:410:G:H1' | 1:AA:432:A:H61 | 1.66 | 0.58 |
| 1:AA:819:A:H4' | 1:AA:820:U:OP2 | 2.01 | 0.58 |
| 1:AA:857:C:O2 | 1:AA:858:G:H1' | 2.02 | 0.58 |
| 2:AB:228:GLY:O | 2:AB:230:VAL:HG13 | 2.02 | 0.58 |
| 3:AC:7:PRO:O | 3:AC:11:ARG:HG2 | 2.02 | 0.58 |
| 1:AA:1278:U:O4 | 10:AJ:99:LYS:HE3 | 2.03 | 0.58 |
| 13:AM:15:VAL:HG12 | 13:AM:45:VAL:HG22 | 1.85 | 0.58 |
| 24:B2:57:ILE:HG21 | 24:B2:59:ARG:HH11 | 1.67 | 0.58 |
| 31:BA:1108:U:C2' | 31:BA:1109:C:H5' | 2.33 | 0.58 |
| 31:BA:551:G:O2' | 31:BA:1220:A:N3 | 2.27 | 0.58 |
| 31:BA:1278:A:OP1 | 43:BR:36:THR:CG2 | 2.50 | 0.58 |
| 31:BA:1451:C:N3 | 31:BA:1459:G:O6 | 2.36 | 0.58 |
| 31:BA:2197:U:H1' | 31:BA:2198:A:C8 | 2.38 | 0.58 |
| 23:B1:21:ARG:NH1 | 31:BA:380:U:OP1 | 2.35 | 0.58 |
| 31:BA:626:U:H3 | 41:BP:105:LEU:HG | 1.68 | 0.58 |
| 41:BP:14:LYS:O | 41:BP:15:ARG:HB2 | 2.03 | 0.58 |
| 42:BQ:75:THR:HA | 42:BQ:88:GLY:CA | 2.33 | 0.58 |
| 1:CA:713:G:H2' | 1:CA:714:G:C8 | 2.37 | 0.58 |
| 7:CG:150:ALA:O | 11:CK:57:THR:HG21 | 2.03 | 0.58 |
| 31:DA:2055:C:H5' | 31:DA:2056:G:O5' | 2.03 | 0.58 |
| 31:DA:543:C:C6 | 31:DA:547:A:N7 | 2.71 | 0.58 |
| 31:DA:649:G:H2' | 31:DA:650:C:C6 | 2.38 | 0.58 |
| 37:DH:158:HIS:CE1 | 37:DH:169:VAL:C | 2.77 | 0.58 |
| 37:DH:99:VAL:HG12 | 37:DH:99:VAL:O | 2.03 | 0.58 |
| 39:DN:2:LYS:HZ3 | 46:DU:94:ASN:ND2 | 2.00 | 0.58 |
| 47:DV:73:SER:OG | 47:DV:74:LYS:N | 2.36 | 0.58 |
| 31:DA:309:G:O3' | 50:DY:18:GLY:CA | 2.50 | 0.58 |
| 1:AA:187:C:H2' | 1:AA:188:C:H6 | 1.67 | 0.58 |
| 1:AA:539:A:OP2 | 12:AL:115:LYS:HE3 | 2.03 | 0.58 |
| 1:AA:721:G:H4' | 1:AA:722:A:O4' | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:187:LEU:HD11 | 2:AB:204:ASN:O | 2.02 | 0.58 |
| 4:AD:17:VAL:HG11 | 4:AD:197:PRO:CB | 2.33 | 0.58 |
| 8:AH:114:THR:HG23 | 8:AH:117:GLY:O | 2.02 | 0.58 |
| 17:AQ:40:LYS:HD2 | 17:AQ:42:TYR:CZ | 2.38 | 0.58 |
| 28:B6:10:LEU:CD2 | 28:B6:10:LEU:H | 2.15 | 0.58 |
| 31:BA:2660:A:H5'' | 31:BA:2661:G:C2 | 2.39 | 0.58 |
| 31:BA:642:G:H21 | 31:BA:646:A:H2 | 1.51 | 0.58 |
| 38:BI:109:ILE:HG22 | 38:BI:130:TYR:OH | 2.03 | 0.58 |
| 44:BS:83:LYS:CE | 44:BS:105:ALA:HB2 | 2.33 | 0.58 |
| 45:BT:129:ARG:CZ | 45:BT:131:ALA:HB3 | 2.33 | 0.58 |
| 45:BT:78:LEU:C | 45:BT:79:HIS:ND1 | 2.56 | 0.58 |
| 48:BW:10:VAL:O | 48:BW:11:ARG:CB | 2.51 | 0.58 |
| 1:CA:1026:G:N3 | 1:CA:1026:G:H2' | 2.18 | 0.58 |
| 1:CA:967:C:H5'' | 1:CA:968:A:OP2 | 2.03 | 0.58 |
| 8:CH:6:ILE:HD12 | 8:CH:6:ILE:N | 2.17 | 0.58 |
| 1:CA:957:U:H4' | 19:CS:79:THR:HB | 1.85 | 0.58 |
| 31:DA:1112:G:H1' | 31:DA:1113:U:OP1 | 2.03 | 0.58 |
| 31:DA:528:A:N1 | 31:DA:2042:A:H2' | 2.18 | 0.58 |
| 31:DA:2197:U:H1' | 31:DA:2198:A:C8 | 2.38 | 0.58 |
| 31:DA:2205:C:O2 | 31:DA:2220:G:C2 | 2.56 | 0.58 |
| 31:DA:528:A:H2' | 31:DA:529:A:H5' | 1.84 | 0.58 |
| 33:DD:35:LYS:CG | 33:DD:64:ILE:N | 2.66 | 0.58 |
| 35:DF:22:ALA:C | 35:DF:26:ALA:HB2 | 2.23 | 0.58 |
| 39:DN:28:THR:HA | 39:DN:106:MET:HE2 | 1.85 | 0.58 |
| 40:DO:13:ASN:ND2 | 40:DO:96:THR:H | 2.00 | 0.58 |
| 44:DS:97:ARG:HD2 | 44:DS:97:ARG:C | 2.24 | 0.58 |
| 31:DA:1225:G:OP1 | 47:DV:88:ARG:HD2 | 2.03 | 0.58 |
| 48:DW:9:TYR:N | 48:DW:102:HIS:HD2 | 1.94 | 0.58 |
| 1:AA:1321:C:H5'' | 1:AA:1322:C:H5'' | 1.85 | 0.58 |
| 1:AA:938:A:N6 | 1:AA:939:G:C6 | 2.72 | 0.58 |
| 4:AD:33:MET:CE | 4:AD:37:PRO:HA | 2.34 | 0.58 |
| 4:AD:73:ARG:HD2 | 4:AD:77:ASN:HD21 | 1.69 | 0.58 |
| 8:AH:17:THR:HB | 8:AH:78:GLN:OE1 | 2.03 | 0.58 |
| 9:AI:48:GLU:N | 9:AI:49:PRO:HD2 | 2.17 | 0.58 |
| 20:AT:39:LYS:O | 20:AT:43:LEU:HG | 2.02 | 0.58 |
| 31:BA:1112:G:H1' | 31:BA:1113:U:OP1 | 2.03 | 0.58 |
| 31:BA:1204:A:N1 | 31:BA:1241:A:C2 | 2.68 | 0.58 |
| 31:BA:1963:U:H4' | 31:BA:1964:G:OP1 | 2.02 | 0.58 |
| 30:B8:35:GLN:OE1 | 31:BA:2421:G:OP2 | 2.21 | 0.58 |
| 31:BA:271(K):U:H3' | 31:BA:271(L):U:C5' | 2.32 | 0.58 |
| 33:BD:255:LYS:N | 33:BD:255:LYS:NZ | 2.51 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BH:137:ASP:HB3 | 37:BH:140:LYS:HB2 | 1.83 | 0.58 |
| 44:BS:97:ARG:O | 44:BS:98:VAL:HG23 | 2.04 | 0.58 |
| 50:BY:45:VAL:CG2 | 50:BY:62:GLU:H | 2.16 | 0.58 |
| 1:CA:564:C:C2 | 17:CQ:31:LEU:HD11 | 2.39 | 0.58 |
| 1:CA:709:G:H2' | 1:CA:710:G:H8 | 1.67 | 0.58 |
| 1:CA:757:U:H2' | 1:CA:758:G:O4' | 2.03 | 0.58 |
| 2:CB:61:LEU:HA | 2:CB:64:ARG:HG2 | 1.85 | 0.58 |
| 9:CI:46:ALA:O | 9:CI:49:PRO:HD2 | 2.02 | 0.58 |
| 1:CA:1250:A:H4' | 9:CI:68:GLY:N | 2.18 | 0.58 |
| 11:CK:31:THR:HA | 11:CK:42:TRP:HA | 1.86 | 0.58 |
| 20:CT:89:ARG:HH21 | 20:CT:104:LEU:HD21 | 1.68 | 0.58 |
| 28:D6:42:TRP:CZ2 | 31:DA:642:G:O3' | 2.57 | 0.58 |
| 30:D8:32:LEU:HG | 30:D8:34:TRP:CE3 | 2.38 | 0.58 |
| 30:D8:34:TRP:HZ3 | 30:D8:41:ILE:CG2 | 2.16 | 0.58 |
| 31:DA:83:G:H1 | 31:DA:102:G:H2' | 1.68 | 0.58 |
| 31:DA:150:C:H2' | 31:DA:151:C:C6 | 2.38 | 0.58 |
| 31:DA:1693:U:OP2 | 31:DA:1694:C:H5 | 1.87 | 0.58 |
| 31:DA:1722:A:N6 | 31:DA:1741:A:C2 | 2.72 | 0.58 |
| 31:DA:2092:U:H4' | 31:DA:2093:G:O5' | 2.04 | 0.58 |
| 31:DA:2309:A:C2 | 31:DA:2310:A:H2 | 2.20 | 0.58 |
| 31:DA:542:C:C2' | 31:DA:543:C:OP1 | 2.51 | 0.58 |
| 31:DA:814:C:H5 | 41:DP:27:HIS:NE2 | 2.02 | 0.58 |
| 31:DA:992:C:O2' | 31:DA:993:G:H5' | 2.03 | 0.58 |
| 32:DB:28:C:H2' | 32:DB:29:A:H8 | 1.69 | 0.58 |
| 34:DE:101:ARG:HB3 | 34:DE:169:ASN:HD22 | 1.69 | 0.58 |
| 48:DW:18:ARG:CG | 48:DW:18:ARG:HH11 | 2.17 | 0.58 |
| 49:DX:60:ARG:CB | 49:DX:72:LYS:H | 2.16 | 0.58 |
| 1:AA:1256:A:N6 | 1:AA:1278:U:H1' | 2.15 | 0.58 |
| 1:AA:1315:U:H2' | 1:AA:1316:G:O4' | 2.03 | 0.58 |
| 1:AA:833:U:H2' | 1:AA:834:C:C6 | 2.37 | 0.58 |
| 22:B0:36:ILE:HD13 | 22:B0:36:ILE:C | 2.24 | 0.58 |
| 23:B1:26:ARG:HB3 | 23:B1:35:THR:H | 1.69 | 0.58 |
| 31:BA:1484:G:N2 | 31:BA:1505:C:C5 | 2.70 | 0.58 |
| 31:BA:1885:A:H5' | 31:BA:1885:A:H8 | 1.69 | 0.58 |
| 31:BA:2262:U:H2' | 31:BA:2263:C:H5'' | 1.86 | 0.58 |
| 31:BA:2532:G:O2' | 31:BA:2657:A:N6 | 2.37 | 0.58 |
| 31:BA:430:G:H5'' | 31:BA:431:U:OP2 | 2.03 | 0.58 |
| 31:BA:542:C:C2' | 31:BA:543:C:OP1 | 2.51 | 0.58 |
| 33:BD:166:GLN:HB3 | 33:BD:174:ILE:HG22 | 1.85 | 0.58 |
| 39:BN:78:TYR:CE1 | 39:BN:79:PRO:HB3 | 2.38 | 0.58 |
| 43:BR:33:ARG:HG2 | 43:BR:115:GLU:CG | 2.24 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:BT:45:PHE:HE2 | 45:BT:63:VAL:HG22 | 1.68 | 0.58 |
| 1:CA:1478:C:H2' | 1:CA:1479:C:H6 | 1.68 | 0.58 |
| 1:CA:927:G:OP2 | 1:CA:1503:A:C4 | 2.56 | 0.58 |
| 1:CA:624:C:H2' | 1:CA:625:G:H8 | 1.68 | 0.58 |
| 1:CA:949:A:N6 | 1:CA:1232:U:H3 | 2.01 | 0.58 |
| 4:CD:108:LEU:HD13 | 4:CD:174:LEU:HD13 | 1.86 | 0.58 |
| 4:CD:141:ARG:HB3 | 4:CD:142:PRO:CD | 2.34 | 0.58 |
| 4:CD:156:GLU:O | 4:CD:159:ARG:HB2 | 2.04 | 0.58 |
| 6:CF:89:MET:SD | 18:CR:76:LEU:HD21 | 2.44 | 0.58 |
| 11:CK:84:VAL:O | 11:CK:85:ARG:HG3 | 2.03 | 0.58 |
| 14:CN:44:LEU:O | 14:CN:44:LEU:HD12 | 2.04 | 0.58 |
| 23:D1:70:VAL:O | 23:D1:73:LEU:HB2 | 2.03 | 0.58 |
| 24:D2:26:ARG:HA | 24:D2:29:LYS:HE3 | 1.85 | 0.58 |
| 30:D8:32:LEU:HB3 | 30:D8:34:TRP:CB | 2.28 | 0.58 |
| 31:DA:1488:G:C2 | 31:DA:1489:U:O2 | 2.56 | 0.58 |
| 31:DA:157:U:H5' | 31:DA:171:G:N2 | 2.17 | 0.58 |
| 31:DA:2652:C:H2' | 31:DA:2653:U:H5' | 1.85 | 0.58 |
| 33:DD:173:VAL:CG2 | 33:DD:174:ILE:N | 2.65 | 0.58 |
| 33:DD:68:LYS:HB3 | 33:DD:70:TRP:CH2 | 2.37 | 0.58 |
| 34:DE:59:VAL:CG2 | 34:DE:63:LEU:HA | 2.31 | 0.58 |
| 35:DF:83:PHE:O | 35:DF:84:VAL:CB | 2.51 | 0.58 |
| 41:DP:10:PRO:CD | 41:DP:11:GLY:H | 2.15 | 0.58 |
| 46:DU:90:VAL:HG13 | 47:DV:39:LEU:HG | 1.83 | 0.58 |
| 49:DX:36:LYS:NZ | 49:DX:38:GLU:C | 2.56 | 0.58 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:C8 | 2.38 | 0.58 |
| 1:AA:1325:C:H4' | 21:AU:17:THR:HG21 | 1.84 | 0.58 |
| 1:AA:344:A:O2' | 1:AA:346:G:N7 | 2.33 | 0.58 |
| 1:AA:437:U:O2' | 1:AA:438:G:H5' | 2.03 | 0.58 |
| 10:AJ:78:ASN:O | 10:AJ:82:ILE:HG12 | 2.04 | 0.58 |
| 14:AN:44:LEU:HD12 | 14:AN:44:LEU:O | 2.03 | 0.58 |
| 6:AF:49:ALA:HB2 | 18:AR:78:LEU:O | 2.02 | 0.58 |
| 23:B1:26:ARG:HG2 | 23:B1:34:THR:HB | 1.86 | 0.58 |
| 31:BA:1839:G:N7 | 31:BA:1927:A:H1' | 2.19 | 0.58 |
| 31:BA:2577:A:H5'' | 31:BA:2578:G:C5' | 2.31 | 0.58 |
| 31:BA:2580:U:H5' | 34:BE:131:ALA:HB2 | 1.83 | 0.58 |
| 31:BA:2619:C:O2' | 31:BA:2620:C:H5' | 2.04 | 0.58 |
| 31:BA:52:A:O2' | 31:BA:53:A:H5' | 2.04 | 0.58 |
| 33:BD:140:THR:O | 33:BD:165:ILE:HG12 | 2.04 | 0.58 |
| 34:BE:14:ILE:HG12 | 34:BE:21:VAL:HG22 | 1.86 | 0.58 |
| 31:BA:2312:U:O3' | 36:BG:71:THR:HG21 | 2.04 | 0.58 |
| 39:BN:75:TYR:CD1 | 39:BN:75:TYR:N | 2.71 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:BV:69:LYS:O | 47:BV:70:ILE:CG2 | 2.51 | 0.58 |
| 1:CA:101:A:C2' | 1:CA:102:G:H5' | 2.34 | 0.58 |
| 3:CC:83:ARG:O | 3:CC:86:VAL:HG22 | 2.02 | 0.58 |
| 5:CE:11:ILE:HD11 | 5:CE:108:ALA:HB3 | 1.85 | 0.58 |
| 6:CF:82:ARG:HA | 6:CF:82:ARG:HH11 | 1.68 | 0.58 |
| 20:CT:26:ASN:O | 20:CT:30:LYS:HB2 | 2.04 | 0.58 |
| 23:D1:85:LEU:C | 23:D1:87:PRO:CD | 2.71 | 0.58 |
| 25:D3:54:VAL:CG1 | 25:D3:55:ARG:N | 2.66 | 0.58 |
| 29:D7:5:TRP:NE1 | 29:D7:7:PRO:HG3 | 2.17 | 0.58 |
| 31:DA:1332:G:H22 | 31:DA:1609:A:H2' | 1.67 | 0.58 |
| 31:DA:1777:U:O2' | 31:DA:1778:U:H5' | 2.04 | 0.58 |
| 31:DA:389:G:H1 | 41:DP:71:VAL:H | 1.50 | 0.58 |
| 31:DA:542:C:H42 | 31:DA:543:C:H42 | 1.50 | 0.58 |
| 34:DE:111:ARG:HB2 | 34:DE:160:TYR:O | 2.04 | 0.58 |
| 41:DP:83:VAL:CG1 | 41:DP:112:LEU:HD21 | 2.34 | 0.58 |
| 34:DE:111:ARG:CZ | 43:DR:2:ARG:HH21 | 2.17 | 0.58 |
| 46:DU:74:LEU:N | 46:DU:74:LEU:HD12 | 2.19 | 0.58 |
| 1:AA:357:G:C2 | 1:AA:358:U:C6 | 2.92 | 0.58 |
| 1:AA:750:G:C2 | 1:AA:751:U:C6 | 2.91 | 0.58 |
| 1:AA:1191:A:P | 3:AC:3:ASN:HD21 | 2.27 | 0.58 |
| 1:AA:546:G:P | 4:AD:72:GLU:HB3 | 2.43 | 0.58 |
| 12:AL:24:VAL:O | 12:AL:24:VAL:HG12 | 2.02 | 0.58 |
| 12:AL:46:LYS:HG2 | 12:AL:47:LYS:N | 2.19 | 0.58 |
| 28:B6:9:LEU:C | 28:B6:9:LEU:HD13 | 2.23 | 0.58 |
| 31:BA:500:G:N2 | 31:BA:502:A:H3' | 2.19 | 0.58 |
| 31:BA:958:U:O2' | 31:BA:959:A:P | 2.61 | 0.58 |
| 33:BD:118:VAL:HG22 | 33:BD:119:ALA:H | 1.67 | 0.58 |
| 34:BE:120:TRP:CE3 | 34:BE:155:LYS:HD3 | 2.38 | 0.58 |
| 37:BH:158:HIS:CE1 | 37:BH:169:VAL:C | 2.76 | 0.58 |
| 39:BN:57:ALA:O | 39:BN:58:ASP:O | 2.22 | 0.58 |
| 41:BP:105:LEU:O | 41:BP:106:LEU:CB | 2.51 | 0.58 |
| 43:BR:9:LYS:C | 43:BR:10:LEU:HG | 2.23 | 0.58 |
| 43:BR:74:LYS:HD2 | 43:BR:77:ARG:HH21 | 1.68 | 0.58 |
| 44:BS:88:ASP:O | 44:BS:89:ARG:O | 2.22 | 0.58 |
| 44:BS:97:ARG:C | 44:BS:97:ARG:CD | 2.72 | 0.58 |
| 1:CA:1264:C:H2' | 1:CA:1265:G:H8 | 1.68 | 0.58 |
| 1:CA:505:G:C6 | 1:CA:535:A:C2 | 2.91 | 0.58 |
| 3:CC:150:LYS:HE2 | 3:CC:152:ILE:HD11 | 1.85 | 0.58 |
| 7:CG:62:PHE:HA | 7:CG:124:LEU:HD22 | 1.86 | 0.58 |
| 9:CI:3:GLN:HB3 | 9:CI:20:ARG:CZ | 2.33 | 0.58 |
| 1:CA:1278:U:O4 | 10:CJ:99:LYS:HE3 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CP:48:TRP:HD1 | 16:CP:48:TRP:H | 1.46 | 0.58 |
| 17:CQ:45:HIS:HD2 | 17:CQ:47:PRO:HD3 | 1.68 | 0.58 |
| 24:D2:18:PRO:O | 24:D2:22:GLU:HB2 | 2.04 | 0.58 |
| 31:DA:1839:G:N7 | 31:DA:1927:A:H1' | 2.19 | 0.58 |
| 31:DA:1893:C:C5 | 31:DA:1894:C:C5 | 2.91 | 0.58 |
| 31:DA:2661:G:C8 | 31:DA:2662:A:C2 | 2.91 | 0.58 |
| 31:DA:271(K):U:H3' | 31:DA:271(L):U:C5' | 2.34 | 0.58 |
| 31:DA:479:A:N3 | 31:DA:481:G:H5'' | 2.17 | 0.58 |
| 31:DA:848:G:N9 | 31:DA:933:A:H8 | 2.02 | 0.58 |
| 31:DA:9:U:N3 | 31:DA:2629:A:N6 | 2.51 | 0.58 |
| 34:DE:200:GLU:N | 34:DE:200:GLU:OE2 | 2.36 | 0.58 |
| 39:DN:67:LEU:HB3 | 39:DN:88:GLU:CD | 2.24 | 0.58 |
| 42:DQ:38:GLU:HB2 | 42:DQ:127:ILE:HG22 | 1.85 | 0.58 |
| 44:DS:74:ALA:HB2 | 44:DS:101:LEU:HD11 | 1.84 | 0.58 |
| 44:DS:95:HIS:O | 44:DS:98:VAL:HG23 | 2.04 | 0.58 |
| 47:DV:38:LEU:HG | 47:DV:39:LEU:H | 1.68 | 0.58 |
| 48:DW:10:VAL:O | 48:DW:11:ARG:CB | 2.51 | 0.58 |
| 49:DX:23:GLU:HG3 | 49:DX:24:GLY:N | 2.19 | 0.58 |
| 50:DY:68:HIS:ND1 | 50:DY:70:SER:HB3 | 2.19 | 0.58 |
| 1:AA:101:A:C2' | 1:AA:102:G:H5' | 2.34 | 0.58 |
| 1:AA:1072:G:H2' | 1:AA:1073:U:C6 | 2.38 | 0.58 |
| 3:AC:152:ILE:HB | 3:AC:199:LYS:HB2 | 1.86 | 0.58 |
| 4:AD:108:LEU:HB3 | 4:AD:110:PHE:CE1 | 2.38 | 0.58 |
| 8:AH:112:LEU:HD12 | 8:AH:112:LEU:O | 2.03 | 0.58 |
| 8:AH:69:ARG:HD3 | 8:AH:75:ARG:O | 2.03 | 0.58 |
| 31:BA:1040:C:O2' | 31:BA:1041:C:P | 2.61 | 0.58 |
| 31:BA:1138:G:H21 | 39:BN:106:MET:HE3 | 1.69 | 0.58 |
| 31:BA:2309:A:C2 | 31:BA:2310:A:H2 | 2.21 | 0.58 |
| 33:BD:70:TRP:HZ3 | 33:BD:146:GLU:OE2 | 1.87 | 0.58 |
| 35:BF:66:PRO:O | 35:BF:67:GLN:CB | 2.48 | 0.58 |
| 38:BI:85:GLU:O | 38:BI:123:LEU:HD12 | 2.03 | 0.58 |
| 31:BA:2875:C:O2' | 45:BT:5:ALA:HB3 | 2.03 | 0.58 |
| 42:BQ:140:ALA:CB | 51:BZ:99:TYR:HB2 | 2.33 | 0.58 |
| 1:CA:1058:G:H2' | 1:CA:1059:C:O4' | 2.04 | 0.58 |
| 1:CA:1281:U:H5' | 1:CA:1282:C:C5 | 2.30 | 0.58 |
| 1:CA:152:A:N6 | 1:CA:170:U:C2 | 2.72 | 0.58 |
| 1:CA:659:U:O2' | 1:CA:660:G:H5' | 2.04 | 0.58 |
| 1:CA:765:G:H5'' | 1:CA:766:A:OP1 | 2.04 | 0.58 |
| 1:CA:937:A:H1' | 1:CA:1379:G:H22 | 1.68 | 0.58 |
| 3:CC:181:ASN:O | 3:CC:204:LEU:HB2 | 2.04 | 0.58 |
| 4:CD:17:VAL:HG11 | 4:CD:197:PRO:CB | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:31:CYS:C | 4:CD:33:MET:N | 2.57 | 0.58 |
| 23:D1:88:LYS:O | 23:D1:92:LYS:HB2 | 2.04 | 0.58 |
| 31:DA:1108:U:C2' | 31:DA:1109:C:H5' | 2.33 | 0.58 |
| 31:DA:128:C:C6 | 31:DA:128:C:C3' | 2.87 | 0.58 |
| 31:DA:1963:U:O2 | 31:DA:1963:U:H2' | 2.03 | 0.58 |
| 31:DA:2094:G:H2' | 31:DA:2095:C:H5' | 1.85 | 0.58 |
| 28:D6:27:LYS:HE3 | 31:DA:2285:C:C5 | 2.38 | 0.58 |
| 31:DA:2308:G:H2' | 31:DA:2309:A:C8 | 2.38 | 0.58 |
| 31:DA:466:A:H5'' | 31:DA:467:G:OP2 | 2.03 | 0.58 |
| 31:DA:542:C:N4 | 31:DA:543:C:H42 | 2.02 | 0.58 |
| 33:DD:83:GLU:HB2 | 33:DD:92:ILE:HD11 | 1.84 | 0.58 |
| 34:DE:61:ARG:N | 34:DE:62:PRO:HD2 | 2.17 | 0.58 |
| 38:DI:83:ALA:HA | 38:DI:89:TYR:CD1 | 2.39 | 0.58 |
| 39:DN:78:TYR:CD1 | 39:DN:79:PRO:HB3 | 2.39 | 0.58 |
| 41:DP:36:LYS:O | 41:DP:38:GLN:HG2 | 2.02 | 0.58 |
| 46:DU:112:ARG:O | 46:DU:115:ALA:HB3 | 2.04 | 0.58 |
| 49:DX:63:LYS:O | 49:DX:68:ARG:HA | 2.04 | 0.58 |
| 49:DX:82:GLN:HB3 | 49:DX:85:PRO:HG2 | 1.84 | 0.58 |
| 50:DY:28:LYS:HD2 | 50:DY:37:VAL:HG12 | 1.84 | 0.58 |
| 50:DY:8:LYS:NZ | 50:DY:73:ARG:HA | 2.16 | 0.58 |
| 1:AA:1190:G:H3' | 3:AC:3:ASN:HD21 | 1.69 | 0.58 |
| 1:AA:594:G:H1 | 1:AA:645:C:N4 | 2.00 | 0.58 |
| 5:AE:36:ASP:OD1 | 5:AE:37:ARG:N | 2.36 | 0.58 |
| 13:AM:86:CYS:HB2 | 19:AS:73:GLU:HB3 | 1.85 | 0.58 |
| 24:B2:49:LYS:O | 24:B2:50:ILE:C | 2.42 | 0.58 |
| 31:BA:1291:C:H2' | 31:BA:1292:U:C6 | 2.39 | 0.58 |
| 31:BA:1486:A:H2' | 31:BA:1487:G:H8 | 1.69 | 0.58 |
| 31:BA:1528(A):A:C5 | 31:BA:1529:G:C8 | 2.92 | 0.58 |
| 31:BA:236:C:H2' | 31:BA:237:C:C6 | 2.38 | 0.58 |
| 32:BB:29:A:C2 | 32:BB:30:C:C2 | 2.92 | 0.58 |
| 38:BI:63:ALA:O | 38:BI:67:ARG:HD2 | 2.04 | 0.58 |
| 38:BI:98:ALA:HA | 38:BI:109:ILE:HD11 | 1.84 | 0.58 |
| 39:BN:39:ARG:CD | 39:BN:41:ASP:HB2 | 2.34 | 0.58 |
| 31:BA:806:C:OP2 | 41:BP:39:LYS:HD2 | 2.04 | 0.58 |
| 47:BV:61:VAL:C | 47:BV:62:LEU:HD23 | 2.24 | 0.58 |
| 1:CA:1468:A:H2' | 1:CA:1469:G:O4' | 2.03 | 0.58 |
| 1:CA:25:C:H2' | 1:CA:26:A:C8 | 2.39 | 0.58 |
| 1:CA:509:A:H4' | 1:CA:510:A:OP1 | 2.02 | 0.58 |
| 23:D1:19:GLN:HE21 | 31:DA:379:G:N2 | 1.93 | 0.58 |
| 30:D8:58:ILE:HG22 | 41:DP:49:ARG:CD | 2.32 | 0.58 |
| 31:DA:1407:C:O2 | 31:DA:1407:C:H2' | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:DA:2065:C:H2' | 31:DA:2066:C:C6 | 2.38 | 0.58 |
| 31:DA:2478:A:C2' | 31:DA:2479:G:H5' | 2.34 | 0.58 |
| 31:DA:2657:A:C2 | 31:DA:2664:G:N2 | 2.71 | 0.58 |
| 31:DA:2801(A):A:C4' | 31:DA:2802:G:H2' | 2.33 | 0.58 |
| 32:DB:49:C:H2' | 32:DB:50:G:C8 | 2.39 | 0.58 |
| 35:DF:198:ALA:O | 35:DF:201:VAL:HG12 | 2.03 | 0.58 |
| 36:DG:16:ARG:O | 36:DG:20:ILE:HG13 | 2.03 | 0.58 |
| 36:DG:120:LEU:HB2 | 36:DG:179:PRO:O | 2.04 | 0.58 |
| 37:DH:149:ARG:HD3 | 37:DH:164:TYR:CE1 | 2.39 | 0.58 |
| 41:DP:38:GLN:CG | 41:DP:39:LYS:H | 2.14 | 0.58 |
| 44:DS:89:ARG:HE | 44:DS:90:GLY:H | 1.52 | 0.58 |
| 31:DA:2683:C:OP1 | 45:DT:53:ARG:NH2 | 2.37 | 0.58 |
| 1:AA:1250:A:H4' | 9:AI:68:GLY:N | 2.19 | 0.58 |
| 1:AA:180:U:C2' | 1:AA:181:G:H5' | 2.33 | 0.58 |
| 1:AA:356:A:H2' | 1:AA:357:G:H8 | 1.67 | 0.58 |
| 1:AA:501:C:H2' | 1:AA:502:G:C8 | 2.38 | 0.58 |
| 1:AA:937:A:H1' | 1:AA:1379:G:N2 | 2.18 | 0.58 |
| 2:AB:158:LEU:H | 2:AB:158:LEU:HD12 | 1.68 | 0.58 |
| 3:AC:23:TYR:CG | 3:AC:24:ALA:N | 2.71 | 0.58 |
| 7:AG:32:ARG:O | 7:AG:33:ASP:HB2 | 2.04 | 0.58 |
| 9:AI:114:TYR:N | 9:AI:114:TYR:CD2 | 2.67 | 0.58 |
| 13:AM:66:LEU:HD12 | 13:AM:66:LEU:N | 2.18 | 0.58 |
| 24:B2:14:ARG:O | 24:B2:18:PRO:CD | 2.52 | 0.58 |
| 28:B6:14:THR:O | 28:B6:49:HIS:HA | 2.04 | 0.58 |
| 31:BA:340:A:C2' | 31:BA:341:G:H5' | 2.34 | 0.58 |
| 31:BA:576:U:H2' | 31:BA:577:G:C8 | 2.39 | 0.58 |
| 39:BN:65:LYS:CD | 39:BN:67:LEU:HG | 2.33 | 0.58 |
| 43:BR:67:LEU:CD1 | 43:BR:76:VAL:HG21 | 2.28 | 0.58 |
| 49:BX:82:GLN:HB3 | 49:BX:85:PRO:HG2 | 1.86 | 0.58 |
| 1:CA:1256:A:H5' | 1:CA:1257:U:OP1 | 2.04 | 0.58 |
| 1:CA:738:C:H2' | 1:CA:739:C:H6 | 1.69 | 0.58 |
| 1:CA:868:C:H2' | 1:CA:869:G:O4' | 2.03 | 0.58 |
| 12:CL:102:ARG:CG | 12:CL:102:ARG:HH11 | 2.17 | 0.58 |
| 12:CL:41:ARG:CG | 12:CL:42:THR:H | 2.16 | 0.58 |
| 13:CM:25:ILE:HD11 | 13:CM:66:LEU:HD23 | 1.86 | 0.58 |
| 23:D1:76:ARG:HB3 | 23:D1:78:LYS:HE3 | 1.86 | 0.58 |
| 24:D2:45:SER:O | 24:D2:48:HIS:CB | 2.49 | 0.58 |
| 28:D6:15:GLU:OE1 | 28:D6:43:CYS:SG | 2.62 | 0.58 |
| 31:DA:1025:G:C4 | 31:DA:1135:C:H1' | 2.39 | 0.58 |
| 31:DA:1378:A:H4' | 31:DA:1379:A:OP1 | 2.04 | 0.58 |
| 31:DA:363(E):U:H2' | 31:DA:363(F):A:O4' | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:430:G:H5'' | 31:DA:431:U:OP2 | 2.04 | 0.58 |
| 36:DG:71:THR:HG22 | 36:DG:72:ARG:N | 2.18 | 0.58 |
| 38:DI:131:LYS:CG | 38:DI:132:PRO:HA | 2.34 | 0.58 |
| 38:DI:130:TYR:CB | 38:DI:136:VAL:HG13 | 2.27 | 0.58 |
| 38:DI:29:TYR:C | 38:DI:32:PRO:HD2 | 2.23 | 0.58 |
| 41:DP:14:LYS:O | 41:DP:15:ARG:HB2 | 2.03 | 0.58 |
| 41:DP:50:ARG:O | 41:DP:57:THR:HG23 | 2.04 | 0.58 |
| 42:DQ:12:GLN:HG2 | 42:DQ:73:PRO:HD2 | 1.86 | 0.58 |
| 44:DS:67:ARG:H | 44:DS:69:VAL:HG13 | 1.68 | 0.58 |
| 45:DT:28:VAL:HG22 | 45:DT:46:GLU:HG3 | 1.85 | 0.58 |
| 49:DX:35:THR:O | 49:DX:36:LYS:C | 2.41 | 0.58 |
| 1:AA:1150:U:O4 | 1:AA:1151:A:N6 | 2.35 | 0.57 |
| 1:AA:69:G:C2 | 1:AA:70:G:N7 | 2.72 | 0.57 |
| 1:AA:863:U:H2' | 1:AA:865:A:OP2 | 2.03 | 0.57 |
| 1:AA:963:G:N3 | 10:AJ:55:LYS:NZ | 2.49 | 0.57 |
| 2:AB:67:THR:HG22 | 2:AB:90:MET:HE1 | 1.85 | 0.57 |
| 3:AC:181:ASN:O | 3:AC:204:LEU:HB2 | 2.03 | 0.57 |
| 3:AC:32:LEU:HD22 | 3:AC:59:ARG:NH1 | 2.19 | 0.57 |
| 5:AE:57:LYS:O | 5:AE:61:TYR:HD2 | 1.87 | 0.57 |
| 13:AM:31:LYS:HA | 13:AM:34:LEU:HD12 | 1.84 | 0.57 |
| 15:AO:37:ASN:HD22 | 15:AO:37:ASN:N | 2.00 | 0.57 |
| 24:B2:26:ARG:NH1 | 24:B2:29:LYS:HE2 | 2.19 | 0.57 |
| 25:B3:6:VAL:HG12 | 25:B3:54:VAL:HG11 | 1.86 | 0.57 |
| 28:B6:20:ASN:O | 28:B6:21:TYR:CD1 | 2.57 | 0.57 |
| 31:BA:2646:C:H6 | 31:BA:2646:C:O5' | 1.87 | 0.57 |
| 31:BA:794:G:O2' | 31:BA:795:C:H5' | 2.04 | 0.57 |
| 33:BD:16:MET:HG3 | 33:BD:206:LEU:O | 2.04 | 0.57 |
| 34:BE:59:VAL:CG2 | 34:BE:63:LEU:HA | 2.31 | 0.57 |
| 34:BE:36:ARG:HH21 | 34:BE:88:GLY:HA2 | 1.65 | 0.57 |
| 31:BA:2562:U:H1' | 40:BO:23:ARG:NH1 | 2.17 | 0.57 |
| 31:BA:662:G:P | 41:BP:18:ARG:HD2 | 2.44 | 0.57 |
| 41:BP:45:LEU:HD22 | 41:BP:46:LYS:H | 1.68 | 0.57 |
| 44:BS:89:ARG:HE | 44:BS:90:GLY:H | 1.52 | 0.57 |
| 1:CA:721:G:H4' | 1:CA:722:A:O4' | 2.04 | 0.57 |
| 2:CB:71:VAL:O | 2:CB:164:VAL:HG22 | 2.03 | 0.57 |
| 13:CM:66:LEU:HD12 | 13:CM:66:LEU:N | 2.17 | 0.57 |
| 31:DA:2309:A:C2 | 31:DA:2310:A:C2 | 2.92 | 0.57 |
| 31:DA:2488:A:H2' | 31:DA:2489:G:O4' | 2.03 | 0.57 |
| 31:DA:280:C:H2' | 31:DA:281:G:O5' | 2.04 | 0.57 |
| 31:DA:352:G:O2' | 31:DA:353:G:O5' | 2.22 | 0.57 |
| 34:DE:101:ARG:HB3 | 34:DE:169:ASN:ND2 | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DG:57:ALA:HB2 | 36:DG:90:LEU:HD21 | 1.86 | 0.57 |
| 42:DQ:141:GLN:CG | 51:DZ:72:ARG:HH11 | 2.16 | 0.57 |
| 44:DS:35:ILE:H | 44:DS:53:SER:HB3 | 1.69 | 0.57 |
| 46:DU:90:VAL:HG12 | 46:DU:91:ASP:H | 1.69 | 0.57 |
| 1:AA:1452:C:H5' | 1:AA:1456:G:C4 | 2.39 | 0.57 |
| 1:AA:375:U:C2 | 1:AA:376:G:C8 | 2.92 | 0.57 |
| 1:AA:748:C:H1' | 1:AA:749:C:OP2 | 2.04 | 0.57 |
| 9:AI:3:GLN:HB3 | 9:AI:20:ARG:CZ | 2.33 | 0.57 |
| 23:B1:92:LYS:C | 23:B1:94:LEU:H | 2.08 | 0.57 |
| 24:B2:46:GLN:C | 24:B2:46:GLN:HE21 | 2.07 | 0.57 |
| 28:B6:51:GLU:O | 28:B6:52:VAL:HB | 2.03 | 0.57 |
| 31:BA:212:G:C2' | 31:BA:213:A:H5' | 2.33 | 0.57 |
| 31:BA:352:G:O2' | 31:BA:353:G:O5' | 2.22 | 0.57 |
| 31:BA:548:A:O2' | 31:BA:549:G:OP1 | 2.20 | 0.57 |
| 32:BB:15:A:H1' | 32:BB:110:G:N9 | 2.18 | 0.57 |
| 32:BB:6:C:C2 | 32:BB:116:G:N2 | 2.71 | 0.57 |
| 33:BD:35:LYS:N | 33:BD:64:ILE:HG23 | 2.19 | 0.57 |
| 40:BO:34:THR:OG1 | 40:BO:35:VAL:N | 2.36 | 0.57 |
| 44:BS:61:ASN:HD22 | 44:BS:62:LYS:N | 2.02 | 0.57 |
| 1:CA:1101:A:H4' | 1:CA:1102:A:O5' | 2.04 | 0.57 |
| 1:CA:1315:U:H2' | 1:CA:1316:G:O4' | 2.05 | 0.57 |
| 1:CA:1479:C:O2' | 1:CA:1480:G:H5' | 2.04 | 0.57 |
| 1:CA:832:C:N4 | 1:CA:855:G:C6 | 2.73 | 0.57 |
| 2:CB:163:PHE:HD2 | 2:CB:185:ILE:HG13 | 1.68 | 0.57 |
| 3:CC:32:LEU:HD22 | 3:CC:59:ARG:NH1 | 2.19 | 0.57 |
| 4:CD:126:ILE:HG22 | 4:CD:127:THR:N | 2.15 | 0.57 |
| 4:CD:58:LEU:HD23 | 4:CD:206:PHE:CE1 | 2.39 | 0.57 |
| 5:CE:101:ILE:HG12 | 5:CE:101:ILE:O | 2.02 | 0.57 |
| 15:CO:74:ASP:OD2 | 15:CO:76:GLU:HB3 | 2.05 | 0.57 |
| 18:CR:43:PHE:O | 18:CR:44:LEU:HD12 | 2.04 | 0.57 |
| 28:D6:15:GLU:HG2 | 28:D6:18:ARG:NE | 2.06 | 0.57 |
| 28:D6:30:THR:O | 28:D6:31:PRO:C | 2.41 | 0.57 |
| 30:D8:35:GLN:CB | 31:DA:2420:C:OP1 | 2.52 | 0.57 |
| 31:DA:1515:G:H2' | 31:DA:1516:C:C6 | 2.39 | 0.57 |
| 31:DA:860:U:C5 | 31:DA:2268:A:C8 | 2.92 | 0.57 |
| 31:DA:2334:G:H21 | 44:DS:18:ILE:CD1 | 2.04 | 0.57 |
| 31:DA:2562:U:H1' | 40:DO:23:ARG:NH1 | 2.15 | 0.57 |
| 31:DA:288:C:O2 | 31:DA:288:C:H2' | 2.03 | 0.57 |
| 31:DA:528:A:C2' | 31:DA:529:A:H5' | 2.34 | 0.57 |
| 32:DB:28:C:H2' | 32:DB:29:A:C8 | 2.39 | 0.57 |
| 43:DR:59:ASP:OD1 | 43:DR:61:HIS:HB3 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:DT:91:ARG:HB2 | 45:DT:115:ARG:O | 2.05 | 0.57 |
| 45:DT:17:THR:O | 45:DT:18:ASP:CB | 2.46 | 0.57 |
| 51:DZ:71:VAL:HG22 | 51:DZ:88:PHE:HE2 | 1.68 | 0.57 |
| 1:AA:1470:G:O2' | 1:AA:1471:G:H5' | 2.03 | 0.57 |
| 1:AA:1471:G:O2' | 1:AA:1472:U:H5' | 2.04 | 0.57 |
| 1:AA:937:A:H1' | 1:AA:1379:G:H22 | 1.70 | 0.57 |
| 4:AD:17:VAL:HG11 | 4:AD:197:PRO:HB2 | 1.85 | 0.57 |
| 6:AF:37:VAL:HG12 | 6:AF:38:GLU:N | 2.19 | 0.57 |
| 7:AG:69:VAL:HA | 7:AG:138:LYS:HD2 | 1.86 | 0.57 |
| 12:AL:110:VAL:HG21 | 12:AL:120:TYR:HB3 | 1.86 | 0.57 |
| 24:B2:14:ARG:CZ | 24:B2:57:ILE:CG2 | 2.82 | 0.57 |
| 30:B8:52:LYS:N | 30:B8:53:PRO:CD | 2.63 | 0.57 |
| 22:B0:2:ALA:H | 31:BA:2602:A:H61 | 1.51 | 0.57 |
| 31:BA:2881:C:H2' | 31:BA:2882:A:O4' | 2.04 | 0.57 |
| 31:BA:314:A:O2' | 31:BA:315:G:H5' | 2.04 | 0.57 |
| 31:BA:528:A:H2 | 31:BA:2043:C:C5' | 2.17 | 0.57 |
| 31:BA:579:G:H2' | 31:BA:580:C:C6 | 2.40 | 0.57 |
| 31:BA:848:G:N9 | 31:BA:933:A:H8 | 2.01 | 0.57 |
| 32:BB:13:A:H2' | 32:BB:70:C:O2' | 2.04 | 0.57 |
| 33:BD:58:HIS:CD2 | 33:BD:59:LYS:N | 2.73 | 0.57 |
| 35:BF:198:ALA:O | 35:BF:201:VAL:HG12 | 2.04 | 0.57 |
| 39:BN:3:THR:CA | 39:BN:4:TYR:CE1 | 2.79 | 0.57 |
| 41:BP:26:GLY:HA2 | 41:BP:30:THR:HG21 | 1.84 | 0.57 |
| 41:BP:23:PRO:O | 41:BP:33:ARG:HG3 | 2.04 | 0.57 |
| 31:BA:2690:C:OP1 | 43:BR:17:ARG:NH1 | 2.37 | 0.57 |
| 45:BT:50:ILE:HA | 45:BT:99:LEU:CD1 | 2.34 | 0.57 |
| 49:BX:35:THR:CB | 49:BX:75:ASP:OD2 | 2.50 | 0.57 |
| 1:CA:706:A:C5 | 1:CA:707:C:H5 | 2.22 | 0.57 |
| 2:CB:228:GLY:O | 2:CB:230:VAL:HG13 | 2.04 | 0.57 |
| 2:CB:61:LEU:HD23 | 2:CB:68:ILE:HD11 | 1.87 | 0.57 |
| 10:CJ:78:ASN:O | 10:CJ:82:ILE:HG12 | 2.04 | 0.57 |
| 12:CL:115:LYS:O | 12:CL:117:ARG:HG3 | 2.04 | 0.57 |
| 13:CM:44:ARG:HB2 | 13:CM:46:LYS:HG2 | 1.86 | 0.57 |
| 16:CP:50:LYS:C | 16:CP:50:LYS:HD3 | 2.25 | 0.57 |
| 31:DA:196:A:C4 | 31:DA:805:G:O6 | 2.57 | 0.57 |
| 31:DA:2313:C:H2' | 31:DA:2314:C:H6 | 1.67 | 0.57 |
| 31:DA:2875:C:O2' | 45:DT:5:ALA:HB3 | 2.04 | 0.57 |
| 34:DE:116:VAL:HG13 | 34:DE:122:PHE:CG | 2.39 | 0.57 |
| 39:DN:90:MET:O | 39:DN:93:THR:O | 2.22 | 0.57 |
| 41:DP:24:GLY:HA3 | 41:DP:33:ARG:NH2 | 2.13 | 0.57 |
| 43:DR:38:VAL:HB | 43:DR:39:PRO:HD3 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:DV:19:LYS:CE | 47:DV:20:LEU:N | 2.67 | 0.57 |
| 46:DU:102:GLU:HG3 | 47:DV:2:PHE:CE2 | 2.39 | 0.57 |
| 1:AA:1256:A:H5' | 1:AA:1257:U:OP1 | 2.05 | 0.57 |
| 1:AA:254:G:O2' | 1:AA:255:G:H5' | 2.04 | 0.57 |
| 1:AA:509:A:O2' | 1:AA:510:A:P | 2.62 | 0.57 |
| 1:AA:612:C:O2' | 1:AA:613:C:H5' | 2.04 | 0.57 |
| 8:AH:21:LYS:O | 8:AH:63:LEU:HD23 | 2.04 | 0.57 |
| 13:AM:69:GLU:HB3 | 13:AM:72:ALA:HB3 | 1.85 | 0.57 |
| 23:B1:85:LEU:C | 23:B1:87:PRO:CD | 2.71 | 0.57 |
| 31:BA:2074:U:H2' | 31:BA:2075:U:C6 | 2.39 | 0.57 |
| 31:BA:649:G:H2' | 31:BA:650:C:C6 | 2.39 | 0.57 |
| 34:BE:93:VAL:H | 34:BE:95:ILE:CD1 | 2.16 | 0.57 |
| 39:BN:67:LEU:C | 39:BN:69:GLN:H | 2.07 | 0.57 |
| 41:BP:121:LYS:HB3 | 41:BP:123:LEU:CD2 | 2.34 | 0.57 |
| 43:BR:100:LEU:HD11 | 43:BR:113:LEU:HD13 | 1.86 | 0.57 |
| 49:BX:31:HIS:CD2 | 49:BX:33:LYS:H | 2.23 | 0.57 |
| 49:BX:73:ARG:N | 49:BX:74:PRO:CD | 2.65 | 0.57 |
| 1:CA:1068:G:N3 | 1:CA:1191:A:C2 | 2.72 | 0.57 |
| 1:CA:159:G:O2' | 1:CA:160:A:C8 | 2.57 | 0.57 |
| 2:CB:97:TRP:HH2 | 2:CB:176:GLU:HG3 | 1.68 | 0.57 |
| 8:CH:51:VAL:HG11 | 8:CH:60:ARG:CG | 2.34 | 0.57 |
| 13:CM:69:GLU:HB3 | 13:CM:72:ALA:HB3 | 1.86 | 0.57 |
| 20:CT:11:SER:HA | 20:CT:13:LEU:HD13 | 1.85 | 0.57 |
| 23:D1:53:VAL:HG21 | 23:D1:74:VAL:HG21 | 1.86 | 0.57 |
| 31:DA:2656:U:H2' | 31:DA:2657:A:H5'' | 1.86 | 0.57 |
| 31:DA:271(A):A:H2 | 31:DA:272(D):G:N3 | 2.02 | 0.57 |
| 31:DA:2895:U:H5 | 31:DA:2896:C:C5 | 2.22 | 0.57 |
| 31:DA:715:G:O2' | 31:DA:716:A:H5' | 2.05 | 0.57 |
| 1:CA:1422:G:H4' | 40:DO:49:ARG:HH12 | 1.69 | 0.57 |
| 40:DO:50:GLY:C | 40:DO:52:VAL:H | 2.08 | 0.57 |
| 40:DO:73:ASP:OD2 | 45:DT:32:TYR:CE1 | 2.57 | 0.57 |
| 41:DP:16:ARG:O | 41:DP:16:ARG:NH1 | 2.37 | 0.57 |
| 42:DQ:75:THR:HA | 42:DQ:88:GLY:CA | 2.32 | 0.57 |
| 45:DT:90:GLN:HG2 | 45:DT:120:ARG:NH2 | 2.20 | 0.57 |
| 49:DX:73:ARG:O | 49:DX:74:PRO:O | 2.22 | 0.57 |
| 1:AA:1423:G:H5'' | 40:BO:49:ARG:NH2 | 2.18 | 0.57 |
| 1:AA:342:C:O2' | 1:AA:343:U:H5' | 2.05 | 0.57 |
| 1:AA:659:U:O2' | 1:AA:660:G:H5' | 2.04 | 0.57 |
| 2:AB:74:LYS:NZ | 2:AB:76:GLN:HB2 | 2.20 | 0.57 |
| 3:AC:34:LEU:HD23 | 3:AC:34:LEU:O | 2.04 | 0.57 |
| 4:AD:126:ILE:HG22 | 4:AD:127:THR:N | 2.19 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:AF:19:LEU:HD23 | 6:AF:19:LEU:O | 2.04 | 0.57 |
| 8:AH:88:LYS:O | 8:AH:92:ARG:HD2 | 2.04 | 0.57 |
| 10:AJ:61:GLU:OE1 | 14:AN:58:LYS:HE2 | 2.05 | 0.57 |
| 20:AT:11:SER:HA | 20:AT:13:LEU:CD1 | 2.35 | 0.57 |
| 23:B1:26:ARG:HG2 | 23:B1:34:THR:CB | 2.34 | 0.57 |
| 23:B1:76:ARG:HB3 | 23:B1:78:LYS:HE3 | 1.85 | 0.57 |
| 30:B8:62:LEU:O | 30:B8:64:TYR:N | 2.37 | 0.57 |
| 31:BA:2478:A:H2' | 31:BA:2479:G:H5' | 1.86 | 0.57 |
| 31:BA:2652:C:H2' | 31:BA:2653:U:H5' | 1.84 | 0.57 |
| 31:BA:2657:A:H2 | 31:BA:2664:G:H21 | 1.50 | 0.57 |
| 32:BB:60:C:C2 | 32:BB:61:G:C8 | 2.93 | 0.57 |
| 39:BN:78:TYR:CD1 | 39:BN:79:PRO:HB3 | 2.39 | 0.57 |
| 40:BO:98:VAL:HG13 | 40:BO:117:LEU:HB3 | 1.84 | 0.57 |
| 42:BQ:39:PRO:HA | 42:BQ:97:VAL:O | 2.05 | 0.57 |
| 1:CA:1084:G:C5 | 1:CA:1085:U:C4 | 2.93 | 0.57 |
| 1:CA:1256:A:O3' | 1:CA:1257:U:H4' | 2.05 | 0.57 |
| 1:CA:159:G:N2 | 1:CA:161:A:H3' | 2.19 | 0.57 |
| 1:CA:707:C:O2' | 1:CA:708:C:H5' | 2.04 | 0.57 |
| 1:CA:748:C:H1' | 1:CA:749:C:OP2 | 2.04 | 0.57 |
| 1:CA:980:C:H5' | 1:CA:981:U:C5 | 2.40 | 0.57 |
| 3:CC:111:LEU:HD22 | 3:CC:204:LEU:HD21 | 1.85 | 0.57 |
| 4:CD:19:LEU:HB2 | 4:CD:21:LEU:HD21 | 1.85 | 0.57 |
| 12:CL:75:HIS:HD2 | 12:CL:77:LEU:H | 1.53 | 0.57 |
| 31:DA:1309:G:O2' | 31:DA:1310:G:H5' | 2.04 | 0.57 |
| 31:DA:1412:A:H2' | 31:DA:1413:G:C8 | 2.39 | 0.57 |
| 31:DA:1762:A:H8 | 31:DA:1762:A:O5' | 1.87 | 0.57 |
| 31:DA:671:C:H2' | 31:DA:672:C:C6 | 2.39 | 0.57 |
| 36:DG:19:LEU:HD13 | 36:DG:32:PRO:HG2 | 1.87 | 0.57 |
| 42:DQ:34:LEU:HD11 | 42:DQ:129:THR:HB | 1.86 | 0.57 |
| 50:DY:96:ILE:HG13 | 50:DY:99:CYS:C | 2.25 | 0.57 |
| 1:AA:509:A:H4' | 1:AA:510:A:OP1 | 2.04 | 0.57 |
| 2:AB:19:HIS:O | 2:AB:39:ILE:HG23 | 2.04 | 0.57 |
| 2:AB:97:TRP:HH2 | 2:AB:176:GLU:HG3 | 1.69 | 0.57 |
| 3:AC:150:LYS:HE2 | 3:AC:152:ILE:HD11 | 1.85 | 0.57 |
| 7:AG:70:LYS:HB3 | 7:AG:96:GLN:OE1 | 2.04 | 0.57 |
| 23:B1:70:VAL:O | 23:B1:73:LEU:HB2 | 2.04 | 0.57 |
| 31:BA:1252:G:C2 | 31:BA:1253:A:C2 | 2.93 | 0.57 |
| 31:BA:1372:U:H2' | 31:BA:1373:A:O4' | 2.05 | 0.57 |
| 33:BD:43:ARG:HH11 | 33:BD:44:ASN:CG | 2.07 | 0.57 |
| 38:BI:130:TYR:CB | 38:BI:136:VAL:HG13 | 2.27 | 0.57 |
| 42:BQ:12:GLN:HG2 | 42:BQ:73:PRO:HD2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BQ:42:ILE:HD13 | 42:BQ:97:VAL:HG21 | 1.87 | 0.57 |
| 49:BX:73:ARG:O | 49:BX:74:PRO:C | 2.42 | 0.57 |
| 1:CA:1190:G:H3' | 3:CC:3:ASN:HD21 | 1.70 | 0.57 |
| 1:CA:1248:A:C2' | 1:CA:1249:C:H5' | 2.35 | 0.57 |
| 1:CA:1346:A:N1 | 1:CA:1374:A:H5'' | 2.19 | 0.57 |
| 1:CA:186:C:C2 | 1:CA:187:C:C5 | 2.92 | 0.57 |
| 1:CA:833:U:H2' | 1:CA:834:C:C6 | 2.39 | 0.57 |
| 1:CA:938:A:N6 | 1:CA:939:G:C6 | 2.73 | 0.57 |
| 1:CA:979:C:H3' | 1:CA:980:C:H5'' | 1.87 | 0.57 |
| 4:CD:194:LEU:N | 4:CD:194:LEU:HD22 | 2.20 | 0.57 |
| 23:D1:26:ARG:HG2 | 23:D1:34:THR:CB | 2.34 | 0.57 |
| 31:DA:1204:A:H61 | 31:DA:1240:U:H2' | 1.69 | 0.57 |
| 31:DA:1418:G:H8 | 31:DA:1418:G:O5' | 1.87 | 0.57 |
| 31:DA:2532:G:O2' | 31:DA:2657:A:N6 | 2.37 | 0.57 |
| 31:DA:2580:U:H4' | 34:DE:131:ALA:H | 1.68 | 0.57 |
| 36:DG:71:THR:HB | 36:DG:89:GLY:CA | 2.34 | 0.57 |
| 37:DH:163:TYR:N | 37:DH:163:TYR:CD1 | 2.72 | 0.57 |
| 39:DN:3:THR:CA | 39:DN:4:TYR:CE1 | 2.77 | 0.57 |
| 41:DP:101:VAL:C | 41:DP:103:ALA:H | 2.07 | 0.57 |
| 31:DA:661:C:C4' | 41:DP:16:ARG:HH12 | 2.18 | 0.57 |
| 43:DR:95:THR:HA | 43:DR:116:LEU:O | 2.05 | 0.57 |
| 43:DR:33:ARG:HG2 | 43:DR:115:GLU:CG | 2.23 | 0.57 |
| 46:DU:85:LYS:O | 46:DU:116:ALA:HB1 | 2.04 | 0.57 |
| 1:AA:1084:G:C5 | 1:AA:1085:U:C4 | 2.92 | 0.57 |
| 1:AA:505:G:C6 | 1:AA:535:A:C2 | 2.93 | 0.57 |
| 1:AA:68:G:H5' | 1:AA:171:A:H1' | 1.87 | 0.57 |
| 1:AA:706:A:C5 | 1:AA:707:C:H5 | 2.22 | 0.57 |
| 6:AF:69:GLU:HG2 | 6:AF:70:ASP:H | 1.70 | 0.57 |
| 12:AL:82:VAL:O | 12:AL:83:VAL:HB | 2.05 | 0.57 |
| 16:AP:22:THR:HG22 | 16:AP:32:TYR:HA | 1.86 | 0.57 |
| 27:B5:51:TYR:HB3 | 27:B5:52:TYR:CD2 | 2.40 | 0.57 |
| 31:BA:1359:A:C8 | 31:BA:1372:U:O4 | 2.57 | 0.57 |
| 31:BA:1952:A:C5 | 40:BO:22:ILE:HD11 | 2.40 | 0.57 |
| 31:BA:2309:A:C2 | 31:BA:2310:A:C2 | 2.93 | 0.57 |
| 31:BA:2476:A:C2 | 31:BA:2477:C:C6 | 2.92 | 0.57 |
| 31:BA:280:C:H2' | 31:BA:281:G:O5' | 2.05 | 0.57 |
| 31:BA:825:C:C2' | 31:BA:826:U:O5' | 2.52 | 0.57 |
| 31:BA:993:G:C5' | 47:BV:75:PHE:CZ | 2.85 | 0.57 |
| 33:BD:35:LYS:CE | 33:BD:64:ILE:C | 2.71 | 0.57 |
| 35:BF:88:VAL:HG11 | 35:BF:91:GLY:HA3 | 1.87 | 0.57 |
| 36:BG:39:ILE:HB | 36:BG:157:ILE:HG22 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BH:138:LYS:O | 37:BH:139:GLN:C | 2.42 | 0.57 |
| 38:BI:29:TYR:C | 38:BI:32:PRO:HD2 | 2.25 | 0.57 |
| 41:BP:62:LEU:N | 41:BP:62:LEU:HD13 | 2.19 | 0.57 |
| 43:BR:95:THR:HA | 43:BR:116:LEU:O | 2.04 | 0.57 |
| 44:BS:74:ALA:HB2 | 44:BS:101:LEU:HD11 | 1.85 | 0.57 |
| 50:BY:44:ILE:HG22 | 50:BY:45:VAL:N | 2.20 | 0.57 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:C6 | 2.40 | 0.57 |
| 1:CA:1072:G:C5 | 1:CA:1073:U:C4 | 2.92 | 0.57 |
| 1:CA:675:A:H61 | 1:CA:715:A:H61 | 1.53 | 0.57 |
| 2:CB:158:LEU:HD12 | 2:CB:158:LEU:H | 1.70 | 0.57 |
| 4:CD:108:LEU:HB3 | 4:CD:110:PHE:CE1 | 2.40 | 0.57 |
| 7:CG:32:ARG:O | 7:CG:33:ASP:HB2 | 2.04 | 0.57 |
| 7:CG:69:VAL:HG13 | 7:CG:134:ALA:O | 2.05 | 0.57 |
| 8:CH:88:LYS:O | 8:CH:92:ARG:HD2 | 2.05 | 0.57 |
| 10:CJ:40:LEU:HD23 | 10:CJ:40:LEU:H | 1.68 | 0.57 |
| 15:CO:25:THR:HG21 | 15:CO:70:LEU:HB2 | 1.87 | 0.57 |
| 30:D8:32:LEU:CB | 30:D8:34:TRP:H | 2.17 | 0.57 |
| 31:DA:11:G:C2' | 31:DA:12:U:H5' | 2.34 | 0.57 |
| 31:DA:2656:U:N3 | 31:DA:2665:A:H2 | 2.01 | 0.57 |
| 31:DA:543:C:N3 | 31:DA:551:G:C2 | 2.73 | 0.57 |
| 31:DA:985:C:H2' | 31:DA:986:C:H6 | 1.70 | 0.57 |
| 33:DD:186:HIS:CD2 | 33:DD:187:GLY:N | 2.73 | 0.57 |
| 36:DG:131:TYR:HB3 | 36:DG:159:VAL:CG1 | 2.34 | 0.57 |
| 37:DH:88:LEU:O | 37:DH:89:ILE:HG23 | 2.05 | 0.57 |
| 31:DA:389:G:N2 | 41:DP:71:VAL:HG12 | 2.20 | 0.57 |
| 45:DT:93:ARG:O | 45:DT:94:ALA:C | 2.41 | 0.57 |
| 49:DX:73:ARG:N | 49:DX:74:PRO:CD | 2.66 | 0.57 |
| 1:AA:1101:A:H4' | 1:AA:1102:A:O5' | 2.04 | 0.57 |
| 1:AA:1228:C:H2' | 1:AA:1229:A:C8 | 2.38 | 0.57 |
| 1:AA:1321:C:H3' | 1:AA:1322:C:H5'' | 1.84 | 0.57 |
| 12:AL:102:ARG:CG | 12:AL:102:ARG:HH11 | 2.18 | 0.57 |
| 17:AQ:45:HIS:HD2 | 17:AQ:47:PRO:HD3 | 1.69 | 0.57 |
| 24:B2:41:ILE:O | 24:B2:43:GLN:N | 2.37 | 0.57 |
| 27:B5:40:LYS:NZ | 27:B5:46:CYS:O | 2.30 | 0.57 |
| 27:B5:36:CYS:CB | 27:B5:49:CYS:SG | 2.93 | 0.57 |
| 27:B5:57:VAL:CG2 | 27:B5:58:LEU:H | 2.16 | 0.57 |
| 30:B8:27:THR:HA | 41:BP:62:LEU:CD1 | 2.35 | 0.57 |
| 31:BA:1717:G:C2 | 31:BA:1718:G:C8 | 2.93 | 0.57 |
| 31:BA:1803:A:H4' | 33:BD:259:THR:HG23 | 1.87 | 0.57 |
| 33:BD:35:LYS:HE2 | 33:BD:104:TYR:CB | 2.33 | 0.57 |
| 34:BE:111:ARG:CZ | 43:BR:2:ARG:HH21 | 2.17 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 31:BA:1279:G:H5' | 43:BR:34:ILE:HD11 | 1.87 | 0.57 |
| 45:BT:29:ARG:HB2 | 45:BT:86:ILE:H | 1.70 | 0.57 |
| 1:CA:79:G:C4' | 1:CA:80:G:OP1 | 2.52 | 0.57 |
| 1:CA:854:G:H3' | 1:CA:871:U:O4 | 2.05 | 0.57 |
| 2:CB:27:LYS:HD2 | 2:CB:193:ASP:HB2 | 1.87 | 0.57 |
| 3:CC:152:ILE:HB | 3:CC:199:LYS:HB2 | 1.87 | 0.57 |
| 23:D1:25:LYS:C | 23:D1:26:ARG:HG3 | 2.24 | 0.57 |
| 27:D5:2:ALA:N | 31:DA:747:U:C4 | 2.73 | 0.57 |
| 30:D8:61:LEU:HD13 | 31:DA:593:G:O2' | 2.05 | 0.57 |
| 31:DA:1210:A:C5' | 31:DA:1210:A:C8 | 2.79 | 0.57 |
| 31:DA:2655:G:N3 | 31:DA:2664:G:O6 | 2.38 | 0.57 |
| 31:DA:995:C:C2 | 39:DN:4:TYR:OH | 2.42 | 0.57 |
| 37:DH:156:ALA:C | 37:DH:158:HIS:N | 2.58 | 0.57 |
| 30:D8:46:ARG:NH2 | 41:DP:65:ARG:NH2 | 2.41 | 0.57 |
| 40:DO:107:ARG:NH2 | 45:DT:35:LYS:HD2 | 2.18 | 0.57 |
| 40:DO:77:ILE:HB | 45:DT:74:ARG:HD3 | 1.87 | 0.57 |
| 2:AB:168:THR:HG21 | 2:AB:192:SER:HA | 1.86 | 0.57 |
| 2:AB:28:PHE:CD1 | 2:AB:190:THR:HA | 2.39 | 0.57 |
| 1:AA:1206:G:O4' | 3:AC:194:GLY:HA2 | 2.05 | 0.57 |
| 4:AD:128:VAL:CG1 | 4:AD:129:ASN:HD22 | 2.06 | 0.57 |
| 4:AD:156:GLU:O | 4:AD:159:ARG:HB2 | 2.05 | 0.57 |
| 7:AG:32:ARG:O | 7:AG:33:ASP:CB | 2.53 | 0.57 |
| 23:B1:88:LYS:O | 23:B1:92:LYS:HB2 | 2.05 | 0.57 |
| 28:B6:40:CYS:SG | 28:B6:45:LYS:HD3 | 2.45 | 0.57 |
| 31:BA:1820:U:C2 | 33:BD:202:LYS:HB3 | 2.40 | 0.57 |
| 31:BA:2801(A):A:C4' | 31:BA:2802:G:H2' | 2.33 | 0.57 |
| 31:BA:518:G:H2' | 31:BA:519:U:C6 | 2.39 | 0.57 |
| 31:BA:2591:C:OP2 | 33:BD:239:ARG:HB2 | 2.05 | 0.57 |
| 33:BD:31:LYS:O | 33:BD:35:LYS:O | 2.23 | 0.57 |
| 36:BG:39:ILE:HA | 36:BG:157:ILE:HA | 1.86 | 0.57 |
| 49:BX:60:ARG:CG | 49:BX:71:GLY:HA3 | 2.35 | 0.57 |
| 50:BY:75:ILE:O | 50:BY:76:CYS:HB2 | 2.05 | 0.57 |
| 51:BZ:23:LYS:HE3 | 51:BZ:40:ASP:OD2 | 2.05 | 0.57 |
| 1:CA:1172:C:H2' | 1:CA:1173:G:H8 | 1.68 | 0.57 |
| 1:CA:1248:A:H2' | 1:CA:1249:C:H5' | 1.87 | 0.57 |
| 3:CC:89:GLU:O | 3:CC:93:LYS:HB2 | 2.05 | 0.57 |
| 23:D1:85:LEU:HB3 | 23:D1:87:PRO:CD | 2.35 | 0.57 |
| 31:DA:1786:A:H1' | 31:DA:1938:A:N6 | 2.19 | 0.57 |
| 31:DA:1980:G:O2' | 31:DA:1982:C:OP2 | 2.15 | 0.57 |
| 31:DA:2386:C:H2' | 31:DA:2387:U:C6 | 2.40 | 0.57 |
| 31:DA:2657:A:H2 | 31:DA:2664:G:N2 | 2.02 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:52:A:C2' | 31:DA:53:A:H5' | 2.35 | 0.57 |
| 35:DF:205:ARG:C | 35:DF:206:ILE:HG13 | 2.25 | 0.57 |
| 38:DI:62:LYS:HE2 | 38:DI:134:PRO:CG | 2.35 | 0.57 |
| 44:DS:87:PHE:CE2 | 44:DS:97:ARG:NH2 | 2.71 | 0.57 |
| 45:DT:80:SER:HB3 | 45:DT:81:PRO:HD3 | 1.86 | 0.57 |
| 50:DY:37:VAL:HG23 | 50:DY:38:ILE:N | 2.20 | 0.57 |
| 50:DY:46:LYS:C | 50:DY:47:LYS:HD2 | 2.25 | 0.57 |
| 1:AA:1072:G:C5 | 1:AA:1073:U:C4 | 2.93 | 0.57 |
| 1:AA:32:A:H2' | 1:AA:33:A:C8 | 2.40 | 0.57 |
| 1:AA:979:C:H3' | 1:AA:980:C:H5'' | 1.86 | 0.57 |
| 13:AM:91:ARG:HB2 | 13:AM:98:VAL:HG21 | 1.87 | 0.57 |
| 17:AQ:68:ARG:O | 17:AQ:68:ARG:HG3 | 2.04 | 0.57 |
| 23:B1:33:LYS:HZ1 | 23:B1:35:THR:HG21 | 1.70 | 0.57 |
| 28:B6:32:ASN:OD1 | 28:B6:33:LYS:N | 2.38 | 0.57 |
| 31:BA:142:A:H8 | 31:BA:1595:G:N2 | 2.00 | 0.57 |
| 33:BD:35:LYS:CE | 33:BD:65:ILE:HA | 2.35 | 0.57 |
| 35:BF:141:ALA:O | 35:BF:144:LYS:HB3 | 2.05 | 0.57 |
| 39:BN:131:GLN:NE2 | 39:BN:134:ARG:HA | 2.19 | 0.57 |
| 39:BN:78:TYR:HD1 | 39:BN:79:PRO:HD3 | 1.70 | 0.57 |
| 42:BQ:34:LEU:HD11 | 42:BQ:129:THR:HB | 1.86 | 0.57 |
| 1:CA:1154:G:H2' | 1:CA:1155:G:C8 | 2.40 | 0.57 |
| 1:CA:356:A:H2' | 1:CA:357:G:H8 | 1.69 | 0.57 |
| 1:CA:376:G:OP1 | 16:CP:5:ARG:HB2 | 2.05 | 0.57 |
| 1:CA:69:G:C2 | 1:CA:70:G:N7 | 2.73 | 0.57 |
| 9:CI:10:ARG:HG2 | 9:CI:104:ARG:O | 2.05 | 0.57 |
| 12:CL:82:VAL:O | 12:CL:83:VAL:HB | 2.04 | 0.57 |
| 22:D0:41:ARG:CD | 22:D0:41:ARG:H | 2.16 | 0.57 |
| 31:DA:2300:G:H1 | 31:DA:2316:C:H42 | 1.52 | 0.57 |
| 28:D6:19:ARG:NH1 | 31:DA:2400:G:H4' | 2.20 | 0.57 |
| 31:DA:773:U:H5' | 33:DD:47:GLY:HA2 | 1.86 | 0.57 |
| 37:DH:85:LYS:CE | 37:DH:133:VAL:HB | 2.35 | 0.57 |
| 41:DP:13:ASN:C | 41:DP:13:ASN:HD22 | 2.07 | 0.57 |
| 43:DR:50:HIS:O | 43:DR:54:LEU:HD22 | 2.04 | 0.57 |
| 44:DS:28:VAL:O | 44:DS:89:ARG:CD | 2.52 | 0.57 |
| 1:AA:1097:C:O2' | 1:AA:1098:C:H5' | 2.05 | 0.56 |
| 1:AA:1256:A:O3' | 1:AA:1257:U:H4' | 2.05 | 0.56 |
| 1:AA:1343:G:H2' | 1:AA:1344:C:C6 | 2.40 | 0.56 |
| 1:AA:193:C:H2' | 1:AA:194:C:H6 | 1.70 | 0.56 |
| 1:AA:227:G:O2' | 1:AA:228:A:H5' | 2.05 | 0.56 |
| 1:AA:657:G:C2 | 1:AA:658:G:C8 | 2.93 | 0.56 |
| 2:AB:7:VAL:O | 2:AB:11:LEU:HG | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:163:PHE:HD2 | 2:AB:185:ILE:HG13 | 1.69 | 0.56 |
| 4:AD:4:TYR:O | 4:AD:5:ILE:HB | 2.05 | 0.56 |
| 1:AA:939:G:H5'' | 7:AG:102:ARG:CZ | 2.34 | 0.56 |
| 25:B3:6:VAL:HG13 | 25:B3:54:VAL:HG11 | 1.86 | 0.56 |
| 31:BA:1497:U:C5' | 31:BA:1498:C:C5 | 2.88 | 0.56 |
| 31:BA:1590:U:C2' | 31:BA:1591:G:H5'' | 2.34 | 0.56 |
| 31:BA:154(A):C:H5 | 31:BA:171:G:N1 | 2.03 | 0.56 |
| 31:BA:307:G:H22 | 31:BA:310:A:H5'' | 1.69 | 0.56 |
| 31:BA:754:C:H2' | 31:BA:755:C:H6 | 1.70 | 0.56 |
| 35:BF:9:ILE:HG12 | 35:BF:14:PRO:C | 2.25 | 0.56 |
| 37:BH:163:TYR:CD1 | 37:BH:163:TYR:N | 2.73 | 0.56 |
| 39:BN:74:ARG:NH2 | 39:BN:101:HIS:HB3 | 2.19 | 0.56 |
| 42:BQ:75:THR:HG22 | 42:BQ:88:GLY:HA3 | 1.86 | 0.56 |
| 31:BA:559:G:H22 | 46:BU:49:HIS:CD2 | 2.22 | 0.56 |
| 47:BV:72:VAL:CG1 | 47:BV:88:ARG:HH22 | 2.12 | 0.56 |
| 1:CA:1096:C:H2' | 1:CA:1097:C:C6 | 2.37 | 0.56 |
| 1:CA:1471:G:O2' | 1:CA:1472:U:H5' | 2.04 | 0.56 |
| 1:CA:175:C:H2' | 1:CA:176:C:C6 | 2.39 | 0.56 |
| 1:CA:830:G:H2' | 1:CA:831:U:H6 | 1.70 | 0.56 |
| 4:CD:112:VAL:HG13 | 4:CD:113:SER:H | 1.69 | 0.56 |
| 24:D2:47:ASN:HA | 24:D2:50:ILE:O | 2.05 | 0.56 |
| 31:DA:1372:U:H2' | 31:DA:1373:A:O4' | 2.04 | 0.56 |
| 31:DA:1563:G:H2' | 31:DA:1564:C:H6 | 1.68 | 0.56 |
| 31:DA:2233:U:H2' | 31:DA:2234:G:C8 | 2.39 | 0.56 |
| 31:DA:2360:A:O2' | 31:DA:2361:A:O5' | 2.23 | 0.56 |
| 31:DA:2646:C:O5' | 31:DA:2646:C:H6 | 1.87 | 0.56 |
| 31:DA:272(D):G:H1 | 31:DA:364:C:H42 | 1.53 | 0.56 |
| 32:DB:94:C:H2' | 32:DB:95:C:H6 | 1.70 | 0.56 |
| 34:DE:128:SER:O | 34:DE:130:GLY:N | 2.38 | 0.56 |
| 36:DG:121:ASN:OD1 | 36:DG:123:ASN:HB2 | 2.05 | 0.56 |
| 44:DS:38:GLN:HG2 | 44:DS:47:THR:HG21 | 1.86 | 0.56 |
| 50:DY:28:LYS:CD | 50:DY:37:VAL:HG12 | 2.35 | 0.56 |
| 50:DY:45:VAL:HG22 | 50:DY:62:GLU:HB2 | 1.87 | 0.56 |
| 1:AA:1392:G:N2 | 1:AA:1502:A:H8 | 2.02 | 0.56 |
| 1:AA:52:G:O2' | 1:AA:53:A:H5' | 2.05 | 0.56 |
| 1:AA:818:G:O2' | 1:AA:819:A:H5' | 2.05 | 0.56 |
| 4:AD:58:LEU:HD23 | 4:AD:206:PHE:CE1 | 2.40 | 0.56 |
| 6:AF:86:ARG:O | 6:AF:87:ARG:HG2 | 2.05 | 0.56 |
| 24:B2:47:ASN:HA | 24:B2:50:ILE:O | 2.05 | 0.56 |
| 30:B8:14:VAL:HG13 | 30:B8:22:VAL:HG13 | 1.86 | 0.56 |
| 31:BA:1952:A:C6 | 31:BA:1953:A:N1 | 2.72 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:2252:G:H2' | 31:BA:2253:G:C8 | 2.40 | 0.56 |
| 31:BA:2360:A:O2' | 31:BA:2361:A:OP2 | 2.21 | 0.56 |
| 31:BA:2703:C:H2' | 31:BA:2704:C:H6 | 1.69 | 0.56 |
| 31:BA:2713:A:C3' | 31:BA:2714:G:C5' | 2.83 | 0.56 |
| 31:BA:298:G:H5' | 31:BA:299:A:OP1 | 2.05 | 0.56 |
| 31:BA:301:G:C4 | 31:BA:302:C:C5 | 2.93 | 0.56 |
| 31:BA:479:A:N3 | 31:BA:481:G:H5'' | 2.20 | 0.56 |
| 31:BA:547:A:H8 | 31:BA:549:G:C6 | 2.23 | 0.56 |
| 31:BA:68:G:H2' | 31:BA:69:C:H6 | 1.69 | 0.56 |
| 31:BA:2580:U:H4' | 34:BE:131:ALA:H | 1.70 | 0.56 |
| 35:BF:178:PRO:HB2 | 35:BF:201:VAL:CG1 | 2.29 | 0.56 |
| 36:BG:114:ILE:HB | 36:BG:117:PHE:HB2 | 1.87 | 0.56 |
| 39:BN:40:PRO:HA | 46:BU:64:ARG:NH2 | 2.15 | 0.56 |
| 42:BQ:141:GLN:CA | 51:BZ:53:ILE:HB | 2.36 | 0.56 |
| 43:BR:4:LEU:O | 43:BR:6:SER:N | 2.33 | 0.56 |
| 32:BB:30:C:OP2 | 44:BS:32:LEU:HD11 | 2.05 | 0.56 |
| 45:BT:57:PHE:O | 45:BT:58:ASN:ND2 | 2.38 | 0.56 |
| 45:BT:32:TYR:HB3 | 45:BT:81:PRO:CB | 2.35 | 0.56 |
| 45:BT:93:ARG:O | 45:BT:94:ALA:O | 2.23 | 0.56 |
| 49:BX:33:LYS:C | 49:BX:35:THR:HG22 | 2.24 | 0.56 |
| 51:BZ:30:ASN:ND2 | 51:BZ:32:HIS:H | 2.02 | 0.56 |
| 1:CA:1074:G:C4 | 1:CA:1102:A:C2 | 2.94 | 0.56 |
| 1:CA:920:U:C1' | 1:CA:1080:A:C2 | 2.88 | 0.56 |
| 1:CA:159:G:H21 | 1:CA:161:A:H3' | 1.70 | 0.56 |
| 1:CA:187:C:H2' | 1:CA:188:C:H6 | 1.69 | 0.56 |
| 1:CA:227:G:O2' | 1:CA:228:A:H5' | 2.04 | 0.56 |
| 1:CA:32:A:H2' | 1:CA:33:A:C8 | 2.41 | 0.56 |
| 2:CB:44:LEU:O | 2:CB:47:THR:HB | 2.06 | 0.56 |
| 5:CE:78:HIS:CE1 | 5:CE:142:LEU:HA | 2.34 | 0.56 |
| 12:CL:24:VAL:HG12 | 12:CL:24:VAL:O | 2.05 | 0.56 |
| 23:D1:40:ARG:CD | 23:D1:41:ARG:H | 2.17 | 0.56 |
| 26:D4:5:ILE:CB | 36:DG:67:LYS:HG2 | 2.35 | 0.56 |
| 28:D6:42:TRP:HA | 28:D6:42:TRP:CE3 | 2.39 | 0.56 |
| 31:DA:454:A:H4' | 31:DA:455:C:OP2 | 2.05 | 0.56 |
| 31:DA:952:G:C6 | 31:DA:953:A:N7 | 2.74 | 0.56 |
| 32:DB:82:G:H2' | 32:DB:83:G:C5' | 2.33 | 0.56 |
| 33:DD:35:LYS:CE | 33:DD:65:ILE:HA | 2.34 | 0.56 |
| 34:DE:15:PHE:HA | 34:DE:19:ARG:O | 2.05 | 0.56 |
| 36:DG:106:LEU:HD12 | 36:DG:110:ALA:CB | 2.35 | 0.56 |
| 36:DG:47:LYS:CD | 36:DG:81:LYS:HD2 | 2.29 | 0.56 |
| 41:DP:17:LYS:O | 41:DP:17:LYS:HG2 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:DR:75:LEU:HD13 | 43:DR:75:LEU:O | 2.04 | 0.56 |
| 49:DX:88:LYS:HD2 | 49:DX:88:LYS:N | 2.20 | 0.56 |
| 50:DY:45:VAL:CG1 | 50:DY:62:GLU:HB2 | 2.30 | 0.56 |
| 1:AA:1072:G:C6 | 1:AA:1073:U:C4 | 2.94 | 0.56 |
| 1:AA:135:C:H2' | 1:AA:136:C:H5' | 1.86 | 0.56 |
| 1:AA:234:C:H2' | 1:AA:235:C:H6 | 1.70 | 0.56 |
| 3:AC:16:ARG:NH1 | 3:AC:16:ARG:HB2 | 2.20 | 0.56 |
| 10:AJ:39:PRO:HB3 | 10:AJ:70:ARG:NH1 | 2.21 | 0.56 |
| 16:AP:48:TRP:HD1 | 16:AP:48:TRP:H | 1.47 | 0.56 |
| 30:B8:32:LEU:CD1 | 30:B8:32:LEU:H | 2.12 | 0.56 |
| 31:BA:1510:G:O2' | 31:BA:1511:C:H5' | 2.04 | 0.56 |
| 31:BA:1796:U:H2' | 31:BA:1797:C:C6 | 2.40 | 0.56 |
| 31:BA:257:A:C2' | 31:BA:258:G:H5' | 2.35 | 0.56 |
| 31:BA:675:A:C8 | 31:BA:804:A:C6 | 2.92 | 0.56 |
| 33:BD:28:GLU:HB2 | 33:BD:29:PRO:CD | 2.34 | 0.56 |
| 34:BE:6:GLY:O | 34:BE:195:LEU:HD12 | 2.05 | 0.56 |
| 34:BE:200:GLU:OE2 | 34:BE:200:GLU:N | 2.38 | 0.56 |
| 43:BR:9:LYS:O | 43:BR:10:LEU:HG | 2.05 | 0.56 |
| 48:BW:20:VAL:O | 48:BW:23:LEU:HB2 | 2.05 | 0.56 |
| 51:BZ:124:ILE:HG13 | 51:BZ:125:LEU:N | 2.20 | 0.56 |
| 51:BZ:165:VAL:HG12 | 51:BZ:166:SER:N | 2.18 | 0.56 |
| 1:CA:1064:G:H5' | 1:CA:1066:C:H1' | 1.87 | 0.56 |
| 1:CA:1321:C:H5'' | 1:CA:1322:C:H5'' | 1.86 | 0.56 |
| 1:CA:621:A:C2' | 1:CA:622:A:H5' | 2.35 | 0.56 |
| 2:CB:168:THR:HG21 | 2:CB:192:SER:HA | 1.87 | 0.56 |
| 4:CD:108:LEU:O | 4:CD:110:PHE:CD1 | 2.57 | 0.56 |
| 4:CD:17:VAL:HG11 | 4:CD:197:PRO:HB2 | 1.86 | 0.56 |
| 4:CD:88:VAL:HG13 | 5:CE:97:GLY:HA3 | 1.86 | 0.56 |
| 8:CH:25:ASP:HB3 | 8:CH:58:TYR:HB3 | 1.86 | 0.56 |
| 10:CJ:49:VAL:HG13 | 14:CN:41:ARG:HB2 | 1.86 | 0.56 |
| 20:CT:61:SER:O | 20:CT:65:LYS:HG3 | 2.05 | 0.56 |
| 31:DA:1022:G:C6 | 31:DA:1140:C:C4 | 2.93 | 0.56 |
| 31:DA:1141:U:OP2 | 39:DN:63:THR:OG1 | 2.18 | 0.56 |
| 31:DA:1590:U:C2' | 31:DA:1591:G:H5'' | 2.36 | 0.56 |
| 31:DA:1885:A:H5' | 31:DA:1885:A:H8 | 1.70 | 0.56 |
| 31:DA:2584:U:O5' | 31:DA:2584:U:O2 | 2.23 | 0.56 |
| 31:DA:536:A:H2' | 31:DA:537:C:C6 | 2.40 | 0.56 |
| 31:DA:838:C:O2' | 31:DA:839:U:H5' | 2.04 | 0.56 |
| 32:DB:21:G:O2' | 32:DB:22:U:H6 | 1.88 | 0.56 |
| 32:DB:29:A:C2 | 32:DB:30:C:C2 | 2.92 | 0.56 |
| 34:DE:56:PRO:O | 34:DE:58:ARG:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:DG:171:ALA:O | 36:DG:175:LEU:HG | 2.05 | 0.56 |
| 39:DN:42:TRP:HA | 39:DN:48:MET:CE | 2.31 | 0.56 |
| 46:DU:76:TYR:CZ | 46:DU:80:ILE:HG13 | 2.41 | 0.56 |
| 46:DU:88:ILE:HD13 | 46:DU:88:ILE:O | 2.05 | 0.56 |
| 49:DX:83:VAL:O | 49:DX:84:ALA:CB | 2.54 | 0.56 |
| 51:DZ:23:LYS:HE3 | 51:DZ:40:ASP:OD2 | 2.05 | 0.56 |
| 1:AA:1510:U:H2' | 1:AA:1511:G:C8 | 2.40 | 0.56 |
| 1:AA:564:C:C2 | 17:AQ:31:LEU:HD11 | 2.41 | 0.56 |
| 1:AA:713:G:H2' | 1:AA:714:G:C8 | 2.40 | 0.56 |
| 4:AD:110:PHE:H | 4:AD:110:PHE:HD1 | 1.52 | 0.56 |
| 20:AT:61:SER:O | 20:AT:65:LYS:HG3 | 2.05 | 0.56 |
| 31:BA:171:G:H2' | 31:BA:172:C:C1' | 2.35 | 0.56 |
| 31:BA:2418:A:H2' | 31:BA:2419:U:H6 | 1.70 | 0.56 |
| 27:B5:16:ARG:NH2 | 31:BA:517:C:OP1 | 2.38 | 0.56 |
| 31:BA:916:G:H2' | 31:BA:917:A:H5'' | 1.88 | 0.56 |
| 33:BD:125:ILE:O | 33:BD:125:ILE:HG22 | 2.04 | 0.56 |
| 41:BP:17:LYS:HG2 | 41:BP:17:LYS:O | 2.05 | 0.56 |
| 1:CA:189(C):C:H2' | 1:CA:189(D):C:O4' | 2.05 | 0.56 |
| 1:CA:308:C:H2' | 1:CA:309:G:H8 | 1.68 | 0.56 |
| 1:CA:52:G:O2' | 1:CA:53:A:H5' | 2.06 | 0.56 |
| 1:CA:857:C:O2 | 1:CA:858:G:H1' | 2.04 | 0.56 |
| 2:CB:74:LYS:O | 2:CB:78:GLN:HG3 | 2.05 | 0.56 |
| 4:CD:28:SER:HB3 | 4:CD:30:LYS:HG2 | 1.86 | 0.56 |
| 1:CA:1048:G:OP1 | 14:CN:4:LYS:HB2 | 2.05 | 0.56 |
| 15:CO:37:ASN:HD22 | 15:CO:37:ASN:N | 2.01 | 0.56 |
| 31:DA:218:A:C2 | 31:DA:235:U:H4' | 2.39 | 0.56 |
| 32:DB:86:G:H3' | 32:DB:87:G:C8 | 2.41 | 0.56 |
| 35:DF:129:PHE:CD2 | 35:DF:163:VAL:HG21 | 2.40 | 0.56 |
| 35:DF:9:ILE:HG12 | 35:DF:14:PRO:C | 2.25 | 0.56 |
| 37:DH:127:GLU:OE1 | 37:DH:127:GLU:HA | 2.05 | 0.56 |
| 38:DI:76:THR:HG22 | 38:DI:139:GLN:HB3 | 1.87 | 0.56 |
| 44:DS:57:LYS:HG2 | 44:DS:58:LEU:H | 1.70 | 0.56 |
| 44:DS:61:ASN:HD22 | 44:DS:62:LYS:N | 2.03 | 0.56 |
| 46:DU:40:PHE:HB3 | 47:DV:78:LYS:HD2 | 1.86 | 0.56 |
| 46:DU:88:ILE:CD1 | 46:DU:88:ILE:O | 2.53 | 0.56 |
| 46:DU:65:ILE:CG1 | 46:DU:96:ALA:HB3 | 2.35 | 0.56 |
| 51:DZ:101:PRO:O | 51:DZ:102:LEU:CD2 | 2.52 | 0.56 |
| 1:AA:195:A:C6 | 1:AA:196:A:N1 | 2.73 | 0.56 |
| 1:AA:425:G:N2 | 1:AA:426:G:H1' | 2.20 | 0.56 |
| 2:AB:88:ALA:HB2 | 2:AB:219:VAL:CG1 | 2.35 | 0.56 |
| 3:AC:89:GLU:O | 3:AC:93:LYS:HB2 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:AD:108:LEU:HD13 | 4:AD:174:LEU:HD13 | 1.86 | 0.56 |
| 6:AF:12:PRO:HG2 | 6:AF:55:ASP:OD1 | 2.06 | 0.56 |
| 33:BD:25:THR:CG2 | 33:BD:82:ILE:H | 2.19 | 0.56 |
| 35:BF:2:LYS:HG3 | 35:BF:25:PRO:HB2 | 1.85 | 0.56 |
| 26:B4:5:ILE:CB | 36:BG:67:LYS:HG2 | 2.34 | 0.56 |
| 39:BN:18:ALA:CB | 39:BN:26:LEU:HD22 | 2.24 | 0.56 |
| 39:BN:45:ASN:N | 39:BN:45:ASN:HD22 | 1.91 | 0.56 |
| 41:BP:24:GLY:HA3 | 41:BP:33:ARG:NH2 | 2.12 | 0.56 |
| 46:BU:69:CYS:HB3 | 46:BU:106:PHE:HZ | 1.70 | 0.56 |
| 47:BV:66:ARG:HD3 | 47:BV:67:GLY:N | 2.21 | 0.56 |
| 47:BV:83:ARG:CG | 47:BV:83:ARG:NH1 | 2.63 | 0.56 |
| 1:CA:328:C:C2' | 1:CA:328:C:O2 | 2.52 | 0.56 |
| 2:CB:7:VAL:O | 2:CB:11:LEU:HG | 2.04 | 0.56 |
| 4:CD:106:TYR:HE1 | 4:CD:113:SER:HA | 1.70 | 0.56 |
| 17:CQ:10:VAL:HG13 | 17:CQ:19:VAL:HB | 1.87 | 0.56 |
| 24:D2:14:ARG:CZ | 24:D2:57:ILE:CG2 | 2.84 | 0.56 |
| 41:BP:121:LYS:HD2 | 25:D3:2:PRO:HD3 | 1.87 | 0.56 |
| 28:D6:32:ASN:OD1 | 28:D6:33:LYS:N | 2.39 | 0.56 |
| 31:DA:1512:U:C2' | 31:DA:1513:C:H5' | 2.35 | 0.56 |
| 31:DA:1887:C:H2' | 31:DA:1888:G:H5' | 1.85 | 0.56 |
| 31:DA:231:C:C2' | 31:DA:232:G:H5' | 2.35 | 0.56 |
| 31:DA:494:G:H8 | 31:DA:494:G:H5'' | 1.70 | 0.56 |
| 31:DA:603:A:O2' | 31:DA:604:G:OP2 | 2.16 | 0.56 |
| 31:DA:635:C:O2' | 31:DA:639:U:OP1 | 2.24 | 0.56 |
| 31:DA:1568:G:H5'' | 33:DD:61:LEU:HD22 | 1.87 | 0.56 |
| 42:DQ:43:THR:HG22 | 42:DQ:94:VAL:HG12 | 1.88 | 0.56 |
| 44:DS:97:ARG:O | 44:DS:98:VAL:HG23 | 2.04 | 0.56 |
| 45:DT:32:TYR:CD2 | 45:DT:81:PRO:HB2 | 2.40 | 0.56 |
| 45:DT:29:ARG:HB2 | 45:DT:86:ILE:H | 1.70 | 0.56 |
| 51:DZ:92:SER:O | 51:DZ:130:PRO:HG2 | 2.06 | 0.56 |
| 42:DQ:137:TYR:HB2 | 51:DZ:76:LEU:HD11 | 1.87 | 0.56 |
| 1:AA:1096:C:H2' | 1:AA:1097:C:C6 | 2.37 | 0.56 |
| 1:AA:1346:A:N1 | 1:AA:1374:A:H5'' | 2.20 | 0.56 |
| 1:AA:683:G:C2 | 1:AA:708:C:N3 | 2.74 | 0.56 |
| 18:AR:58:LEU:HB3 | 18:AR:62:GLU:HB2 | 1.88 | 0.56 |
| 31:BA:102:G:O2' | 31:BA:103:A:P | 2.63 | 0.56 |
| 31:BA:1385:G:H4' | 31:BA:1386:C:OP1 | 2.06 | 0.56 |
| 31:BA:2300:G:H1 | 31:BA:2316:C:H42 | 1.52 | 0.56 |
| 33:BD:210:GLY:O | 33:BD:212:SER:N | 2.39 | 0.56 |
| 36:BG:171:ALA:O | 36:BG:175:LEU:HG | 2.05 | 0.56 |
| 38:BI:6:LEU:O | 38:BI:15:VAL:HB | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BQ:76:LYS:H | 42:BQ:88:GLY:HA2 | 1.70 | 0.56 |
| 47:BV:19:LYS:CE | 47:BV:20:LEU:N | 2.68 | 0.56 |
| 49:BX:66:LEU:HD23 | 49:BX:66:LEU:O | 2.06 | 0.56 |
| 50:BY:8:LYS:NZ | 50:BY:73:ARG:HA | 2.15 | 0.56 |
| 42:BQ:137:TYR:HB2 | 51:BZ:76:LEU:HD11 | 1.86 | 0.56 |
| 1:CA:1391:U:H2' | 1:CA:1392:G:C8 | 2.41 | 0.56 |
| 6:CF:69:GLU:H | 6:CF:69:GLU:CD | 2.09 | 0.56 |
| 7:CG:40:ALA:O | 7:CG:44:TYR:CD1 | 2.59 | 0.56 |
| 12:CL:87:GLY:HA2 | 12:CL:98:TYR:HA | 1.86 | 0.56 |
| 16:CP:28:ARG:NH1 | 16:CP:29:ASP:OD2 | 2.38 | 0.56 |
| 24:D2:41:ILE:O | 24:D2:43:GLN:N | 2.39 | 0.56 |
| 37:DH:121:ILE:HD11 | 37:DH:140:LYS:HB3 | 1.88 | 0.56 |
| 42:DQ:141:GLN:O | 51:DZ:70:LEU:HD22 | 2.05 | 0.56 |
| 43:DR:116:LEU:O | 43:DR:117:VAL:HB | 2.05 | 0.56 |
| 45:DT:50:ILE:HD13 | 45:DT:64:ARG:HB3 | 1.87 | 0.56 |
| 47:DV:6:LYS:HG3 | 47:DV:6:LYS:O | 2.04 | 0.56 |
| 42:DQ:141:GLN:HE22 | 51:DZ:89:PHE:HB3 | 1.70 | 0.56 |
| 1:AA:189(C):C:H2' | 1:AA:189(D):C:O4' | 2.05 | 0.56 |
| 1:AA:675:A:H61 | 1:AA:715:A:H61 | 1.53 | 0.56 |
| 3:AC:180:ALA:HB1 | 3:AC:182:ILE:HG13 | 1.88 | 0.56 |
| 25:B3:49:LYS:HE2 | 31:BA:850:C:O3' | 2.06 | 0.56 |
| 31:BA:1179:C:C3' | 31:BA:1180:C:H5'' | 2.36 | 0.56 |
| 31:BA:1406:U:H2' | 31:BA:1407:C:C6 | 2.41 | 0.56 |
| 31:BA:218:A:C2 | 31:BA:235:U:H4' | 2.40 | 0.56 |
| 31:BA:2756:U:H4' | 31:BA:2757:A:OP1 | 2.05 | 0.56 |
| 31:BA:363(E):U:H2' | 31:BA:363(F):A:O4' | 2.05 | 0.56 |
| 36:BG:58:GLN:HA | 36:BG:61:ALA:HB3 | 1.88 | 0.56 |
| 40:BO:107:ARG:NH2 | 45:BT:35:LYS:HD2 | 2.20 | 0.56 |
| 40:BO:50:GLY:C | 40:BO:52:VAL:H | 2.08 | 0.56 |
| 49:BX:41:ASN:O | 49:BX:45:THR:HG23 | 2.05 | 0.56 |
| 51:BZ:152:ALA:HB1 | 51:BZ:167:PRO:HB2 | 1.86 | 0.56 |
| 1:CA:1054:C:O2' | 1:CA:1055:A:H5'' | 2.06 | 0.56 |
| 2:CB:67:THR:HG22 | 2:CB:90:MET:HE1 | 1.87 | 0.56 |
| 10:CJ:7:LYS:HD3 | 10:CJ:71:LEU:CD1 | 2.35 | 0.56 |
| 24:D2:26:ARG:NH1 | 24:D2:29:LYS:HE2 | 2.20 | 0.56 |
| 27:D5:11:THR:HG23 | 31:DA:1263:U:O2' | 2.05 | 0.56 |
| 27:D5:46:CYS:O | 27:D5:48:GLU:N | 2.38 | 0.56 |
| 31:DA:1312:U:H4' | 31:DA:1313:U:O5' | 2.06 | 0.56 |
| 31:DA:171:G:H2' | 31:DA:172:C:C1' | 2.35 | 0.56 |
| 31:DA:1783:A:C2 | 31:DA:2587:A:C5 | 2.93 | 0.56 |
| 31:DA:2619:C:H2' | 31:DA:2620:C:H6 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:2716:U:O2' | 31:DA:2717:G:H5' | 2.05 | 0.56 |
| 31:DA:774:A:C2 | 31:DA:787:U:O2' | 2.53 | 0.56 |
| 31:DA:861:A:C2 | 31:DA:917:A:C4 | 2.94 | 0.56 |
| 31:DA:92:A:O2' | 31:DA:93:G:H5' | 2.05 | 0.56 |
| 34:DE:132:HIS:HA | 34:DE:135:HIS:CE1 | 2.41 | 0.56 |
| 42:DQ:20:ALA:C | 42:DQ:22:LYS:H | 2.08 | 0.56 |
| 46:DU:60:LEU:O | 46:DU:64:ARG:HG2 | 2.05 | 0.56 |
| 51:DZ:165:VAL:HG12 | 51:DZ:166:SER:N | 2.21 | 0.56 |
| 51:DZ:6:LYS:HB3 | 51:DZ:8:TYR:CE1 | 2.41 | 0.56 |
| 1:AA:1074:G:C4 | 1:AA:1102:A:C2 | 2.94 | 0.56 |
| 1:AA:110:C:H2' | 1:AA:111:G:O4' | 2.05 | 0.56 |
| 1:AA:1154:G:H2' | 1:AA:1155:G:C8 | 2.40 | 0.56 |
| 1:AA:685:G:N2 | 1:AA:686:U:C4 | 2.74 | 0.56 |
| 2:AB:204:ASN:HD21 | 2:AB:207:ALA:N | 2.04 | 0.56 |
| 4:AD:88:VAL:O | 4:AD:92:VAL:HG23 | 2.06 | 0.56 |
| 17:AQ:23:VAL:O | 17:AQ:39:SER:HB2 | 2.06 | 0.56 |
| 20:AT:10:LEU:O | 20:AT:12:ALA:N | 2.39 | 0.56 |
| 31:BA:1496:A:C8 | 31:BA:1577:C:O2' | 2.59 | 0.56 |
| 31:BA:1444:G:N2 | 31:BA:1548:C:C2 | 2.74 | 0.56 |
| 31:BA:1742:G:H8 | 31:BA:1742:G:H3' | 1.71 | 0.56 |
| 31:BA:1884:A:O2' | 31:BA:1885:A:H5'' | 2.05 | 0.56 |
| 31:BA:1750:G:O2' | 31:BA:2860:A:N1 | 2.37 | 0.56 |
| 31:BA:344:G:O2' | 31:BA:345:A:H5' | 2.04 | 0.56 |
| 32:BB:75:G:C5' | 32:BB:75:G:H8 | 2.19 | 0.56 |
| 37:BH:44:VAL:O | 37:BH:46:GLU:OE2 | 2.24 | 0.56 |
| 39:BN:28:THR:HA | 39:BN:106:MET:HE2 | 1.86 | 0.56 |
| 39:BN:131:GLN:HG2 | 39:BN:133:GLN:O | 2.05 | 0.56 |
| 44:BS:35:ILE:H | 44:BS:53:SER:HB3 | 1.71 | 0.56 |
| 45:BT:33:LYS:N | 45:BT:33:LYS:HZ3 | 2.02 | 0.56 |
| 45:BT:3:ARG:HB2 | 45:BT:6:LEU:CB | 2.33 | 0.56 |
| 48:BW:10:VAL:O | 48:BW:11:ARG:HB2 | 2.04 | 0.56 |
| 1:CA:1191:A:P | 3:CC:3:ASN:HD21 | 2.29 | 0.56 |
| 1:CA:1252:A:H2' | 1:CA:1253:G:O4' | 2.06 | 0.56 |
| 1:CA:145:G:C2 | 1:CA:146:G:H1' | 2.40 | 0.56 |
| 2:CB:88:ALA:HB2 | 2:CB:219:VAL:CG1 | 2.35 | 0.56 |
| 6:CF:6:VAL:HG13 | 6:CF:90:VAL:HG22 | 1.88 | 0.56 |
| 6:CF:8:ILE:HG22 | 6:CF:9:VAL:N | 2.20 | 0.56 |
| 8:CH:10:LEU:HD13 | 8:CH:83:ILE:HD11 | 1.87 | 0.56 |
| 17:CQ:68:ARG:HG3 | 17:CQ:68:ARG:O | 2.04 | 0.56 |
| 18:CR:58:LEU:HB3 | 18:CR:62:GLU:HB2 | 1.87 | 0.56 |
| 31:DA:1164:G:H2' | 31:DA:1165:U:C6 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:1527:G:H5'' | 31:DA:1528:A:OP1 | 2.05 | 0.56 |
| 31:DA:1528(A):A:C5 | 31:DA:1529:G:C8 | 2.93 | 0.56 |
| 31:DA:1884:A:O2' | 31:DA:1885:A:H5'' | 2.05 | 0.56 |
| 31:DA:2461:C:H2' | 31:DA:2462:U:C6 | 2.40 | 0.56 |
| 31:DA:2870:C:C2' | 31:DA:2871:C:H5' | 2.35 | 0.56 |
| 31:DA:953:A:C2' | 31:DA:954:G:H5' | 2.36 | 0.56 |
| 32:DB:45:A:C2 | 32:DB:46:A:C1' | 2.88 | 0.56 |
| 43:DR:52:ILE:O | 43:DR:55:ALA:N | 2.39 | 0.56 |
| 1:AA:949:A:N6 | 1:AA:1232:U:H3 | 2.02 | 0.56 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.41 | 0.56 |
| 1:AA:1399:C:C2 | 1:AA:1502:A:N6 | 2.74 | 0.56 |
| 1:AA:322:C:C5 | 1:AA:328:C:H5 | 2.20 | 0.56 |
| 1:AA:624:C:H2' | 1:AA:625:G:H8 | 1.70 | 0.56 |
| 4:AD:131:ARG:HD3 | 4:AD:131:ARG:H | 1.71 | 0.56 |
| 4:AD:88:VAL:HG13 | 5:AE:97:GLY:HA3 | 1.87 | 0.56 |
| 6:AF:69:GLU:CD | 6:AF:69:GLU:H | 2.09 | 0.56 |
| 28:B6:42:TRP:CE3 | 28:B6:42:TRP:HA | 2.40 | 0.56 |
| 30:B8:35:GLN:HE21 | 30:B8:36:LYS:HG3 | 1.70 | 0.56 |
| 31:BA:1488:G:C2 | 31:BA:1489:U:O2 | 2.59 | 0.56 |
| 31:BA:150:C:H2' | 31:BA:151:C:C6 | 2.41 | 0.56 |
| 31:BA:2469:A:H2 | 31:BA:2481:G:N2 | 1.96 | 0.56 |
| 31:BA:271(A):A:H2 | 31:BA:272(D):G:N3 | 2.03 | 0.56 |
| 33:BD:133:LEU:HB3 | 33:BD:173:VAL:HG11 | 1.86 | 0.56 |
| 34:BE:39:PRO:HD3 | 34:BE:45:THR:OG1 | 2.06 | 0.56 |
| 34:BE:75:VAL:O | 34:BE:77:ILE:N | 2.39 | 0.56 |
| 35:BF:80:ALA:O | 35:BF:83:PHE:HB2 | 2.06 | 0.56 |
| 37:BH:89:ILE:O | 37:BH:90:LYS:CB | 2.53 | 0.56 |
| 38:BI:5:LEU:HD23 | 38:BI:5:LEU:N | 2.19 | 0.56 |
| 40:BO:73:ASP:OD2 | 45:BT:32:TYR:CE1 | 2.59 | 0.56 |
| 44:BS:87:PHE:HE2 | 44:BS:97:ARG:NH2 | 2.03 | 0.56 |
| 45:BT:28:VAL:HG22 | 45:BT:46:GLU:HG3 | 1.87 | 0.56 |
| 31:BA:995:C:N3 | 46:BU:57:PHE:CE2 | 2.74 | 0.56 |
| 47:BV:61:VAL:O | 47:BV:62:LEU:HD23 | 2.06 | 0.56 |
| 1:CA:1510:U:H2' | 1:CA:1511:G:C8 | 2.40 | 0.56 |
| 1:CA:551:U:O2' | 12:CL:86:ARG:HD2 | 2.06 | 0.56 |
| 1:CA:626:U:C2 | 1:CA:627:G:C8 | 2.94 | 0.56 |
| 2:CB:87:ARG:HD2 | 2:CB:87:ARG:O | 2.06 | 0.56 |
| 31:DA:1317:A:H2' | 31:DA:1318:C:H6 | 1.70 | 0.56 |
| 31:DA:1510:G:O2' | 31:DA:1511:C:H5' | 2.05 | 0.56 |
| 31:DA:2206:G:N3 | 31:DA:2206:G:H3' | 2.21 | 0.56 |
| 31:DA:2315:G:H2' | 31:DA:2316:C:C6 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:D6:19:ARG:HH11 | 31:DA:2400:G:H4' | 1.71 | 0.56 |
| 31:DA:287:C:C4 | 31:DA:288:C:C5 | 2.94 | 0.56 |
| 31:DA:661:C:H2' | 31:DA:662:G:H8 | 1.71 | 0.56 |
| 31:DA:708:C:O2 | 31:DA:708:C:H2' | 2.06 | 0.56 |
| 37:DH:85:LYS:NZ | 37:DH:133:VAL:HB | 2.21 | 0.56 |
| 45:DT:33:LYS:NZ | 45:DT:33:LYS:HA | 2.21 | 0.56 |
| 46:DU:88:ILE:O | 46:DU:90:VAL:N | 2.39 | 0.56 |
| 47:DV:2:PHE:CE1 | 47:DV:13:ARG:NE | 2.74 | 0.56 |
| 51:DZ:145:GLU:HG3 | 51:DZ:146:ILE:H | 1.71 | 0.56 |
| 1:AA:262:A:C6 | 1:AA:263:A:C6 | 2.94 | 0.56 |
| 1:AA:660:G:H2' | 1:AA:661:G:O4' | 2.06 | 0.56 |
| 1:AA:763:G:H2' | 1:AA:764:C:H6 | 1.71 | 0.56 |
| 3:AC:11:ARG:O | 3:AC:14:ILE:O | 2.24 | 0.56 |
| 5:AE:96:PRO:HA | 5:AE:117:ASP:OD2 | 2.06 | 0.56 |
| 7:AG:40:ALA:O | 7:AG:44:TYR:CD1 | 2.59 | 0.56 |
| 9:AI:105:ASP:OD1 | 9:AI:107:ARG:HD3 | 2.06 | 0.56 |
| 1:AA:1216:G:OP1 | 14:AN:2:ALA:HA | 2.06 | 0.56 |
| 1:AA:472:A:C4' | 16:AP:82:GLN:HE22 | 2.19 | 0.56 |
| 24:B2:30:ARG:CG | 24:B2:30:ARG:HH11 | 2.17 | 0.56 |
| 31:BA:1945:G:H2' | 31:BA:1946:U:C6 | 2.40 | 0.56 |
| 31:BA:2584:U:O5' | 31:BA:2584:U:O2 | 2.24 | 0.56 |
| 31:BA:272(J):C:C2' | 31:BA:274:G:OP1 | 2.53 | 0.56 |
| 33:BD:249:PRO:HD2 | 33:BD:250:TRP:CE3 | 2.40 | 0.56 |
| 35:BF:21:ALA:C | 35:BF:23:ASP:H | 2.09 | 0.56 |
| 37:BH:92:ILE:O | 37:BH:94:TYR:N | 2.39 | 0.56 |
| 41:BP:36:LYS:O | 41:BP:38:GLN:HG2 | 2.05 | 0.56 |
| 45:BT:26:ASP:HB3 | 45:BT:89:VAL:O | 2.06 | 0.56 |
| 46:BU:101:ARG:O | 46:BU:102:GLU:C | 2.44 | 0.56 |
| 48:BW:56:ALA:O | 48:BW:57:ASN:C | 2.44 | 0.56 |
| 49:BX:23:GLU:HG3 | 49:BX:24:GLY:N | 2.19 | 0.56 |
| 1:CA:110:C:H2' | 1:CA:111:G:O4' | 2.05 | 0.56 |
| 1:CA:1256:A:N6 | 1:CA:1278:U:H1' | 2.15 | 0.56 |
| 1:CA:1442(B):A:OP1 | 1:CA:1442(B):A:H4' | 2.06 | 0.56 |
| 1:CA:623:C:C4 | 1:CA:624:C:C4 | 2.94 | 0.56 |
| 1:CA:685:G:C2 | 1:CA:686:U:C4 | 2.94 | 0.56 |
| 1:CA:872:A:C4 | 1:CA:874:G:N7 | 2.74 | 0.56 |
| 2:CB:67:THR:HG21 | 2:CB:155:LEU:CD2 | 2.36 | 0.56 |
| 8:CH:21:LYS:O | 8:CH:63:LEU:HD23 | 2.06 | 0.56 |
| 27:D5:51:TYR:CD2 | 27:D5:52:TYR:CZ | 2.94 | 0.56 |
| 31:DA:1459:G:H2' | 31:DA:1459:G:N3 | 2.20 | 0.56 |
| 31:DA:17:G:H2' | 31:DA:18:C:C6 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:2360:A:O2' | 31:DA:2361:A:OP2 | 2.24 | 0.56 |
| 31:DA:272(J):C:C2' | 31:DA:274:G:OP1 | 2.54 | 0.56 |
| 31:DA:2859:G:C8 | 31:DA:2859:G:C3' | 2.89 | 0.56 |
| 41:DP:33:ARG:O | 41:DP:35:HIS:N | 2.39 | 0.56 |
| 44:DS:26:LEU:HA | 44:DS:39:ILE:HD13 | 1.88 | 0.56 |
| 44:DS:89:ARG:O | 44:DS:90:GLY:O | 2.23 | 0.56 |
| 46:DU:47:TYR:HA | 46:DU:50:ARG:NH2 | 2.20 | 0.56 |
| 1:AA:131:C:H2' | 1:AA:132:C:C6 | 2.41 | 0.56 |
| 1:AA:1441:G:H5'' | 1:AA:1442:G:H5' | 1.88 | 0.56 |
| 1:AA:559:A:C4' | 1:AA:560:U:H3' | 2.36 | 0.56 |
| 4:AD:9:CYS:HA | 4:AD:12:CYS:HB2 | 1.87 | 0.56 |
| 16:AP:28:ARG:NH1 | 16:AP:29:ASP:OD2 | 2.39 | 0.56 |
| 30:B8:6:THR:CG2 | 31:BA:243:U:OP1 | 2.54 | 0.56 |
| 22:B0:18:ALA:HB1 | 31:BA:2271:G:OP1 | 2.06 | 0.56 |
| 31:BA:2272:U:H5'' | 31:BA:2273:A:OP1 | 2.07 | 0.56 |
| 31:BA:234:C:H2' | 31:BA:235:U:H6 | 1.71 | 0.56 |
| 31:BA:2859:G:C8 | 31:BA:2859:G:C3' | 2.89 | 0.56 |
| 31:BA:259:G:N2 | 31:BA:621:A:H8 | 2.02 | 0.56 |
| 31:BA:829:A:N7 | 31:BA:2248:C:H5' | 2.20 | 0.56 |
| 36:BG:71:THR:HB | 36:BG:89:GLY:CA | 2.35 | 0.56 |
| 42:BQ:37:LEU:HB2 | 42:BQ:128:LYS:O | 2.05 | 0.56 |
| 44:BS:38:GLN:HG2 | 44:BS:47:THR:HG21 | 1.88 | 0.56 |
| 45:BT:33:LYS:NZ | 45:BT:33:LYS:H | 2.03 | 0.56 |
| 50:BY:45:VAL:CG2 | 50:BY:62:GLU:N | 2.69 | 0.56 |
| 1:CA:1158:C:N3 | 1:CA:1181:G:N2 | 2.52 | 0.56 |
| 1:CA:1201:A:C1' | 1:CA:1202:G:OP2 | 2.52 | 0.56 |
| 1:CA:1470:G:O2' | 1:CA:1471:G:H5' | 2.06 | 0.56 |
| 1:CA:189(B):C:H42 | 1:CA:189(I):G:H1 | 1.53 | 0.56 |
| 2:CB:204:ASN:HD21 | 2:CB:207:ALA:N | 2.04 | 0.56 |
| 2:CB:28:PHE:CD1 | 2:CB:190:THR:HA | 2.41 | 0.56 |
| 3:CC:20:SER:CB | 3:CC:40:ARG:HH22 | 2.17 | 0.56 |
| 12:CL:46:LYS:HD3 | 12:CL:94:PRO:CG | 2.36 | 0.56 |
| 22:D0:53:MET:HB2 | 22:D0:59:LEU:CD2 | 2.36 | 0.56 |
| 24:D2:14:ARG:CZ | 24:D2:57:ILE:HB | 2.37 | 0.56 |
| 27:D5:40:LYS:NZ | 27:D5:46:CYS:O | 2.36 | 0.56 |
| 31:DA:2511:U:O4 | 31:DA:2575:C:N3 | 2.39 | 0.56 |
| 31:DA:2660:A:H3' | 31:DA:2661:G:O4' | 2.06 | 0.56 |
| 31:DA:836:G:H2' | 31:DA:837:C:C6 | 2.41 | 0.56 |
| 32:DB:81:G:O6 | 32:DB:96:U:O2 | 2.23 | 0.56 |
| 33:DD:172:TYR:CD1 | 33:DD:186:HIS:CA | 2.88 | 0.56 |
| 33:DD:246:PRO:HB2 | 33:DD:255:LYS:HG3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DD:247:ALA:HA | 33:DD:254:THR:HG22 | 1.86 | 0.56 |
| 39:DN:111:PRO:HA | 39:DN:114:ARG:NH1 | 2.21 | 0.56 |
| 42:DQ:29:PHE:CD1 | 42:DQ:29:PHE:N | 2.74 | 0.56 |
| 47:DV:54:GLY:O | 47:DV:56:SER:N | 2.39 | 0.56 |
| 51:DZ:125:LEU:HD23 | 51:DZ:126:VAL:N | 2.20 | 0.56 |
| 1:AA:1483:A:H1' | 31:BA:1948:G:O4' | 2.06 | 0.55 |
| 11:AK:31:THR:HA | 11:AK:42:TRP:HA | 1.86 | 0.55 |
| 14:AN:51:GLY:C | 14:AN:53:LEU:H | 2.10 | 0.55 |
| 19:AS:51:VAL:HG21 | 19:AS:71:LEU:HB3 | 1.88 | 0.55 |
| 27:B5:47:PRO:O | 27:B5:48:GLU:HG3 | 2.06 | 0.55 |
| 28:B6:25:LYS:O | 31:BA:2286:A:H2 | 1.89 | 0.55 |
| 31:BA:1109:C:C5 | 31:BA:1110:G:C4 | 2.95 | 0.55 |
| 31:BA:2376:A:OP1 | 31:BA:2376:A:H8 | 1.89 | 0.55 |
| 31:BA:2404:C:C2' | 31:BA:2405:G:H5' | 2.35 | 0.55 |
| 31:BA:2655:G:N3 | 31:BA:2664:G:O6 | 2.39 | 0.55 |
| 31:BA:2702:U:OP1 | 31:BA:2702:U:O2 | 2.24 | 0.55 |
| 31:BA:271(M):G:H4' | 38:BI:53:ALA:HB1 | 1.88 | 0.55 |
| 31:BA:543:C:N3 | 31:BA:551:G:C2 | 2.73 | 0.55 |
| 34:BE:111:ARG:HB2 | 34:BE:160:TYR:O | 2.06 | 0.55 |
| 37:BH:98:LEU:HD13 | 37:BH:125:VAL:HG23 | 1.88 | 0.55 |
| 41:BP:27:HIS:C | 41:BP:27:HIS:CD2 | 2.79 | 0.55 |
| 42:BQ:141:GLN:HE22 | 51:BZ:89:PHE:HB3 | 1.71 | 0.55 |
| 31:BA:956:G:OP2 | 42:BQ:14:ARG:NH2 | 2.38 | 0.55 |
| 43:BR:13:HIS:HE1 | 43:BR:15:SER:OG | 1.89 | 0.55 |
| 45:BT:78:LEU:O | 45:BT:79:HIS:ND1 | 2.38 | 0.55 |
| 1:CA:109:A:C6 | 1:CA:326:G:C6 | 2.94 | 0.55 |
| 1:CA:339:C:OP2 | 40:DO:97:ARG:NH1 | 2.38 | 0.55 |
| 1:CA:559:A:C4' | 1:CA:560:U:H3' | 2.36 | 0.55 |
| 1:CA:929:G:C6 | 1:CA:930:C:N4 | 2.74 | 0.55 |
| 1:CA:951:G:H1' | 1:CA:970:C:O2' | 2.05 | 0.55 |
| 2:CB:11:LEU:HB3 | 2:CB:213:LEU:HD11 | 1.88 | 0.55 |
| 3:CC:180:ALA:HB1 | 3:CC:182:ILE:HG13 | 1.87 | 0.55 |
| 7:CG:85:TYR:CD1 | 7:CG:154:TYR:HE1 | 2.24 | 0.55 |
| 11:CK:21:ILE:HD12 | 11:CK:21:ILE:N | 2.21 | 0.55 |
| 14:CN:51:GLY:C | 14:CN:53:LEU:H | 2.08 | 0.55 |
| 19:CS:69:HIS:HB2 | 19:CS:74:PHE:HE2 | 1.71 | 0.55 |
| 23:D1:86:SER:N | 23:D1:87:PRO:CD | 2.69 | 0.55 |
| 23:D1:87:PRO:HD2 | 23:D1:88:LYS:H | 1.70 | 0.55 |
| 24:D2:25:VAL:C | 24:D2:27:GLU:H | 2.10 | 0.55 |
| 31:DA:2580:U:H5' | 34:DE:131:ALA:HB2 | 1.87 | 0.55 |
| 31:DA:2652:C:O2' | 31:DA:2653:U:H5' | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:271(P):C:H2' | 31:DA:271(Q):G:H5' | 1.88 | 0.55 |
| 31:DA:288:C:N4 | 31:DA:353:G:H1 | 2.04 | 0.55 |
| 35:DF:123:LEU:HD12 | 35:DF:124:LEU:H | 1.71 | 0.55 |
| 36:DG:114:ILE:HB | 36:DG:117:PHE:HB2 | 1.88 | 0.55 |
| 36:DG:60:LEU:O | 36:DG:60:LEU:HD22 | 2.06 | 0.55 |
| 37:DH:98:LEU:HD13 | 37:DH:125:VAL:HG23 | 1.87 | 0.55 |
| 45:DT:48:ILE:HG22 | 45:DT:50:ILE:HD12 | 1.88 | 0.55 |
| 45:DT:16:ARG:H | 45:DT:79:HIS:CD2 | 2.22 | 0.55 |
| 47:DV:47:VAL:HG22 | 47:DV:48:GLY:N | 2.21 | 0.55 |
| 47:DV:61:VAL:C | 47:DV:62:LEU:HD23 | 2.25 | 0.55 |
| 1:AA:386:C:H2' | 1:AA:387:U:C5' | 2.33 | 0.55 |
| 1:AA:948:C:OP1 | 13:AM:107:ALA:HA | 2.07 | 0.55 |
| 31:BA:203:C:H3' | 31:BA:204:A:H5'' | 1.89 | 0.55 |
| 32:BB:81:G:O6 | 32:BB:96:U:O2 | 2.24 | 0.55 |
| 40:BO:10:VAL:HG22 | 40:BO:17:ARG:O | 2.06 | 0.55 |
| 31:BA:2684:U:H1' | 40:BO:70:LYS:HD2 | 1.88 | 0.55 |
| 31:BA:446:G:OP1 | 46:BU:3:ARG:NH1 | 2.40 | 0.55 |
| 31:BA:1187:G:H5'' | 47:BV:82:ARG:NH1 | 2.21 | 0.55 |
| 7:CG:46:ALA:O | 7:CG:50:ILE:HG12 | 2.06 | 0.55 |
| 7:CG:69:VAL:O | 7:CG:71:PRO:HD3 | 2.06 | 0.55 |
| 10:CJ:7:LYS:O | 10:CJ:96:ILE:HA | 2.06 | 0.55 |
| 12:CL:92:ASP:C | 12:CL:93:LEU:HD23 | 2.26 | 0.55 |
| 1:CA:1330:U:H4' | 13:CM:23:TYR:CE2 | 2.41 | 0.55 |
| 15:CO:82:ILE:HD11 | 15:CO:87:ILE:O | 2.07 | 0.55 |
| 19:CS:42:PRO:O | 19:CS:43:GLU:HB3 | 2.06 | 0.55 |
| 20:CT:56:MET:CG | 20:CT:88:VAL:HG21 | 2.36 | 0.55 |
| 22:D0:48:GLY:HA3 | 22:D0:80:HIS:CE1 | 2.40 | 0.55 |
| 24:D2:50:ILE:O | 24:D2:51:ARG:HB3 | 2.06 | 0.55 |
| 27:D5:51:TYR:CD2 | 27:D5:52:TYR:CE2 | 2.94 | 0.55 |
| 28:D6:36:LEU:O | 28:D6:36:LEU:HG | 2.06 | 0.55 |
| 31:DA:1657:C:H2' | 31:DA:1658:C:C6 | 2.42 | 0.55 |
| 31:DA:2810:A:C2' | 34:DE:61:ARG:NH2 | 2.69 | 0.55 |
| 31:DA:307:G:N2 | 31:DA:310:A:H5'' | 2.21 | 0.55 |
| 31:DA:910:A:C4 | 42:DQ:13:GLN:OE1 | 2.60 | 0.55 |
| 33:DD:210:GLY:O | 33:DD:212:SER:N | 2.39 | 0.55 |
| 33:DD:35:LYS:CE | 33:DD:64:ILE:O | 2.54 | 0.55 |
| 34:DE:39:PRO:HD3 | 34:DE:45:THR:OG1 | 2.05 | 0.55 |
| 35:DF:24:LEU:O | 35:DF:26:ALA:N | 2.39 | 0.55 |
| 36:DG:39:ILE:HA | 36:DG:157:ILE:HA | 1.88 | 0.55 |
| 39:DN:56:ASN:C | 39:DN:57:ALA:O | 2.43 | 0.55 |
| 41:DP:5:ASP:O | 41:DP:6:LEU:HB3 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:DV:19:LYS:HG2 | 47:DV:96:ILE:CB | 2.35 | 0.55 |
| 1:AA:1074:G:N3 | 1:AA:1102:A:C2 | 2.74 | 0.55 |
| 1:AA:1479:C:O2' | 1:AA:1480:G:H5' | 2.05 | 0.55 |
| 1:AA:542:G:H5' | 4:AD:41:GLY:HA3 | 1.89 | 0.55 |
| 2:AB:61:LEU:HA | 2:AB:64:ARG:HG2 | 1.87 | 0.55 |
| 2:AB:61:LEU:HD23 | 2:AB:68:ILE:HD11 | 1.88 | 0.55 |
| 4:AD:49:ARG:HA | 4:AD:49:ARG:NE | 2.18 | 0.55 |
| 5:AE:145:LYS:O | 5:AE:149:GLU:HG2 | 2.07 | 0.55 |
| 7:AG:97:GLN:HE21 | 7:AG:101:LEU:HD11 | 1.71 | 0.55 |
| 10:AJ:7:LYS:HD3 | 10:AJ:71:LEU:CD1 | 2.36 | 0.55 |
| 28:B6:40:CYS:SG | 28:B6:45:LYS:NZ | 2.60 | 0.55 |
| 31:BA:1021:A:C3' | 31:BA:1021:A:C8 | 2.89 | 0.55 |
| 31:BA:128:C:C3' | 31:BA:128:C:C6 | 2.89 | 0.55 |
| 31:BA:1499:C:C2' | 31:BA:1500:G:H5' | 2.36 | 0.55 |
| 31:BA:1741:A:N7 | 31:BA:1742:G:C2 | 2.74 | 0.55 |
| 31:BA:1839:G:H5' | 31:BA:1839:G:H8 | 1.71 | 0.55 |
| 31:BA:298:G:C5' | 31:BA:299:A:OP1 | 2.55 | 0.55 |
| 36:BG:5:VAL:HB | 36:BG:104:GLU:OE2 | 2.07 | 0.55 |
| 37:BH:149:ARG:HD3 | 37:BH:164:TYR:CE1 | 2.41 | 0.55 |
| 46:BU:65:ILE:HG12 | 46:BU:96:ALA:CB | 2.36 | 0.55 |
| 48:BW:54:ALA:HB1 | 48:BW:107:LEU:HD22 | 1.88 | 0.55 |
| 49:BX:40:LYS:O | 49:BX:42:ALA:N | 2.40 | 0.55 |
| 50:BY:71:LYS:HZ2 | 50:BY:71:LYS:HB2 | 1.66 | 0.55 |
| 50:BY:37:VAL:HG11 | 50:BY:72:VAL:HG21 | 1.89 | 0.55 |
| 51:BZ:73:GLN:HG2 | 51:BZ:87:ASP:OD2 | 2.07 | 0.55 |
| 51:BZ:71:VAL:HG22 | 51:BZ:88:PHE:CE2 | 2.42 | 0.55 |
| 1:CA:1258:G:O2' | 1:CA:1259:C:H5' | 2.06 | 0.55 |
| 1:CA:243:A:H4' | 1:CA:244:U:O5' | 2.05 | 0.55 |
| 1:CA:791:G:C6 | 1:CA:792:A:N7 | 2.74 | 0.55 |
| 1:CA:971:G:H3' | 1:CA:971:G:OP1 | 2.07 | 0.55 |
| 5:CE:96:PRO:HA | 5:CE:117:ASP:OD2 | 2.07 | 0.55 |
| 7:CG:32:ARG:O | 7:CG:33:ASP:CB | 2.54 | 0.55 |
| 13:CM:91:ARG:HB2 | 13:CM:98:VAL:HG21 | 1.88 | 0.55 |
| 1:CA:1216:G:OP1 | 14:CN:2:ALA:HA | 2.06 | 0.55 |
| 41:BP:120:ALA:O | 25:D3:1:MET:CG | 2.53 | 0.55 |
| 31:DA:1588:C:O2 | 31:DA:1588:C:H2' | 2.04 | 0.55 |
| 31:DA:2335:A:C8 | 31:DA:2337:G:N7 | 2.74 | 0.55 |
| 31:DA:2498:C:O2' | 31:DA:2499:C:H5' | 2.05 | 0.55 |
| 31:DA:340:A:C2' | 31:DA:341:G:H5' | 2.36 | 0.55 |
| 31:DA:27:G:C2 | 31:DA:512:G:N3 | 2.75 | 0.55 |
| 31:DA:580:C:H2' | 31:DA:581:C:C6 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:634:C:H2' | 31:DA:635:C:C6 | 2.41 | 0.55 |
| 31:DA:883:G:H1 | 31:DA:893:C:H41 | 1.54 | 0.55 |
| 33:DD:17:THR:CG2 | 33:DD:204:ILE:HA | 2.36 | 0.55 |
| 33:DD:28:GLU:HB2 | 33:DD:29:PRO:CD | 2.35 | 0.55 |
| 33:DD:35:LYS:HE3 | 33:DD:65:ILE:HA | 1.88 | 0.55 |
| 37:DH:138:LYS:H | 37:DH:141:VAL:H | 1.52 | 0.55 |
| 37:DH:154:PRO:O | 37:DH:156:ALA:N | 2.37 | 0.55 |
| 39:DN:67:LEU:C | 39:DN:69:GLN:N | 2.59 | 0.55 |
| 45:DT:3:ARG:HB2 | 45:DT:6:LEU:CB | 2.32 | 0.55 |
| 46:DU:87:GLY:CA | 47:DV:52:VAL:HG13 | 2.28 | 0.55 |
| 47:DV:53:GLU:O | 47:DV:55:ALA:N | 2.40 | 0.55 |
| 49:DX:30:VAL:HG23 | 49:DX:76:ARG:HA | 1.87 | 0.55 |
| 1:AA:1068:G:N3 | 1:AA:1191:A:C2 | 2.74 | 0.55 |
| 1:AA:1201:A:C1' | 1:AA:1202:G:OP2 | 2.53 | 0.55 |
| 1:AA:1248:A:C2' | 1:AA:1249:C:H5' | 2.36 | 0.55 |
| 1:AA:1366:C:OP1 | 9:AI:117:HIS:CE1 | 2.59 | 0.55 |
| 14:AN:48:ALA:HB2 | 14:AN:53:LEU:HD12 | 1.89 | 0.55 |
| 27:B5:33:CYS:SG | 27:B5:40:LYS:HE3 | 2.46 | 0.55 |
| 27:B5:55:ARG:C | 27:B5:56:LYS:HG3 | 2.26 | 0.55 |
| 28:B6:15:GLU:OE2 | 28:B6:43:CYS:HB3 | 2.07 | 0.55 |
| 28:B6:29:ASN:O | 28:B6:30:THR:C | 2.44 | 0.55 |
| 30:B8:35:GLN:CB | 31:BA:2420:C:OP1 | 2.54 | 0.55 |
| 31:BA:1332:G:H22 | 31:BA:1609:A:H2' | 1.71 | 0.55 |
| 31:BA:1495:A:H5'' | 31:BA:1496:A:OP2 | 2.05 | 0.55 |
| 31:BA:1833:U:O2' | 31:BA:1969:A:N1 | 2.36 | 0.55 |
| 31:BA:2350:C:H2' | 31:BA:2351:G:O4' | 2.06 | 0.55 |
| 31:BA:2444:G:OP2 | 35:BF:68:LYS:HE2 | 2.06 | 0.55 |
| 36:BG:120:LEU:HB2 | 36:BG:179:PRO:O | 2.05 | 0.55 |
| 38:BI:131:LYS:CG | 38:BI:132:PRO:HA | 2.37 | 0.55 |
| 41:BP:5:ASP:O | 41:BP:6:LEU:HB3 | 2.06 | 0.55 |
| 43:BR:53:HIS:CD2 | 43:BR:94:TYR:OH | 2.58 | 0.55 |
| 31:BA:71:A:C2 | 49:BX:31:HIS:CE1 | 2.75 | 0.55 |
| 1:CA:1343:G:H2' | 1:CA:1344:C:C6 | 2.41 | 0.55 |
| 1:CA:386:C:H2' | 1:CA:387:U:C5' | 2.33 | 0.55 |
| 1:CA:503:C:H2' | 1:CA:504:C:C6 | 2.40 | 0.55 |
| 1:CA:97:G:O2' | 1:CA:98:G:O5' | 2.24 | 0.55 |
| 3:CC:52:LEU:H | 3:CC:52:LEU:CD2 | 2.18 | 0.55 |
| 1:CA:437:U:OP1 | 4:CD:155:LEU:HD22 | 2.07 | 0.55 |
| 5:CE:45:PHE:CE2 | 5:CE:47:LYS:HD2 | 2.42 | 0.55 |
| 15:CO:23:GLY:O | 15:CO:27:VAL:HB | 2.06 | 0.55 |
| 23:D1:26:ARG:HB3 | 23:D1:35:THR:H | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 23:D1:20:ARG:HD3 | 23:D1:41:ARG:HD3 | 1.88 | 0.55 |
| 27:D5:52:TYR:O | 27:D5:52:TYR:CD1 | 2.60 | 0.55 |
| 31:DA:142:A:H1' | 31:DA:1408:C:O4' | 2.06 | 0.55 |
| 31:DA:207:A:H2' | 31:DA:208:C:O4' | 2.07 | 0.55 |
| 31:DA:271(J):C:H5' | 31:DA:271(K):U:OP2 | 2.06 | 0.55 |
| 31:DA:271(X):G:C2' | 31:DA:271(Y):U:H5'' | 2.37 | 0.55 |
| 33:DD:255:LYS:NZ | 33:DD:255:LYS:N | 2.52 | 0.55 |
| 34:DE:3:GLY:CA | 34:DE:81:ILE:HG21 | 2.37 | 0.55 |
| 38:DI:56:LYS:HZ3 | 38:DI:56:LYS:C | 2.09 | 0.55 |
| 39:DN:43:THR:HG22 | 39:DN:45:ASN:ND2 | 2.21 | 0.55 |
| 31:DA:870:A:C5' | 42:DQ:7:MET:HB2 | 2.22 | 0.55 |
| 45:DT:53:ARG:O | 45:DT:53:ARG:HG3 | 2.07 | 0.55 |
| 45:DT:93:ARG:O | 45:DT:94:ALA:O | 2.25 | 0.55 |
| 48:DW:4:LYS:CE | 48:DW:6:ILE:HD11 | 2.37 | 0.55 |
| 1:AA:1248:A:H2' | 1:AA:1249:C:H5' | 1.88 | 0.55 |
| 1:AA:145:G:C2 | 1:AA:146:G:H1' | 2.42 | 0.55 |
| 1:AA:192:U:O2' | 1:AA:193:C:H5' | 2.06 | 0.55 |
| 1:AA:79:G:C4' | 1:AA:80:G:OP1 | 2.53 | 0.55 |
| 2:AB:67:THR:HG21 | 2:AB:155:LEU:CD2 | 2.36 | 0.55 |
| 4:AD:13:ARG:O | 4:AD:15:GLU:N | 2.39 | 0.55 |
| 4:AD:141:ARG:HB3 | 4:AD:142:PRO:CD | 2.36 | 0.55 |
| 4:AD:19:LEU:HD13 | 4:AD:21:LEU:HD21 | 1.88 | 0.55 |
| 5:AE:18:ARG:NH2 | 5:AE:25:ARG:HG2 | 2.21 | 0.55 |
| 7:AG:85:TYR:CD1 | 7:AG:154:TYR:HE1 | 2.25 | 0.55 |
| 10:AJ:7:LYS:O | 10:AJ:96:ILE:HA | 2.06 | 0.55 |
| 22:B0:68:GLU:CG | 22:B0:80:HIS:HB2 | 2.36 | 0.55 |
| 30:B8:35:GLN:NE2 | 30:B8:36:LYS:NZ | 2.55 | 0.55 |
| 30:B8:34:TRP:HZ3 | 30:B8:41:ILE:CG2 | 2.20 | 0.55 |
| 31:BA:173:G:C6 | 31:BA:174:C:C4 | 2.95 | 0.55 |
| 31:BA:1947:C:C2' | 31:BA:1948:G:H5' | 2.36 | 0.55 |
| 31:BA:2206:G:N3 | 31:BA:2206:G:H3' | 2.22 | 0.55 |
| 31:BA:2478:A:C2' | 31:BA:2479:G:H5' | 2.37 | 0.55 |
| 31:BA:2022:U:O2' | 31:BA:2617:C:H5' | 2.06 | 0.55 |
| 31:BA:884:C:O2' | 31:BA:892:G:C8 | 2.51 | 0.55 |
| 31:BA:930:U:O4' | 31:BA:930:U:O2 | 2.24 | 0.55 |
| 32:BB:21:G:O2' | 32:BB:22:U:H6 | 1.90 | 0.55 |
| 33:BD:146:GLU:HB2 | 33:BD:189:CYS:HB3 | 1.88 | 0.55 |
| 34:BE:134:ILE:H | 34:BE:134:ILE:HD13 | 1.71 | 0.55 |
| 36:BG:16:ARG:O | 36:BG:20:ILE:HG13 | 2.06 | 0.55 |
| 31:BA:814:C:H5 | 41:BP:27:HIS:CD2 | 2.24 | 0.55 |
| 41:BP:33:ARG:O | 41:BP:35:HIS:N | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BQ:22:LYS:NZ | 42:BQ:25:ASP:OD1 | 2.39 | 0.55 |
| 43:BR:38:VAL:HB | 43:BR:39:PRO:HD3 | 1.86 | 0.55 |
| 44:BS:56:LEU:C | 44:BS:56:LEU:HD23 | 2.27 | 0.55 |
| 45:BT:91:ARG:HB2 | 45:BT:115:ARG:O | 2.06 | 0.55 |
| 47:BV:44:LYS:HG2 | 47:BV:45:THR:H | 1.72 | 0.55 |
| 49:BX:72:LYS:HG3 | 49:BX:73:ARG:N | 2.17 | 0.55 |
| 50:BY:52:SER:O | 50:BY:54:LYS:N | 2.39 | 0.55 |
| 42:BQ:141:GLN:HG2 | 51:BZ:72:ARG:HA | 1.88 | 0.55 |
| 1:CA:1113:C:H2' | 1:CA:1114:C:C6 | 2.42 | 0.55 |
| 1:CA:445:G:C4 | 1:CA:446:G:C8 | 2.94 | 0.55 |
| 1:CA:658:G:C4 | 1:CA:659:U:C5 | 2.94 | 0.55 |
| 1:CA:659:U:H2' | 1:CA:660:G:C5' | 2.37 | 0.55 |
| 6:CF:12:PRO:CB | 6:CF:57:GLN:HB2 | 2.35 | 0.55 |
| 6:CF:39:LYS:HB2 | 6:CF:62:TRP:CZ3 | 2.42 | 0.55 |
| 7:CG:75:VAL:HG21 | 7:CG:144:MET:HB3 | 1.89 | 0.55 |
| 13:CM:106:ASN:O | 13:CM:107:ALA:HB3 | 2.07 | 0.55 |
| 16:CP:22:THR:HG22 | 16:CP:32:TYR:HA | 1.89 | 0.55 |
| 24:D2:46:GLN:C | 24:D2:46:GLN:HE21 | 2.09 | 0.55 |
| 28:D6:11:LEU:CD2 | 28:D6:26:ASN:H | 2.19 | 0.55 |
| 29:D7:48:LYS:N | 29:D7:48:LYS:HD3 | 2.22 | 0.55 |
| 31:DA:1266:G:O5' | 48:DW:15:ARG:NH2 | 2.40 | 0.55 |
| 31:DA:271(P):C:H2' | 31:DA:271(Q):G:C5' | 2.37 | 0.55 |
| 30:D8:61:LEU:HD22 | 31:DA:593:G:O3' | 2.06 | 0.55 |
| 31:DA:90:U:H1' | 31:DA:92:A:H5'' | 1.88 | 0.55 |
| 33:DD:145:VAL:HG12 | 33:DD:146:GLU:O | 2.07 | 0.55 |
| 41:DP:84:ASN:HA | 41:DP:115:LEU:O | 2.06 | 0.55 |
| 41:DP:121:LYS:HB3 | 41:DP:123:LEU:CD2 | 2.36 | 0.55 |
| 41:DP:23:PRO:O | 41:DP:33:ARG:HG3 | 2.07 | 0.55 |
| 41:DP:27:HIS:CD2 | 41:DP:27:HIS:C | 2.80 | 0.55 |
| 42:DQ:57:HIS:CE1 | 42:DQ:116:GLU:HB3 | 2.41 | 0.55 |
| 48:DW:95:ILE:O | 48:DW:95:ILE:HG13 | 2.07 | 0.55 |
| 49:DX:33:LYS:C | 49:DX:35:THR:HG22 | 2.27 | 0.55 |
| 31:DA:106:C:H1' | 50:DY:2:ARG:HE | 1.72 | 0.55 |
| 31:DA:875:G:C4' | 51:DZ:170:THR:HG21 | 2.33 | 0.55 |
| 1:AA:1252:A:H2' | 1:AA:1253:G:O4' | 2.07 | 0.55 |
| 1:AA:1492:A:H5' | 1:AA:1493:A:OP2 | 2.06 | 0.55 |
| 1:AA:370:C:H2' | 1:AA:371:G:H8 | 1.71 | 0.55 |
| 9:AI:8:GLY:HA2 | 9:AI:79:LEU:HD12 | 1.89 | 0.55 |
| 13:AM:25:ILE:CD1 | 13:AM:66:LEU:HD23 | 2.36 | 0.55 |
| 19:AS:42:PRO:O | 19:AS:43:GLU:HB3 | 2.05 | 0.55 |
| 24:B2:26:ARG:HG3 | 24:B2:29:LYS:NZ | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:B2:52:ASP:O | 24:B2:56:GLN:NE2 | 2.39 | 0.55 |
| 25:B3:19:GLN:HE22 | 25:B3:52:HIS:CE1 | 2.21 | 0.55 |
| 31:BA:1164:G:H2' | 31:BA:1165:U:C6 | 2.42 | 0.55 |
| 31:BA:1247:A:OP1 | 35:BF:95:ARG:NH2 | 2.37 | 0.55 |
| 31:BA:11:G:C2' | 31:BA:12:U:H5' | 2.36 | 0.55 |
| 31:BA:1505:C:H2' | 31:BA:1506:C:O4' | 2.06 | 0.55 |
| 31:BA:2186:G:H2' | 31:BA:2187:G:H5'' | 1.88 | 0.55 |
| 31:BA:790:C:O2' | 31:BA:791:C:H5' | 2.07 | 0.55 |
| 31:BA:855:G:C4 | 31:BA:856:C:C5 | 2.94 | 0.55 |
| 35:BF:53:THR:HG22 | 35:BF:55:GLY:CA | 2.37 | 0.55 |
| 37:BH:144:VAL:O | 37:BH:148:ILE:HG12 | 2.06 | 0.55 |
| 31:BA:389:G:H22 | 41:BP:71:VAL:HG12 | 1.71 | 0.55 |
| 44:BS:83:LYS:HE2 | 44:BS:105:ALA:HB2 | 1.89 | 0.55 |
| 49:BX:85:PRO:O | 49:BX:87:GLN:N | 2.40 | 0.55 |
| 51:BZ:144:LEU:N | 51:BZ:144:LEU:HD22 | 2.21 | 0.55 |
| 1:CA:961:U:OP2 | 1:CA:1223:C:H4' | 2.06 | 0.55 |
| 1:CA:375:U:C2 | 1:CA:376:G:C8 | 2.95 | 0.55 |
| 1:CA:428:G:C4' | 1:CA:429:U:O5' | 2.55 | 0.55 |
| 2:CB:19:HIS:O | 2:CB:39:ILE:HG23 | 2.06 | 0.55 |
| 2:CB:74:LYS:NZ | 2:CB:76:GLN:HB2 | 2.21 | 0.55 |
| 24:D2:26:ARG:HG2 | 49:DX:5:TYR:CB | 2.37 | 0.55 |
| 28:D6:16:CYS:O | 28:D6:18:ARG:NH2 | 2.39 | 0.55 |
| 30:D8:32:LEU:N | 30:D8:32:LEU:HD13 | 2.05 | 0.55 |
| 31:DA:271(E):U:H2' | 31:DA:271(F):C:C6 | 2.41 | 0.55 |
| 31:DA:2854:G:H2' | 31:DA:2855:C:C6 | 2.41 | 0.55 |
| 31:DA:776:G:H4' | 31:DA:777:A:O5' | 2.06 | 0.55 |
| 31:DA:828:U:C3' | 31:DA:828:U:O2 | 2.54 | 0.55 |
| 38:DI:56:LYS:C | 38:DI:56:LYS:NZ | 2.59 | 0.55 |
| 40:DO:24:VAL:HB | 40:DO:33:ALA:HB2 | 1.88 | 0.55 |
| 42:DQ:141:GLN:HG2 | 51:DZ:72:ARG:HA | 1.88 | 0.55 |
| 42:DQ:75:THR:HG22 | 42:DQ:88:GLY:HA3 | 1.89 | 0.55 |
| 43:DR:9:LYS:C | 43:DR:10:LEU:HG | 2.26 | 0.55 |
| 49:DX:76:ARG:O | 49:DX:77:LYS:HB2 | 2.07 | 0.55 |
| 50:DY:45:VAL:CG2 | 50:DY:62:GLU:H | 2.20 | 0.55 |
| 51:DZ:105:VAL:HG12 | 51:DZ:139:VAL:O | 2.06 | 0.55 |
| 1:AA:1190:G:OP1 | 3:AC:4:LYS:HA | 2.06 | 0.55 |
| 1:AA:308:C:H2' | 1:AA:309:G:H8 | 1.70 | 0.55 |
| 1:AA:445:G:C4 | 1:AA:446:G:C8 | 2.94 | 0.55 |
| 1:AA:552:U:O2' | 1:AA:553:A:H5' | 2.06 | 0.55 |
| 1:AA:868:C:H2' | 1:AA:869:G:O4' | 2.06 | 0.55 |
| 5:AE:78:HIS:CE1 | 5:AE:142:LEU:HA | 2.33 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AF:11:ASN:O | 6:AF:14:LEU:HB2 | 2.06 | 0.55 |
| 6:AF:39:LYS:CB | 6:AF:62:TRP:HZ3 | 2.20 | 0.55 |
| 1:AA:1348:U:H4' | 9:AI:120:ARG:HD2 | 1.87 | 0.55 |
| 11:AK:41:THR:CG2 | 11:AK:42:TRP:N | 2.69 | 0.55 |
| 17:AQ:65:ILE:H | 17:AQ:65:ILE:HD12 | 1.72 | 0.55 |
| 19:AS:69:HIS:HB2 | 19:AS:74:PHE:HE2 | 1.71 | 0.55 |
| 28:B6:36:LEU:HG | 28:B6:36:LEU:O | 2.06 | 0.55 |
| 31:BA:1027:A:C6 | 31:BA:1126:A:C4 | 2.94 | 0.55 |
| 31:BA:1434:A:H2' | 31:BA:1435:G:C8 | 2.42 | 0.55 |
| 31:BA:2252:G:H2' | 31:BA:2253:G:H8 | 1.71 | 0.55 |
| 31:BA:2359:C:H2' | 31:BA:2360:A:C5' | 2.27 | 0.55 |
| 31:BA:2364:C:C2' | 31:BA:2365:G:H5' | 2.37 | 0.55 |
| 31:BA:2473:U:N3 | 31:BA:2474:C:C6 | 2.75 | 0.55 |
| 31:BA:2582:G:C2 | 31:BA:2583:G:C8 | 2.94 | 0.55 |
| 31:BA:322:A:H3' | 35:BF:169:ASN:ND2 | 2.22 | 0.55 |
| 31:BA:573:G:O2' | 31:BA:574:C:H3' | 2.07 | 0.55 |
| 31:BA:883:G:H1 | 31:BA:893:C:H41 | 1.55 | 0.55 |
| 31:BA:706:A:OP1 | 33:BD:7:LYS:HE3 | 2.07 | 0.55 |
| 34:BE:50:GLY:HA3 | 34:BE:74:PRO:HG3 | 1.89 | 0.55 |
| 41:BP:26:GLY:HA2 | 41:BP:30:THR:CG2 | 2.37 | 0.55 |
| 41:BP:88:LEU:C | 41:BP:90:ARG:H | 2.09 | 0.55 |
| 31:BA:1276:A:O2' | 43:BR:16:HIS:HE1 | 1.89 | 0.55 |
| 45:BT:28:VAL:HG11 | 45:BT:46:GLU:OE1 | 2.05 | 0.55 |
| 49:BX:63:LYS:HD2 | 49:BX:70:LEU:HD13 | 1.87 | 0.55 |
| 50:BY:20:TYR:CD2 | 50:BY:41:GLY:HA2 | 2.42 | 0.55 |
| 50:BY:39:VAL:O | 50:BY:40:GLU:CD | 2.45 | 0.55 |
| 51:BZ:166:SER:OG | 51:BZ:167:PRO:CA | 2.54 | 0.55 |
| 51:BZ:45:ASP:O | 51:BZ:46:LYS:C | 2.43 | 0.55 |
| 1:CA:192:U:O2' | 1:CA:193:C:H5' | 2.06 | 0.55 |
| 1:CA:878:G:C5' | 8:CH:89:PRO:HG2 | 2.37 | 0.55 |
| 4:CD:131:ARG:HD3 | 4:CD:131:ARG:H | 1.71 | 0.55 |
| 12:CL:32:PHE:HD1 | 12:CL:86:ARG:HA | 1.72 | 0.55 |
| 15:CO:63:ARG:HG2 | 15:CO:67:LEU:HD12 | 1.89 | 0.55 |
| 30:D8:6:THR:HB | 30:D8:63:PRO:HG3 | 1.88 | 0.55 |
| 31:DA:1106:A:C2' | 31:DA:1107:G:O5' | 2.55 | 0.55 |
| 31:DA:1224:C:O3' | 47:DV:88:ARG:HB3 | 2.07 | 0.55 |
| 31:DA:2020:A:HO2' | 31:DA:2021:C:H5' | 1.67 | 0.55 |
| 33:DD:27:THR:CG2 | 33:DD:28:GLU:H | 2.19 | 0.55 |
| 40:DO:26:LYS:HB2 | 40:DO:30:ALA:HB2 | 1.88 | 0.55 |
| 44:DS:56:LEU:O | 44:DS:57:LYS:HB2 | 2.06 | 0.55 |
| 46:DU:64:ARG:CA | 46:DU:64:ARG:CZ | 2.73 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:AA:328:C:O2 | 1:AA:328:C:C2' | 2.55 | 0.55 |
| 1:AA:353:A:C5' | 1:AA:353:A:C8 | 2.83 | 0.55 |
| 2:AB:121:LEU:O | 2:AB:121:LEU:HD23 | 2.07 | 0.55 |
| 4:AD:10:ARG:HA | 4:AD:13:ARG:HG3 | 1.87 | 0.55 |
| 4:AD:106:TYR:HE1 | 4:AD:113:SER:HA | 1.72 | 0.55 |
| 5:AE:68:GLU:O | 5:AE:70:PRO:HD3 | 2.06 | 0.55 |
| 12:AL:41:ARG:HG2 | 12:AL:42:THR:H | 1.71 | 0.55 |
| 12:AL:32:PHE:HD1 | 12:AL:86:ARG:HA | 1.72 | 0.55 |
| 22:B0:41:ARG:H | 22:B0:41:ARG:CD | 2.19 | 0.55 |
| 23:B1:33:LYS:NZ | 23:B1:35:THR:HG21 | 2.22 | 0.55 |
| 28:B6:19:ARG:NH1 | 31:BA:2400:G:H4' | 2.22 | 0.55 |
| 31:BA:1204:A:H61 | 31:BA:1240:U:H2' | 1.72 | 0.55 |
| 1:AA:1494:G:N2 | 31:BA:1912:A:N3 | 2.54 | 0.55 |
| 31:BA:2488:A:H2' | 31:BA:2489:G:O4' | 2.07 | 0.55 |
| 31:BA:271(H):G:O2' | 31:BA:271(I):G:H5'' | 2.07 | 0.55 |
| 31:BA:479:A:H4' | 31:BA:480:A:OP1 | 2.07 | 0.55 |
| 31:BA:828:U:C3' | 31:BA:828:U:O2 | 2.55 | 0.55 |
| 33:BD:35:LYS:HE3 | 33:BD:65:ILE:HA | 1.89 | 0.55 |
| 31:BA:2572:A:C8 | 34:BE:144:ARG:HD2 | 2.42 | 0.55 |
| 36:BG:106:LEU:O | 36:BG:110:ALA:HB3 | 2.07 | 0.55 |
| 39:BN:56:ASN:C | 39:BN:57:ALA:O | 2.42 | 0.55 |
| 1:AA:1422:G:H4' | 40:BO:49:ARG:NH1 | 2.22 | 0.55 |
| 42:BQ:108:GLY:HA3 | 51:BZ:116:VAL:HG21 | 1.89 | 0.55 |
| 44:BS:28:VAL:O | 44:BS:89:ARG:HB2 | 2.06 | 0.55 |
| 45:BT:45:PHE:CE2 | 45:BT:63:VAL:HG22 | 2.42 | 0.55 |
| 1:CA:1097:C:O2' | 1:CA:1098:C:H5' | 2.06 | 0.55 |
| 1:CA:1103:C:H2' | 1:CA:1104:G:O4' | 2.07 | 0.55 |
| 1:CA:510:A:H5'' | 1:CA:511:C:OP2 | 2.06 | 0.55 |
| 7:CG:146:GLU:OE2 | 7:CG:149:ARG:HD2 | 2.07 | 0.55 |
| 10:CJ:29:ARG:HG2 | 10:CJ:29:ARG:O | 2.07 | 0.55 |
| 17:CQ:21:VAL:HG21 | 17:CQ:59:ILE:HD11 | 1.89 | 0.55 |
| 23:D1:21:ARG:HD3 | 23:D1:21:ARG:O | 2.06 | 0.55 |
| 26:D4:29:PRO:C | 26:D4:31:ILE:H | 2.10 | 0.55 |
| 27:D5:51:TYR:HB3 | 27:D5:52:TYR:CD2 | 2.42 | 0.55 |
| 28:D6:16:CYS:O | 28:D6:18:ARG:CZ | 2.55 | 0.55 |
| 30:D8:62:LEU:O | 30:D8:64:TYR:N | 2.40 | 0.55 |
| 31:DA:1288:U:C2 | 31:DA:1327:C:C2 | 2.95 | 0.55 |
| 31:DA:2660:A:H5'' | 31:DA:2661:G:C2 | 2.41 | 0.55 |
| 32:DB:86:G:H2' | 32:DB:87:G:C8 | 2.42 | 0.55 |
| 39:DN:131:GLN:HG2 | 39:DN:133:GLN:O | 2.07 | 0.55 |
| 31:DA:1141:U:OP1 | 39:DN:25:ARG:NH1 | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 41:DP:105:LEU:O | 41:DP:106:LEU:CB | 2.52 | 0.55 |
| 42:DQ:78:PRO:O | 42:DQ:79:LEU:CG | 2.54 | 0.55 |
| 44:DS:59:LYS:HE3 | 44:DS:68:GLN:HE22 | 1.72 | 0.55 |
| 49:DX:80:ILE:O | 49:DX:81:VAL:HB | 2.06 | 0.55 |
| 42:DQ:141:GLN:CA | 51:DZ:53:ILE:HB | 2.36 | 0.55 |
| 42:DQ:140:ALA:CB | 51:DZ:99:TYR:HB2 | 2.36 | 0.55 |
| 1:AA:961:U:OP2 | 1:AA:1223:C:H4' | 2.07 | 0.55 |
| 1:AA:1477:C:H2' | 1:AA:1478:C:C6 | 2.41 | 0.55 |
| 1:AA:187:C:H2' | 1:AA:188:C:C6 | 2.41 | 0.55 |
| 1:AA:380:G:C2 | 1:AA:384:G:C6 | 2.95 | 0.55 |
| 1:AA:620:C:H2' | 1:AA:621:A:O4' | 2.07 | 0.55 |
| 2:AB:163:PHE:O | 2:AB:164:VAL:HG23 | 2.07 | 0.55 |
| 12:AL:62:SER:C | 12:AL:64:TYR:H | 2.10 | 0.55 |
| 12:AL:82:VAL:CG1 | 12:AL:83:VAL:H | 2.15 | 0.55 |
| 12:AL:6:THR:OG1 | 12:AL:9:GLN:HG3 | 2.07 | 0.55 |
| 1:AA:1330:U:H4' | 13:AM:23:TYR:CE2 | 2.42 | 0.55 |
| 22:B0:65:GLY:HA2 | 22:B0:84:LEU:HD21 | 1.89 | 0.55 |
| 31:BA:128:C:H2' | 31:BA:129:C:O4' | 2.06 | 0.55 |
| 31:BA:174:C:H3' | 31:BA:175:G:H5'' | 1.89 | 0.55 |
| 31:BA:1946:U:H2' | 31:BA:1947:C:C6 | 2.42 | 0.55 |
| 31:BA:2262:U:C2' | 31:BA:2263:C:C5' | 2.84 | 0.55 |
| 31:BA:229:A:H3' | 31:BA:230:U:H5' | 1.89 | 0.55 |
| 31:BA:2801(A):A:C3' | 31:BA:2802:G:H5' | 2.37 | 0.55 |
| 31:BA:2032:G:H21 | 34:BE:146:THR:HG23 | 1.71 | 0.55 |
| 34:BE:174:ASP:OD2 | 34:BE:175:VAL:N | 2.40 | 0.55 |
| 36:BG:60:LEU:O | 36:BG:60:LEU:HD22 | 2.07 | 0.55 |
| 31:BA:2376:A:O2' | 44:BS:108:GLY:HA2 | 2.07 | 0.55 |
| 44:BS:53:SER:O | 44:BS:55:ALA:N | 2.40 | 0.55 |
| 49:BX:60:ARG:HH21 | 49:BX:74:PRO:HG2 | 1.72 | 0.55 |
| 1:CA:380:G:C2 | 1:CA:384:G:C6 | 2.94 | 0.55 |
| 1:CA:491:G:H2' | 1:CA:492:G:H8 | 1.71 | 0.55 |
| 7:CG:115:ARG:HB2 | 7:CG:118:VAL:HG22 | 1.89 | 0.55 |
| 17:CQ:97:SER:O | 17:CQ:98:LEU:HD23 | 2.07 | 0.55 |
| 23:D1:87:PRO:HB2 | 23:D1:91:LYS:CE | 2.37 | 0.55 |
| 24:D2:26:ARG:HG3 | 24:D2:29:LYS:NZ | 2.22 | 0.55 |
| 31:DA:1040:C:O2' | 31:DA:1041:C:P | 2.64 | 0.55 |
| 31:DA:1179:C:C3' | 31:DA:1180:C:H5'' | 2.36 | 0.55 |
| 31:DA:1209:G:H21 | 31:DA:1210:A:N6 | 2.04 | 0.55 |
| 31:DA:196:A:H2' | 31:DA:196:A:N3 | 2.22 | 0.55 |
| 31:DA:234:C:H2' | 31:DA:235:U:H6 | 1.71 | 0.55 |
| 31:DA:2661:G:N7 | 31:DA:2662:A:C2 | 2.75 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DB:27:C:C4 | 32:DB:28:C:C4 | 2.95 | 0.55 |
| 39:DN:128:HIS:NE2 | 39:DN:131:GLN:OE1 | 2.40 | 0.55 |
| 50:DY:77:PRO:O | 50:DY:78:ALA:HB2 | 2.07 | 0.55 |
| 1:AA:1356:G:H2' | 1:AA:1357:A:C8 | 2.42 | 0.55 |
| 1:AA:1112:C:N3 | 3:AC:178:LEU:HD23 | 2.22 | 0.55 |
| 5:AE:77:PRO:HG2 | 5:AE:142:LEU:HD22 | 1.89 | 0.55 |
| 7:AG:46:ALA:O | 7:AG:50:ILE:HG12 | 2.07 | 0.55 |
| 13:AM:44:ARG:HB2 | 13:AM:46:LYS:HG2 | 1.88 | 0.55 |
| 30:B8:6:THR:HB | 30:B8:63:PRO:HG3 | 1.89 | 0.55 |
| 31:BA:142:A:N6 | 31:BA:1595:G:O2' | 2.40 | 0.55 |
| 32:BB:86:G:H2' | 32:BB:87:G:C8 | 2.42 | 0.55 |
| 33:BD:39:LYS:HB2 | 33:BD:62:TYR:HB2 | 1.89 | 0.55 |
| 38:BI:38:LEU:H | 38:BI:38:LEU:CD1 | 2.12 | 0.55 |
| 39:BN:57:ALA:O | 39:BN:58:ASP:C | 2.44 | 0.55 |
| 47:BV:85:LYS:C | 47:BV:87:HIS:H | 2.05 | 0.55 |
| 49:BX:23:GLU:CG | 49:BX:24:GLY:N | 2.69 | 0.55 |
| 51:BZ:6:LYS:HB3 | 51:BZ:8:TYR:CE1 | 2.42 | 0.55 |
| 1:CA:135:C:H2' | 1:CA:136:C:H5' | 1.87 | 0.55 |
| 1:CA:620:C:H2' | 1:CA:621:A:O4' | 2.07 | 0.55 |
| 1:CA:939:G:H5'' | 7:CG:102:ARG:CZ | 2.36 | 0.55 |
| 2:CB:32:ILE:HD12 | 2:CB:42:ILE:HA | 1.87 | 0.55 |
| 1:CA:1206:G:O4' | 3:CC:194:GLY:HA2 | 2.06 | 0.55 |
| 3:CC:95:THR:HG22 | 3:CC:97:LYS:H | 1.71 | 0.55 |
| 4:CD:19:LEU:HD13 | 4:CD:21:LEU:HD21 | 1.89 | 0.55 |
| 5:CE:147:ASP:HA | 5:CE:150:ARG:HB3 | 1.89 | 0.55 |
| 31:DA:102:G:C8 | 31:DA:102:G:C5' | 2.70 | 0.55 |
| 31:DA:1210:A:H5'' | 31:DA:1212:G:O4' | 2.07 | 0.55 |
| 31:DA:142:A:H5'' | 31:DA:142(A):C:C5 | 2.41 | 0.55 |
| 31:DA:1925:C:C2' | 31:DA:1926:U:H5' | 2.37 | 0.55 |
| 31:DA:2376:A:O2' | 44:DS:108:GLY:HA2 | 2.07 | 0.55 |
| 27:D5:7:PRO:HA | 31:DA:2615:U:C2 | 2.42 | 0.55 |
| 31:DA:484:C:H2' | 31:DA:485:C:H6 | 1.68 | 0.55 |
| 31:DA:573:G:O2' | 31:DA:574:C:H3' | 2.07 | 0.55 |
| 31:DA:836:G:C5 | 31:DA:837:C:C4 | 2.94 | 0.55 |
| 33:DD:158:ALA:O | 33:DD:159:ALA:HB2 | 2.06 | 0.55 |
| 33:DD:175:LEU:HD12 | 33:DD:185:VAL:HG21 | 1.89 | 0.55 |
| 33:DD:24:ILE:O | 33:DD:24:ILE:HG22 | 2.06 | 0.55 |
| 42:DQ:35:VAL:CG1 | 42:DQ:130:LYS:HB3 | 2.32 | 0.55 |
| 45:DT:31:SER:CA | 45:DT:32:TYR:CD2 | 2.90 | 0.55 |
| 50:DY:10:GLY:CA | 50:DY:27:VAL:HG13 | 2.22 | 0.55 |
| 42:DQ:137:TYR:HE2 | 51:DZ:74:VAL:O | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1147:C:C5 | 1:AA:1148:U:C4 | 2.95 | 0.54 |
| 1:AA:343:U:C2 | 1:AA:347:G:C2 | 2.96 | 0.54 |
| 1:AA:437:U:OP1 | 4:AD:155:LEU:HD22 | 2.06 | 0.54 |
| 5:AE:105:VAL:O | 5:AE:109:ILE:HG13 | 2.06 | 0.54 |
| 8:AH:25:ASP:HB3 | 8:AH:58:TYR:HB3 | 1.89 | 0.54 |
| 18:AR:50:ILE:CD1 | 18:AR:70:ILE:HG21 | 2.37 | 0.54 |
| 22:B0:53:MET:HB2 | 22:B0:59:LEU:CD2 | 2.36 | 0.54 |
| 28:B6:10:LEU:HD22 | 28:B6:10:LEU:H | 1.73 | 0.54 |
| 29:B7:48:LYS:HD3 | 29:B7:48:LYS:N | 2.22 | 0.54 |
| 30:B8:39:LYS:HD3 | 30:B8:39:LYS:C | 2.28 | 0.54 |
| 31:BA:1022:G:N2 | 31:BA:1142(A):A:H2 | 1.99 | 0.54 |
| 31:BA:1339:G:H21 | 31:BA:1603:A:H1' | 1.71 | 0.54 |
| 31:BA:860:U:C5 | 31:BA:2268:A:C8 | 2.95 | 0.54 |
| 31:BA:2315:G:H2' | 31:BA:2316:C:C6 | 2.42 | 0.54 |
| 28:B6:42:TRP:CZ2 | 31:BA:642:G:O3' | 2.60 | 0.54 |
| 33:BD:31:LYS:O | 33:BD:32:SER:C | 2.45 | 0.54 |
| 35:BF:21:ALA:HB3 | 35:BF:23:ASP:OD2 | 2.06 | 0.54 |
| 37:BH:105:LEU:H | 37:BH:105:LEU:HD22 | 1.72 | 0.54 |
| 38:BI:38:LEU:HB2 | 38:BI:40:THR:HG22 | 1.89 | 0.54 |
| 42:BQ:16:ARG:NH1 | 42:BQ:16:ARG:HB2 | 2.22 | 0.54 |
| 43:BR:71:GLN:CA | 43:BR:71:GLN:HE21 | 2.14 | 0.54 |
| 31:BA:993:G:C5' | 47:BV:75:PHE:CE2 | 2.84 | 0.54 |
| 48:BW:59:VAL:HG12 | 48:BW:60:ASN:N | 2.20 | 0.54 |
| 51:BZ:27:VAL:HG23 | 51:BZ:36:LYS:HA | 1.89 | 0.54 |
| 51:BZ:51:ALA:O | 51:BZ:52:SER:HB3 | 2.07 | 0.54 |
| 1:CA:1422:G:H4' | 40:DO:49:ARG:NH1 | 2.22 | 0.54 |
| 1:CA:427:U:P | 4:CD:13:ARG:HH22 | 2.31 | 0.54 |
| 2:CB:144:ARG:HA | 2:CB:147:LYS:HB2 | 1.90 | 0.54 |
| 5:CE:51:VAL:HB | 5:CE:52:PRO:CD | 2.35 | 0.54 |
| 6:CF:19:LEU:HD23 | 6:CF:19:LEU:O | 2.07 | 0.54 |
| 23:D1:19:GLN:CG | 23:D1:44:PRO:HG3 | 2.37 | 0.54 |
| 30:D8:34:TRP:CZ3 | 30:D8:41:ILE:HG23 | 2.38 | 0.54 |
| 31:DA:1502:C:H2' | 31:DA:1502:C:O2 | 2.06 | 0.54 |
| 31:DA:175:G:H5' | 31:DA:175:G:H8 | 1.72 | 0.54 |
| 31:DA:185:U:H4' | 31:DA:218:A:H4' | 1.88 | 0.54 |
| 31:DA:2818:G:C2' | 31:DA:2819:G:H5' | 2.38 | 0.54 |
| 31:DA:807:U:H2' | 31:DA:808:G:O5' | 2.06 | 0.54 |
| 38:DI:38:LEU:HB2 | 38:DI:40:THR:HG22 | 1.89 | 0.54 |
| 38:DI:72:LEU:HD12 | 38:DI:138:ILE:CG2 | 2.32 | 0.54 |
| 42:DQ:54:MET:HB3 | 42:DQ:64:ILE:CD1 | 2.37 | 0.54 |
| 49:DX:60:ARG:NH2 | 49:DX:74:PRO:HG2 | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:DZ:45:ASP:O | 51:DZ:46:LYS:C | 2.44 | 0.54 |
| 1:AA:370:C:H2' | 1:AA:371:G:C8 | 2.42 | 0.54 |
| 1:AA:491:G:H2' | 1:AA:492:G:C8 | 2.41 | 0.54 |
| 4:AD:62:GLN:NE2 | 4:AD:65:ARG:HE | 2.05 | 0.54 |
| 7:AG:69:VAL:HG13 | 7:AG:134:ALA:O | 2.07 | 0.54 |
| 9:AI:114:TYR:HE1 | 10:AJ:60:ARG:O | 1.90 | 0.54 |
| 15:AO:67:LEU:HD22 | 15:AO:78:TYR:CE1 | 2.42 | 0.54 |
| 23:B1:21:ARG:HD3 | 23:B1:21:ARG:O | 2.08 | 0.54 |
| 31:BA:1161:C:O2' | 47:BV:8:GLY:HA2 | 2.08 | 0.54 |
| 31:BA:1568:G:H5'' | 33:BD:61:LEU:HD22 | 1.88 | 0.54 |
| 31:BA:1692:U:H2' | 31:BA:1694:C:C5 | 2.43 | 0.54 |
| 31:BA:2360:A:O2' | 31:BA:2361:A:O5' | 2.26 | 0.54 |
| 31:BA:2632:A:H1' | 34:BE:61:ARG:NH1 | 2.22 | 0.54 |
| 31:BA:362:U:H6 | 31:BA:362:U:H3' | 1.72 | 0.54 |
| 31:BA:527:C:O2 | 31:BA:527:C:O4' | 2.18 | 0.54 |
| 31:BA:614:U:O2 | 31:BA:614:U:O5' | 2.25 | 0.54 |
| 31:BA:824:A:O2' | 31:BA:825:C:H5' | 2.07 | 0.54 |
| 34:BE:3:GLY:HA3 | 34:BE:81:ILE:HG21 | 1.89 | 0.54 |
| 34:BE:61:ARG:H | 34:BE:62:PRO:CD | 2.19 | 0.54 |
| 35:BF:110:LEU:HD21 | 35:BF:181:LEU:HD23 | 1.88 | 0.54 |
| 31:BA:389:G:N2 | 41:BP:71:VAL:HG12 | 2.22 | 0.54 |
| 45:BT:38:ASN:HD22 | 45:BT:40:THR:N | 2.03 | 0.54 |
| 45:BT:53:ARG:O | 45:BT:53:ARG:HG3 | 2.06 | 0.54 |
| 47:BV:2:PHE:CE1 | 47:BV:13:ARG:NE | 2.74 | 0.54 |
| 48:BW:9:TYR:N | 48:BW:102:HIS:HD2 | 1.99 | 0.54 |
| 1:CA:1147:C:C5 | 1:CA:1148:U:C4 | 2.96 | 0.54 |
| 1:CA:1392:G:H21 | 1:CA:1502:A:H8 | 1.55 | 0.54 |
| 1:CA:664:G:H22 | 1:CA:741:G:H1 | 1.55 | 0.54 |
| 2:CB:135:GLN:O | 2:CB:139:LYS:HB2 | 2.07 | 0.54 |
| 1:CA:1190:G:OP1 | 3:CC:4:LYS:HA | 2.07 | 0.54 |
| 5:CE:18:ARG:NH2 | 5:CE:25:ARG:HG2 | 2.22 | 0.54 |
| 5:CE:57:LYS:HB3 | 5:CE:61:TYR:HE2 | 1.72 | 0.54 |
| 8:CH:95:VAL:HG12 | 8:CH:99:GLU:HB2 | 1.88 | 0.54 |
| 9:CI:8:GLY:HA2 | 9:CI:79:LEU:HD12 | 1.90 | 0.54 |
| 13:CM:25:ILE:CD1 | 13:CM:66:LEU:HD23 | 2.37 | 0.54 |
| 17:CQ:23:VAL:O | 17:CQ:39:SER:HB2 | 2.06 | 0.54 |
| 17:CQ:86:GLU:O | 17:CQ:90:ILE:HG12 | 2.07 | 0.54 |
| 22:D0:36:ILE:C | 22:D0:36:ILE:HD13 | 2.27 | 0.54 |
| 24:D2:49:LYS:O | 24:D2:50:ILE:C | 2.46 | 0.54 |
| 28:D6:42:TRP:HA | 28:D6:42:TRP:HE3 | 1.72 | 0.54 |
| 31:DA:1106:A:H2' | 31:DA:1107:G:O5' | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:2394:C:P | 41:DP:63:PRO:HD2 | 2.47 | 0.54 |
| 31:DA:344:G:O2' | 31:DA:345:A:H5' | 2.07 | 0.54 |
| 31:DA:828:U:H4' | 31:DA:831:G:N1 | 2.23 | 0.54 |
| 33:DD:35:LYS:CE | 33:DD:64:ILE:C | 2.73 | 0.54 |
| 36:DG:12:TYR:HA | 36:DG:16:ARG:HG3 | 1.89 | 0.54 |
| 40:DO:112:MET:HA | 40:DO:112:MET:HE3 | 1.89 | 0.54 |
| 45:DT:26:ASP:HB3 | 45:DT:89:VAL:O | 2.07 | 0.54 |
| 46:DU:92:ARG:HD2 | 47:DV:11:GLN:CG | 2.37 | 0.54 |
| 49:DX:85:PRO:O | 49:DX:86:GLY:C | 2.44 | 0.54 |
| 51:DZ:27:VAL:HG23 | 51:DZ:36:LYS:HA | 1.89 | 0.54 |
| 1:AA:191:G:H1' | 20:AT:105:SER:HA | 1.89 | 0.54 |
| 2:AB:14:GLY:O | 2:AB:15:VAL:HG13 | 2.08 | 0.54 |
| 3:AC:102:ASN:O | 3:AC:103:VAL:HG23 | 2.08 | 0.54 |
| 4:AD:108:LEU:O | 4:AD:110:PHE:CD1 | 2.60 | 0.54 |
| 4:AD:31:CYS:C | 4:AD:33:MET:N | 2.58 | 0.54 |
| 20:AT:56:MET:CG | 20:AT:88:VAL:HG21 | 2.37 | 0.54 |
| 31:BA:1803:A:O2' | 33:BD:259:THR:HG21 | 2.07 | 0.54 |
| 31:BA:2660:A:H5'' | 31:BA:2661:G:H21 | 1.73 | 0.54 |
| 31:BA:2795:G:N2 | 31:BA:2796:U:O2' | 2.40 | 0.54 |
| 31:BA:2884:U:H2' | 31:BA:2885:C:H5' | 1.88 | 0.54 |
| 31:BA:985:C:H2' | 31:BA:986:C:H6 | 1.72 | 0.54 |
| 34:BE:103:ASP:OD2 | 34:BE:168:MET:HE1 | 2.08 | 0.54 |
| 38:BI:110:ASP:C | 38:BI:112:LYS:H | 2.11 | 0.54 |
| 43:BR:103:ARG:NH1 | 43:BR:108:GLY:O | 2.40 | 0.54 |
| 46:BU:92:ARG:CZ | 47:BV:11:GLN:HG2 | 2.38 | 0.54 |
| 51:BZ:165:VAL:HG12 | 51:BZ:166:SER:HG | 1.73 | 0.54 |
| 1:CA:1366:C:OP1 | 9:CI:117:HIS:CE1 | 2.60 | 0.54 |
| 1:CA:1492:A:H5' | 1:CA:1493:A:OP2 | 2.06 | 0.54 |
| 1:CA:425:G:H2' | 1:CA:426:G:H5' | 1.89 | 0.54 |
| 1:CA:832:C:O2' | 1:CA:833:U:P | 2.65 | 0.54 |
| 1:CA:92:C:H2' | 1:CA:93:G:C8 | 2.43 | 0.54 |
| 2:CB:84:GLU:OE1 | 2:CB:219:VAL:HB | 2.07 | 0.54 |
| 1:CA:412:A:C8 | 4:CD:35:ARG:NH2 | 2.75 | 0.54 |
| 4:CD:9:CYS:HA | 4:CD:12:CYS:HB2 | 1.89 | 0.54 |
| 6:CF:39:LYS:CB | 6:CF:62:TRP:HZ3 | 2.20 | 0.54 |
| 7:CG:50:ILE:HD12 | 7:CG:61:VAL:HG11 | 1.90 | 0.54 |
| 1:CA:1348:U:H4' | 9:CI:120:ARG:HD2 | 1.89 | 0.54 |
| 16:CP:17:TYR:CE1 | 16:CP:41:PRO:HG3 | 2.42 | 0.54 |
| 28:D6:32:ASN:O | 28:D6:33:LYS:HB2 | 2.07 | 0.54 |
| 31:DA:1288:U:H4' | 31:DA:1289:C:OP2 | 2.08 | 0.54 |
| 31:DA:1417:C:C2' | 31:DA:1418:G:H5' | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:1578:U:OP2 | 31:DA:1578:U:H6 | 1.91 | 0.54 |
| 31:DA:559:G:H22 | 46:DU:49:HIS:CD2 | 2.26 | 0.54 |
| 35:DF:65:TRP:CZ3 | 35:DF:72:ARG:HB3 | 2.42 | 0.54 |
| 39:DN:65:LYS:HD2 | 39:DN:67:LEU:HG | 1.89 | 0.54 |
| 39:DN:68:GLU:HG2 | 39:DN:86:PRO:HG3 | 1.90 | 0.54 |
| 42:DQ:16:ARG:NH1 | 42:DQ:16:ARG:HB2 | 2.20 | 0.54 |
| 44:DS:76:LYS:O | 44:DS:79:ALA:HB3 | 2.08 | 0.54 |
| 44:DS:97:ARG:CD | 44:DS:97:ARG:C | 2.75 | 0.54 |
| 48:DW:20:VAL:O | 48:DW:23:LEU:HB2 | 2.07 | 0.54 |
| 1:AA:159:G:H2' | 1:AA:161:A:OP2 | 2.08 | 0.54 |
| 1:AA:159:G:N2 | 1:AA:161:A:H3' | 2.21 | 0.54 |
| 1:AA:165:C:H2' | 1:AA:166:G:C8 | 2.42 | 0.54 |
| 1:AA:242:C:H2' | 1:AA:243:A:H5' | 1.88 | 0.54 |
| 1:AA:590:C:H2' | 1:AA:591:U:H6 | 1.73 | 0.54 |
| 1:AA:951:G:H1' | 1:AA:970:C:O2' | 2.07 | 0.54 |
| 1:AA:986:A:H2' | 1:AA:987:G:O4' | 2.08 | 0.54 |
| 5:AE:79:GLU:HB3 | 5:AE:92:LYS:HG3 | 1.89 | 0.54 |
| 6:AF:39:LYS:HB2 | 6:AF:62:TRP:HZ3 | 1.73 | 0.54 |
| 7:AG:75:VAL:HG21 | 7:AG:144:MET:HB3 | 1.88 | 0.54 |
| 8:AH:51:VAL:HG11 | 8:AH:60:ARG:CG | 2.37 | 0.54 |
| 15:AO:82:ILE:HD11 | 15:AO:87:ILE:O | 2.08 | 0.54 |
| 27:B5:50:GLY:O | 27:B5:51:TYR:CD1 | 2.60 | 0.54 |
| 31:BA:1526:G:C6 | 31:BA:1527:G:C2 | 2.95 | 0.54 |
| 31:BA:1858:G:O2' | 31:BA:1884:A:N6 | 2.40 | 0.54 |
| 23:B1:47:GLN:CG | 31:BA:2230:G:H1' | 2.28 | 0.54 |
| 31:BA:2342:C:H6 | 31:BA:2342:C:OP2 | 1.90 | 0.54 |
| 31:BA:2661:G:N7 | 31:BA:2662:A:C2 | 2.75 | 0.54 |
| 31:BA:271(T):C:H2' | 31:BA:271(T):C:O2 | 2.07 | 0.54 |
| 31:BA:531:C:H4' | 31:BA:532:A:H5'' | 1.90 | 0.54 |
| 31:BA:607:U:OP1 | 35:BF:102:PRO:HA | 2.06 | 0.54 |
| 31:BA:863:A:C2' | 31:BA:864:G:H5' | 2.36 | 0.54 |
| 31:BA:90:U:H1' | 31:BA:92:A:H5'' | 1.89 | 0.54 |
| 31:BA:910:A:C4 | 42:BQ:13:GLN:OE1 | 2.61 | 0.54 |
| 33:BD:132:PRO:O | 33:BD:136:ILE:HD12 | 2.07 | 0.54 |
| 37:BH:153:LYS:HG2 | 37:BH:154:PRO:N | 2.23 | 0.54 |
| 38:BI:61:ARG:O | 38:BI:133:HIS:CE1 | 2.60 | 0.54 |
| 39:BN:128:HIS:NE2 | 39:BN:131:GLN:OE1 | 2.40 | 0.54 |
| 39:BN:68:GLU:HG2 | 39:BN:86:PRO:HG3 | 1.89 | 0.54 |
| 40:BO:13:ASN:HD21 | 40:BO:97:ARG:N | 2.02 | 0.54 |
| 41:BP:16:ARG:O | 41:BP:16:ARG:NH1 | 2.41 | 0.54 |
| 42:BQ:78:PRO:O | 42:BQ:79:LEU:CG | 2.55 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 44:BS:28:VAL:O | 44:BS:89:ARG:CD | 2.55 | 0.54 |
| 46:BU:88:ILE:O | 46:BU:90:VAL:N | 2.40 | 0.54 |
| 47:BV:19:LYS:CD | 47:BV:20:LEU:H | 2.21 | 0.54 |
| 51:BZ:102:LEU:HD11 | 51:BZ:124:ILE:HG22 | 1.89 | 0.54 |
| 51:BZ:145:GLU:HG3 | 51:BZ:146:ILE:H | 1.73 | 0.54 |
| 1:CA:1442(B):A:N1 | 45:DT:118:ARG:NH2 | 2.54 | 0.54 |
| 1:CA:1452:C:H5' | 1:CA:1456:G:C4 | 2.41 | 0.54 |
| 1:CA:660:G:H2' | 1:CA:661:G:O4' | 2.06 | 0.54 |
| 1:CA:683:G:C6 | 1:CA:684:A:C5 | 2.95 | 0.54 |
| 2:CB:71:VAL:HG22 | 2:CB:93:VAL:HB | 1.90 | 0.54 |
| 3:CC:126:ARG:O | 3:CC:127:ARG:HB2 | 2.08 | 0.54 |
| 4:CD:90:GLY:O | 4:CD:94:LEU:HD12 | 2.07 | 0.54 |
| 9:CI:17:VAL:HG22 | 9:CI:63:ILE:HG12 | 1.90 | 0.54 |
| 12:CL:62:SER:C | 12:CL:64:TYR:H | 2.10 | 0.54 |
| 16:CP:21:VAL:HG22 | 16:CP:34:GLU:O | 2.08 | 0.54 |
| 23:D1:89:GLU:O | 23:D1:93:GLU:N | 2.39 | 0.54 |
| 27:D5:11:THR:CG2 | 31:DA:1264:G:H5' | 2.38 | 0.54 |
| 30:D8:35:GLN:HA | 31:DA:2420:C:P | 2.48 | 0.54 |
| 31:DA:146:G:H2' | 31:DA:147:U:O4' | 2.07 | 0.54 |
| 31:DA:2557:G:H2' | 31:DA:2558:C:C6 | 2.43 | 0.54 |
| 31:DA:1051:G:H5' | 31:DA:2752:C:O2' | 2.07 | 0.54 |
| 31:DA:2801(A):A:C3' | 31:DA:2802:G:H5' | 2.37 | 0.54 |
| 31:DA:708:C:H42 | 31:DA:723:G:H1 | 1.55 | 0.54 |
| 33:DD:209:ALA:C | 33:DD:210:GLY:O | 2.42 | 0.54 |
| 33:DD:8:PRO:HB3 | 33:DD:14:ARG:CB | 2.34 | 0.54 |
| 35:DF:53:THR:HG22 | 35:DF:55:GLY:CA | 2.37 | 0.54 |
| 36:DG:20:ILE:O | 36:DG:24:GLY:HA2 | 2.07 | 0.54 |
| 41:DP:108:LYS:C | 41:DP:110:TYR:H | 2.10 | 0.54 |
| 41:DP:112:LEU:H | 41:DP:128:HIS:CD2 | 2.23 | 0.54 |
| 41:DP:71:VAL:CG1 | 41:DP:72:PRO:CD | 2.86 | 0.54 |
| 44:DS:95:HIS:CG | 44:DS:96:GLY:N | 2.76 | 0.54 |
| 47:DV:47:VAL:HG21 | 47:DV:49:THR:HB | 1.88 | 0.54 |
| 47:DV:72:VAL:CA | 47:DV:88:ARG:HH12 | 2.15 | 0.54 |
| 49:DX:60:ARG:CG | 49:DX:71:GLY:HA3 | 2.36 | 0.54 |
| 50:DY:13:VAL:HG12 | 50:DY:73:ARG:C | 2.28 | 0.54 |
| 50:DY:61:ILE:N | 50:DY:61:ILE:HD12 | 2.23 | 0.54 |
| 1:AA:37:U:O2' | 1:AA:38:G:H5' | 2.06 | 0.54 |
| 1:AA:425:G:H2' | 1:AA:426:G:H5' | 1.88 | 0.54 |
| 1:AA:719:C:H5 | 1:AA:720:C:C4 | 2.25 | 0.54 |
| 3:AC:138:VAL:HG22 | 3:AC:151:VAL:CG2 | 2.36 | 0.54 |
| 26:B4:29:PRO:C | 26:B4:31:ILE:H | 2.10 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:B6:19:ARG:HH11 | 31:BA:2400:G:H4' | 1.73 | 0.54 |
| 28:B6:28:ARG:CA | 28:B6:32:ASN:HB3 | 2.36 | 0.54 |
| 31:BA:142:A:C8 | 31:BA:1595:G:N2 | 2.61 | 0.54 |
| 31:BA:1657:C:H2' | 31:BA:1658:C:C6 | 2.42 | 0.54 |
| 31:BA:2464:C:O2' | 31:BA:2465:C:P | 2.65 | 0.54 |
| 35:BF:119:ARG:HG2 | 35:BF:119:ARG:O | 2.06 | 0.54 |
| 37:BH:158:HIS:CE1 | 37:BH:168:PRO:C | 2.81 | 0.54 |
| 39:BN:45:ASN:ND2 | 39:BN:45:ASN:H | 1.98 | 0.54 |
| 31:BA:587:C:H5 | 41:BP:33:ARG:HH11 | 1.55 | 0.54 |
| 31:BA:2394:C:P | 41:BP:63:PRO:HD2 | 2.47 | 0.54 |
| 44:BS:34:HIS:N | 44:BS:34:HIS:CD2 | 2.73 | 0.54 |
| 45:BT:16:ARG:H | 45:BT:79:HIS:CD2 | 2.25 | 0.54 |
| 45:BT:32:TYR:HD2 | 45:BT:81:PRO:O | 1.90 | 0.54 |
| 49:BX:53:LYS:N | 49:BX:80:ILE:HG22 | 2.21 | 0.54 |
| 51:BZ:101:PRO:O | 51:BZ:102:LEU:CD2 | 2.52 | 0.54 |
| 1:CA:159:G:H2' | 1:CA:161:A:OP2 | 2.08 | 0.54 |
| 1:CA:189:G:C6 | 1:CA:189(A):C:N4 | 2.76 | 0.54 |
| 2:CB:121:LEU:O | 2:CB:121:LEU:HD23 | 2.07 | 0.54 |
| 8:CH:44:PHE:HA | 8:CH:79:VAL:HG11 | 1.89 | 0.54 |
| 9:CI:122:ALA:HB1 | 9:CI:123:PRO:HD2 | 1.88 | 0.54 |
| 23:D1:19:GLN:CD | 23:D1:44:PRO:HB3 | 2.27 | 0.54 |
| 24:D2:30:ARG:H | 24:D2:30:ARG:CD | 2.15 | 0.54 |
| 31:DA:1486:A:H2' | 31:DA:1487:G:H8 | 1.72 | 0.54 |
| 31:DA:2756:U:H4' | 31:DA:2757:A:OP1 | 2.07 | 0.54 |
| 33:DD:35:LYS:N | 33:DD:64:ILE:HG23 | 2.22 | 0.54 |
| 34:DE:51:PHE:CD1 | 34:DE:52:LEU:N | 2.75 | 0.54 |
| 35:DF:53:THR:H | 35:DF:56:GLU:HB2 | 1.73 | 0.54 |
| 42:DQ:29:PHE:HD1 | 42:DQ:29:PHE:N | 2.06 | 0.54 |
| 45:DT:33:LYS:NZ | 45:DT:33:LYS:CA | 2.71 | 0.54 |
| 45:DT:33:LYS:NZ | 45:DT:33:LYS:H | 2.05 | 0.54 |
| 42:DQ:108:GLY:HA3 | 51:DZ:116:VAL:HG21 | 1.89 | 0.54 |
| 1:AA:1113:C:H2' | 1:AA:1114:C:C6 | 2.42 | 0.54 |
| 4:AD:31:CYS:O | 4:AD:31:CYS:SG | 2.65 | 0.54 |
| 6:AF:50:TYR:CE2 | 6:AF:52:ILE:HD11 | 2.42 | 0.54 |
| 7:AG:69:VAL:O | 7:AG:71:PRO:HD3 | 2.07 | 0.54 |
| 9:AI:17:VAL:HG22 | 9:AI:63:ILE:HG12 | 1.88 | 0.54 |
| 10:AJ:40:LEU:HD21 | 10:AJ:69:ASN:HB3 | 1.90 | 0.54 |
| 30:B8:35:GLN:NE2 | 30:B8:36:LYS:HZ2 | 2.05 | 0.54 |
| 31:BA:1309:G:O2' | 31:BA:1310:G:H5' | 2.08 | 0.54 |
| 31:BA:864:G:C6 | 31:BA:865:C:N4 | 2.76 | 0.54 |
| 33:BD:255:LYS:HZ2 | 33:BD:255:LYS:C | 2.11 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:BA:773:U:H5' | 33:BD:47:GLY:HA2 | 1.90 | 0.54 |
| 31:BA:320:A:OP2 | 35:BF:137:LYS:HE2 | 2.08 | 0.54 |
| 36:BG:81:LYS:O | 36:BG:82:LEU:O | 2.26 | 0.54 |
| 39:BN:65:LYS:HD2 | 39:BN:67:LEU:HG | 1.90 | 0.54 |
| 49:BX:80:ILE:HG23 | 49:BX:81:VAL:N | 2.22 | 0.54 |
| 50:BY:37:VAL:HG11 | 50:BY:72:VAL:CG2 | 2.38 | 0.54 |
| 1:CA:1386:G:C2 | 1:CA:1387:G:C8 | 2.95 | 0.54 |
| 1:CA:542:G:P | 4:CD:10:ARG:HH21 | 2.30 | 0.54 |
| 1:CA:707:C:O2 | 1:CA:708:C:C6 | 2.61 | 0.54 |
| 1:CA:811:C:O2' | 1:CA:901:A:N1 | 2.39 | 0.54 |
| 1:CA:1112:C:N3 | 3:CC:178:LEU:HD23 | 2.23 | 0.54 |
| 5:CE:145:LYS:O | 5:CE:149:GLU:HG2 | 2.07 | 0.54 |
| 6:CF:89:MET:HG2 | 6:CF:91:VAL:HG23 | 1.87 | 0.54 |
| 7:CG:70:LYS:HB3 | 7:CG:96:GLN:OE1 | 2.08 | 0.54 |
| 9:CI:53:VAL:CG1 | 9:CI:95:LYS:HE3 | 2.38 | 0.54 |
| 10:CJ:40:LEU:HD21 | 10:CJ:69:ASN:HB3 | 1.90 | 0.54 |
| 12:CL:92:ASP:O | 12:CL:93:LEU:HD23 | 2.08 | 0.54 |
| 13:CM:68:GLY:O | 13:CM:69:GLU:HB2 | 2.07 | 0.54 |
| 1:CA:310:G:H5'' | 16:CP:31:LYS:HB2 | 1.89 | 0.54 |
| 31:DA:1179:C:H3' | 31:DA:1180:C:H5'' | 1.90 | 0.54 |
| 31:DA:1568:G:OP2 | 33:DD:63:ARG:NH2 | 2.41 | 0.54 |
| 31:DA:1742:G:H8 | 31:DA:1742:G:H3' | 1.73 | 0.54 |
| 31:DA:2025:C:H2' | 31:DA:2026:C:C6 | 2.43 | 0.54 |
| 31:DA:2286:A:H5'' | 31:DA:2287:A:O4' | 2.07 | 0.54 |
| 31:DA:271(H):G:O2' | 31:DA:271(I):G:H5'' | 2.07 | 0.54 |
| 31:DA:548:A:O2' | 31:DA:549:G:OP1 | 2.22 | 0.54 |
| 31:DA:855:G:C4 | 31:DA:856:C:C5 | 2.96 | 0.54 |
| 36:DG:5:VAL:HB | 36:DG:104:GLU:OE2 | 2.08 | 0.54 |
| 37:DH:92:ILE:O | 37:DH:94:TYR:N | 2.40 | 0.54 |
| 38:DI:15:VAL:HG23 | 38:DI:16:GLY:N | 2.22 | 0.54 |
| 39:DN:13:TRP:O | 39:DN:135:PRO:HG2 | 2.08 | 0.54 |
| 39:DN:74:ARG:NH2 | 39:DN:101:HIS:HB3 | 2.22 | 0.54 |
| 31:DA:833:U:H5'' | 41:DP:48:PRO:HB3 | 1.89 | 0.54 |
| 43:DR:10:LEU:HD22 | 43:DR:17:ARG:HD2 | 1.89 | 0.54 |
| 45:DT:42:ILE:HG13 | 45:DT:42:ILE:O | 2.07 | 0.54 |
| 24:D2:55:ARG:HH22 | 49:DX:3:THR:CG2 | 2.21 | 0.54 |
| 50:DY:20:TYR:CD2 | 50:DY:41:GLY:HA2 | 2.43 | 0.54 |
| 51:DZ:40:ASP:HB3 | 51:DZ:43:GLU:HB2 | 1.89 | 0.54 |
| 1:AA:1312:G:N2 | 1:AA:1326:C:C2 | 2.75 | 0.54 |
| 1:AA:1410:G:O2' | 1:AA:1411:C:H5' | 2.08 | 0.54 |
| 1:AA:200:G:H1 | 1:AA:217:C:N4 | 1.99 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:310:G:H5'' | 16:AP:31:LYS:HB2 | 1.88 | 0.54 |
| 2:AB:144:ARG:HA | 2:AB:147:LYS:HB2 | 1.89 | 0.54 |
| 1:AA:542:G:P | 4:AD:10:ARG:HH21 | 2.30 | 0.54 |
| 4:AD:79:PHE:CG | 4:AD:207:TYR:HD1 | 2.25 | 0.54 |
| 8:AH:95:VAL:HG12 | 8:AH:99:GLU:HB2 | 1.88 | 0.54 |
| 12:AL:110:VAL:CG2 | 12:AL:120:TYR:HB3 | 2.37 | 0.54 |
| 12:AL:46:LYS:HD3 | 12:AL:94:PRO:CG | 2.38 | 0.54 |
| 31:BA:1396:U:O2 | 31:BA:1396:U:C2' | 2.56 | 0.54 |
| 31:BA:1515:G:H2' | 31:BA:1516:C:H6 | 1.72 | 0.54 |
| 31:BA:2075:U:H2' | 31:BA:2238:G:N2 | 2.22 | 0.54 |
| 31:BA:2660:A:H3' | 31:BA:2661:G:O4' | 2.07 | 0.54 |
| 31:BA:836:G:C5 | 31:BA:837:C:C4 | 2.96 | 0.54 |
| 31:BA:876:C:C4 | 31:BA:877:U:C5 | 2.96 | 0.54 |
| 36:BG:19:LEU:HD13 | 36:BG:32:PRO:HG2 | 1.89 | 0.54 |
| 36:BG:91:ARG:C | 36:BG:91:ARG:HD2 | 2.28 | 0.54 |
| 1:AA:1422:G:O3' | 40:BO:49:ARG:NH2 | 2.40 | 0.54 |
| 41:BP:88:LEU:HD11 | 41:BP:95:VAL:HG21 | 1.88 | 0.54 |
| 31:BA:106:C:H1' | 50:BY:2:ARG:HE | 1.72 | 0.54 |
| 1:CA:1079:G:O3' | 5:CE:14:ARG:NH2 | 2.41 | 0.54 |
| 1:CA:1312:G:N2 | 1:CA:1326:C:C2 | 2.76 | 0.54 |
| 1:CA:189:G:C6 | 1:CA:189(A):C:C4 | 2.95 | 0.54 |
| 2:CB:14:GLY:O | 2:CB:15:VAL:HG13 | 2.07 | 0.54 |
| 3:CC:11:ARG:O | 3:CC:14:ILE:O | 2.25 | 0.54 |
| 1:CA:673:G:O3' | 6:CF:87:ARG:NH2 | 2.41 | 0.54 |
| 12:CL:46:LYS:HG2 | 12:CL:47:LYS:N | 2.22 | 0.54 |
| 1:CA:235:C:H5' | 17:CQ:70:ARG:HG2 | 1.88 | 0.54 |
| 31:DA:1328:G:H2' | 31:DA:1330:C:C5 | 2.43 | 0.54 |
| 31:DA:2272:U:H5'' | 31:DA:2273:A:OP1 | 2.06 | 0.54 |
| 31:DA:2404:C:C2' | 31:DA:2405:G:H5' | 2.37 | 0.54 |
| 31:DA:301:G:C4 | 31:DA:302:C:C5 | 2.96 | 0.54 |
| 31:DA:577:G:O2' | 31:DA:1254:A:OP1 | 2.26 | 0.54 |
| 31:DA:68:G:H2' | 31:DA:69:C:C6 | 2.42 | 0.54 |
| 31:DA:870:A:C2 | 31:DA:908:C:C2 | 2.96 | 0.54 |
| 32:DB:66:A:C5 | 32:DB:109:C:C5 | 2.96 | 0.54 |
| 39:DN:130:HIS:O | 39:DN:130:HIS:CD2 | 2.61 | 0.54 |
| 40:DO:104:ARG:O | 40:DO:107:ARG:HB3 | 2.08 | 0.54 |
| 43:DR:116:LEU:O | 43:DR:117:VAL:CB | 2.55 | 0.54 |
| 43:DR:18:LEU:O | 43:DR:19:ALA:C | 2.43 | 0.54 |
| 45:DT:23:ARG:HB2 | 45:DT:24:PRO:CD | 2.37 | 0.54 |
| 45:DT:40:THR:O | 45:DT:41:ARG:HB2 | 2.08 | 0.54 |
| 46:DU:83:LEU:CB | 46:DU:88:ILE:HD11 | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:DX:41:ASN:O | 49:DX:45:THR:HG23 | 2.06 | 0.54 |
| 1:AA:327:A:O2' | 1:AA:329:A:H8 | 1.91 | 0.54 |
| 2:AB:32:ILE:HD12 | 2:AB:42:ILE:HA | 1.89 | 0.54 |
| 2:AB:74:LYS:O | 2:AB:78:GLN:HG3 | 2.08 | 0.54 |
| 4:AD:14:ARG:HA | 4:AD:39:PRO:HG3 | 1.89 | 0.54 |
| 6:AF:12:PRO:CB | 6:AF:57:GLN:HB2 | 2.36 | 0.54 |
| 9:AI:53:VAL:CG1 | 9:AI:95:LYS:HE3 | 2.38 | 0.54 |
| 6:AF:89:MET:SD | 18:AR:76:LEU:HD21 | 2.48 | 0.54 |
| 23:B1:94:LEU:HD22 | 23:B1:95:LEU:HB2 | 1.90 | 0.54 |
| 30:B8:60:LEU:C | 30:B8:63:PRO:HD2 | 2.28 | 0.54 |
| 31:BA:1270:C:H5'' | 31:BA:1271:G:O5' | 2.08 | 0.54 |
| 31:BA:562:U:C4 | 31:BA:2036:C:O4' | 2.61 | 0.54 |
| 31:BA:271(P):C:H2' | 31:BA:271(Q):G:H5' | 1.90 | 0.54 |
| 31:BA:52:A:C2' | 31:BA:53:A:H5' | 2.38 | 0.54 |
| 33:BD:35:LYS:CE | 33:BD:64:ILE:O | 2.56 | 0.54 |
| 34:BE:34:VAL:CG2 | 34:BE:48:GLN:HE21 | 2.20 | 0.54 |
| 35:BF:185:ASP:HA | 35:BF:188:ARG:HG2 | 1.89 | 0.54 |
| 37:BH:85:LYS:CE | 37:BH:133:VAL:HB | 2.37 | 0.54 |
| 37:BH:85:LYS:HE2 | 37:BH:145:ALA:HB2 | 1.89 | 0.54 |
| 45:BT:91:ARG:HB2 | 45:BT:116:ALA:HA | 1.89 | 0.54 |
| 45:BT:68:TYR:N | 45:BT:68:TYR:CD2 | 2.75 | 0.54 |
| 1:CA:1428:A:H2' | 1:CA:1429:C:C6 | 2.42 | 0.54 |
| 1:CA:189(J):G:O2' | 1:CA:189(K):U:H5' | 2.07 | 0.54 |
| 2:CB:20:GLU:HG3 | 2:CB:189:ASP:OD2 | 2.08 | 0.54 |
| 4:CD:13:ARG:O | 4:CD:15:GLU:N | 2.41 | 0.54 |
| 30:D8:14:VAL:CG1 | 30:D8:22:VAL:HG13 | 2.37 | 0.54 |
| 31:DA:1001:A:H2' | 31:DA:1002:G:O4' | 2.06 | 0.54 |
| 31:DA:1109:C:C5 | 31:DA:1110:G:C4 | 2.96 | 0.54 |
| 31:DA:1142(A):A:C4 | 31:DA:1144:G:C8 | 2.96 | 0.54 |
| 31:DA:2000:G:OP2 | 43:DR:3:HIS:CE1 | 2.61 | 0.54 |
| 31:DA:2496:C:OP1 | 42:DQ:82:ARG:HD3 | 2.08 | 0.54 |
| 31:DA:307:G:H22 | 31:DA:310:A:H5'' | 1.73 | 0.54 |
| 31:DA:90:U:O2 | 31:DA:90:U:C2' | 2.51 | 0.54 |
| 31:DA:966:G:H2' | 31:DA:967:C:H6 | 1.72 | 0.54 |
| 31:DA:2579:C:O3' | 34:DE:131:ALA:HB3 | 2.08 | 0.54 |
| 34:DE:160:TYR:CD2 | 34:DE:161:GLY:N | 2.76 | 0.54 |
| 41:DP:105:LEU:HD12 | 41:DP:105:LEU:N | 2.22 | 0.54 |
| 42:DQ:38:GLU:OE2 | 42:DQ:127:ILE:HG22 | 2.08 | 0.54 |
| 43:DR:101:ALA:O | 43:DR:102:GLU:HB2 | 2.08 | 0.54 |
| 32:DB:117:G:H4' | 44:DS:55:ALA:HB1 | 1.90 | 0.54 |
| 45:DT:78:LEU:C | 45:DT:79:HIS:ND1 | 2.61 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:329:G:OP2 | 50:DY:71:LYS:HE2 | 2.07 | 0.54 |
| 50:DY:8:LYS:H | 50:DY:8:LYS:HD2 | 1.73 | 0.54 |
| 51:DZ:65:GLN:OE1 | 51:DZ:67:LEU:HD11 | 2.08 | 0.54 |
| 1:AA:1258:G:O2' | 1:AA:1259:C:H5' | 2.07 | 0.54 |
| 1:AA:1385:G:C2 | 1:AA:1386:G:C8 | 2.96 | 0.54 |
| 1:AA:189(B):C:H42 | 1:AA:189(I):G:H1 | 1.56 | 0.54 |
| 1:AA:551:U:O2' | 12:AL:86:ARG:HD2 | 2.08 | 0.54 |
| 1:AA:658:G:C4 | 1:AA:659:U:C5 | 2.95 | 0.54 |
| 1:AA:69:G:C2 | 1:AA:70:G:C5 | 2.96 | 0.54 |
| 1:AA:832:C:O2' | 1:AA:833:U:P | 2.65 | 0.54 |
| 3:AC:52:LEU:CD2 | 3:AC:52:LEU:H | 2.19 | 0.54 |
| 1:AA:7:G:H21 | 5:AE:121:LYS:HG2 | 1.72 | 0.54 |
| 6:AF:8:ILE:HG22 | 6:AF:9:VAL:N | 2.22 | 0.54 |
| 17:AQ:21:VAL:HG21 | 17:AQ:59:ILE:HD11 | 1.89 | 0.54 |
| 18:AR:57:GLY:C | 18:AR:58:LEU:HD12 | 2.29 | 0.54 |
| 20:AT:14:LYS:O | 20:AT:18:GLN:HG3 | 2.07 | 0.54 |
| 31:BA:1459:G:N3 | 31:BA:1459:G:H2' | 2.21 | 0.54 |
| 31:BA:2359:C:C2' | 31:BA:2360:A:C5' | 2.84 | 0.54 |
| 31:BA:2660:A:C2' | 31:BA:2661:G:O5' | 2.55 | 0.54 |
| 31:BA:287:C:C4 | 31:BA:288:C:C5 | 2.96 | 0.54 |
| 34:BE:48:GLN:CG | 34:BE:78:LEU:HB3 | 2.38 | 0.54 |
| 31:BA:322:A:H3' | 35:BF:169:ASN:HD21 | 1.73 | 0.54 |
| 38:BI:13:GLY:O | 38:BI:14:ASP:C | 2.46 | 0.54 |
| 41:BP:146:VAL:HG13 | 41:BP:147:LEU:H | 1.73 | 0.54 |
| 44:BS:54:LEU:HA | 44:BS:57:LYS:O | 2.07 | 0.54 |
| 47:BV:67:GLY:O | 47:BV:69:LYS:N | 2.41 | 0.54 |
| 1:CA:1184:G:H2' | 1:CA:1185:G:C8 | 2.42 | 0.54 |
| 1:CA:173:U:O4' | 1:CA:197:A:C4 | 2.61 | 0.54 |
| 1:CA:510:A:H5'' | 1:CA:511:C:P | 2.48 | 0.54 |
| 1:CA:986:A:H2' | 1:CA:987:G:O4' | 2.08 | 0.54 |
| 4:CD:49:ARG:NE | 4:CD:49:ARG:HA | 2.20 | 0.54 |
| 6:CF:61:LEU:HD23 | 6:CF:63:TYR:OH | 2.07 | 0.54 |
| 10:CJ:61:GLU:OE1 | 14:CN:58:LYS:HE2 | 2.08 | 0.54 |
| 20:CT:93:GLU:O | 20:CT:93:GLU:HG2 | 2.06 | 0.54 |
| 31:DA:1579:A:H2' | 31:DA:1580:A:C8 | 2.43 | 0.54 |
| 31:DA:229:A:H3' | 31:DA:230:U:H5' | 1.89 | 0.54 |
| 31:DA:2762:G:H8 | 31:DA:2762:G:H5' | 1.73 | 0.54 |
| 31:DA:2795:G:N2 | 31:DA:2796:U:O2' | 2.41 | 0.54 |
| 31:DA:477:A:H2' | 31:DA:478:A:C8 | 2.43 | 0.54 |
| 31:DA:661:C:H2' | 31:DA:662:G:C8 | 2.43 | 0.54 |
| 32:DB:43:C:H4' | 36:DG:66:GLN:NE2 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DD:16:MET:HG3 | 33:DD:206:LEU:O | 2.08 | 0.54 |
| 34:DE:93:VAL:N | 34:DE:95:ILE:HD13 | 2.22 | 0.54 |
| 36:DG:58:GLN:HA | 36:DG:61:ALA:HB3 | 1.89 | 0.54 |
| 37:DH:89:ILE:O | 37:DH:90:LYS:CB | 2.56 | 0.54 |
| 38:DI:1:MET:O | 38:DI:20:ASP:HA | 2.08 | 0.54 |
| 41:DP:83:VAL:HG12 | 41:DP:112:LEU:HD21 | 1.89 | 0.54 |
| 44:DS:34:HIS:CD2 | 44:DS:34:HIS:N | 2.76 | 0.54 |
| 47:DV:44:LYS:HG2 | 47:DV:45:THR:H | 1.72 | 0.54 |
| 49:DX:23:GLU:CG | 49:DX:24:GLY:N | 2.70 | 0.54 |
| 1:AA:129:U:O2 | 1:AA:131:C:C5 | 2.60 | 0.54 |
| 1:AA:1371:G:C6 | 1:AA:1372:U:C4 | 2.96 | 0.54 |
| 1:AA:950:U:H2' | 1:AA:951:G:C8 | 2.41 | 0.54 |
| 5:AE:147:ASP:HA | 5:AE:150:ARG:HB3 | 1.89 | 0.54 |
| 5:AE:57:LYS:HB3 | 5:AE:61:TYR:HE2 | 1.73 | 0.54 |
| 6:AF:39:LYS:HB2 | 6:AF:62:TRP:CZ3 | 2.42 | 0.54 |
| 13:AM:106:ASN:O | 13:AM:107:ALA:HB3 | 2.08 | 0.54 |
| 15:AO:74:ASP:OD2 | 15:AO:76:GLU:HB3 | 2.08 | 0.54 |
| 17:AQ:99:SER:O | 17:AQ:100:LYS:HD3 | 2.08 | 0.54 |
| 23:B1:56:GLN:HA | 23:B1:56:GLN:OE1 | 2.06 | 0.54 |
| 23:B1:94:LEU:O | 23:B1:95:LEU:HG | 2.07 | 0.54 |
| 24:B2:34:GLU:N | 24:B2:34:GLU:OE2 | 2.39 | 0.54 |
| 31:BA:1043:C:O2' | 31:BA:1044:G:C8 | 2.58 | 0.54 |
| 31:BA:146:G:H2' | 31:BA:147:U:O4' | 2.08 | 0.54 |
| 31:BA:1859:A:C2 | 31:BA:1884:A:H1' | 2.43 | 0.54 |
| 31:BA:271(J):C:H5' | 31:BA:271(K):U:OP2 | 2.07 | 0.54 |
| 31:BA:661:C:O3' | 41:BP:18:ARG:HD2 | 2.08 | 0.54 |
| 32:BB:31:C:H4' | 36:BG:29:TRP:CH2 | 2.44 | 0.54 |
| 33:BD:35:LYS:HA | 33:BD:64:ILE:CG2 | 2.38 | 0.54 |
| 31:BA:1670:C:O2 | 34:BE:129:HIS:HE1 | 1.91 | 0.54 |
| 36:BG:56:ALA:HA | 36:BG:59:GLU:OE1 | 2.07 | 0.54 |
| 38:BI:125:GLU:OE1 | 38:BI:141:LYS:HG2 | 2.07 | 0.54 |
| 31:BA:661:C:C4' | 41:BP:16:ARG:HH12 | 2.21 | 0.54 |
| 42:BQ:38:GLU:HB2 | 42:BQ:127:ILE:HG22 | 1.88 | 0.54 |
| 42:BQ:18:LYS:O | 42:BQ:19:GLY:C | 2.45 | 0.54 |
| 48:BW:2:GLU:OE1 | 48:BW:72:LYS:NZ | 2.41 | 0.54 |
| 24:B2:26:ARG:HG2 | 49:BX:5:TYR:CB | 2.36 | 0.54 |
| 50:BY:13:VAL:HG12 | 50:BY:73:ARG:C | 2.28 | 0.54 |
| 1:CA:450:G:H1 | 1:CA:483:C:H42 | 1.55 | 0.54 |
| 6:CF:37:VAL:HG12 | 6:CF:38:GLU:N | 2.23 | 0.54 |
| 8:CH:86:ILE:HG22 | 8:CH:87:SER:N | 2.21 | 0.54 |
| 9:CI:105:ASP:OD1 | 9:CI:107:ARG:HD3 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:CM:81:LEU:HD21 | 13:CM:88:ARG:HH22 | 1.73 | 0.54 |
| 1:CA:472:A:C4' | 16:CP:82:GLN:HE22 | 2.19 | 0.54 |
| 24:D2:43:GLN:O | 24:D2:46:GLN:HB3 | 2.08 | 0.54 |
| 24:D2:49:LYS:HE2 | 31:DA:76:C:OP1 | 2.07 | 0.54 |
| 27:D5:41:PRO:HG2 | 27:D5:44:THR:OG1 | 2.08 | 0.54 |
| 30:D8:35:GLN:HE21 | 30:D8:36:LYS:HG3 | 1.73 | 0.54 |
| 30:D8:6:THR:CG2 | 31:DA:243:U:OP1 | 2.55 | 0.54 |
| 31:DA:1947:C:C2' | 31:DA:1948:G:H5'' | 2.38 | 0.54 |
| 31:DA:2186:G:H2' | 31:DA:2187:G:H5'' | 1.90 | 0.54 |
| 31:DA:257:A:H2' | 31:DA:258:G:H5' | 1.90 | 0.54 |
| 23:D1:34:THR:HG23 | 31:DA:388:G:P | 2.47 | 0.54 |
| 31:DA:547:A:C8 | 31:DA:549:G:C6 | 2.96 | 0.54 |
| 33:DD:118:VAL:HG22 | 33:DD:119:ALA:H | 1.73 | 0.54 |
| 33:DD:39:LYS:HB2 | 33:DD:62:TYR:HB2 | 1.90 | 0.54 |
| 37:DH:153:LYS:CD | 37:DH:153:LYS:N | 2.71 | 0.54 |
| 39:DN:15:LEU:HD22 | 39:DN:16:ILE:H | 1.73 | 0.54 |
| 41:DP:23:PRO:HB2 | 41:DP:33:ARG:HG3 | 1.90 | 0.54 |
| 44:DS:63:THR:O | 44:DS:66:ALA:O | 2.26 | 0.54 |
| 45:DT:32:TYR:HB3 | 45:DT:81:PRO:CB | 2.38 | 0.54 |
| 49:DX:63:LYS:HE3 | 49:DX:70:LEU:CD2 | 2.34 | 0.54 |
| 51:DZ:124:ILE:HG13 | 51:DZ:125:LEU:N | 2.23 | 0.54 |
| 51:DZ:144:LEU:HD22 | 51:DZ:144:LEU:N | 2.23 | 0.54 |
| 1:AA:1399:C:H4' | 1:AA:1400:C:H5'' | 1.90 | 0.53 |
| 1:AA:377:G:OP1 | 16:AP:3:LYS:HD2 | 2.08 | 0.53 |
| 1:AA:854:G:H3' | 1:AA:871:U:O4 | 2.08 | 0.53 |
| 6:AF:73:ASN:O | 6:AF:76:ALA:HB3 | 2.09 | 0.53 |
| 7:AG:50:ILE:HD12 | 7:AG:61:VAL:HG11 | 1.89 | 0.53 |
| 8:AH:44:PHE:HA | 8:AH:79:VAL:HG11 | 1.90 | 0.53 |
| 11:AK:84:VAL:O | 11:AK:85:ARG:HG3 | 2.08 | 0.53 |
| 12:AL:32:PHE:HB3 | 12:AL:85:ILE:O | 2.08 | 0.53 |
| 13:AM:78:ILE:HA | 13:AM:81:LEU:HD12 | 1.90 | 0.53 |
| 6:AF:96:PRO:HB3 | 18:AR:30:ASP:OD2 | 2.08 | 0.53 |
| 31:BA:1106:A:C2' | 31:BA:1107:G:O5' | 2.56 | 0.53 |
| 31:BA:1268:A:C2 | 31:BA:2013:A:C4 | 2.97 | 0.53 |
| 31:BA:1472:A:H2' | 31:BA:1473:G:H5' | 1.91 | 0.53 |
| 31:BA:175:G:H5' | 31:BA:175:G:H8 | 1.73 | 0.53 |
| 31:BA:1822:G:C5' | 31:BA:1822:G:H8 | 2.12 | 0.53 |
| 31:BA:2461:C:H2' | 31:BA:2462:U:C6 | 2.43 | 0.53 |
| 31:BA:662:G:OP1 | 41:BP:18:ARG:NH1 | 2.42 | 0.53 |
| 31:BA:993:G:OP1 | 47:BV:75:PHE:CE2 | 2.61 | 0.53 |
| 33:BD:255:LYS:O | 33:BD:255:LYS:HD2 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BG:60:LEU:O | 36:BG:64:THR:HG22 | 2.08 | 0.53 |
| 36:BG:47:LYS:CD | 36:BG:81:LYS:HD2 | 2.29 | 0.53 |
| 38:BI:10:GLU:O | 38:BI:12:LEU:HD23 | 2.06 | 0.53 |
| 41:BP:96:THR:HG22 | 41:BP:126:VAL:CG2 | 2.38 | 0.53 |
| 42:BQ:29:PHE:CD1 | 42:BQ:29:PHE:N | 2.76 | 0.53 |
| 44:BS:38:GLN:HG2 | 44:BS:47:THR:CG2 | 2.39 | 0.53 |
| 45:BT:28:VAL:HG21 | 45:BT:46:GLU:HG3 | 1.89 | 0.53 |
| 31:BA:535:C:O3' | 46:BU:53:ARG:NH1 | 2.41 | 0.53 |
| 50:BY:29:GLU:N | 50:BY:29:GLU:OE1 | 2.41 | 0.53 |
| 50:BY:49:VAL:HG12 | 50:BY:53:PRO:HG3 | 1.90 | 0.53 |
| 1:CA:321:A:N6 | 1:CA:328:C:H1' | 2.22 | 0.53 |
| 1:CA:636:U:H2' | 1:CA:637:G:C8 | 2.42 | 0.53 |
| 3:CC:73:PRO:HA | 3:CC:76:VAL:HG13 | 1.89 | 0.53 |
| 4:CD:62:GLN:NE2 | 4:CD:65:ARG:HE | 2.06 | 0.53 |
| 1:CA:450:G:C5' | 16:CP:41:PRO:O | 2.54 | 0.53 |
| 20:CT:11:SER:HA | 20:CT:13:LEU:CD1 | 2.37 | 0.53 |
| 27:D5:55:ARG:C | 27:D5:56:LYS:HG3 | 2.28 | 0.53 |
| 31:DA:999:U:O2' | 31:DA:1000:A:H5' | 2.08 | 0.53 |
| 31:DA:107:C:N3 | 31:DA:108:U:C5 | 2.76 | 0.53 |
| 31:DA:1505:C:H2' | 31:DA:1506:C:O4' | 2.07 | 0.53 |
| 31:DA:271(D):G:H2' | 31:DA:271(E):U:O4' | 2.08 | 0.53 |
| 31:DA:259:G:N2 | 31:DA:621:A:H8 | 2.04 | 0.53 |
| 31:DA:662:G:OP1 | 41:DP:18:ARG:NH1 | 2.41 | 0.53 |
| 33:DD:43:ARG:HD2 | 33:DD:44:ASN:OD1 | 2.08 | 0.53 |
| 34:DE:36:ARG:NH1 | 34:DE:85:ASN:ND2 | 2.56 | 0.53 |
| 34:DE:65:GLY:C | 34:DE:67:PHE:H | 2.11 | 0.53 |
| 34:DE:70:ALA:O | 34:DE:72:VAL:O | 2.25 | 0.53 |
| 36:DG:45:GLU:HB2 | 36:DG:47:LYS:HG3 | 1.90 | 0.53 |
| 31:DA:2690:C:OP1 | 43:DR:17:ARG:NH1 | 2.41 | 0.53 |
| 43:DR:87:TYR:HE1 | 43:DR:117:VAL:HG12 | 1.72 | 0.53 |
| 44:DS:17:ARG:O | 44:DS:18:ILE:HB | 2.07 | 0.53 |
| 45:DT:34:VAL:O | 45:DT:35:LYS:HB3 | 2.08 | 0.53 |
| 45:DT:31:SER:HB3 | 45:DT:43:GLN:O | 2.08 | 0.53 |
| 49:DX:40:LYS:O | 49:DX:42:ALA:N | 2.41 | 0.53 |
| 49:DX:85:PRO:O | 49:DX:87:GLN:N | 2.41 | 0.53 |
| 50:DY:52:SER:C | 50:DY:54:LYS:H | 2.12 | 0.53 |
| 1:AA:1468:A:H2' | 1:AA:1469:G:O4' | 2.08 | 0.53 |
| 1:AA:189(J):G:O2' | 1:AA:189(K):U:H5' | 2.08 | 0.53 |
| 1:AA:62:U:O2' | 1:AA:379:C:H1' | 2.08 | 0.53 |
| 8:AH:103:VAL:CG2 | 8:AH:110:ALA:HB2 | 2.39 | 0.53 |
| 12:AL:58:VAL:O | 12:AL:65:GLU:HA | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:AA:177:C:OP1 | 20:AT:65:LYS:HD3 | 2.08 | 0.53 |
| 23:B1:85:LEU:HB3 | 23:B1:87:PRO:CD | 2.38 | 0.53 |
| 23:B1:86:SER:N | 23:B1:87:PRO:CD | 2.71 | 0.53 |
| 24:B2:43:GLN:O | 24:B2:46:GLN:HB3 | 2.09 | 0.53 |
| 28:B6:28:ARG:HA | 28:B6:32:ASN:ND2 | 2.16 | 0.53 |
| 31:BA:1278:A:O2' | 43:BR:34:ILE:HD11 | 2.08 | 0.53 |
| 31:BA:1662:C:O2' | 31:BA:1663:C:H5' | 2.08 | 0.53 |
| 31:BA:2086:U:H2' | 31:BA:2087:G:C8 | 2.43 | 0.53 |
| 31:BA:2503:A:C8 | 55:BA:3364:ERY:H293 | 2.43 | 0.53 |
| 31:BA:510:C:H2' | 31:BA:511:U:H5' | 1.89 | 0.53 |
| 31:BA:27:G:C2 | 31:BA:512:G:N3 | 2.76 | 0.53 |
| 37:BH:41:MET:HB3 | 37:BH:43:VAL:HG13 | 1.91 | 0.53 |
| 45:BT:30:VAL:HG21 | 45:BT:83:ILE:N | 2.23 | 0.53 |
| 45:BT:40:THR:O | 45:BT:41:ARG:HB2 | 2.06 | 0.53 |
| 47:BV:69:LYS:O | 47:BV:70:ILE:HG23 | 2.08 | 0.53 |
| 48:BW:18:ARG:NH1 | 48:BW:18:ARG:CG | 2.69 | 0.53 |
| 49:BX:63:LYS:HE3 | 49:BX:70:LEU:CD2 | 2.37 | 0.53 |
| 1:CA:254:G:O2' | 1:CA:255:G:H5' | 2.08 | 0.53 |
| 1:CA:370:C:H2' | 1:CA:371:G:H8 | 1.73 | 0.53 |
| 1:CA:585:G:N3 | 1:CA:879:C:H4' | 2.23 | 0.53 |
| 4:CD:79:PHE:CG | 4:CD:207:TYR:HD1 | 2.26 | 0.53 |
| 1:CA:1347:G:C8 | 9:CI:107:ARG:HB3 | 2.43 | 0.53 |
| 10:CJ:32:ALA:HB2 | 10:CJ:76:ASN:HB3 | 1.89 | 0.53 |
| 14:CN:6:LEU:HD23 | 14:CN:9:LYS:HD3 | 1.89 | 0.53 |
| 20:CT:14:LYS:O | 20:CT:18:GLN:HG3 | 2.08 | 0.53 |
| 31:DA:1396:U:C2' | 31:DA:1396:U:O2 | 2.53 | 0.53 |
| 31:DA:1496:A:C8 | 31:DA:1577:C:O2' | 2.58 | 0.53 |
| 31:DA:1657:C:H2' | 31:DA:1658:C:H6 | 1.72 | 0.53 |
| 31:DA:1895:C:C2 | 31:DA:1896:G:C8 | 2.95 | 0.53 |
| 31:DA:2473:U:N3 | 31:DA:2474:C:C6 | 2.77 | 0.53 |
| 31:DA:518:G:H2' | 31:DA:519:U:C6 | 2.43 | 0.53 |
| 34:DE:134:ILE:H | 34:DE:134:ILE:HD13 | 1.72 | 0.53 |
| 35:DF:21:ALA:C | 35:DF:23:ASP:H | 2.10 | 0.53 |
| 41:DP:140:ALA:O | 41:DP:141:ALA:CB | 2.56 | 0.53 |
| 41:DP:148:LEU:O | 41:DP:148:LEU:HD22 | 2.08 | 0.53 |
| 42:DQ:76:LYS:H | 42:DQ:88:GLY:HA2 | 1.73 | 0.53 |
| 47:DV:1:MET:CE | 47:DV:1:MET:HA | 2.37 | 0.53 |
| 31:DA:993:G:C5' | 47:DV:75:PHE:CZ | 2.90 | 0.53 |
| 31:DA:993:G:N3 | 47:DV:91:TYR:CE1 | 2.76 | 0.53 |
| 51:DZ:166:SER:OG | 51:DZ:168:GLU:N | 2.41 | 0.53 |
| 1:AA:765:G:H5'' | 1:AA:766:A:OP1 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 6:AF:91:VAL:HG12 | 6:AF:92:LYS:N | 2.24 | 0.53 |
| 16:AP:17:TYR:CE1 | 16:AP:41:PRO:HG3 | 2.43 | 0.53 |
| 28:B6:15:GLU:OE2 | 28:B6:43:CYS:CB | 2.57 | 0.53 |
| 28:B6:34:LEU:HD22 | 28:B6:50:ARG:NH1 | 2.24 | 0.53 |
| 31:BA:1040:C:O2' | 31:BA:1041:C:OP2 | 2.24 | 0.53 |
| 31:BA:1771:C:O2' | 31:BA:1786:A:C8 | 2.51 | 0.53 |
| 31:BA:2055:C:H5' | 31:BA:2056:G:O5' | 2.08 | 0.53 |
| 33:BD:172:TYR:CD1 | 33:BD:186:HIS:CA | 2.90 | 0.53 |
| 34:BE:128:SER:OG | 34:BE:129:HIS:N | 2.36 | 0.53 |
| 34:BE:167:VAL:CG2 | 34:BE:170:LEU:HD11 | 2.37 | 0.53 |
| 35:BF:178:PRO:HG2 | 35:BF:179:GLU:OE1 | 2.09 | 0.53 |
| 38:BI:56:LYS:C | 38:BI:56:LYS:NZ | 2.62 | 0.53 |
| 31:BA:252:G:P | 41:BP:50:ARG:HH11 | 2.31 | 0.53 |
| 42:BQ:32:TYR:CE2 | 42:BQ:133:ARG:HG2 | 2.43 | 0.53 |
| 45:BT:51:ARG:HG2 | 45:BT:52:ILE:N | 2.23 | 0.53 |
| 45:BT:55:ASN:N | 45:BT:59:THR:HB | 2.23 | 0.53 |
| 50:BY:37:VAL:CG2 | 50:BY:67:LEU:HB3 | 2.38 | 0.53 |
| 2:CB:189:ASP:N | 2:CB:189:ASP:OD1 | 2.41 | 0.53 |
| 12:CL:6:THR:OG1 | 12:CL:9:GLN:HG3 | 2.08 | 0.53 |
| 15:CO:87:ILE:CG2 | 15:CO:88:ARG:N | 2.71 | 0.53 |
| 16:CP:3:LYS:O | 16:CP:21:VAL:HA | 2.08 | 0.53 |
| 20:CT:75:ASN:O | 20:CT:79:ARG:HB2 | 2.07 | 0.53 |
| 31:DA:1161:C:O2' | 47:DV:8:GLY:HA2 | 2.08 | 0.53 |
| 31:DA:1410:G:H1 | 31:DA:1592:C:H42 | 1.56 | 0.53 |
| 31:DA:1677:A:H2' | 31:DA:1678:G:C8 | 2.44 | 0.53 |
| 31:DA:1804:C:O2' | 31:DA:1805:U:H5' | 2.08 | 0.53 |
| 31:DA:1948:G:H5' | 31:DA:1948:G:C8 | 2.39 | 0.53 |
| 31:DA:271(D):G:C6 | 31:DA:271(E):U:C4 | 2.97 | 0.53 |
| 31:DA:2784:C:O2' | 31:DA:2785:C:H5' | 2.09 | 0.53 |
| 31:DA:2801(A):A:H4' | 31:DA:2802:G:C2' | 2.38 | 0.53 |
| 29:D7:40:TRP:CD2 | 31:DA:459:U:H5'' | 2.43 | 0.53 |
| 31:DA:997:G:O2' | 31:DA:998:C:H5' | 2.08 | 0.53 |
| 33:DD:58:HIS:CD2 | 33:DD:59:LYS:N | 2.76 | 0.53 |
| 31:DA:706:A:OP1 | 33:DD:7:LYS:HE3 | 2.08 | 0.53 |
| 34:DE:50:GLY:HA3 | 34:DE:74:PRO:HG3 | 1.90 | 0.53 |
| 44:DS:38:GLN:HG2 | 44:DS:47:THR:CG2 | 2.39 | 0.53 |
| 45:DT:33:LYS:HA | 45:DT:33:LYS:HZ2 | 1.73 | 0.53 |
| 47:DV:19:LYS:HE2 | 47:DV:20:LEU:H | 1.73 | 0.53 |
| 51:DZ:99:TYR:HB3 | 51:DZ:123:ASP:OD1 | 2.08 | 0.53 |
| 1:AA:321:A:N6 | 1:AA:328:C:H1' | 2.23 | 0.53 |
| 1:AA:376:G:O2' | 1:AA:377:G:H5' | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:AA:427:U:P | 4:AD:13:ARG:HH22 | 2.32 | 0.53 |
| 1:AA:658:G:H2' | 1:AA:659:U:H6 | 1.73 | 0.53 |
| 7:AG:152:ALA:O | 7:AG:155:ARG:HG3 | 2.07 | 0.53 |
| 11:AK:21:ILE:N | 11:AK:21:ILE:HD12 | 2.23 | 0.53 |
| 15:AO:17:ARG:CG | 15:AO:17:ARG:NH1 | 2.64 | 0.53 |
| 15:AO:25:THR:HG21 | 15:AO:70:LEU:HB2 | 1.89 | 0.53 |
| 15:AO:81:LEU:HD11 | 15:AO:85:LEU:HD12 | 1.89 | 0.53 |
| 23:B1:20:ARG:HD3 | 23:B1:41:ARG:HD3 | 1.89 | 0.53 |
| 31:BA:196:A:H2' | 31:BA:196:A:N3 | 2.23 | 0.53 |
| 31:BA:2243:U:H2' | 31:BA:2244:U:C6 | 2.43 | 0.53 |
| 31:BA:2475:C:H5'' | 31:BA:2475:C:C6 | 2.43 | 0.53 |
| 31:BA:271(X):G:C2' | 31:BA:271(Y):U:H5'' | 2.39 | 0.53 |
| 31:BA:2801(A):A:H4' | 31:BA:2802:G:C2' | 2.38 | 0.53 |
| 31:BA:607:U:C2 | 31:BA:621:A:N1 | 2.77 | 0.53 |
| 31:BA:775:G:C4 | 31:BA:794:G:C8 | 2.95 | 0.53 |
| 31:BA:675:A:C4 | 31:BA:804:A:C2 | 2.96 | 0.53 |
| 33:BD:143:HIS:HD2 | 33:BD:144:ALA:HB2 | 1.73 | 0.53 |
| 31:BA:2810:A:C2' | 34:BE:61:ARG:NH2 | 2.68 | 0.53 |
| 35:BF:24:LEU:O | 35:BF:26:ALA:N | 2.41 | 0.53 |
| 36:BG:12:TYR:HA | 36:BG:16:ARG:HG3 | 1.91 | 0.53 |
| 36:BG:45:GLU:HB2 | 36:BG:47:LYS:HG3 | 1.89 | 0.53 |
| 38:BI:76:THR:HG22 | 38:BI:139:GLN:HB3 | 1.89 | 0.53 |
| 42:BQ:20:ALA:C | 42:BQ:22:LYS:H | 2.10 | 0.53 |
| 46:BU:57:PHE:O | 46:BU:58:ARG:C | 2.47 | 0.53 |
| 50:BY:8:LYS:H | 50:BY:8:LYS:HD2 | 1.73 | 0.53 |
| 31:BA:875:G:C4' | 51:BZ:170:THR:HG21 | 2.34 | 0.53 |
| 1:CA:1052:U:H2' | 1:CA:1055:A:OP1 | 2.08 | 0.53 |
| 1:CA:125:U:H2' | 1:CA:126:G:C8 | 2.43 | 0.53 |
| 1:CA:250:A:H1' | 1:CA:251:G:OP2 | 2.09 | 0.53 |
| 1:CA:495:A:H4' | 1:CA:496:A:OP1 | 2.08 | 0.53 |
| 4:CD:128:VAL:O | 4:CD:130:GLY:N | 2.41 | 0.53 |
| 6:CF:55:ASP:HB2 | 6:CF:86:ARG:HH12 | 1.73 | 0.53 |
| 9:CI:40:LEU:HD11 | 9:CI:70:LYS:HG2 | 1.91 | 0.53 |
| 1:CA:1320:C:H5' | 19:CS:70:LYS:HG2 | 1.90 | 0.53 |
| 23:D1:60:PHE:HZ | 23:D1:90:ILE:HG21 | 1.73 | 0.53 |
| 24:D2:14:ARG:O | 24:D2:18:PRO:CD | 2.56 | 0.53 |
| 27:D5:4:HIS:HB3 | 27:D5:5:PRO:CD | 2.30 | 0.53 |
| 31:DA:107:C:C2 | 31:DA:108:U:C5 | 2.96 | 0.53 |
| 31:DA:128:C:H6 | 31:DA:128:C:C5' | 2.20 | 0.53 |
| 31:DA:2359:C:C2' | 31:DA:2360:A:C5' | 2.86 | 0.53 |
| 33:DD:35:LYS:NZ | 33:DD:104:TYR:CB | 2.65 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DE:16:ARG:O | 34:DE:18:ASP:N | 2.42 | 0.53 |
| 35:DF:185:ASP:HA | 35:DF:188:ARG:HG2 | 1.89 | 0.53 |
| 35:DF:200:GLU:O | 35:DF:204:ASN:HB2 | 2.09 | 0.53 |
| 38:DI:98:ALA:HA | 38:DI:109:ILE:CD1 | 2.39 | 0.53 |
| 38:DI:78:THR:HA | 38:DI:141:LYS:HB2 | 1.90 | 0.53 |
| 38:DI:82:ARG:HG2 | 38:DI:89:TYR:HD2 | 1.69 | 0.53 |
| 41:DP:98:GLU:HG3 | 41:DP:99:LEU:N | 2.21 | 0.53 |
| 1:CA:346:G:H5'' | 45:DT:41:ARG:NH2 | 2.24 | 0.53 |
| 51:DZ:102:LEU:HG | 51:DZ:123:ASP:HA | 1.90 | 0.53 |
| 51:DZ:150:LEU:N | 51:DZ:150:LEU:HD13 | 2.23 | 0.53 |
| 1:AA:1423:G:P | 40:BO:49:ARG:NH2 | 2.82 | 0.53 |
| 1:AA:1478:C:H2' | 1:AA:1479:C:H6 | 1.73 | 0.53 |
| 1:AA:1497:G:C2' | 1:AA:1498:U:H5' | 2.39 | 0.53 |
| 1:AA:235:C:H5' | 17:AQ:70:ARG:HG2 | 1.90 | 0.53 |
| 1:AA:52:G:C2' | 1:AA:53:A:H5' | 2.39 | 0.53 |
| 1:AA:939:G:H5'' | 7:AG:102:ARG:NH2 | 2.23 | 0.53 |
| 23:B1:40:ARG:HD3 | 23:B1:41:ARG:N | 2.21 | 0.53 |
| 31:BA:1486:A:H2' | 31:BA:1487:G:C8 | 2.43 | 0.53 |
| 31:BA:2306:C:H5'' | 31:BA:2307:G:O4' | 2.08 | 0.53 |
| 30:B8:62:LEU:CD1 | 31:BA:242:G:H5'' | 2.30 | 0.53 |
| 31:BA:310:A:P | 50:BY:18:GLY:HA2 | 2.47 | 0.53 |
| 38:BI:2:LYS:HB2 | 38:BI:39:ALA:CB | 2.38 | 0.53 |
| 40:BO:77:ILE:HB | 45:BT:74:ARG:HD3 | 1.91 | 0.53 |
| 42:BQ:17:LEU:HD23 | 42:BQ:17:LEU:N | 2.22 | 0.53 |
| 43:BR:55:ALA:CB | 43:BR:79:LEU:HD13 | 2.35 | 0.53 |
| 48:BW:4:LYS:CE | 48:BW:6:ILE:HD11 | 2.38 | 0.53 |
| 51:BZ:166:SER:OG | 51:BZ:168:GLU:N | 2.41 | 0.53 |
| 1:CA:1410:G:C4 | 1:CA:1491:G:N2 | 2.76 | 0.53 |
| 4:CD:64:LEU:HD12 | 4:CD:64:LEU:O | 2.08 | 0.53 |
| 8:CH:103:VAL:CG2 | 8:CH:110:ALA:HB2 | 2.38 | 0.53 |
| 12:CL:32:PHE:HB3 | 12:CL:85:ILE:O | 2.09 | 0.53 |
| 28:D6:40:CYS:SG | 28:D6:45:LYS:NZ | 2.62 | 0.53 |
| 31:DA:1495:A:H5'' | 31:DA:1496:A:OP2 | 2.09 | 0.53 |
| 31:DA:154(A):C:H5 | 31:DA:171:G:N1 | 2.07 | 0.53 |
| 31:DA:2001:A:H2' | 31:DA:2002:G:C8 | 2.44 | 0.53 |
| 31:DA:2437:U:H2' | 31:DA:2438:U:C6 | 2.44 | 0.53 |
| 31:DA:614:U:O2 | 31:DA:614:U:O5' | 2.26 | 0.53 |
| 31:DA:943:U:OP2 | 41:DP:38:GLN:OE1 | 2.25 | 0.53 |
| 31:DA:966:G:C4 | 31:DA:967:C:C5 | 2.96 | 0.53 |
| 32:DB:6:C:C2 | 32:DB:116:G:N2 | 2.76 | 0.53 |
| 31:DA:661:C:O3' | 41:DP:18:ARG:HD2 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:DP:88:LEU:C | 41:DP:90:ARG:H | 2.11 | 0.53 |
| 44:DS:16:ASN:C | 44:DS:17:ARG:O | 2.46 | 0.53 |
| 44:DS:34:HIS:CE1 | 44:DS:54:LEU:CB | 2.89 | 0.53 |
| 45:DT:47:GLY:HA3 | 45:DT:63:VAL:HG23 | 1.89 | 0.53 |
| 1:AA:1199:U:H4' | 10:AJ:54:PHE:CE1 | 2.44 | 0.53 |
| 1:AA:409:G:C2' | 1:AA:410:G:H5' | 2.38 | 0.53 |
| 1:AA:460:G:O6 | 1:AA:470:C:H5'' | 2.09 | 0.53 |
| 7:AG:115:ARG:HB2 | 7:AG:118:VAL:HG22 | 1.90 | 0.53 |
| 7:AG:113:GLU:HB2 | 7:AG:119:ARG:CG | 2.38 | 0.53 |
| 8:AH:10:LEU:HD23 | 8:AH:10:LEU:H | 1.72 | 0.53 |
| 9:AI:79:LEU:HD22 | 9:AI:79:LEU:O | 2.08 | 0.53 |
| 17:AQ:33:GLY:O | 17:AQ:34:LYS:C | 2.47 | 0.53 |
| 23:B1:17:SER:O | 23:B1:44:PRO:CD | 2.43 | 0.53 |
| 24:B2:25:VAL:C | 24:B2:27:GLU:H | 2.12 | 0.53 |
| 30:B8:31:HIS:O | 30:B8:32:LEU:C | 2.46 | 0.53 |
| 31:BA:1176:G:C4' | 31:BA:1177:A:OP1 | 2.57 | 0.53 |
| 31:BA:1407:C:O2 | 31:BA:1407:C:H2' | 2.07 | 0.53 |
| 31:BA:151:C:C2' | 31:BA:152:G:H5' | 2.39 | 0.53 |
| 31:BA:1887:C:C2' | 31:BA:1888:G:H5' | 2.38 | 0.53 |
| 31:BA:2463:C:O2' | 31:BA:2464:C:H5' | 2.09 | 0.53 |
| 31:BA:271(P):C:H2' | 31:BA:271(Q):G:C5' | 2.39 | 0.53 |
| 31:BA:838:C:O2' | 31:BA:839:U:H5' | 2.08 | 0.53 |
| 31:BA:866:A:C6 | 31:BA:914:C:C5 | 2.97 | 0.53 |
| 33:BD:167:GLY:C | 33:BD:168:ARG:HG2 | 2.29 | 0.53 |
| 33:BD:8:PRO:HB3 | 33:BD:14:ARG:CB | 2.34 | 0.53 |
| 39:BN:67:LEU:HB3 | 39:BN:88:GLU:CD | 2.29 | 0.53 |
| 41:BP:23:PRO:HB2 | 41:BP:33:ARG:HG3 | 1.91 | 0.53 |
| 44:BS:17:ARG:NE | 44:BS:89:ARG:HH21 | 2.06 | 0.53 |
| 46:BU:75:ASN:HB2 | 46:BU:78:THR:H | 1.73 | 0.53 |
| 47:BV:47:VAL:HG21 | 47:BV:49:THR:HB | 1.89 | 0.53 |
| 49:BX:21:PHE:CD1 | 49:BX:21:PHE:N | 2.76 | 0.53 |
| 50:BY:77:PRO:O | 50:BY:78:ALA:HB2 | 2.09 | 0.53 |
| 51:BZ:102:LEU:HG | 51:BZ:123:ASP:HA | 1.91 | 0.53 |
| 51:BZ:128:VAL:CG2 | 51:BZ:161:VAL:HG22 | 2.39 | 0.53 |
| 1:CA:1371:G:C6 | 1:CA:1372:U:C4 | 2.97 | 0.53 |
| 1:CA:278:G:O4' | 1:CA:282:A:H1' | 2.08 | 0.53 |
| 5:CE:103:GLY:C | 5:CE:106:PRO:HD2 | 2.29 | 0.53 |
| 6:CF:18:GLN:O | 6:CF:21:LEU:HB2 | 2.09 | 0.53 |
| 6:CF:78:GLU:O | 6:CF:81:ILE:HG13 | 2.08 | 0.53 |
| 7:CG:113:GLU:HB2 | 7:CG:119:ARG:CG | 2.39 | 0.53 |
| 7:CG:92:SER:OG | 7:CG:93:PRO:HD2 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:CH:92:ARG:HD2 | 8:CH:92:ARG:N | 2.23 | 0.53 |
| 14:CN:45:ARG:HG2 | 14:CN:49:HIS:CD2 | 2.43 | 0.53 |
| 20:CT:56:MET:HG2 | 20:CT:84:LEU:HD11 | 1.90 | 0.53 |
| 30:D8:30:ARG:O | 30:D8:31:HIS:O | 2.25 | 0.53 |
| 31:DA:109:G:C4 | 31:DA:110:G:C8 | 2.97 | 0.53 |
| 31:DA:1341:U:H3' | 31:DA:1397:U:O2 | 2.09 | 0.53 |
| 31:DA:189:G:H2' | 31:DA:205:G:N2 | 2.23 | 0.53 |
| 31:DA:2884:U:C2' | 31:DA:2885:C:H5' | 2.38 | 0.53 |
| 31:DA:643:A:O2' | 31:DA:644:A:H5' | 2.08 | 0.53 |
| 31:DA:64:A:C2' | 31:DA:65:C:H5' | 2.39 | 0.53 |
| 33:DD:70:TRP:HZ3 | 33:DD:146:GLU:OE2 | 1.92 | 0.53 |
| 33:DD:255:LYS:HD2 | 33:DD:255:LYS:O | 2.09 | 0.53 |
| 35:DF:84:VAL:O | 35:DF:85:GLY:C | 2.46 | 0.53 |
| 36:DG:33:ARG:HB2 | 36:DG:162:THR:OG1 | 2.09 | 0.53 |
| 36:DG:81:LYS:O | 36:DG:82:LEU:O | 2.26 | 0.53 |
| 37:DH:138:LYS:O | 37:DH:139:GLN:C | 2.47 | 0.53 |
| 43:DR:104:ARG:HD2 | 43:DR:111:LEU:HD11 | 1.91 | 0.53 |
| 45:DT:31:SER:HA | 45:DT:32:TYR:CE2 | 2.44 | 0.53 |
| 49:DX:35:THR:CB | 49:DX:75:ASP:OD2 | 2.53 | 0.53 |
| 50:DY:75:ILE:HD11 | 50:DY:80:GLY:N | 2.24 | 0.53 |
| 51:DZ:128:VAL:CG2 | 51:DZ:161:VAL:HG22 | 2.38 | 0.53 |
| 1:AA:1157:A:C1' | 1:AA:1181:G:H21 | 2.21 | 0.53 |
| 1:AA:1410:G:C4 | 1:AA:1491:G:N2 | 2.77 | 0.53 |
| 1:AA:659:U:H2' | 1:AA:660:G:C5' | 2.38 | 0.53 |
| 2:AB:11:LEU:HB3 | 2:AB:213:LEU:HD11 | 1.89 | 0.53 |
| 2:AB:22:LYS:HZ3 | 2:AB:40:HIS:HE1 | 1.55 | 0.53 |
| 2:AB:87:ARG:HD2 | 2:AB:87:ARG:O | 2.09 | 0.53 |
| 6:AF:55:ASP:HB2 | 6:AF:86:ARG:HH12 | 1.74 | 0.53 |
| 13:AM:32:GLU:OE2 | 13:AM:64:TRP:HH2 | 1.92 | 0.53 |
| 17:AQ:10:VAL:HG13 | 17:AQ:19:VAL:HB | 1.91 | 0.53 |
| 20:AT:46:GLU:HG2 | 20:AT:48:LYS:HE2 | 1.90 | 0.53 |
| 20:AT:55:ILE:O | 20:AT:58:LYS:N | 2.41 | 0.53 |
| 24:B2:50:ILE:O | 24:B2:51:ARG:HB3 | 2.08 | 0.53 |
| 24:B2:14:ARG:CZ | 24:B2:57:ILE:HB | 2.38 | 0.53 |
| 30:B8:35:GLN:HE21 | 30:B8:36:LYS:NZ | 2.07 | 0.53 |
| 31:BA:1947:C:C2' | 31:BA:1948:G:C5' | 2.87 | 0.53 |
| 31:BA:2291:U:H5'' | 31:BA:2380:C:O2' | 2.09 | 0.53 |
| 30:B8:35:GLN:HA | 31:BA:2420:C:OP2 | 2.08 | 0.53 |
| 31:BA:2845:G:C2' | 31:BA:2846:G:H5' | 2.39 | 0.53 |
| 31:BA:435:C:C5 | 31:BA:436:C:C5 | 2.97 | 0.53 |
| 31:BA:196:A:C4 | 31:BA:805:G:C6 | 2.96 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:848:G:H2' | 31:BA:849:A:C8 | 2.44 | 0.53 |
| 31:BA:92:A:C2' | 31:BA:93:G:O4' | 2.56 | 0.53 |
| 35:BF:63:LYS:HE2 | 35:BF:67:GLN:HB2 | 1.89 | 0.53 |
| 39:BN:67:LEU:C | 39:BN:69:GLN:N | 2.63 | 0.53 |
| 42:BQ:137:TYR:HE2 | 51:BZ:74:VAL:O | 1.91 | 0.53 |
| 43:BR:101:ALA:O | 43:BR:102:GLU:HB2 | 2.09 | 0.53 |
| 45:BT:47:GLY:HA3 | 45:BT:63:VAL:HG23 | 1.91 | 0.53 |
| 50:BY:68:HIS:N | 50:BY:71:LYS:NZ | 2.57 | 0.53 |
| 42:BQ:140:ALA:CB | 51:BZ:53:ILE:HG13 | 2.30 | 0.53 |
| 1:CA:1157:A:C1' | 1:CA:1181:G:H21 | 2.21 | 0.53 |
| 1:CA:1385:G:C2 | 1:CA:1386:G:C8 | 2.97 | 0.53 |
| 1:CA:1399:C:H4' | 1:CA:1400:C:H5'' | 1.91 | 0.53 |
| 1:CA:457:C:H2' | 1:CA:458:C:H6 | 1.74 | 0.53 |
| 1:CA:945:G:H2' | 1:CA:945:G:N3 | 2.24 | 0.53 |
| 4:CD:176:LEU:HG | 4:CD:178:VAL:HG22 | 1.90 | 0.53 |
| 11:CK:57:THR:HG22 | 11:CK:59:TYR:H | 1.73 | 0.53 |
| 12:CL:58:VAL:O | 12:CL:65:GLU:HA | 2.09 | 0.53 |
| 15:CO:9:GLN:HA | 15:CO:12:ILE:HD12 | 1.91 | 0.53 |
| 22:D0:1:MET:CB | 31:DA:2602:A:H62 | 2.21 | 0.53 |
| 31:DA:102:G:O2' | 31:DA:103:A:P | 2.65 | 0.53 |
| 31:DA:1359:A:H2' | 31:DA:1360:A:H5' | 1.90 | 0.53 |
| 31:DA:154:G:H2' | 31:DA:154(A):C:O2 | 2.09 | 0.53 |
| 31:DA:1587:A:H3' | 31:DA:1588:C:H6 | 1.73 | 0.53 |
| 31:DA:1859:A:C2 | 31:DA:1884:A:H1' | 2.44 | 0.53 |
| 31:DA:1952:A:C6 | 31:DA:1953:A:N1 | 2.76 | 0.53 |
| 31:DA:1935:G:C6 | 31:DA:1962:C:C6 | 2.96 | 0.53 |
| 31:DA:2820:A:H1' | 43:DR:5:LYS:HZ3 | 1.74 | 0.53 |
| 31:DA:824:A:O2' | 31:DA:825:C:H5' | 2.09 | 0.53 |
| 33:DD:43:ARG:NH1 | 33:DD:44:ASN:ND2 | 2.57 | 0.53 |
| 37:DH:118:PRO:HG2 | 37:DH:121:ILE:HD12 | 1.91 | 0.53 |
| 39:DN:75:TYR:N | 39:DN:75:TYR:CD1 | 2.76 | 0.53 |
| 43:DR:9:LYS:O | 43:DR:10:LEU:HG | 2.09 | 0.53 |
| 1:AA:994:A:N6 | 1:AA:1046:A:C2 | 2.77 | 0.53 |
| 1:AA:173:U:O4' | 1:AA:197:A:C4 | 2.62 | 0.53 |
| 1:AA:412:A:C8 | 4:AD:35:ARG:NH2 | 2.76 | 0.53 |
| 1:AA:41:G:H2' | 1:AA:42:G:C8 | 2.43 | 0.53 |
| 1:AA:520:A:H2 | 1:AA:536:C:O2 | 1.91 | 0.53 |
| 1:AA:731:G:H5' | 1:AA:766:A:H4' | 1.91 | 0.53 |
| 1:AA:971:G:H3' | 1:AA:971:G:OP1 | 2.08 | 0.53 |
| 10:AJ:29:ARG:O | 10:AJ:29:ARG:HG2 | 2.07 | 0.53 |
| 10:AJ:32:ALA:HB2 | 10:AJ:76:ASN:HB3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AT:94:ALA:O | 20:AT:95:ALA:HB3 | 2.09 | 0.53 |
| 24:B2:44:LEU:O | 24:B2:44:LEU:HD12 | 2.09 | 0.53 |
| 30:B8:30:ARG:HB2 | 31:BA:2393:A:OP1 | 2.08 | 0.53 |
| 31:BA:1438:U:O2' | 31:BA:1439:A:H5' | 2.08 | 0.53 |
| 31:BA:1515:G:H2' | 31:BA:1516:C:C6 | 2.44 | 0.53 |
| 31:BA:2360:A:O2' | 31:BA:2361:A:H5'' | 2.08 | 0.53 |
| 31:BA:2854:G:H2' | 31:BA:2855:C:C6 | 2.43 | 0.53 |
| 33:BD:267:SER:O | 33:BD:268:ARG:HB2 | 2.08 | 0.53 |
| 33:BD:70:TRP:CD1 | 33:BD:70:TRP:C | 2.82 | 0.53 |
| 33:BD:83:GLU:HB2 | 33:BD:92:ILE:HD11 | 1.90 | 0.53 |
| 36:BG:46:ALA:H | 36:BG:82:LEU:CD1 | 2.22 | 0.53 |
| 39:BN:13:TRP:O | 39:BN:135:PRO:HG2 | 2.09 | 0.53 |
| 42:BQ:16:ARG:CG | 42:BQ:17:LEU:H | 2.21 | 0.53 |
| 42:BQ:16:ARG:CG | 42:BQ:17:LEU:N | 2.72 | 0.53 |
| 46:BU:91:ASP:O | 46:BU:92:ARG:HB3 | 2.08 | 0.53 |
| 50:BY:52:SER:C | 50:BY:54:LYS:H | 2.12 | 0.53 |
| 50:BY:88:LYS:O | 50:BY:89:PHE:HB2 | 2.07 | 0.53 |
| 1:CA:1201:A:H4' | 1:CA:1202:G:O5' | 2.09 | 0.53 |
| 1:CA:343:U:O2' | 1:CA:346:G:O6 | 2.25 | 0.53 |
| 1:CA:380:G:N2 | 1:CA:384:G:C5 | 2.77 | 0.53 |
| 1:CA:380:G:N2 | 1:CA:384:G:C6 | 2.77 | 0.53 |
| 1:CA:460:G:O6 | 1:CA:470:C:H5'' | 2.09 | 0.53 |
| 1:CA:69:G:C2 | 1:CA:70:G:C5 | 2.97 | 0.53 |
| 1:CA:963:G:N3 | 10:CJ:55:LYS:NZ | 2.50 | 0.53 |
| 1:CA:994:A:N6 | 1:CA:1046:A:C2 | 2.76 | 0.53 |
| 3:CC:16:ARG:NH1 | 3:CC:16:ARG:HB2 | 2.24 | 0.53 |
| 4:CD:170:VAL:HG13 | 4:CD:171:GLY:N | 2.22 | 0.53 |
| 7:CG:153:HIS:CE1 | 11:CK:58:PRO:HD2 | 2.42 | 0.53 |
| 12:CL:110:VAL:HG23 | 12:CL:120:TYR:O | 2.08 | 0.53 |
| 14:CN:48:ALA:HB2 | 14:CN:53:LEU:HD12 | 1.91 | 0.53 |
| 23:D1:94:LEU:HD22 | 23:D1:95:LEU:HB2 | 1.89 | 0.53 |
| 29:D7:47:ARG:C | 29:D7:48:LYS:HD3 | 2.29 | 0.53 |
| 31:DA:1802:A:N1 | 31:DA:1822:G:H1' | 2.24 | 0.53 |
| 32:DB:73:A:H3' | 32:DB:74:U:H6 | 1.74 | 0.53 |
| 33:DD:108:PRO:HD2 | 33:DD:111:LEU:HG | 1.90 | 0.53 |
| 34:DE:70:ALA:O | 34:DE:71:GLY:C | 2.47 | 0.53 |
| 39:DN:47:ALA:CB | 39:DN:112:LEU:HD11 | 2.34 | 0.53 |
| 40:DO:98:VAL:HG13 | 40:DO:117:LEU:HB3 | 1.90 | 0.53 |
| 42:DQ:23:GLY:O | 42:DQ:100:GLY:CA | 2.51 | 0.53 |
| 42:DQ:20:ALA:HA | 42:DQ:98:LYS:HD3 | 1.90 | 0.53 |
| 31:DA:2378:A:C2 | 44:DS:20:ARG:NH1 | 2.77 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:DT:45:PHE:HE2 | 45:DT:63:VAL:HG22 | 1.74 | 0.53 |
| 46:DU:50:ARG:CZ | 47:DV:75:PHE:CE2 | 2.92 | 0.53 |
| 47:DV:67:GLY:O | 47:DV:69:LYS:N | 2.42 | 0.53 |
| 50:DY:96:ILE:CG1 | 50:DY:99:CYS:SG | 2.97 | 0.53 |
| 1:AA:1477:C:H2' | 1:AA:1478:C:H6 | 1.72 | 0.53 |
| 1:AA:343:U:N3 | 1:AA:347:G:C6 | 2.76 | 0.53 |
| 1:AA:623:C:C4 | 1:AA:624:C:C4 | 2.97 | 0.53 |
| 1:AA:980:C:H5' | 1:AA:981:U:C5 | 2.43 | 0.53 |
| 6:AF:24:GLU:HG2 | 6:AF:28:ARG:CZ | 2.39 | 0.53 |
| 7:AG:146:GLU:OE2 | 7:AG:149:ARG:HD2 | 2.09 | 0.53 |
| 16:AP:50:LYS:HD3 | 16:AP:50:LYS:C | 2.29 | 0.53 |
| 18:AR:44:LEU:HA | 18:AR:49:LYS:O | 2.09 | 0.53 |
| 20:AT:93:GLU:O | 20:AT:93:GLU:HG2 | 2.09 | 0.53 |
| 31:BA:1282:U:H2' | 31:BA:1283:G:O4' | 2.09 | 0.53 |
| 31:BA:1312:U:H4' | 31:BA:1313:U:O5' | 2.08 | 0.53 |
| 31:BA:1410:G:H1 | 31:BA:1592:C:H42 | 1.55 | 0.53 |
| 31:BA:1693:U:H4' | 31:BA:1694:C:OP2 | 2.09 | 0.53 |
| 27:B5:4:HIS:O | 31:BA:2056:G:N2 | 2.42 | 0.53 |
| 31:BA:2069:G:C2' | 31:BA:2070:G:H5' | 2.38 | 0.53 |
| 31:BA:2646:C:OP2 | 31:BA:2732:G:O2' | 2.18 | 0.53 |
| 31:BA:2657:A:H2 | 31:BA:2664:G:N2 | 2.07 | 0.53 |
| 31:BA:873:G:N2 | 31:BA:905:U:C2 | 2.77 | 0.53 |
| 31:BA:993:G:N2 | 47:BV:91:TYR:OH | 2.42 | 0.53 |
| 34:BE:51:PHE:CE1 | 34:BE:52:LEU:HG | 2.43 | 0.53 |
| 41:BP:62:LEU:CD1 | 41:BP:62:LEU:H | 2.14 | 0.53 |
| 42:BQ:75:THR:HA | 42:BQ:89:ASN:H | 1.74 | 0.53 |
| 42:BQ:78:PRO:O | 42:BQ:79:LEU:CB | 2.57 | 0.53 |
| 43:BR:11:ASN:CG | 43:BR:12:ARG:N | 2.61 | 0.53 |
| 47:BV:56:SER:O | 47:BV:57:VAL:HB | 2.09 | 0.53 |
| 48:BW:71:VAL:HA | 48:BW:107:LEU:HD12 | 1.91 | 0.53 |
| 50:BY:28:LYS:HD2 | 50:BY:37:VAL:CG1 | 2.38 | 0.53 |
| 50:BY:45:VAL:HG11 | 50:BY:60:PHE:C | 2.28 | 0.53 |
| 1:CA:242:C:H2' | 1:CA:243:A:H5' | 1.90 | 0.53 |
| 1:CA:936:C:H2' | 1:CA:937:A:O4' | 2.08 | 0.53 |
| 2:CB:239:VAL:O | 2:CB:239:VAL:HG12 | 2.09 | 0.53 |
| 5:CE:77:PRO:HG2 | 5:CE:142:LEU:HD22 | 1.90 | 0.53 |
| 6:CF:7:ASN:ND2 | 6:CF:7:ASN:N | 2.56 | 0.53 |
| 16:CP:75:ARG:C | 16:CP:77:ALA:H | 2.12 | 0.53 |
| 25:D3:6:VAL:HG12 | 25:D3:54:VAL:HG11 | 1.89 | 0.53 |
| 31:DA:1227:G:OP1 | 46:DU:13:LYS:HG2 | 2.09 | 0.53 |
| 31:DA:1741:A:N7 | 31:DA:1742:G:C2 | 2.77 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:1885:A:H2' | 31:DA:1886:C:O4' | 2.09 | 0.53 |
| 31:DA:2069:G:C2' | 31:DA:2070:G:H5' | 2.39 | 0.53 |
| 30:D8:31:HIS:CD2 | 31:DA:2419:U:O4 | 2.62 | 0.53 |
| 31:DA:2518:A:H5' | 31:DA:2518:A:C8 | 2.44 | 0.53 |
| 31:DA:2543:G:H2' | 31:DA:2544:G:C8 | 2.44 | 0.53 |
| 31:DA:2689:U:H4' | 31:DA:2690:C:OP2 | 2.09 | 0.53 |
| 31:DA:28:A:C2 | 31:DA:513:A:C8 | 2.97 | 0.53 |
| 34:DE:120:TRP:O | 34:DE:121:ASN:HB2 | 2.09 | 0.53 |
| 34:DE:60:ASN:N | 34:DE:60:ASN:HD22 | 2.06 | 0.53 |
| 34:DE:77:ILE:HG23 | 34:DE:78:LEU:N | 2.24 | 0.53 |
| 36:DG:125:PHE:CE2 | 36:DG:173:LEU:HD12 | 2.44 | 0.53 |
| 39:DN:57:ALA:O | 39:DN:58:ASP:C | 2.48 | 0.53 |
| 41:DP:30:THR:CG2 | 41:DP:31:ALA:N | 2.69 | 0.53 |
| 41:DP:62:LEU:N | 41:DP:62:LEU:HD13 | 2.24 | 0.53 |
| 42:DQ:54:MET:HB3 | 42:DQ:64:ILE:HD13 | 1.91 | 0.53 |
| 43:DR:37:THR:OG1 | 43:DR:40:LYS:HG3 | 2.08 | 0.53 |
| 44:DS:56:LEU:O | 44:DS:57:LYS:CB | 2.56 | 0.53 |
| 45:DT:32:TYR:HD2 | 45:DT:81:PRO:O | 1.91 | 0.53 |
| 45:DT:91:ARG:HB2 | 45:DT:116:ALA:HA | 1.91 | 0.53 |
| 50:DY:35:TYR:CD2 | 50:DY:69:ALA:HB3 | 2.43 | 0.53 |
| 1:AA:116:A:H61 | 1:AA:313:A:H1' | 1.73 | 0.53 |
| 1:AA:355:C:C2 | 1:AA:356:A:C8 | 2.96 | 0.53 |
| 1:AA:664:G:H22 | 1:AA:741:G:H1 | 1.57 | 0.53 |
| 4:AD:176:LEU:HG | 4:AD:178:VAL:HG22 | 1.91 | 0.53 |
| 4:AD:22:LYS:HB2 | 4:AD:26:CYS:SG | 2.49 | 0.53 |
| 7:AG:92:SER:OG | 7:AG:93:PRO:HD2 | 2.09 | 0.53 |
| 9:AI:10:ARG:HG2 | 9:AI:104:ARG:O | 2.09 | 0.53 |
| 9:AI:53:VAL:HB | 9:AI:92:TYR:HE2 | 1.74 | 0.53 |
| 13:AM:68:GLY:O | 13:AM:69:GLU:HB2 | 2.07 | 0.53 |
| 14:AN:45:ARG:HG2 | 14:AN:49:HIS:CD2 | 2.44 | 0.53 |
| 15:AO:9:GLN:HA | 15:AO:12:ILE:HD12 | 1.91 | 0.53 |
| 20:AT:73:HIS:O | 20:AT:76:ALA:HB3 | 2.09 | 0.53 |
| 20:AT:56:MET:HG2 | 20:AT:84:LEU:HD11 | 1.91 | 0.53 |
| 28:B6:42:TRP:HA | 28:B6:42:TRP:HE3 | 1.73 | 0.53 |
| 31:BA:1109:C:C5 | 31:BA:1110:G:C5 | 2.96 | 0.53 |
| 31:BA:1332:G:N2 | 31:BA:1609:A:H2' | 2.24 | 0.53 |
| 31:BA:207:A:H2' | 31:BA:208:C:O4' | 2.07 | 0.53 |
| 31:BA:2286:A:H8 | 31:BA:2286:A:HO2' | 1.53 | 0.53 |
| 31:BA:528:A:C2' | 31:BA:529:A:H5' | 2.39 | 0.53 |
| 35:BF:89:VAL:HG12 | 35:BF:90:PHE:H | 1.72 | 0.53 |
| 36:BG:131:TYR:O | 36:BG:159:VAL:HG12 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BI:15:VAL:HG23 | 38:BI:16:GLY:N | 2.23 | 0.53 |
| 41:BP:148:LEU:O | 41:BP:148:LEU:HD22 | 2.09 | 0.53 |
| 44:BS:35:ILE:H | 44:BS:53:SER:CB | 2.22 | 0.53 |
| 47:BV:54:GLY:O | 47:BV:56:SER:OG | 2.17 | 0.53 |
| 31:BA:1225:G:OP1 | 47:BV:88:ARG:HB3 | 2.09 | 0.53 |
| 49:BX:76:ARG:O | 49:BX:77:LYS:HB2 | 2.08 | 0.53 |
| 50:BY:96:ILE:CG1 | 50:BY:99:CYS:SG | 2.97 | 0.53 |
| 1:CA:68:G:H5' | 1:CA:171:A:H1' | 1.90 | 0.53 |
| 1:CA:193:C:H2' | 1:CA:194:C:H6 | 1.74 | 0.53 |
| 1:CA:343:U:N3 | 1:CA:347:G:C6 | 2.77 | 0.53 |
| 1:CA:723:U:H5'' | 1:CA:724:G:OP2 | 2.09 | 0.53 |
| 1:CA:763:G:H2' | 1:CA:764:C:H6 | 1.74 | 0.53 |
| 1:CA:853:G:H2' | 1:CA:854:G:C8 | 2.43 | 0.53 |
| 3:CC:153:VAL:HG12 | 3:CC:154:SER:H | 1.74 | 0.53 |
| 12:CL:32:PHE:CB | 12:CL:84:LEU:HD21 | 2.39 | 0.53 |
| 21:CU:9:ARG:O | 21:CU:13:ILE:HG13 | 2.09 | 0.53 |
| 27:D5:52:TYR:CG | 27:D5:52:TYR:O | 2.62 | 0.53 |
| 31:DA:1109:C:C5 | 31:DA:1110:G:C5 | 2.97 | 0.53 |
| 31:DA:1176:G:C4' | 31:DA:1177:A:OP1 | 2.57 | 0.53 |
| 31:DA:1282:U:H2' | 31:DA:1283:G:O4' | 2.08 | 0.53 |
| 31:DA:2552:U:H2' | 31:DA:2554:U:OP2 | 2.09 | 0.53 |
| 31:DA:2639:A:C2' | 31:DA:2640:G:H5' | 2.39 | 0.53 |
| 31:DA:2845:G:C2' | 31:DA:2846:G:H5' | 2.39 | 0.53 |
| 31:DA:721:C:O2 | 31:DA:721:C:H2' | 2.09 | 0.53 |
| 31:DA:790:C:O2' | 31:DA:791:C:H5' | 2.09 | 0.53 |
| 32:DB:31:C:H4' | 36:DG:29:TRP:CH2 | 2.44 | 0.53 |
| 34:DE:12:THR:O | 34:DE:23:VAL:HG23 | 2.09 | 0.53 |
| 35:DF:113:ALA:HB1 | 35:DF:186:ILE:HG21 | 1.89 | 0.53 |
| 35:DF:141:ALA:O | 35:DF:144:LYS:HB3 | 2.09 | 0.53 |
| 36:DG:98:ARG:O | 36:DG:101:ILE:HG22 | 2.09 | 0.53 |
| 31:DA:995:C:N3 | 46:DU:57:PHE:CE2 | 2.77 | 0.53 |
| 39:DN:2:LYS:NZ | 46:DU:94:ASN:HD21 | 2.07 | 0.53 |
| 50:DY:75:ILE:O | 50:DY:76:CYS:HB2 | 2.09 | 0.53 |
| 1:AA:136:C:H42 | 1:AA:227:G:H1 | 1.56 | 0.52 |
| 1:AA:1452:C:O4' | 1:AA:1456:G:C2 | 2.61 | 0.52 |
| 1:AA:457:C:H2' | 1:AA:458:C:H6 | 1.74 | 0.52 |
| 1:AA:495:A:H4' | 1:AA:496:A:OP1 | 2.09 | 0.52 |
| 1:AA:92:C:H2' | 1:AA:93:G:C8 | 2.43 | 0.52 |
| 6:AF:61:LEU:HD23 | 6:AF:63:TYR:OH | 2.10 | 0.52 |
| 13:AM:32:GLU:OE2 | 13:AM:64:TRP:CH2 | 2.63 | 0.52 |
| 19:AS:63:THR:O | 19:AS:66:MET:HG2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:B2:18:PRO:O | 24:B2:22:GLU:HB2 | 2.09 | 0.52 |
| 31:BA:1925:C:C2' | 31:BA:1926:U:H5' | 2.38 | 0.52 |
| 31:BA:2017:U:H5'' | 31:BA:2018:G:P | 2.49 | 0.52 |
| 31:BA:2092:U:H4' | 31:BA:2093:G:O5' | 2.09 | 0.52 |
| 22:B0:1:MET:CB | 31:BA:2602:A:H62 | 2.22 | 0.52 |
| 31:BA:2652:C:O2' | 31:BA:2653:U:H5' | 2.08 | 0.52 |
| 32:BB:28:C:C2 | 32:BB:29:A:C8 | 2.97 | 0.52 |
| 33:BD:246:PRO:HB2 | 33:BD:255:LYS:HG3 | 1.90 | 0.52 |
| 33:BD:35:LYS:NZ | 33:BD:65:ILE:HA | 2.24 | 0.52 |
| 40:BO:112:MET:HA | 40:BO:112:MET:HE3 | 1.91 | 0.52 |
| 40:BO:35:VAL:HA | 40:BO:62:VAL:HG12 | 1.91 | 0.52 |
| 41:BP:108:LYS:C | 41:BP:110:TYR:H | 2.11 | 0.52 |
| 43:BR:10:LEU:HD22 | 43:BR:17:ARG:HD2 | 1.91 | 0.52 |
| 46:BU:92:ARG:NE | 47:BV:11:GLN:HG2 | 2.23 | 0.52 |
| 1:CA:1255:G:H5' | 1:CA:1256:A:OP1 | 2.09 | 0.52 |
| 1:CA:1236:A:O2' | 1:CA:1304:G:H4' | 2.10 | 0.52 |
| 1:CA:1356:G:H2' | 1:CA:1357:A:C8 | 2.44 | 0.52 |
| 1:CA:322:C:C5 | 1:CA:328:C:H5 | 2.20 | 0.52 |
| 7:CG:113:GLU:HB2 | 7:CG:119:ARG:HG2 | 1.90 | 0.52 |
| 15:CO:67:LEU:HD22 | 15:CO:78:TYR:HE1 | 1.74 | 0.52 |
| 23:D1:40:ARG:HD3 | 23:D1:41:ARG:N | 2.19 | 0.52 |
| 28:D6:19:ARG:O | 28:D6:20:ASN:O | 2.27 | 0.52 |
| 31:DA:1526:G:C6 | 31:DA:1527:G:C2 | 2.97 | 0.52 |
| 31:DA:1820:U:C2 | 33:DD:202:LYS:HB3 | 2.43 | 0.52 |
| 31:DA:1826:G:H2' | 31:DA:1827:C:H6 | 1.74 | 0.52 |
| 31:DA:2086:U:H2' | 31:DA:2087:G:C8 | 2.44 | 0.52 |
| 31:DA:2476:A:C2 | 31:DA:2477:C:H5'' | 2.44 | 0.52 |
| 31:DA:2494:G:C4 | 31:DA:2495:G:C8 | 2.97 | 0.52 |
| 31:DA:271(T):C:C2 | 31:DA:271(U):G:C8 | 2.97 | 0.52 |
| 31:DA:2728:U:O2' | 31:DA:2729:G:H5' | 2.07 | 0.52 |
| 31:DA:387:U:H4' | 31:DA:388:G:O5' | 2.09 | 0.52 |
| 31:DA:693:C:H2' | 31:DA:694:U:C6 | 2.44 | 0.52 |
| 31:DA:706:A:H2' | 31:DA:707:G:O4' | 2.09 | 0.52 |
| 34:DE:36:ARG:HH11 | 34:DE:85:ASN:ND2 | 2.07 | 0.52 |
| 38:DI:144:VAL:HG12 | 38:DI:145:VAL:H | 1.74 | 0.52 |
| 42:DQ:32:TYR:CE2 | 42:DQ:133:ARG:HG2 | 2.43 | 0.52 |
| 44:DS:17:ARG:C | 44:DS:19:LYS:H | 2.12 | 0.52 |
| 44:DS:42:ASP:O | 44:DS:43:GLU:HB2 | 2.08 | 0.52 |
| 44:DS:56:LEU:HD23 | 44:DS:56:LEU:C | 2.30 | 0.52 |
| 31:DA:1162:G:O2' | 47:DV:92:THR:HG23 | 2.07 | 0.52 |
| 49:DX:31:HIS:HD2 | 49:DX:33:LYS:H | 1.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 49:DX:83:VAL:HG23 | 49:DX:83:VAL:O | 2.09 | 0.52 |
| 50:DY:71:LYS:HZ3 | 50:DY:71:LYS:HB2 | 1.72 | 0.52 |
| 51:DZ:10:ARG:HH21 | 51:DZ:26:GLY:H | 1.55 | 0.52 |
| 1:AA:1074:G:C2 | 1:AA:1102:A:C2 | 2.97 | 0.52 |
| 1:AA:1255:G:H5' | 1:AA:1256:A:OP1 | 2.09 | 0.52 |
| 1:AA:343:U:O2 | 1:AA:347:G:C2 | 2.62 | 0.52 |
| 1:AA:353:A:C2' | 1:AA:354:G:OP2 | 2.56 | 0.52 |
| 1:AA:377:G:O2' | 1:AA:378:G:H5' | 2.09 | 0.52 |
| 1:AA:380:G:N2 | 1:AA:384:G:C6 | 2.77 | 0.52 |
| 1:AA:621:A:C2' | 1:AA:622:A:H5' | 2.39 | 0.52 |
| 1:AA:804:U:H5'' | 1:AA:805:C:OP2 | 2.09 | 0.52 |
| 1:AA:858:G:O6 | 1:AA:869:G:H3' | 2.08 | 0.52 |
| 2:AB:98:LEU:HB2 | 2:AB:101:MET:CE | 2.39 | 0.52 |
| 5:AE:126:ARG:HA | 5:AE:131:ILE:HD11 | 1.90 | 0.52 |
| 6:AF:18:GLN:O | 6:AF:21:LEU:HB2 | 2.09 | 0.52 |
| 9:AI:65:VAL:HG21 | 9:AI:73:GLN:HB3 | 1.92 | 0.52 |
| 16:AP:79:VAL:HG12 | 16:AP:80:PHE:CG | 2.44 | 0.52 |
| 18:AR:61:LYS:O | 18:AR:65:ILE:HG13 | 2.09 | 0.52 |
| 18:AR:59:SER:OG | 18:AR:62:GLU:HG3 | 2.09 | 0.52 |
| 24:B2:26:ARG:NE | 24:B2:29:LYS:HE2 | 2.24 | 0.52 |
| 30:B8:22:VAL:O | 30:B8:49:VAL:HG23 | 2.08 | 0.52 |
| 31:BA:481:G:O2' | 31:BA:482:A:P | 2.67 | 0.52 |
| 31:BA:536:A:H2' | 31:BA:537:C:H6 | 1.74 | 0.52 |
| 33:BD:64:ILE:O | 33:BD:64:ILE:HG12 | 2.08 | 0.52 |
| 37:BH:85:LYS:NZ | 37:BH:133:VAL:HB | 2.24 | 0.52 |
| 38:BI:6:LEU:N | 38:BI:6:LEU:HD23 | 2.25 | 0.52 |
| 41:BP:105:LEU:HD12 | 41:BP:105:LEU:N | 2.24 | 0.52 |
| 45:BT:109:GLU:HB3 | 45:BT:113:LYS:HE3 | 1.90 | 0.52 |
| 45:BT:35:LYS:O | 45:BT:37:GLY:N | 2.43 | 0.52 |
| 45:BT:90:GLN:HG2 | 45:BT:120:ARG:NH2 | 2.24 | 0.52 |
| 31:BA:2863:C:OP1 | 45:BT:93:ARG:NH1 | 2.43 | 0.52 |
| 46:BU:85:LYS:O | 46:BU:116:ALA:HB1 | 2.09 | 0.52 |
| 47:BV:53:GLU:O | 47:BV:55:ALA:N | 2.43 | 0.52 |
| 49:BX:88:LYS:HD2 | 49:BX:88:LYS:N | 2.23 | 0.52 |
| 51:BZ:73:GLN:HG2 | 51:BZ:87:ASP:OD1 | 2.10 | 0.52 |
| 1:CA:1410:G:O2' | 1:CA:1411:C:H5' | 2.09 | 0.52 |
| 1:CA:234:C:H2' | 1:CA:235:C:H6 | 1.74 | 0.52 |
| 1:CA:590:C:H2' | 1:CA:591:U:H6 | 1.74 | 0.52 |
| 6:CF:50:TYR:CZ | 18:CR:77:GLY:HA2 | 2.43 | 0.52 |
| 11:CK:20:TYR:C | 11:CK:21:ILE:HD12 | 2.30 | 0.52 |
| 28:D6:34:LEU:HD22 | 28:D6:50:ARG:NH1 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:D8:32:LEU:CD1 | 30:D8:32:LEU:H | 2.11 | 0.52 |
| 31:DA:1420:U:O2' | 31:DA:1421:G:OP1 | 2.26 | 0.52 |
| 31:DA:151:C:C2' | 31:DA:152:G:H5' | 2.40 | 0.52 |
| 31:DA:1947:C:C2' | 31:DA:1948:G:C5' | 2.88 | 0.52 |
| 31:DA:2065:C:H2' | 31:DA:2066:C:H6 | 1.72 | 0.52 |
| 31:DA:2199:A:H5'' | 31:DA:2200:C:OP2 | 2.09 | 0.52 |
| 31:DA:2660:A:C2' | 31:DA:2661:G:O5' | 2.57 | 0.52 |
| 31:DA:2713:A:C3' | 31:DA:2714:G:C5' | 2.86 | 0.52 |
| 31:DA:271(P):C:C2' | 31:DA:271(Q):G:H5' | 2.38 | 0.52 |
| 31:DA:2762:G:H5' | 31:DA:2762:G:C8 | 2.45 | 0.52 |
| 31:DA:315:G:H2' | 31:DA:316:C:C6 | 2.43 | 0.52 |
| 31:DA:643:A:C2' | 31:DA:644:A:O5' | 2.58 | 0.52 |
| 32:DB:60:C:O2 | 32:DB:61:G:C8 | 2.63 | 0.52 |
| 34:DE:31:CYS:HB3 | 34:DE:49:LEU:HD12 | 1.90 | 0.52 |
| 37:DH:148:ILE:O | 37:DH:162:ILE:HD11 | 2.08 | 0.52 |
| 38:DI:125:GLU:OE1 | 38:DI:141:LYS:HG2 | 2.09 | 0.52 |
| 40:DO:42:SER:OG | 40:DO:44:LYS:HE2 | 2.09 | 0.52 |
| 42:DQ:16:ARG:CG | 42:DQ:17:LEU:H | 2.23 | 0.52 |
| 44:DS:28:VAL:O | 44:DS:89:ARG:HB2 | 2.08 | 0.52 |
| 45:DT:33:LYS:H | 45:DT:33:LYS:HZ2 | 1.56 | 0.52 |
| 47:DV:61:VAL:O | 47:DV:62:LEU:HD23 | 2.08 | 0.52 |
| 51:DZ:73:GLN:HG2 | 51:DZ:87:ASP:OD2 | 2.09 | 0.52 |
| 1:AA:1084:G:OP1 | 1:AA:1086:U:C2 | 2.62 | 0.52 |
| 1:AA:1452:C:H4' | 1:AA:1456:G:N3 | 2.24 | 0.52 |
| 1:AA:262:A:C6 | 1:AA:263:A:N6 | 2.77 | 0.52 |
| 1:AA:626:U:C2 | 1:AA:627:G:C8 | 2.98 | 0.52 |
| 2:AB:20:GLU:HG3 | 2:AB:189:ASP:OD2 | 2.09 | 0.52 |
| 2:AB:71:VAL:HG22 | 2:AB:93:VAL:HB | 1.90 | 0.52 |
| 7:AG:113:GLU:HB2 | 7:AG:119:ARG:HG2 | 1.91 | 0.52 |
| 8:AH:123:GLU:O | 8:AH:127:LEU:HB2 | 2.10 | 0.52 |
| 14:AN:6:LEU:HD23 | 14:AN:9:LYS:HD3 | 1.90 | 0.52 |
| 19:AS:29:ARG:HB3 | 19:AS:47:HIS:HA | 1.91 | 0.52 |
| 31:BA:1047:G:H21 | 31:BA:1111:A:N6 | 2.04 | 0.52 |
| 31:BA:1179:C:H3' | 31:BA:1180:C:H5'' | 1.90 | 0.52 |
| 31:BA:143:G:H1' | 49:BX:38:GLU:HG3 | 1.91 | 0.52 |
| 31:BA:1587:A:H3' | 31:BA:1588:C:H6 | 1.74 | 0.52 |
| 31:BA:2660:A:C5' | 31:BA:2661:G:N2 | 2.71 | 0.52 |
| 31:BA:866:A:C6 | 31:BA:914:C:C6 | 2.98 | 0.52 |
| 34:BE:116:VAL:HG13 | 34:BE:122:PHE:HB2 | 1.91 | 0.52 |
| 34:BE:201:THR:CG2 | 34:BE:202:LYS:N | 2.71 | 0.52 |
| 35:BF:200:GLU:O | 35:BF:204:ASN:HB2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BI:144:VAL:HG12 | 38:BI:145:VAL:H | 1.74 | 0.52 |
| 40:BO:24:VAL:HB | 40:BO:33:ALA:HB2 | 1.90 | 0.52 |
| 41:BP:17:LYS:O | 41:BP:19:VAL:HG23 | 2.09 | 0.52 |
| 45:BT:91:ARG:HB3 | 45:BT:116:ALA:HA | 1.90 | 0.52 |
| 50:BY:45:VAL:CG1 | 50:BY:62:GLU:HB2 | 2.33 | 0.52 |
| 1:CA:1125:U:H2' | 1:CA:1126:U:OP2 | 2.10 | 0.52 |
| 1:CA:300:A:H8 | 1:CA:300:A:O5' | 1.91 | 0.52 |
| 1:CA:475:G:H2' | 1:CA:476:G:C8 | 2.41 | 0.52 |
| 1:CA:657:G:C2 | 1:CA:658:G:C8 | 2.97 | 0.52 |
| 3:CC:138:VAL:HG22 | 3:CC:151:VAL:CG2 | 2.38 | 0.52 |
| 8:CH:114:THR:HG23 | 8:CH:117:GLY:O | 2.08 | 0.52 |
| 9:CI:55:ALA:CB | 9:CI:58:ARG:HD2 | 2.40 | 0.52 |
| 15:CO:36:ILE:HG22 | 15:CO:37:ASN:HD22 | 1.74 | 0.52 |
| 20:CT:63:ILE:HD13 | 20:CT:80:ARG:HB2 | 1.90 | 0.52 |
| 20:CT:94:ALA:O | 20:CT:95:ALA:HB3 | 2.09 | 0.52 |
| 22:D0:27:GLU:HB3 | 31:DA:856:C:H1' | 1.92 | 0.52 |
| 22:D0:65:GLY:HA2 | 22:D0:84:LEU:HD21 | 1.90 | 0.52 |
| 28:D6:28:ARG:CA | 28:D6:32:ASN:HB3 | 2.39 | 0.52 |
| 31:DA:991:C:O2 | 31:DA:1164:G:C2 | 2.62 | 0.52 |
| 31:DA:1497:U:H5'' | 31:DA:1498:C:C5 | 2.45 | 0.52 |
| 31:DA:1642:G:C2' | 31:DA:1643:G:H5' | 2.40 | 0.52 |
| 31:DA:2287:A:H61 | 31:DA:2344:U:H3 | 1.49 | 0.52 |
| 31:DA:2291:U:H5'' | 31:DA:2380:C:O2' | 2.09 | 0.52 |
| 31:DA:2410:G:C2 | 31:DA:2411:A:H1' | 2.45 | 0.52 |
| 31:DA:1751:C:HO2' | 31:DA:2861:G:HO2' | 1.55 | 0.52 |
| 31:DA:2865:U:C4 | 31:DA:2866:U:C4 | 2.97 | 0.52 |
| 31:DA:814:C:H5 | 41:DP:27:HIS:CD2 | 2.27 | 0.52 |
| 33:DD:118:VAL:HG22 | 33:DD:119:ALA:N | 2.24 | 0.52 |
| 33:DD:70:TRP:CD1 | 33:DD:70:TRP:C | 2.82 | 0.52 |
| 36:DG:39:ILE:HB | 36:DG:157:ILE:HG22 | 1.90 | 0.52 |
| 37:DH:153:LYS:HG2 | 37:DH:154:PRO:N | 2.25 | 0.52 |
| 39:DN:34:LEU:O | 39:DN:49:GLY:HA3 | 2.08 | 0.52 |
| 45:DT:30:VAL:HG21 | 45:DT:83:ILE:H | 1.73 | 0.52 |
| 45:DT:51:ARG:CG | 45:DT:98:LYS:HE2 | 2.37 | 0.52 |
| 31:DA:495:G:H1' | 48:DW:57:ASN:ND2 | 2.23 | 0.52 |
| 50:DY:44:ILE:HG22 | 50:DY:45:VAL:N | 2.23 | 0.52 |
| 1:AA:1103:C:H2' | 1:AA:1104:G:O4' | 2.10 | 0.52 |
| 1:AA:1392:G:C2' | 1:AA:1393:U:H5' | 2.39 | 0.52 |
| 1:AA:1530:G:OP1 | 1:AA:1530:G:C4' | 2.56 | 0.52 |
| 1:AA:250:A:C4' | 1:AA:251:G:O5' | 2.52 | 0.52 |
| 1:AA:865:A:C2 | 1:AA:918:A:H4' | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AE:148:VAL:HG21 | 8:AH:107:LEU:HD22 | 1.91 | 0.52 |
| 15:AO:23:GLY:O | 15:AO:27:VAL:HB | 2.09 | 0.52 |
| 16:AP:74:LEU:HB3 | 16:AP:79:VAL:HG11 | 1.91 | 0.52 |
| 17:AQ:86:GLU:O | 17:AQ:90:ILE:HG12 | 2.09 | 0.52 |
| 19:AS:24:ALA:O | 19:AS:25:LYS:HB2 | 2.10 | 0.52 |
| 23:B1:10:LYS:O | 23:B1:13:ILE:CG2 | 2.58 | 0.52 |
| 31:BA:142:A:H5'' | 31:BA:142(A):C:C5 | 2.45 | 0.52 |
| 31:BA:1502:C:H2' | 31:BA:1502:C:O2 | 2.09 | 0.52 |
| 31:BA:1512:U:C2' | 31:BA:1513:C:H5' | 2.40 | 0.52 |
| 31:BA:1865:G:H2' | 31:BA:1876:A:N7 | 2.25 | 0.52 |
| 31:BA:2036:C:H6 | 31:BA:2036:C:C5' | 2.18 | 0.52 |
| 31:BA:2069:G:H2' | 31:BA:2070:G:H5' | 1.91 | 0.52 |
| 31:BA:2102:U:C6 | 31:BA:2187:G:O6 | 2.63 | 0.52 |
| 31:BA:2476:A:C6 | 31:BA:2477:C:C5 | 2.97 | 0.52 |
| 31:BA:570:G:H2' | 31:BA:2030:A:C5 | 2.44 | 0.52 |
| 31:BA:643:A:C2' | 31:BA:644:A:O5' | 2.58 | 0.52 |
| 32:BB:21:G:O2' | 32:BB:22:U:OP2 | 2.27 | 0.52 |
| 33:BD:209:ALA:C | 33:BD:210:GLY:O | 2.44 | 0.52 |
| 33:BD:35:LYS:NZ | 33:BD:104:TYR:CB | 2.61 | 0.52 |
| 34:BE:31:CYS:HB3 | 34:BE:49:LEU:HD12 | 1.89 | 0.52 |
| 35:BF:22:ALA:O | 35:BF:26:ALA:CB | 2.43 | 0.52 |
| 37:BH:89:ILE:HG22 | 37:BH:162:ILE:HG22 | 1.91 | 0.52 |
| 38:BI:82:ARG:HG2 | 38:BI:89:TYR:HD2 | 1.71 | 0.52 |
| 42:BQ:85:LYS:HG3 | 42:BQ:86:GLY:N | 2.24 | 0.52 |
| 43:BR:59:ASP:OD1 | 43:BR:61:HIS:HB3 | 2.09 | 0.52 |
| 49:BX:87:GLN:HB2 | 49:BX:88:LYS:HD2 | 1.92 | 0.52 |
| 50:BY:61:ILE:N | 50:BY:61:ILE:HD12 | 2.24 | 0.52 |
| 1:CA:1441:G:H5'' | 1:CA:1442:G:H5' | 1.90 | 0.52 |
| 1:CA:327:A:O2' | 1:CA:329:A:H8 | 1.92 | 0.52 |
| 1:CA:804:U:H5'' | 1:CA:805:C:OP2 | 2.09 | 0.52 |
| 7:CG:97:GLN:HE21 | 7:CG:101:LEU:HD11 | 1.73 | 0.52 |
| 12:CL:34:ARG:O | 12:CL:61:THR:HG23 | 2.10 | 0.52 |
| 13:CM:78:ILE:HA | 13:CM:81:LEU:HD12 | 1.92 | 0.52 |
| 14:CN:22:THR:HB | 14:CN:33:VAL:HG11 | 1.90 | 0.52 |
| 1:CA:375:U:O3' | 16:CP:6:LEU:HB2 | 2.09 | 0.52 |
| 6:CF:100:ASN:H | 18:CR:23:LYS:HZ2 | 1.58 | 0.52 |
| 31:DA:53:A:H61 | 31:DA:117:G:C2' | 2.23 | 0.52 |
| 31:DA:1245:G:OP1 | 41:DP:16:ARG:HD2 | 2.09 | 0.52 |
| 31:DA:1448:G:H1' | 31:DA:1528:A:H61 | 1.71 | 0.52 |
| 31:DA:2324:C:H5'' | 31:DA:2325:G:H5' | 1.91 | 0.52 |
| 31:DA:2639:A:H2' | 31:DA:2640:G:H5' | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:271(P):C:O2' | 31:DA:271(Q):G:H5' | 2.09 | 0.52 |
| 31:DA:271(R):G:C2' | 31:DA:271(S):G:H5' | 2.39 | 0.52 |
| 31:DA:271(T):C:H2' | 31:DA:271(T):C:O2 | 2.09 | 0.52 |
| 31:DA:510:C:H2' | 31:DA:511:U:H5' | 1.91 | 0.52 |
| 31:DA:528:A:C8 | 31:DA:528:A:H3' | 2.45 | 0.52 |
| 38:DI:8:PRO:HA | 38:DI:13:GLY:O | 2.10 | 0.52 |
| 41:DP:146:VAL:HG13 | 41:DP:147:LEU:H | 1.74 | 0.52 |
| 45:DT:109:GLU:HB3 | 45:DT:113:LYS:HE3 | 1.90 | 0.52 |
| 45:DT:91:ARG:HA | 45:DT:117:ASP:H | 1.73 | 0.52 |
| 45:DT:91:ARG:HB3 | 45:DT:116:ALA:HA | 1.91 | 0.52 |
| 45:DT:92:GLY:C | 45:DT:94:ALA:H | 2.13 | 0.52 |
| 49:DX:65:ARG:HA | 49:DX:65:ARG:HE | 1.74 | 0.52 |
| 51:DZ:39:VAL:CG2 | 51:DZ:44:PHE:HB2 | 2.39 | 0.52 |
| 42:DQ:141:GLN:HE21 | 51:DZ:71:VAL:C | 2.11 | 0.52 |
| 1:AA:356:A:H2 | 1:AA:368:U:O2 | 1.93 | 0.52 |
| 1:AA:636:U:H2' | 1:AA:637:G:C8 | 2.44 | 0.52 |
| 9:AI:40:LEU:HD11 | 9:AI:70:LYS:HG2 | 1.90 | 0.52 |
| 13:AM:97:PRO:O | 13:AM:98:VAL:HA | 2.10 | 0.52 |
| 16:AP:75:ARG:C | 16:AP:77:ALA:H | 2.13 | 0.52 |
| 23:B1:10:LYS:CG | 23:B1:11:ARG:H | 2.22 | 0.52 |
| 24:B2:47:ASN:ND2 | 24:B2:48:HIS:N | 2.57 | 0.52 |
| 27:B5:36:CYS:HB2 | 27:B5:49:CYS:SG | 2.50 | 0.52 |
| 27:B5:57:VAL:CB | 27:B5:58:LEU:HD12 | 2.39 | 0.52 |
| 30:B8:32:LEU:N | 30:B8:32:LEU:HD13 | 2.05 | 0.52 |
| 31:BA:1045:A:H3' | 31:BA:1045:A:N3 | 2.25 | 0.52 |
| 30:B8:31:HIS:CD2 | 31:BA:2419:U:O4 | 2.60 | 0.52 |
| 31:BA:582:G:H2' | 31:BA:583:G:C8 | 2.45 | 0.52 |
| 31:BA:643:A:O2' | 31:BA:644:A:H5' | 2.09 | 0.52 |
| 33:BD:96:HIS:CE1 | 33:BD:102:LYS:HD3 | 2.44 | 0.52 |
| 38:BI:1:MET:O | 38:BI:20:ASP:HA | 2.09 | 0.52 |
| 38:BI:69:LYS:O | 38:BI:69:LYS:HG2 | 2.10 | 0.52 |
| 39:BN:78:TYR:CD1 | 39:BN:79:PRO:HD3 | 2.44 | 0.52 |
| 39:BN:90:MET:O | 39:BN:93:THR:O | 2.28 | 0.52 |
| 31:BA:1191:G:OP1 | 41:BP:35:HIS:ND1 | 2.42 | 0.52 |
| 45:BT:31:SER:CA | 45:BT:32:TYR:CD2 | 2.92 | 0.52 |
| 47:BV:38:LEU:HG | 47:BV:39:LEU:H | 1.74 | 0.52 |
| 1:CA:1135:U:H4' | 1:CA:1136:U:H5 | 1.74 | 0.52 |
| 1:CA:304:U:H2' | 1:CA:305:G:C8 | 2.45 | 0.52 |
| 1:CA:336:C:O2' | 1:CA:337:C:H5' | 2.09 | 0.52 |
| 1:CA:356:A:H2 | 1:CA:368:U:O2 | 1.91 | 0.52 |
| 1:CA:523:A:H61 | 12:CL:53:ARG:HH12 | 1.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:163:PHE:O | 2:CB:164:VAL:HG23 | 2.10 | 0.52 |
| 2:CB:97:TRP:HH2 | 2:CB:176:GLU:CG | 2.22 | 0.52 |
| 5:CE:80:ILE:HG22 | 8:CH:104:ARG:CZ | 2.40 | 0.52 |
| 5:CE:79:GLU:HB3 | 5:CE:92:LYS:HG3 | 1.91 | 0.52 |
| 7:CG:121:ALA:O | 7:CG:125:MET:HG3 | 2.10 | 0.52 |
| 9:CI:65:VAL:HG21 | 9:CI:73:GLN:HB3 | 1.92 | 0.52 |
| 28:D6:28:ARG:HA | 28:D6:32:ASN:HB3 | 1.91 | 0.52 |
| 31:DA:1332:G:N2 | 31:DA:1609:A:H2' | 2.24 | 0.52 |
| 31:DA:1833:U:O2' | 31:DA:1969:A:N1 | 2.37 | 0.52 |
| 31:DA:2820:A:O4' | 43:DR:5:LYS:HG3 | 2.08 | 0.52 |
| 33:DD:131:LEU:N | 33:DD:131:LEU:HD12 | 2.25 | 0.52 |
| 33:DD:146:GLU:HB2 | 33:DD:189:CYS:HB3 | 1.90 | 0.52 |
| 33:DD:89:SER:HB2 | 33:DD:159:ALA:HB2 | 1.92 | 0.52 |
| 31:DA:1006:C:C1' | 39:DN:106:MET:HE3 | 2.35 | 0.52 |
| 39:DN:45:ASN:H | 39:DN:45:ASN:ND2 | 2.00 | 0.52 |
| 41:DP:10:PRO:HD2 | 41:DP:11:GLY:H | 1.74 | 0.52 |
| 42:DQ:18:LYS:O | 42:DQ:19:GLY:C | 2.47 | 0.52 |
| 42:DQ:75:THR:HA | 42:DQ:89:ASN:H | 1.74 | 0.52 |
| 47:DV:70:ILE:CB | 47:DV:90:PRO:HB2 | 2.38 | 0.52 |
| 50:DY:68:HIS:N | 50:DY:71:LYS:HZ1 | 2.08 | 0.52 |
| 1:AA:1347:G:C8 | 9:AI:107:ARG:HB3 | 2.44 | 0.52 |
| 2:AB:239:VAL:HG12 | 2:AB:239:VAL:O | 2.09 | 0.52 |
| 3:AC:126:ARG:O | 3:AC:127:ARG:HB2 | 2.08 | 0.52 |
| 7:AG:121:ALA:O | 7:AG:125:MET:HG3 | 2.09 | 0.52 |
| 24:B2:55:ARG:HH22 | 49:BX:3:THR:CG2 | 2.23 | 0.52 |
| 30:B8:32:LEU:CB | 30:B8:35:GLN:N | 2.62 | 0.52 |
| 30:B8:35:GLN:HE21 | 30:B8:36:LYS:HZ3 | 1.57 | 0.52 |
| 31:BA:1138:G:H21 | 39:BN:106:MET:CE | 2.21 | 0.52 |
| 31:BA:2712:U:O2' | 31:BA:2713:A:H5' | 2.10 | 0.52 |
| 31:BA:330:A:H2 | 31:BA:1210:A:C2' | 2.11 | 0.52 |
| 33:BD:255:LYS:CE | 33:BD:255:LYS:H | 2.23 | 0.52 |
| 34:BE:60:ASN:OD1 | 34:BE:62:PRO:HD2 | 2.10 | 0.52 |
| 40:BO:90:GLN:O | 40:BO:91:LEU:HB2 | 2.10 | 0.52 |
| 47:BV:70:ILE:HB | 47:BV:90:PRO:CB | 2.40 | 0.52 |
| 51:BZ:118:GLN:O | 51:BZ:120:ILE:N | 2.40 | 0.52 |
| 1:CA:187:C:H2' | 1:CA:188:C:C6 | 2.44 | 0.52 |
| 1:CA:579:G:H2' | 1:CA:580:U:C6 | 2.44 | 0.52 |
| 1:CA:665:A:C5 | 1:CA:733:A:C5 | 2.98 | 0.52 |
| 1:CA:763:G:O2' | 1:CA:764:C:H5' | 2.09 | 0.52 |
| 6:CF:12:PRO:HG2 | 6:CF:55:ASP:OD1 | 2.09 | 0.52 |
| 6:CF:39:LYS:HB2 | 6:CF:62:TRP:HZ3 | 1.72 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:CF:69:GLU:HG2 | 6:CF:70:ASP:H | 1.73 | 0.52 |
| 19:CS:24:ALA:O | 19:CS:25:LYS:HB2 | 2.10 | 0.52 |
| 27:D5:40:LYS:CE | 27:D5:46:CYS:HB3 | 2.39 | 0.52 |
| 28:D6:20:ASN:O | 28:D6:21:TYR:CD1 | 2.63 | 0.52 |
| 30:D8:35:GLN:NE2 | 30:D8:36:LYS:NZ | 2.58 | 0.52 |
| 31:DA:1138:G:H21 | 39:DN:106:MET:CE | 2.22 | 0.52 |
| 31:DA:1169:G:N2 | 31:DA:1181:C:C2 | 2.78 | 0.52 |
| 31:DA:173:G:C6 | 31:DA:174:C:C4 | 2.98 | 0.52 |
| 31:DA:1839:G:C8 | 31:DA:1927:A:H1' | 2.44 | 0.52 |
| 31:DA:1865:G:H2' | 31:DA:1876:A:N7 | 2.24 | 0.52 |
| 31:DA:784:A:C8 | 31:DA:792:G:C5 | 2.97 | 0.52 |
| 32:DB:41:U:C2' | 32:DB:42:C:OP1 | 2.58 | 0.52 |
| 33:DD:79:VAL:HG21 | 33:DD:111:LEU:HD11 | 1.91 | 0.52 |
| 33:DD:35:LYS:NZ | 33:DD:65:ILE:HA | 2.25 | 0.52 |
| 34:DE:111:ARG:HD2 | 34:DE:160:TYR:CE1 | 2.43 | 0.52 |
| 34:DE:174:ASP:OD2 | 34:DE:175:VAL:N | 2.40 | 0.52 |
| 31:DA:2632:A:H1' | 34:DE:61:ARG:CZ | 2.40 | 0.52 |
| 31:DA:2632:A:N3 | 34:DE:61:ARG:NH1 | 2.58 | 0.52 |
| 37:DH:54:ARG:CG | 37:DH:65:HIS:HD2 | 2.22 | 0.52 |
| 39:DN:95:PRO:HG2 | 39:DN:96:GLU:OE2 | 2.09 | 0.52 |
| 44:DS:26:LEU:HD22 | 44:DS:87:PHE:CD1 | 2.44 | 0.52 |
| 44:DS:35:ILE:C | 44:DS:36:TYR:CD1 | 2.83 | 0.52 |
| 44:DS:83:LYS:HE2 | 44:DS:105:ALA:HB2 | 1.92 | 0.52 |
| 39:DN:2:LYS:NZ | 46:DU:94:ASN:ND2 | 2.57 | 0.52 |
| 46:DU:91:ASP:OD2 | 46:DU:96:ALA:N | 2.42 | 0.52 |
| 47:DV:51:VAL:CG1 | 47:DV:52:VAL:N | 2.72 | 0.52 |
| 47:DV:69:LYS:O | 47:DV:70:ILE:CG2 | 2.57 | 0.52 |
| 50:DY:49:VAL:HG12 | 50:DY:53:PRO:HG3 | 1.92 | 0.52 |
| 51:DZ:152:ALA:HB1 | 51:DZ:167:PRO:HB2 | 1.91 | 0.52 |
| 1:AA:545:C:H5'' | 4:AD:72:GLU:HG2 | 1.92 | 0.52 |
| 1:AA:70:G:H2' | 1:AA:71:C:C6 | 2.45 | 0.52 |
| 1:AA:936:C:H2' | 1:AA:937:A:O4' | 2.10 | 0.52 |
| 3:AC:157:ILE:CD1 | 3:AC:166:GLU:HB2 | 2.39 | 0.52 |
| 11:AK:15:ALA:HA | 11:AK:77:MET:HA | 1.91 | 0.52 |
| 1:AA:1320:C:H5' | 19:AS:70:LYS:HG2 | 1.90 | 0.52 |
| 23:B1:25:LYS:O | 23:B1:26:ARG:HG3 | 2.10 | 0.52 |
| 28:B6:19:ARG:O | 28:B6:20:ASN:O | 2.28 | 0.52 |
| 31:BA:1288:U:H4' | 31:BA:1289:C:OP2 | 2.09 | 0.52 |
| 31:BA:2030:A:C5' | 31:BA:2031:A:OP1 | 2.54 | 0.52 |
| 31:BA:185:U:H4' | 31:BA:218:A:H4' | 1.92 | 0.52 |
| 31:BA:2536:G:C5 | 31:BA:2537:U:C5 | 2.98 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:271(D):G:H2' | 31:BA:271(E):U:O4' | 2.10 | 0.52 |
| 31:BA:2807:G:H3' | 31:BA:2808:U:H5'' | 1.92 | 0.52 |
| 31:BA:790:C:O2' | 31:BA:791:C:C5' | 2.57 | 0.52 |
| 39:BN:47:ALA:CB | 39:BN:112:LEU:HD11 | 2.31 | 0.52 |
| 43:BR:2:ARG:HB2 | 43:BR:5:LYS:HE3 | 1.92 | 0.52 |
| 45:BT:92:GLY:C | 45:BT:94:ALA:H | 2.12 | 0.52 |
| 47:BV:15:GLU:O | 47:BV:98:GLU:OE2 | 2.28 | 0.52 |
| 1:CA:1290:G:N3 | 1:CA:1290:G:H2' | 2.25 | 0.52 |
| 1:CA:1316:G:H2' | 1:CA:1317:C:H5'' | 1.91 | 0.52 |
| 1:CA:1470:G:C2' | 1:CA:1471:G:H5' | 2.39 | 0.52 |
| 1:CA:20:U:H2' | 1:CA:21:G:O4' | 2.09 | 0.52 |
| 1:CA:342:C:C2' | 1:CA:343:U:H5' | 2.39 | 0.52 |
| 1:CA:343:U:C2 | 1:CA:347:G:C2 | 2.97 | 0.52 |
| 1:CA:553:A:H2' | 1:CA:554:C:C6 | 2.45 | 0.52 |
| 3:CC:157:ILE:CD1 | 3:CC:166:GLU:HB2 | 2.39 | 0.52 |
| 4:CD:148:VAL:HG12 | 4:CD:149:ALA:N | 2.25 | 0.52 |
| 9:CI:116:LYS:O | 9:CI:118:LYS:N | 2.42 | 0.52 |
| 9:CI:53:VAL:HB | 9:CI:92:TYR:HE2 | 1.75 | 0.52 |
| 19:CS:29:ARG:HB3 | 19:CS:47:HIS:HA | 1.92 | 0.52 |
| 24:D2:57:ILE:HG21 | 24:D2:59:ARG:NH1 | 2.24 | 0.52 |
| 31:DA:1027:A:N6 | 31:DA:1126:A:C4 | 2.78 | 0.52 |
| 31:DA:2306:C:H5'' | 31:DA:2307:G:O4' | 2.09 | 0.52 |
| 38:DI:109:ILE:HG22 | 38:DI:130:TYR:OH | 2.09 | 0.52 |
| 50:DY:52:SER:O | 50:DY:54:LYS:N | 2.41 | 0.52 |
| 1:AA:376:G:H2' | 1:AA:377:G:H8 | 1.74 | 0.52 |
| 1:AA:707:C:O2 | 1:AA:708:C:C6 | 2.63 | 0.52 |
| 1:AA:929:G:C6 | 1:AA:930:C:N4 | 2.78 | 0.52 |
| 1:AA:989:C:N4 | 1:AA:1216:G:H1 | 2.07 | 0.52 |
| 2:AB:135:GLN:O | 2:AB:139:LYS:HB2 | 2.09 | 0.52 |
| 3:AC:108:ASN:ND2 | 3:AC:111:LEU:HD12 | 2.24 | 0.52 |
| 5:AE:135:THR:O | 5:AE:138:ALA:HB3 | 2.10 | 0.52 |
| 7:AG:111:ARG:HB3 | 7:AG:113:GLU:HG2 | 1.92 | 0.52 |
| 17:AQ:74:LEU:HD12 | 17:AQ:75:ARG:HG2 | 1.92 | 0.52 |
| 20:AT:12:ALA:O | 20:AT:15:ARG:HB2 | 2.10 | 0.52 |
| 20:AT:75:ASN:ND2 | 20:AT:75:ASN:H | 2.07 | 0.52 |
| 24:B2:22:GLU:O | 24:B2:25:VAL:HG12 | 2.10 | 0.52 |
| 31:BA:1330:C:O2' | 31:BA:1331:A:H5' | 2.10 | 0.52 |
| 31:BA:1527:G:C5' | 31:BA:1528:A:OP1 | 2.58 | 0.52 |
| 31:BA:2302:G:C6 | 31:BA:2315:G:C6 | 2.98 | 0.52 |
| 31:BA:1786:A:H2 | 31:BA:2606:C:H1' | 1.75 | 0.52 |
| 31:BA:2660:A:H5'' | 31:BA:2661:G:N2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:BA:2656:U:N3 | 31:BA:2665:A:H2 | 2.05 | 0.52 |
| 31:BA:2779:U:O2 | 31:BA:2779:U:O4' | 2.28 | 0.52 |
| 31:BA:309:G:N3 | 31:BA:329:G:O2' | 2.41 | 0.52 |
| 31:BA:357:A:C2 | 31:BA:358:U:O2 | 2.63 | 0.52 |
| 31:BA:693:C:O2' | 31:BA:694:U:H5' | 2.09 | 0.52 |
| 31:BA:971:C:H2' | 31:BA:972:G:H5' | 1.91 | 0.52 |
| 50:BY:9:LYS:HA | 50:BY:30:VAL:HG21 | 1.92 | 0.52 |
| 1:CA:1452:C:O4' | 1:CA:1456:G:C2 | 2.63 | 0.52 |
| 1:CA:377:G:O2' | 1:CA:378:G:H5' | 2.10 | 0.52 |
| 1:CA:52:G:C2' | 1:CA:53:A:H5' | 2.39 | 0.52 |
| 1:CA:542:G:H5' | 4:CD:41:GLY:HA3 | 1.91 | 0.52 |
| 1:CA:719:C:H5 | 1:CA:720:C:C4 | 2.27 | 0.52 |
| 7:CG:111:ARG:HB3 | 7:CG:113:GLU:HG2 | 1.92 | 0.52 |
| 9:CI:79:LEU:O | 9:CI:79:LEU:HD22 | 2.09 | 0.52 |
| 1:CA:1199:U:H4' | 10:CJ:54:PHE:CE1 | 2.44 | 0.52 |
| 15:CO:8:LYS:HG2 | 15:CO:12:ILE:HD11 | 1.92 | 0.52 |
| 18:CR:57:GLY:C | 18:CR:58:LEU:HD12 | 2.29 | 0.52 |
| 30:D8:31:HIS:O | 30:D8:32:LEU:C | 2.47 | 0.52 |
| 31:DA:1497:U:H3 | 31:DA:1578:U:P | 2.32 | 0.52 |
| 31:DA:2016:U:H2' | 31:DA:2017:U:C6 | 2.44 | 0.52 |
| 31:DA:2102:U:C6 | 31:DA:2187:G:O6 | 2.62 | 0.52 |
| 22:D0:43:THR:HG22 | 31:DA:2331:G:O3' | 2.09 | 0.52 |
| 31:DA:2335:A:N7 | 31:DA:2337:G:C5 | 2.78 | 0.52 |
| 31:DA:2646:C:H2' | 31:DA:2647:U:O4' | 2.09 | 0.52 |
| 31:DA:639:U:H2' | 31:DA:640:C:H6 | 1.73 | 0.52 |
| 33:DD:131:LEU:HB2 | 33:DD:136:ILE:CD1 | 2.38 | 0.52 |
| 33:DD:255:LYS:CE | 33:DD:255:LYS:H | 2.21 | 0.52 |
| 35:DF:63:LYS:HE2 | 35:DF:67:GLN:HB2 | 1.91 | 0.52 |
| 35:DF:65:TRP:O | 35:DF:67:GLN:N | 2.43 | 0.52 |
| 36:DG:52:ILE:HG22 | 36:DG:54:GLU:CG | 2.39 | 0.52 |
| 32:DB:42:C:O4' | 36:DG:69:ALA:HB2 | 2.10 | 0.52 |
| 37:DH:54:ARG:HB3 | 37:DH:65:HIS:CD2 | 2.45 | 0.52 |
| 39:DN:131:GLN:NE2 | 39:DN:134:ARG:HA | 2.24 | 0.52 |
| 39:DN:39:ARG:HD3 | 39:DN:41:ASP:HB2 | 1.91 | 0.52 |
| 41:DP:108:LYS:O | 41:DP:110:TYR:N | 2.41 | 0.52 |
| 41:DP:17:LYS:C | 41:DP:19:VAL:N | 2.62 | 0.52 |
| 44:DS:35:ILE:H | 44:DS:53:SER:CB | 2.23 | 0.52 |
| 45:DT:35:LYS:O | 45:DT:37:GLY:N | 2.43 | 0.52 |
| 45:DT:38:ASN:HD22 | 45:DT:40:THR:N | 2.07 | 0.52 |
| 47:DV:83:ARG:CG | 47:DV:83:ARG:NH1 | 2.64 | 0.52 |
| 1:AA:1052:U:H2' | 1:AA:1055:A:OP1 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1184:G:H2' | 1:AA:1185:G:C8 | 2.42 | 0.52 |
| 1:AA:38:G:N1 | 1:AA:397:A:C2 | 2.78 | 0.52 |
| 1:AA:683:G:C6 | 1:AA:684:A:C5 | 2.98 | 0.52 |
| 1:AA:657:G:C2 | 1:AA:750:G:C5 | 2.98 | 0.52 |
| 6:AF:7:ASN:ND2 | 6:AF:7:ASN:N | 2.56 | 0.52 |
| 8:AH:6:ILE:H | 8:AH:6:ILE:CD1 | 2.23 | 0.52 |
| 10:AJ:48:THR:HA | 10:AJ:62:HIS:HB3 | 1.91 | 0.52 |
| 22:B0:11:ARG:O | 22:B0:14:ARG:NH2 | 2.43 | 0.52 |
| 23:B1:26:ARG:CD | 23:B1:34:THR:HB | 2.40 | 0.52 |
| 23:B1:33:LYS:HB3 | 31:BA:2395:C:O2' | 2.10 | 0.52 |
| 25:B3:13:ILE:HD13 | 25:B3:13:ILE:N | 2.25 | 0.52 |
| 31:BA:1015:G:C2' | 31:BA:1016:G:H5' | 2.40 | 0.52 |
| 31:BA:1047:G:N2 | 31:BA:1111:A:N6 | 2.54 | 0.52 |
| 31:BA:768:G:O2' | 31:BA:1379:A:N6 | 2.42 | 0.52 |
| 31:BA:2394:C:OP1 | 41:BP:63:PRO:CD | 2.50 | 0.52 |
| 31:BA:2632:A:N3 | 34:BE:61:ARG:NH1 | 2.58 | 0.52 |
| 31:BA:300:A:H2' | 31:BA:334:C:H1' | 1.92 | 0.52 |
| 31:BA:995:C:O2 | 39:BN:4:TYR:OH | 2.25 | 0.52 |
| 33:BD:43:ARG:HD2 | 33:BD:44:ASN:OD1 | 2.10 | 0.52 |
| 34:BE:70:ALA:O | 34:BE:71:GLY:C | 2.48 | 0.52 |
| 39:BN:43:THR:HG22 | 39:BN:45:ASN:ND2 | 2.24 | 0.52 |
| 39:BN:98:VAL:HG23 | 39:BN:99:LEU:H | 1.74 | 0.52 |
| 40:BO:69:ILE:O | 40:BO:76:ALA:HA | 2.10 | 0.52 |
| 41:BP:47:ASP:CB | 41:BP:48:PRO:O | 2.46 | 0.52 |
| 31:BA:2870:C:H5'' | 43:BR:65:LEU:HD21 | 1.91 | 0.52 |
| 45:BT:33:LYS:H | 45:BT:33:LYS:HZ2 | 1.58 | 0.52 |
| 1:CA:1410:G:C2 | 1:CA:1411:C:C2 | 2.98 | 0.52 |
| 1:CA:376:G:O2' | 1:CA:377:G:H5' | 2.10 | 0.52 |
| 1:CA:560:U:H5' | 1:CA:566:G:N2 | 2.24 | 0.52 |
| 1:CA:621:A:O2' | 1:CA:622:A:H5' | 2.10 | 0.52 |
| 1:CA:624:C:H2' | 1:CA:625:G:C8 | 2.44 | 0.52 |
| 1:CA:70:G:H2' | 1:CA:71:C:C6 | 2.45 | 0.52 |
| 1:CA:826:C:H2' | 1:CA:827:U:C6 | 2.44 | 0.52 |
| 2:CB:71:VAL:HB | 2:CB:164:VAL:HG22 | 1.92 | 0.52 |
| 2:CB:170:GLU:O | 2:CB:174:VAL:HG23 | 2.10 | 0.52 |
| 7:CG:66:VAL:O | 7:CG:70:LYS:HG3 | 2.09 | 0.52 |
| 5:CE:148:VAL:HG21 | 8:CH:107:LEU:HD22 | 1.92 | 0.52 |
| 19:CS:51:VAL:HG21 | 19:CS:71:LEU:HB3 | 1.91 | 0.52 |
| 1:CA:192:U:H4' | 20:CT:103:GLY:HA2 | 1.92 | 0.52 |
| 25:D3:45:GLY:O | 25:D3:48:GLU:HB2 | 2.10 | 0.52 |
| 27:D5:16:ARG:NH2 | 31:DA:517:C:OP1 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:D5:50:GLY:O | 27:D5:51:TYR:CD1 | 2.62 | 0.52 |
| 31:DA:1578:U:O2 | 31:DA:1578:U:H2' | 2.09 | 0.52 |
| 31:DA:1836:C:H2' | 31:DA:1837:C:H6 | 1.75 | 0.52 |
| 31:DA:1856:G:H2' | 31:DA:1857:G:H5' | 1.92 | 0.52 |
| 31:DA:2017:U:H5'' | 31:DA:2018:G:P | 2.49 | 0.52 |
| 31:DA:2567:G:H2' | 31:DA:2568:C:H6 | 1.70 | 0.52 |
| 31:DA:562:U:C4 | 31:DA:2036:C:O4' | 2.63 | 0.52 |
| 31:DA:582:G:H2' | 31:DA:583:G:C8 | 2.45 | 0.52 |
| 31:DA:768:G:O2' | 31:DA:1379:A:N6 | 2.43 | 0.52 |
| 31:DA:664:C:H4' | 31:DA:941:A:OP1 | 2.10 | 0.52 |
| 42:DQ:58:PHE:CD1 | 42:DQ:58:PHE:O | 2.62 | 0.52 |
| 45:DT:106:SER:O | 45:DT:107:ASP:CB | 2.58 | 0.52 |
| 49:DX:62:LYS:CB | 49:DX:69:TYR:H | 2.18 | 0.52 |
| 49:DX:72:LYS:HG3 | 49:DX:73:ARG:N | 2.19 | 0.52 |
| 50:DY:2:ARG:C | 50:DY:4:LYS:N | 2.62 | 0.52 |
| 1:AA:1001(A):G:H2' | 1:AA:1002:G:O4' | 2.10 | 0.52 |
| 1:AA:1103:C:H5'' | 2:AB:98:LEU:HD13 | 1.92 | 0.52 |
| 1:AA:355:C:O2' | 1:AA:356:A:H5' | 2.10 | 0.52 |
| 1:AA:450:G:H1 | 1:AA:483:C:H42 | 1.58 | 0.52 |
| 3:AC:46:GLU:O | 3:AC:47:LEU:HB2 | 2.10 | 0.52 |
| 5:AE:36:ASP:O | 5:AE:37:ARG:HB2 | 2.09 | 0.52 |
| 5:AE:80:ILE:HG22 | 8:AH:104:ARG:CZ | 2.39 | 0.52 |
| 6:AF:89:MET:HG2 | 6:AF:91:VAL:HG23 | 1.92 | 0.52 |
| 8:AH:10:LEU:HD13 | 8:AH:83:ILE:HD11 | 1.92 | 0.52 |
| 9:AI:99:LEU:HD12 | 9:AI:101:PHE:CE1 | 2.44 | 0.52 |
| 16:AP:49:LEU:HG | 16:AP:50:LYS:N | 2.25 | 0.52 |
| 31:BA:1051:G:H5' | 31:BA:2752:C:O2' | 2.10 | 0.52 |
| 31:BA:1141:U:OP1 | 39:BN:25:ARG:NH1 | 2.43 | 0.52 |
| 31:BA:1446:C:O2 | 31:BA:1447:G:C8 | 2.63 | 0.52 |
| 31:BA:1495:A:H2' | 31:BA:1495:A:N3 | 2.25 | 0.52 |
| 31:BA:1820:U:H4' | 31:BA:1821:A:OP2 | 2.10 | 0.52 |
| 31:BA:1839:G:C8 | 31:BA:1927:A:H1' | 2.45 | 0.52 |
| 31:BA:272(D):G:H1 | 31:BA:364:C:H42 | 1.56 | 0.52 |
| 33:BD:173:VAL:HG23 | 33:BD:174:ILE:N | 2.25 | 0.52 |
| 31:BA:2810:A:H2' | 34:BE:61:ARG:HH21 | 1.75 | 0.52 |
| 34:BE:87:GLU:HG3 | 34:BE:87:GLU:O | 2.10 | 0.52 |
| 35:BF:199:TRP:CH2 | 35:BF:203:GLN:NE2 | 2.77 | 0.52 |
| 31:BA:449:A:OP1 | 35:BF:84:VAL:O | 2.28 | 0.52 |
| 36:BG:52:ILE:HG22 | 36:BG:54:GLU:CG | 2.39 | 0.52 |
| 31:BA:2000:G:OP2 | 43:BR:3:HIS:CE1 | 2.63 | 0.52 |
| 44:BS:56:LEU:O | 44:BS:57:LYS:CB | 2.58 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 45:BT:28:VAL:O | 45:BT:29:ARG:HD2 | 2.09 | 0.52 |
| 45:BT:32:TYR:CD2 | 45:BT:81:PRO:HB2 | 2.45 | 0.52 |
| 51:BZ:54:HIS:HE1 | 51:BZ:123:ASP:CG | 2.14 | 0.52 |
| 1:CA:1128:C:H1' | 1:CA:1146:A:H61 | 1.75 | 0.52 |
| 1:CA:134:A:H1' | 1:CA:325:A:C5 | 2.45 | 0.52 |
| 1:CA:552:U:O2' | 1:CA:553:A:H5' | 2.09 | 0.52 |
| 1:CA:577:G:C8 | 1:CA:816:A:C6 | 2.98 | 0.52 |
| 1:CA:96:U:O2' | 1:CA:97:G:P | 2.68 | 0.52 |
| 3:CC:46:GLU:O | 3:CC:47:LEU:HB2 | 2.10 | 0.52 |
| 4:CD:106:TYR:CE1 | 4:CD:112:VAL:O | 2.63 | 0.52 |
| 9:CI:99:LEU:HD12 | 9:CI:101:PHE:CE1 | 2.44 | 0.52 |
| 17:CQ:65:ILE:HD12 | 17:CQ:69:LYS:O | 2.10 | 0.52 |
| 23:D1:26:ARG:CD | 23:D1:34:THR:HB | 2.39 | 0.52 |
| 24:D2:22:GLU:O | 24:D2:25:VAL:HG12 | 2.10 | 0.52 |
| 31:DA:1300:U:C3' | 31:DA:1301:A:C5' | 2.88 | 0.52 |
| 31:DA:142:A:N6 | 31:DA:1595:G:O2' | 2.42 | 0.52 |
| 31:DA:1495:A:H2' | 31:DA:1495:A:N3 | 2.24 | 0.52 |
| 31:DA:2021:C:H4' | 31:DA:2022:U:OP2 | 2.09 | 0.52 |
| 31:DA:271(X):G:H2' | 31:DA:271(Y):U:H5'' | 1.92 | 0.52 |
| 34:DE:116:VAL:HG13 | 34:DE:122:PHE:HB2 | 1.92 | 0.52 |
| 34:DE:119:ARG:HB3 | 34:DE:120:TRP:CD1 | 2.45 | 0.52 |
| 31:DA:1670:C:O2 | 34:DE:129:HIS:CE1 | 2.62 | 0.52 |
| 36:DG:37:VAL:HG23 | 36:DG:99:MET:HG3 | 1.92 | 0.52 |
| 42:DQ:42:ILE:HD13 | 42:DQ:97:VAL:CG2 | 2.40 | 0.52 |
| 45:DT:100:TYR:HD2 | 45:DT:103:ARG:HH21 | 1.53 | 0.52 |
| 49:DX:37:THR:HG23 | 49:DX:54:VAL:HB | 1.91 | 0.52 |
| 49:DX:55:ASN:HB2 | 49:DX:78:LYS:CD | 2.40 | 0.52 |
| 50:DY:88:LYS:O | 50:DY:89:PHE:HB2 | 2.09 | 0.52 |
| 1:AA:1386:G:C2 | 1:AA:1387:G:C8 | 2.98 | 0.51 |
| 1:AA:189:G:C6 | 1:AA:189(A):C:C4 | 2.98 | 0.51 |
| 1:AA:304:U:H2' | 1:AA:305:G:C8 | 2.45 | 0.51 |
| 2:AB:170:GLU:O | 2:AB:174:VAL:HG23 | 2.09 | 0.51 |
| 3:AC:111:LEU:HD21 | 3:AC:145:GLY:O | 2.10 | 0.51 |
| 6:AF:6:VAL:HG13 | 6:AF:90:VAL:HG22 | 1.92 | 0.51 |
| 1:AA:1372:U:OP1 | 9:AI:72:GLY:N | 2.43 | 0.51 |
| 10:AJ:96:ILE:N | 10:AJ:96:ILE:HD13 | 2.25 | 0.51 |
| 17:AQ:76:LEU:HD12 | 17:AQ:77:VAL:H | 1.75 | 0.51 |
| 19:AS:65:ASN:HB2 | 19:AS:66:MET:HE3 | 1.91 | 0.51 |
| 21:AU:9:ARG:O | 21:AU:13:ILE:HG13 | 2.10 | 0.51 |
| 28:B6:32:ASN:O | 28:B6:33:LYS:CB | 2.59 | 0.51 |
| 31:BA:1109:C:H5 | 31:BA:1110:G:C8 | 2.28 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:BA:1323:U:H2' | 31:BA:1324:G:H5' | 1.91 | 0.51 |
| 31:BA:1657:C:H2' | 31:BA:1658:C:H6 | 1.74 | 0.51 |
| 31:BA:236:C:H2' | 31:BA:237:C:H6 | 1.75 | 0.51 |
| 31:BA:2700:C:C2' | 31:BA:2701:C:H5' | 2.40 | 0.51 |
| 31:BA:547:A:C8 | 31:BA:549:G:C6 | 2.98 | 0.51 |
| 31:BA:892:G:H3' | 31:BA:892:G:N3 | 2.26 | 0.51 |
| 41:BP:17:LYS:C | 41:BP:19:VAL:N | 2.60 | 0.51 |
| 42:BQ:54:MET:HB3 | 42:BQ:64:ILE:CD1 | 2.40 | 0.51 |
| 46:BU:92:ARG:HH22 | 47:BV:10:LYS:CB | 2.23 | 0.51 |
| 49:BX:60:ARG:NH2 | 49:BX:74:PRO:HG2 | 2.25 | 0.51 |
| 51:BZ:40:ASP:HB3 | 51:BZ:43:GLU:HB2 | 1.90 | 0.51 |
| 1:CA:1003:G:C2' | 1:CA:1004:A:H4' | 2.33 | 0.51 |
| 1:CA:1189:C:H5'' | 3:CC:5:ILE:HG21 | 1.91 | 0.51 |
| 1:CA:1416:G:H2' | 1:CA:1417:G:O4' | 2.10 | 0.51 |
| 1:CA:327:A:H3' | 1:CA:328:C:H5'' | 1.92 | 0.51 |
| 1:CA:353:A:C2' | 1:CA:354:G:OP2 | 2.58 | 0.51 |
| 1:CA:370:C:H2' | 1:CA:371:G:C8 | 2.44 | 0.51 |
| 1:CA:696:A:H8 | 1:CA:696:A:O5' | 1.93 | 0.51 |
| 1:CA:858:G:O6 | 1:CA:869:G:H3' | 2.09 | 0.51 |
| 5:CE:12:LEU:C | 5:CE:12:LEU:HD22 | 2.30 | 0.51 |
| 1:CA:710:G:OP1 | 6:CF:54:LYS:HE3 | 2.09 | 0.51 |
| 2:CB:178:ARG:HH21 | 8:CH:68:ARG:HH22 | 1.57 | 0.51 |
| 1:CA:522:C:H41 | 12:CL:53:ARG:HH22 | 1.58 | 0.51 |
| 13:CM:32:GLU:OE2 | 13:CM:64:TRP:HH2 | 1.93 | 0.51 |
| 19:CS:22:LEU:HD13 | 19:CS:27:GLU:HB2 | 1.92 | 0.51 |
| 28:D6:15:GLU:OE2 | 28:D6:43:CYS:HB3 | 2.10 | 0.51 |
| 31:DA:1486:A:H2' | 31:DA:1487:G:C8 | 2.45 | 0.51 |
| 31:DA:1935:G:H1' | 31:DA:1964:G:N2 | 2.26 | 0.51 |
| 31:DA:228:A:H2' | 31:DA:230:U:O4' | 2.10 | 0.51 |
| 27:D5:34:PRO:HG3 | 31:DA:2885:C:O2' | 2.10 | 0.51 |
| 31:DA:506:G:O3' | 31:DA:507:A:H8 | 1.93 | 0.51 |
| 31:DA:993:G:N2 | 47:DV:91:TYR:OH | 2.43 | 0.51 |
| 38:DI:5:LEU:N | 38:DI:5:LEU:HD23 | 2.25 | 0.51 |
| 1:AA:1233:G:H2' | 1:AA:1234:C:C6 | 2.45 | 0.51 |
| 1:AA:1316:G:H2' | 1:AA:1317:C:H5'' | 1.92 | 0.51 |
| 1:AA:1409:C:N4 | 1:AA:1491:G:H1 | 2.07 | 0.51 |
| 1:AA:278:G:O4' | 1:AA:282:A:H1' | 2.10 | 0.51 |
| 1:AA:781:A:C3' | 1:AA:782:A:H5' | 2.39 | 0.51 |
| 1:AA:816:A:OP2 | 1:AA:1527:C:H5' | 2.10 | 0.51 |
| 1:AA:811:C:O2' | 1:AA:901:A:N1 | 2.42 | 0.51 |
| 3:AC:73:PRO:HA | 3:AC:76:VAL:HG13 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:30:LYS:C | 4:AD:32:ALA:H | 2.14 | 0.51 |
| 5:AE:45:PHE:CE2 | 5:AE:47:LYS:HD2 | 2.44 | 0.51 |
| 7:AG:22:LEU:HG | 7:AG:62:PHE:HE2 | 1.75 | 0.51 |
| 1:AA:375:U:O3' | 16:AP:6:LEU:HB2 | 2.10 | 0.51 |
| 22:B0:48:GLY:HA3 | 22:B0:80:HIS:CE1 | 2.45 | 0.51 |
| 23:B1:19:GLN:CD | 23:B1:44:PRO:HB3 | 2.30 | 0.51 |
| 31:BA:1420:U:O2' | 31:BA:1421:G:OP1 | 2.27 | 0.51 |
| 31:BA:1531:C:H3' | 31:BA:1532:C:C4' | 2.40 | 0.51 |
| 31:BA:1439:A:C2 | 31:BA:1553:A:C4 | 2.98 | 0.51 |
| 31:BA:228:A:H2' | 31:BA:230:U:O4' | 2.10 | 0.51 |
| 31:BA:542:C:N4 | 31:BA:543:C:H42 | 1.96 | 0.51 |
| 34:BE:201:THR:HG22 | 34:BE:203:LYS:N | 2.25 | 0.51 |
| 36:BG:125:PHE:CE2 | 36:BG:173:LEU:HD12 | 2.45 | 0.51 |
| 38:BI:62:LYS:HE2 | 38:BI:134:PRO:CG | 2.40 | 0.51 |
| 44:BS:16:ASN:C | 44:BS:17:ARG:O | 2.46 | 0.51 |
| 45:BT:100:TYR:HB3 | 45:BT:103:ARG:HE | 1.76 | 0.51 |
| 46:BU:104:GLN:HB2 | 47:BV:43:GLU:OE2 | 2.10 | 0.51 |
| 49:BX:8:ILE:H | 49:BX:8:ILE:HD12 | 1.75 | 0.51 |
| 50:BY:45:VAL:HG22 | 50:BY:62:GLU:HB2 | 1.91 | 0.51 |
| 51:BZ:150:LEU:N | 51:BZ:150:LEU:HD13 | 2.25 | 0.51 |
| 1:CA:81:U:C4 | 1:CA:83:U:C5 | 2.99 | 0.51 |
| 2:CB:84:GLU:HB3 | 2:CB:219:VAL:CG2 | 2.29 | 0.51 |
| 3:CC:102:ASN:O | 3:CC:103:VAL:HG23 | 2.11 | 0.51 |
| 5:CE:34:VAL:O | 5:CE:41:VAL:HG12 | 2.10 | 0.51 |
| 10:CJ:7:LYS:HB2 | 10:CJ:97:GLU:HB2 | 1.92 | 0.51 |
| 12:CL:102:ARG:HD2 | 12:CL:108:ALA:O | 2.10 | 0.51 |
| 14:CN:40:CYS:SG | 14:CN:42:ILE:HG12 | 2.50 | 0.51 |
| 1:CA:1216:G:H5'' | 14:CN:5:ALA:CB | 2.40 | 0.51 |
| 16:CP:39:TYR:CD2 | 16:CP:73:LEU:HD13 | 2.46 | 0.51 |
| 31:DA:1171:G:N7 | 31:DA:1173:G:H1' | 2.25 | 0.51 |
| 31:DA:1198:U:H2' | 31:DA:1199:U:C6 | 2.46 | 0.51 |
| 31:DA:1531:C:H3' | 31:DA:1532:C:C4' | 2.41 | 0.51 |
| 31:DA:2019:A:H2' | 31:DA:2020:A:O5' | 2.10 | 0.51 |
| 31:DA:2484:G:C2 | 31:DA:2485:G:C8 | 2.98 | 0.51 |
| 31:DA:527:C:O4' | 31:DA:527:C:O2 | 2.27 | 0.51 |
| 31:DA:782:A:H5' | 31:DA:783:A:C2 | 2.45 | 0.51 |
| 31:DA:786:C:O2' | 31:DA:787:U:H5' | 2.09 | 0.51 |
| 34:DE:108:SER:HB3 | 34:DE:165:VAL:HG21 | 1.92 | 0.51 |
| 37:DH:126:PRO:HB2 | 37:DH:130:ARG:NH1 | 2.25 | 0.51 |
| 37:DH:41:MET:HE1 | 37:DH:54:ARG:HA | 1.91 | 0.51 |
| 38:DI:110:ASP:C | 38:DI:112:LYS:H | 2.13 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DI:45:LYS:O | 38:DI:48:GLU:N | 2.44 | 0.51 |
| 41:DP:108:LYS:C | 41:DP:110:TYR:N | 2.64 | 0.51 |
| 49:DX:35:THR:O | 49:DX:39:ILE:CG2 | 2.58 | 0.51 |
| 1:AA:1003:G:N3 | 1:AA:1004:A:H1' | 2.26 | 0.51 |
| 1:AA:1148:U:H2' | 1:AA:1149:C:O4' | 2.11 | 0.51 |
| 1:AA:1290:G:N3 | 1:AA:1290:G:H2' | 2.24 | 0.51 |
| 1:AA:22:G:O2' | 1:AA:23:C:H5' | 2.11 | 0.51 |
| 1:AA:246:A:C4 | 1:AA:282:A:N6 | 2.78 | 0.51 |
| 1:AA:27:G:O2' | 1:AA:28:G:H5' | 2.10 | 0.51 |
| 1:AA:585:G:N3 | 1:AA:879:C:H4' | 2.25 | 0.51 |
| 1:AA:66:G:C4' | 1:AA:173:U:C4 | 2.94 | 0.51 |
| 1:AA:723:U:H5'' | 1:AA:724:G:OP2 | 2.08 | 0.51 |
| 1:AA:79:G:H4' | 1:AA:80:G:OP1 | 2.10 | 0.51 |
| 1:AA:97:G:O2' | 1:AA:98:G:O5' | 2.28 | 0.51 |
| 2:AB:84:GLU:OE1 | 2:AB:219:VAL:HB | 2.10 | 0.51 |
| 2:AB:27:LYS:HD2 | 2:AB:193:ASP:HB2 | 1.90 | 0.51 |
| 5:AE:34:VAL:O | 5:AE:41:VAL:HG12 | 2.11 | 0.51 |
| 6:AF:50:TYR:CZ | 18:AR:77:GLY:HA2 | 2.45 | 0.51 |
| 12:AL:32:PHE:CB | 12:AL:84:LEU:HD21 | 2.40 | 0.51 |
| 13:AM:81:LEU:HD21 | 13:AM:88:ARG:HH22 | 1.75 | 0.51 |
| 16:AP:39:TYR:CE1 | 16:AP:41:PRO:HA | 2.46 | 0.51 |
| 19:AS:22:LEU:HD13 | 19:AS:27:GLU:HB2 | 1.92 | 0.51 |
| 29:B7:47:ARG:C | 29:B7:48:LYS:HD3 | 2.30 | 0.51 |
| 31:BA:117:G:H5'' | 31:BA:118:A:OP2 | 2.10 | 0.51 |
| 31:BA:1499:C:O2' | 31:BA:1500:G:H5' | 2.09 | 0.51 |
| 31:BA:1786:A:C2 | 31:BA:2606:C:H1' | 2.44 | 0.51 |
| 31:BA:1935:G:C6 | 31:BA:1962:C:C6 | 2.97 | 0.51 |
| 31:BA:2065:C:H2' | 31:BA:2066:C:C6 | 2.45 | 0.51 |
| 31:BA:2308:G:H2' | 31:BA:2309:A:N7 | 2.26 | 0.51 |
| 31:BA:2386:C:H2' | 31:BA:2387:U:C6 | 2.45 | 0.51 |
| 31:BA:2646:C:H2' | 31:BA:2647:U:O4' | 2.10 | 0.51 |
| 31:BA:271(P):C:H2' | 31:BA:271(Q):G:O5' | 2.10 | 0.51 |
| 31:BA:271(R):G:C2' | 31:BA:271(S):G:H5' | 2.40 | 0.51 |
| 31:BA:995:C:N3 | 39:BN:4:TYR:HE1 | 2.08 | 0.51 |
| 34:BE:179:GLU:HB3 | 34:BE:181:LEU:CD2 | 2.40 | 0.51 |
| 34:BE:93:VAL:H | 34:BE:95:ILE:HD13 | 1.75 | 0.51 |
| 35:BF:1:MET:O | 35:BF:2:LYS:C | 2.48 | 0.51 |
| 35:BF:2:LYS:O | 35:BF:25:PRO:HG2 | 2.11 | 0.51 |
| 36:BG:133:LEU:HD12 | 36:BG:133:LEU:C | 2.30 | 0.51 |
| 37:BH:54:ARG:CG | 37:BH:65:HIS:HD2 | 2.22 | 0.51 |
| 44:BS:26:LEU:HA | 44:BS:39:ILE:HD13 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BT:106:SER:O | 45:BT:107:ASP:CB | 2.58 | 0.51 |
| 45:BT:91:ARG:HA | 45:BT:117:ASP:H | 1.76 | 0.51 |
| 45:BT:33:LYS:HZ2 | 45:BT:33:LYS:HA | 1.75 | 0.51 |
| 45:BT:56:GLY:O | 45:BT:59:THR:CG2 | 2.58 | 0.51 |
| 46:BU:64:ARG:CA | 46:BU:64:ARG:CZ | 2.70 | 0.51 |
| 47:BV:43:GLU:N | 47:BV:48:GLY:HA2 | 2.25 | 0.51 |
| 31:BA:310:A:OP1 | 50:BY:18:GLY:HA2 | 2.11 | 0.51 |
| 31:BA:106:C:H1' | 50:BY:2:ARG:NE | 2.25 | 0.51 |
| 50:BY:28:LYS:CE | 50:BY:30:VAL:HG22 | 2.28 | 0.51 |
| 51:BZ:99:TYR:HB3 | 51:BZ:123:ASP:OD1 | 2.11 | 0.51 |
| 1:CA:1074:G:N3 | 1:CA:1102:A:C2 | 2.78 | 0.51 |
| 1:CA:1233:G:H2' | 1:CA:1234:C:C6 | 2.45 | 0.51 |
| 1:CA:55:A:C4 | 1:CA:56:U:C6 | 2.99 | 0.51 |
| 1:CA:80:G:N1 | 1:CA:89:C:N4 | 2.57 | 0.51 |
| 2:CB:178:ARG:NH2 | 8:CH:68:ARG:HH22 | 2.08 | 0.51 |
| 3:CC:36:ASP:HB3 | 3:CC:40:ARG:HH12 | 1.75 | 0.51 |
| 10:CJ:48:THR:HA | 10:CJ:62:HIS:HB3 | 1.91 | 0.51 |
| 12:CL:18:VAL:O | 12:CL:19:ARG:HB3 | 2.10 | 0.51 |
| 15:CO:87:ILE:HG22 | 15:CO:88:ARG:HG3 | 1.92 | 0.51 |
| 16:CP:49:LEU:HG | 16:CP:50:LYS:N | 2.25 | 0.51 |
| 27:D5:32:PRO:HD2 | 31:DA:2886:G:O2' | 2.10 | 0.51 |
| 27:D5:11:THR:HG23 | 31:DA:1264:G:H5' | 1.92 | 0.51 |
| 31:DA:1859:A:C6 | 31:DA:1884:A:C8 | 2.98 | 0.51 |
| 31:DA:2023:G:C2 | 31:DA:2024:G:C8 | 2.98 | 0.51 |
| 31:DA:363(C):G:H2' | 31:DA:363(D):G:O4' | 2.11 | 0.51 |
| 31:DA:466:A:H1' | 31:DA:683:C:O4' | 2.10 | 0.51 |
| 31:DA:467:G:H2' | 31:DA:468:G:H5' | 1.92 | 0.51 |
| 32:DB:52:A:O2' | 32:DB:53:A:C8 | 2.58 | 0.51 |
| 35:DF:1:MET:O | 35:DF:2:LYS:C | 2.48 | 0.51 |
| 40:DO:35:VAL:HA | 40:DO:62:VAL:HG12 | 1.92 | 0.51 |
| 49:DX:40:LYS:C | 49:DX:42:ALA:H | 2.13 | 0.51 |
| 1:AA:1238:A:N6 | 1:AA:1299:A:H62 | 2.07 | 0.51 |
| 1:AA:1410:G:C2 | 1:AA:1411:C:C2 | 2.99 | 0.51 |
| 1:AA:189:G:C6 | 1:AA:189(A):C:N4 | 2.79 | 0.51 |
| 1:AA:264:U:O2' | 17:AQ:64:PRO:HB2 | 2.10 | 0.51 |
| 1:AA:342:C:C2' | 1:AA:343:U:H5' | 2.40 | 0.51 |
| 1:AA:428:G:C4' | 1:AA:429:U:O5' | 2.58 | 0.51 |
| 1:AA:503:C:H2' | 1:AA:504:C:C6 | 2.43 | 0.51 |
| 1:AA:649:G:H2' | 1:AA:650:G:H8 | 1.75 | 0.51 |
| 1:AA:832:C:N4 | 1:AA:855:G:C6 | 2.79 | 0.51 |
| 1:AA:945:G:N3 | 1:AA:945:G:H2' | 2.24 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:AI:116:LYS:O | 9:AI:118:LYS:N | 2.43 | 0.51 |
| 12:AL:55:VAL:HG13 | 12:AL:68:ALA:O | 2.10 | 0.51 |
| 13:AM:68:GLY:HA2 | 13:AM:71:ARG:HB3 | 1.93 | 0.51 |
| 15:AO:8:LYS:HG2 | 15:AO:12:ILE:HD11 | 1.91 | 0.51 |
| 15:AO:87:ILE:CG2 | 15:AO:88:ARG:N | 2.73 | 0.51 |
| 1:AA:564:C:C4 | 17:AQ:31:LEU:HD11 | 2.46 | 0.51 |
| 22:B0:43:THR:HG22 | 31:BA:2331:G:O3' | 2.09 | 0.51 |
| 31:BA:1001:A:H2' | 31:BA:1002:G:O4' | 2.10 | 0.51 |
| 31:BA:2689:U:C4' | 31:BA:2690:C:OP2 | 2.59 | 0.51 |
| 31:BA:271(X):G:H2' | 31:BA:271(Y):U:H5'' | 1.92 | 0.51 |
| 37:BH:153:LYS:N | 37:BH:153:LYS:CD | 2.73 | 0.51 |
| 41:BP:112:LEU:H | 41:BP:128:HIS:CD2 | 2.25 | 0.51 |
| 42:BQ:7:MET:O | 42:BQ:10:ARG:NH2 | 2.43 | 0.51 |
| 49:BX:38:GLU:OE1 | 49:BX:38:GLU:CA | 2.58 | 0.51 |
| 49:BX:73:ARG:N | 49:BX:74:PRO:HD3 | 2.25 | 0.51 |
| 50:BY:2:ARG:C | 50:BY:4:LYS:N | 2.62 | 0.51 |
| 1:CA:1001(A):G:H2' | 1:CA:1002:G:O4' | 2.09 | 0.51 |
| 1:CA:1003:G:N3 | 1:CA:1004:A:H1' | 2.25 | 0.51 |
| 1:CA:989:C:N4 | 1:CA:1216:G:H1 | 2.08 | 0.51 |
| 1:CA:229:U:C2' | 1:CA:230:G:H5' | 2.40 | 0.51 |
| 1:CA:532:A:H61 | 3:CC:193:TYR:CB | 2.19 | 0.51 |
| 1:CA:561:U:O2' | 1:CA:562:C:OP2 | 2.26 | 0.51 |
| 2:CB:115:LEU:HB2 | 2:CB:145:LEU:HD12 | 1.92 | 0.51 |
| 3:CC:64:VAL:HB | 3:CC:99:VAL:HG12 | 1.93 | 0.51 |
| 5:CE:34:VAL:O | 5:CE:41:VAL:HA | 2.11 | 0.51 |
| 10:CJ:84:GLN:O | 10:CJ:88:LEU:HB2 | 2.09 | 0.51 |
| 12:CL:82:VAL:CG1 | 12:CL:83:VAL:H | 2.16 | 0.51 |
| 18:CR:44:LEU:HA | 18:CR:49:LYS:O | 2.11 | 0.51 |
| 24:D2:23:LYS:HB2 | 49:DX:5:TYR:CE1 | 2.46 | 0.51 |
| 28:D6:29:ASN:O | 28:D6:30:THR:C | 2.49 | 0.51 |
| 30:D8:22:VAL:O | 30:D8:49:VAL:HG23 | 2.09 | 0.51 |
| 31:DA:1040:C:O2' | 31:DA:1041:C:OP2 | 2.26 | 0.51 |
| 31:DA:1495:A:H2' | 31:DA:1496:A:N3 | 2.25 | 0.51 |
| 31:DA:175:G:C5' | 31:DA:175:G:H8 | 2.23 | 0.51 |
| 31:DA:2394:C:OP1 | 41:DP:63:PRO:CD | 2.52 | 0.51 |
| 31:DA:2557:G:H2' | 31:DA:2558:C:H6 | 1.76 | 0.51 |
| 31:DA:1786:A:C2 | 31:DA:2606:C:H1' | 2.44 | 0.51 |
| 31:DA:1786:A:H2 | 31:DA:2606:C:H1' | 1.76 | 0.51 |
| 31:DA:2880:C:O2' | 43:DR:90:ARG:HD3 | 2.10 | 0.51 |
| 31:DA:676:A:C2 | 31:DA:802:A:N6 | 2.69 | 0.51 |
| 31:DA:780:G:C2 | 31:DA:782:A:C2 | 2.98 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:975:C:H2' | 31:DA:975:C:O2 | 2.10 | 0.51 |
| 36:DG:91:ARG:C | 36:DG:91:ARG:HD2 | 2.31 | 0.51 |
| 38:DI:13:GLY:O | 38:DI:14:ASP:C | 2.49 | 0.51 |
| 39:DN:78:TYR:HD1 | 39:DN:79:PRO:HD3 | 1.75 | 0.51 |
| 39:DN:78:TYR:CD1 | 39:DN:79:PRO:CD | 2.89 | 0.51 |
| 45:DT:28:VAL:HB | 45:DT:88:ILE:HG13 | 1.91 | 0.51 |
| 47:DV:75:PHE:CE1 | 47:DV:89:GLN:CB | 2.84 | 0.51 |
| 49:DX:38:GLU:OE1 | 49:DX:38:GLU:CA | 2.58 | 0.51 |
| 50:DY:95:LYS:HD3 | 50:DY:100:ALA:CB | 2.14 | 0.51 |
| 51:DZ:27:VAL:HG13 | 51:DZ:29:TYR:HD2 | 1.75 | 0.51 |
| 51:DZ:30:ASN:ND2 | 51:DZ:32:HIS:H | 2.07 | 0.51 |
| 1:AA:590:C:H2' | 1:AA:591:U:C6 | 2.46 | 0.51 |
| 1:AA:930:C:O2' | 1:AA:931:C:H5' | 2.10 | 0.51 |
| 3:AC:121:ALA:HB2 | 3:AC:187:ALA:HB1 | 1.93 | 0.51 |
| 4:AD:23:GLY:HA3 | 4:AD:112:VAL:HG22 | 1.91 | 0.51 |
| 4:AD:74:GLN:O | 4:AD:78:LEU:HG | 2.10 | 0.51 |
| 23:B1:19:GLN:CG | 23:B1:44:PRO:HG3 | 2.40 | 0.51 |
| 24:B2:57:ILE:HG21 | 24:B2:59:ARG:NH1 | 2.26 | 0.51 |
| 31:BA:1588:C:O2 | 31:BA:1588:C:H2' | 2.10 | 0.51 |
| 31:BA:1895:C:C2 | 31:BA:1896:G:C8 | 2.99 | 0.51 |
| 31:BA:1973:G:C4 | 31:BA:1974:C:C5 | 2.98 | 0.51 |
| 31:BA:2321:G:H5'' | 31:BA:2322:A:OP2 | 2.10 | 0.51 |
| 31:BA:2335:A:C8 | 31:BA:2337:G:N7 | 2.79 | 0.51 |
| 31:BA:2521:C:H42 | 31:BA:2544:G:H1 | 1.58 | 0.51 |
| 31:BA:2683:C:OP1 | 45:BT:53:ARG:NH2 | 2.43 | 0.51 |
| 31:BA:953:A:C2 | 31:BA:954:G:C8 | 2.98 | 0.51 |
| 34:BE:70:ALA:O | 34:BE:72:VAL:O | 2.28 | 0.51 |
| 36:BG:20:ILE:O | 36:BG:24:GLY:HA2 | 2.10 | 0.51 |
| 38:BI:124:GLY:H | 38:BI:142:VAL:HG23 | 1.76 | 0.51 |
| 41:BP:95:VAL:HG13 | 41:BP:123:LEU:HD11 | 1.91 | 0.51 |
| 45:BT:100:TYR:HD2 | 45:BT:103:ARG:NH2 | 2.08 | 0.51 |
| 49:BX:21:PHE:HB3 | 49:BX:90:GLU:HG3 | 1.91 | 0.51 |
| 50:BY:28:LYS:HE3 | 50:BY:37:VAL:HG12 | 1.92 | 0.51 |
| 51:BZ:19:ARG:HA | 51:BZ:23:LYS:O | 2.10 | 0.51 |
| 1:CA:1006:C:H42 | 1:CA:1024:G:H21 | 1.58 | 0.51 |
| 1:CA:1452:C:H4' | 1:CA:1456:G:N3 | 2.25 | 0.51 |
| 1:CA:678:U:H2' | 1:CA:679:C:C6 | 2.45 | 0.51 |
| 2:CB:116:GLU:HA | 2:CB:119:GLU:HB2 | 1.92 | 0.51 |
| 5:CE:75:THR:HG23 | 5:CE:76:ILE:H | 1.75 | 0.51 |
| 9:CI:114:TYR:HE1 | 10:CJ:60:ARG:O | 1.93 | 0.51 |
| 13:CM:32:GLU:OE2 | 13:CM:64:TRP:CH2 | 2.63 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:71:ARG:HG3 | 13:CM:71:ARG:O | 2.10 | 0.51 |
| 31:DA:1045:A:H3' | 31:DA:1045:A:N3 | 2.25 | 0.51 |
| 31:DA:1256:G:H5' | 31:DA:1257:C:OP2 | 2.11 | 0.51 |
| 31:DA:213:A:H2' | 31:DA:214:G:O4' | 2.11 | 0.51 |
| 31:DA:2199:A:C5' | 31:DA:2200:C:OP2 | 2.58 | 0.51 |
| 31:DA:271(K):U:H2' | 31:DA:271(M):G:N2 | 2.24 | 0.51 |
| 31:DA:271(P):C:H2' | 31:DA:271(Q):G:O5' | 2.10 | 0.51 |
| 31:DA:1750:G:O2' | 31:DA:2860:A:N1 | 2.40 | 0.51 |
| 31:DA:548:A:HO2' | 31:DA:549:G:P | 2.32 | 0.51 |
| 31:DA:825:C:C2' | 31:DA:826:U:O5' | 2.58 | 0.51 |
| 31:DA:824:A:C2' | 31:DA:825:C:H5' | 2.40 | 0.51 |
| 25:D3:52:HIS:CD2 | 32:DB:83:G:H4' | 2.45 | 0.51 |
| 34:DE:60:ASN:OD1 | 34:DE:62:PRO:HD2 | 2.11 | 0.51 |
| 34:DE:87:GLU:HG3 | 34:DE:87:GLU:O | 2.09 | 0.51 |
| 36:DG:39:ILE:HD12 | 36:DG:40:ASN:N | 2.25 | 0.51 |
| 36:DG:56:ALA:HA | 36:DG:59:GLU:OE1 | 2.10 | 0.51 |
| 38:DI:73:GLU:O | 38:DI:73:GLU:HG3 | 2.11 | 0.51 |
| 41:DP:48:PRO:O | 41:DP:49:ARG:C | 2.47 | 0.51 |
| 46:DU:75:ASN:HB2 | 46:DU:78:THR:H | 1.74 | 0.51 |
| 48:DW:10:VAL:O | 48:DW:11:ARG:HB2 | 2.09 | 0.51 |
| 49:DX:65:ARG:HA | 49:DX:65:ARG:NE | 2.25 | 0.51 |
| 51:DZ:166:SER:OG | 51:DZ:167:PRO:CA | 2.56 | 0.51 |
| 1:AA:1003:G:C2' | 1:AA:1004:A:H4' | 2.32 | 0.51 |
| 1:AA:192:U:C1' | 20:AT:103:GLY:HA2 | 2.41 | 0.51 |
| 1:AA:475:G:O2' | 1:AA:476:G:H5' | 2.11 | 0.51 |
| 1:AA:705:U:C5 | 1:AA:706:A:C5 | 2.99 | 0.51 |
| 1:AA:80:G:N1 | 1:AA:89:C:N4 | 2.58 | 0.51 |
| 2:AB:71:VAL:HB | 2:AB:164:VAL:HG22 | 1.92 | 0.51 |
| 5:AE:139:LEU:HA | 5:AE:142:LEU:HD12 | 1.92 | 0.51 |
| 10:AJ:7:LYS:HB2 | 10:AJ:97:GLU:HB2 | 1.92 | 0.51 |
| 16:AP:1:MET:HG2 | 16:AP:2:VAL:O | 2.10 | 0.51 |
| 23:B1:40:ARG:CD | 23:B1:41:ARG:H | 2.21 | 0.51 |
| 23:B1:87:PRO:HB2 | 23:B1:91:LYS:CE | 2.40 | 0.51 |
| 24:B2:18:PRO:O | 24:B2:19:VAL:C | 2.47 | 0.51 |
| 30:B8:62:LEU:N | 30:B8:63:PRO:HD2 | 2.25 | 0.51 |
| 31:BA:1568:G:OP2 | 33:BD:63:ARG:NH2 | 2.43 | 0.51 |
| 31:BA:1784:A:H4' | 31:BA:1785:A:C5' | 2.41 | 0.51 |
| 31:BA:1856:G:H2' | 31:BA:1857:G:H5' | 1.92 | 0.51 |
| 31:BA:1858:G:H1' | 31:BA:1884:A:N6 | 2.26 | 0.51 |
| 31:BA:194:G:H2' | 31:BA:195:A:O4' | 2.11 | 0.51 |
| 31:BA:2565:A:C5' | 31:BA:2566:A:OP2 | 2.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:2787:C:O2 | 34:BE:61:ARG:NH1 | 2.44 | 0.51 |
| 31:BA:649:G:H2' | 31:BA:650:C:H6 | 1.75 | 0.51 |
| 31:BA:796:C:H2' | 31:BA:797:C:H6 | 1.71 | 0.51 |
| 32:BB:41:U:C2' | 32:BB:42:C:OP1 | 2.58 | 0.51 |
| 32:BB:50:G:O5' | 32:BB:50:G:H8 | 1.93 | 0.51 |
| 33:BD:17:THR:CG2 | 33:BD:204:ILE:HA | 2.40 | 0.51 |
| 33:BD:186:HIS:CD2 | 33:BD:187:GLY:N | 2.79 | 0.51 |
| 38:BI:78:THR:HA | 38:BI:141:LYS:HB2 | 1.92 | 0.51 |
| 40:BO:26:LYS:HB2 | 40:BO:30:ALA:HB2 | 1.92 | 0.51 |
| 41:BP:108:LYS:O | 41:BP:110:TYR:N | 2.44 | 0.51 |
| 1:CA:1442:G:O2' | 1:CA:1442(A):G:C5' | 2.48 | 0.51 |
| 1:CA:166:G:C4 | 1:CA:167:G:C8 | 2.99 | 0.51 |
| 1:CA:343:U:O2 | 1:CA:347:G:C2 | 2.64 | 0.51 |
| 1:CA:365:U:H5'' | 1:CA:366:C:OP1 | 2.11 | 0.51 |
| 1:CA:377:G:OP1 | 16:CP:3:LYS:HD2 | 2.11 | 0.51 |
| 1:CA:475:G:O2' | 1:CA:476:G:H5' | 2.10 | 0.51 |
| 1:CA:987:G:N2 | 1:CA:1219:U:C2 | 2.79 | 0.51 |
| 2:CB:97:TRP:CH2 | 2:CB:176:GLU:OE2 | 2.64 | 0.51 |
| 4:CD:23:GLY:HA3 | 4:CD:112:VAL:HG22 | 1.91 | 0.51 |
| 5:CE:33:VAL:HG12 | 5:CE:34:VAL:N | 2.26 | 0.51 |
| 10:CJ:24:VAL:HG21 | 10:CJ:37:PRO:HD3 | 1.92 | 0.51 |
| 22:D0:68:GLU:CG | 22:D0:80:HIS:HB2 | 2.40 | 0.51 |
| 23:D1:9:GLY:O | 23:D1:10:LYS:CB | 2.59 | 0.51 |
| 31:DA:1490:A:H5' | 31:DA:1491:G:OP2 | 2.10 | 0.51 |
| 31:DA:1659:U:C4 | 31:DA:1660:C:C5 | 2.99 | 0.51 |
| 31:DA:2723:C:H5'' | 43:DR:2:ARG:CD | 2.40 | 0.51 |
| 31:DA:547:A:C8 | 31:DA:549:G:O6 | 2.63 | 0.51 |
| 31:DA:596:G:C5 | 31:DA:597:U:C5 | 2.99 | 0.51 |
| 31:DA:729:G:O5' | 33:DD:208:LYS:NZ | 2.38 | 0.51 |
| 31:DA:84:A:H5'' | 50:DY:9:LYS:HD3 | 1.92 | 0.51 |
| 31:DA:934:G:H2' | 31:DA:935:C:C6 | 2.46 | 0.51 |
| 33:DD:132:PRO:HG3 | 33:DD:190:TYR:CE1 | 2.45 | 0.51 |
| 36:DG:120:LEU:O | 36:DG:122:PRO:HD3 | 2.11 | 0.51 |
| 45:DT:28:VAL:HG21 | 45:DT:46:GLU:HG3 | 1.92 | 0.51 |
| 47:DV:73:SER:OG | 47:DV:75:PHE:HE1 | 1.91 | 0.51 |
| 50:DY:86:ARG:HG2 | 50:DY:87:LYS:N | 2.24 | 0.51 |
| 1:AA:1054:C:H3' | 1:AA:1054:C:O2 | 2.11 | 0.51 |
| 1:AA:109:A:C6 | 1:AA:326:G:C6 | 2.99 | 0.51 |
| 1:AA:1252:A:H61 | 1:AA:1285:A:H61 | 1.58 | 0.51 |
| 1:AA:323:U:OP1 | 20:AT:26:ASN:ND2 | 2.44 | 0.51 |
| 1:AA:458:C:H2' | 1:AA:460:G:H8 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:552:U:H2' | 1:AA:553:A:H5' | 1.92 | 0.51 |
| 1:AA:665:A:C5 | 1:AA:733:A:C5 | 2.99 | 0.51 |
| 1:AA:791:G:C6 | 1:AA:792:A:N7 | 2.79 | 0.51 |
| 2:AB:17:PHE:O | 2:AB:18:GLY:O | 2.28 | 0.51 |
| 1:AA:878:G:C5' | 8:AH:89:PRO:HG2 | 2.41 | 0.51 |
| 9:AI:55:ALA:CB | 9:AI:58:ARG:HD2 | 2.40 | 0.51 |
| 12:AL:75:HIS:HD2 | 12:AL:77:LEU:H | 1.57 | 0.51 |
| 30:B8:39:LYS:CD | 30:B8:39:LYS:C | 2.79 | 0.51 |
| 31:BA:83:G:H1 | 31:BA:102:G:H2' | 1.76 | 0.51 |
| 31:BA:1341:U:H3' | 31:BA:1397:U:O2 | 2.11 | 0.51 |
| 31:BA:2199:A:OP2 | 31:BA:2200:C:C5 | 2.61 | 0.51 |
| 31:BA:2286:A:H5'' | 31:BA:2287:A:O4' | 2.10 | 0.51 |
| 31:BA:2639:A:C2' | 31:BA:2640:G:H5' | 2.41 | 0.51 |
| 31:BA:2639:A:H2' | 31:BA:2640:G:H5' | 1.92 | 0.51 |
| 31:BA:271(K):U:H2' | 31:BA:271(M):G:N2 | 2.26 | 0.51 |
| 31:BA:2722:G:H2' | 31:BA:2723:C:C6 | 2.45 | 0.51 |
| 31:BA:2791:C:H4' | 31:BA:2792:G:O5' | 2.11 | 0.51 |
| 31:BA:807:U:C2' | 31:BA:808:G:O5' | 2.57 | 0.51 |
| 31:BA:917:A:H5' | 31:BA:917:A:H8 | 1.75 | 0.51 |
| 32:BB:82:G:H2' | 32:BB:83:G:C5' | 2.37 | 0.51 |
| 33:BD:224:ALA:O | 33:BD:225:ALA:HB2 | 2.10 | 0.51 |
| 36:BG:98:ARG:O | 36:BG:101:ILE:HG22 | 2.10 | 0.51 |
| 39:BN:17:ASP:CG | 39:BN:17:ASP:O | 2.44 | 0.51 |
| 39:BN:2:LYS:NZ | 46:BU:94:ASN:ND2 | 2.59 | 0.51 |
| 39:BN:78:TYR:HD1 | 39:BN:79:PRO:CG | 2.23 | 0.51 |
| 44:BS:57:LYS:CG | 44:BS:58:LEU:H | 2.24 | 0.51 |
| 50:BY:81:LYS:HD3 | 50:BY:97:ARG:HG3 | 1.93 | 0.51 |
| 42:BQ:141:GLN:O | 51:BZ:70:LEU:HD22 | 2.11 | 0.51 |
| 1:CA:1084:G:OP1 | 1:CA:1086:U:C2 | 2.64 | 0.51 |
| 1:CA:1478:C:O2' | 1:CA:1479:C:H5' | 2.11 | 0.51 |
| 1:CA:1504:G:OP1 | 1:CA:1507:A:H4' | 2.11 | 0.51 |
| 1:CA:1508:G:H2' | 1:CA:1509:C:C6 | 2.45 | 0.51 |
| 1:CA:22:G:O2' | 1:CA:23:C:H5' | 2.11 | 0.51 |
| 3:CC:121:ALA:HB2 | 3:CC:187:ALA:HB1 | 1.92 | 0.51 |
| 6:CF:17:SER:O | 6:CF:21:LEU:HD22 | 2.11 | 0.51 |
| 13:CM:83:ASP:CG | 13:CM:84:ILE:H | 2.14 | 0.51 |
| 1:CA:376:G:O3' | 16:CP:5:ARG:HD2 | 2.10 | 0.51 |
| 24:D2:26:ARG:NE | 24:D2:29:LYS:HE2 | 2.24 | 0.51 |
| 24:D2:34:GLU:O | 24:D2:36:ARG:HB2 | 2.11 | 0.51 |
| 31:DA:1301:A:C8 | 31:DA:1303:G:C8 | 2.99 | 0.51 |
| 31:DA:1902:C:H2' | 31:DA:1903:G:O5' | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:1946:U:H2' | 31:DA:1947:C:H6 | 1.75 | 0.51 |
| 31:DA:826:U:OP1 | 31:DA:2428:G:H3' | 2.10 | 0.51 |
| 31:DA:2870:C:H2' | 31:DA:2871:C:H5' | 1.93 | 0.51 |
| 31:DA:455:C:N3 | 31:DA:473:G:H5' | 2.26 | 0.51 |
| 31:DA:607:U:O2 | 31:DA:621:A:N1 | 2.43 | 0.51 |
| 31:DA:686:G:N2 | 31:DA:788:A:H61 | 2.08 | 0.51 |
| 31:DA:740:U:H2' | 31:DA:741:G:C8 | 2.46 | 0.51 |
| 31:DA:753:C:O5' | 31:DA:753:C:H6 | 1.92 | 0.51 |
| 34:DE:52:LEU:O | 34:DE:74:PRO:CA | 2.59 | 0.51 |
| 35:DF:21:ALA:HB3 | 35:DF:23:ASP:OD2 | 2.10 | 0.51 |
| 36:DG:152:LEU:O | 36:DG:153:ARG:HB2 | 2.09 | 0.51 |
| 39:DN:78:TYR:HD1 | 39:DN:79:PRO:N | 2.08 | 0.51 |
| 42:DQ:42:ILE:HD13 | 42:DQ:97:VAL:HG21 | 1.92 | 0.51 |
| 44:DS:54:LEU:HA | 44:DS:57:LYS:O | 2.09 | 0.51 |
| 48:DW:54:ALA:HB1 | 48:DW:107:LEU:HD22 | 1.92 | 0.51 |
| 1:AA:1211:U:H5' | 1:AA:1212:U:OP1 | 2.11 | 0.51 |
| 1:AA:394:G:H2' | 1:AA:395:C:H6 | 1.76 | 0.51 |
| 5:AE:139:LEU:HA | 5:AE:142:LEU:CD1 | 2.41 | 0.51 |
| 6:AF:5:GLU:HB3 | 6:AF:62:TRP:NE1 | 2.25 | 0.51 |
| 9:AI:83:ARG:O | 9:AI:86:VAL:HG12 | 2.11 | 0.51 |
| 15:AO:51:HIS:O | 15:AO:54:ARG:HB3 | 2.11 | 0.51 |
| 24:B2:37:PHE:CD2 | 24:B2:37:PHE:O | 2.64 | 0.51 |
| 27:B5:42:PRO:HB2 | 27:B5:43:HIS:HD2 | 1.75 | 0.51 |
| 27:B5:52:TYR:CD1 | 27:B5:52:TYR:O | 2.63 | 0.51 |
| 31:BA:1171:G:N7 | 31:BA:1173:G:H1' | 2.25 | 0.51 |
| 31:BA:2320:A:H2' | 31:BA:2320:A:N3 | 2.25 | 0.51 |
| 30:B8:35:GLN:CG | 31:BA:2420:C:OP1 | 2.59 | 0.51 |
| 22:B0:1:MET:HA | 31:BA:2451:A:H4' | 1.93 | 0.51 |
| 31:BA:271(E):U:H2' | 31:BA:271(F):C:C6 | 2.46 | 0.51 |
| 31:BA:340:A:H2' | 31:BA:341:G:C5' | 2.41 | 0.51 |
| 31:BA:494:G:C8 | 31:BA:494:G:H5'' | 2.45 | 0.51 |
| 31:BA:743:G:C2' | 31:BA:744:G:H5' | 2.41 | 0.51 |
| 31:BA:92:A:H2' | 31:BA:93:G:H8 | 1.75 | 0.51 |
| 34:BE:96:PHE:HA | 34:BE:100:GLU:OE1 | 2.11 | 0.51 |
| 35:BF:203:GLN:O | 35:BF:206:ILE:C | 2.49 | 0.51 |
| 41:BP:16:ARG:O | 41:BP:18:ARG:N | 2.44 | 0.51 |
| 42:BQ:27:VAL:HA | 42:BQ:105:GLU:OE1 | 2.11 | 0.51 |
| 43:BR:53:HIS:O | 43:BR:56:LYS:HB3 | 2.11 | 0.51 |
| 46:BU:83:LEU:CB | 46:BU:88:ILE:HD11 | 2.39 | 0.51 |
| 49:BX:21:PHE:N | 49:BX:21:PHE:HD1 | 2.09 | 0.51 |
| 50:BY:7:VAL:CB | 50:BY:8:LYS:NZ | 2.72 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1211:U:H5' | 1:CA:1212:U:OP1 | 2.11 | 0.51 |
| 1:CA:147:G:N2 | 1:CA:148:G:H1' | 2.26 | 0.51 |
| 1:CA:1497:G:C2' | 1:CA:1498:U:H5' | 2.41 | 0.51 |
| 1:CA:542:G:H2' | 1:CA:543:C:C6 | 2.44 | 0.51 |
| 1:CA:944:G:H5'' | 1:CA:945:G:OP2 | 2.11 | 0.51 |
| 2:CB:139:LYS:O | 2:CB:143:GLU:HG2 | 2.10 | 0.51 |
| 4:CD:30:LYS:C | 4:CD:32:ALA:H | 2.14 | 0.51 |
| 1:CA:545:C:H5'' | 4:CD:72:GLU:HG2 | 1.92 | 0.51 |
| 5:CE:80:ILE:HD11 | 5:CE:138:ALA:HB1 | 1.91 | 0.51 |
| 6:CF:3:ARG:HB3 | 6:CF:93:SER:HB2 | 1.93 | 0.51 |
| 11:CK:41:THR:CG2 | 11:CK:42:TRP:N | 2.73 | 0.51 |
| 14:CN:24:CYS:HB3 | 14:CN:27:CYS:O | 2.11 | 0.51 |
| 27:D5:36:CYS:C | 27:D5:38:ALA:N | 2.64 | 0.51 |
| 27:D5:47:PRO:O | 27:D5:48:GLU:HG3 | 2.11 | 0.51 |
| 31:DA:2476:A:C2 | 31:DA:2477:C:C6 | 2.98 | 0.51 |
| 31:DA:272(B):G:O2' | 31:DA:272(C):G:O4' | 2.29 | 0.51 |
| 31:DA:27:G:C4 | 31:DA:512:G:N2 | 2.78 | 0.51 |
| 31:DA:363(C):G:C4 | 31:DA:363(D):G:C8 | 2.98 | 0.51 |
| 31:DA:479:A:H4' | 31:DA:480:A:OP1 | 2.09 | 0.51 |
| 31:DA:693:C:O2' | 31:DA:694:U:H5' | 2.11 | 0.51 |
| 35:DF:4:VAL:O | 35:DF:4:VAL:HG12 | 2.11 | 0.51 |
| 35:DF:70:THR:HG21 | 35:DF:72:ARG:HB2 | 1.92 | 0.51 |
| 31:DA:1131:G:H4' | 39:DN:82:LEU:HG | 1.93 | 0.51 |
| 42:DQ:70:PRO:HA | 42:DQ:95:ALA:HB2 | 1.92 | 0.51 |
| 31:DA:993:G:H1' | 47:DV:91:TYR:CE1 | 2.45 | 0.51 |
| 1:AA:1201:A:H4' | 1:AA:1202:G:O5' | 2.11 | 0.51 |
| 1:AA:1218:C:H2' | 1:AA:1219:U:C6 | 2.45 | 0.51 |
| 1:AA:132:C:O2' | 1:AA:133:U:H5' | 2.10 | 0.51 |
| 1:AA:1478:C:O2' | 1:AA:1479:C:H5' | 2.11 | 0.51 |
| 1:AA:149:A:HO2' | 1:AA:150:C:H6 | 1.52 | 0.51 |
| 1:AA:299:G:C6 | 1:AA:300:A:C6 | 2.99 | 0.51 |
| 2:AB:97:TRP:HH2 | 2:AB:176:GLU:CG | 2.24 | 0.51 |
| 10:AJ:82:ILE:O | 10:AJ:86:MET:HB3 | 2.11 | 0.51 |
| 13:AM:3:ARG:HG2 | 13:AM:9:ILE:CG1 | 2.41 | 0.51 |
| 1:AA:310:G:C5' | 16:AP:31:LYS:HB2 | 2.41 | 0.51 |
| 17:AQ:65:ILE:HD12 | 17:AQ:69:LYS:O | 2.10 | 0.51 |
| 24:B2:41:ILE:O | 24:B2:44:LEU:N | 2.41 | 0.51 |
| 24:B2:47:ASN:HD22 | 24:B2:47:ASN:N | 2.09 | 0.51 |
| 28:B6:28:ARG:HA | 28:B6:32:ASN:HB3 | 1.91 | 0.51 |
| 29:B7:19:ARG:HH11 | 29:B7:19:ARG:HG2 | 1.76 | 0.51 |
| 30:B8:10:ALA:HB2 | 30:B8:59:LYS:HZ2 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:BA:1171:G:H3' | 31:BA:1173:G:O4' | 2.11 | 0.51 |
| 31:BA:1256:G:H5' | 31:BA:1257:C:OP2 | 2.11 | 0.51 |
| 31:BA:1416:G:O2' | 31:BA:1417:C:P | 2.69 | 0.51 |
| 31:BA:1578:U:O2 | 31:BA:1578:U:H2' | 2.10 | 0.51 |
| 28:B6:23:THR:HG21 | 31:BA:2419:U:H4' | 1.93 | 0.51 |
| 31:BA:2753:A:O2' | 31:BA:2754:U:P | 2.69 | 0.51 |
| 31:BA:288:C:N4 | 31:BA:353:G:H1 | 2.08 | 0.51 |
| 33:BD:24:ILE:HG22 | 33:BD:24:ILE:O | 2.11 | 0.51 |
| 34:BE:132:HIS:HA | 34:BE:135:HIS:CE1 | 2.46 | 0.51 |
| 38:BI:79:ILE:HG22 | 38:BI:81:VAL:HG23 | 1.93 | 0.51 |
| 44:BS:56:LEU:O | 44:BS:57:LYS:HB2 | 2.09 | 0.51 |
| 45:BT:28:VAL:HG22 | 45:BT:46:GLU:HA | 1.92 | 0.51 |
| 46:BU:92:ARG:NH2 | 47:BV:10:LYS:CA | 2.74 | 0.51 |
| 50:BY:90:LEU:HD12 | 50:BY:91:GLU:HG2 | 1.92 | 0.51 |
| 1:CA:165:C:H2' | 1:CA:166:G:C8 | 2.46 | 0.51 |
| 1:CA:195:A:C5 | 1:CA:196:A:N1 | 2.78 | 0.51 |
| 1:CA:950:U:H2' | 1:CA:951:G:C8 | 2.43 | 0.51 |
| 10:CJ:82:ILE:O | 10:CJ:86:MET:HB3 | 2.11 | 0.51 |
| 30:D8:31:HIS:HB3 | 31:DA:2420:C:H41 | 1.76 | 0.51 |
| 31:DA:1024:G:C3' | 31:DA:1025:G:H5'' | 2.33 | 0.51 |
| 31:DA:1191:G:OP1 | 41:DP:35:HIS:ND1 | 2.43 | 0.51 |
| 31:DA:1330:C:O2' | 31:DA:1331:A:H5' | 2.10 | 0.51 |
| 31:DA:1487:G:C2 | 31:DA:1488:G:C4 | 2.99 | 0.51 |
| 31:DA:1796:U:H2' | 31:DA:1797:C:H6 | 1.72 | 0.51 |
| 31:DA:241:A:O4' | 31:DA:243:U:C6 | 2.63 | 0.51 |
| 31:DA:2656:U:C2' | 31:DA:2657:A:H5'' | 2.40 | 0.51 |
| 31:DA:576:U:H2' | 31:DA:577:G:C8 | 2.46 | 0.51 |
| 31:DA:588:U:O4 | 31:DA:670:A:H1' | 2.10 | 0.51 |
| 33:DD:64:ILE:O | 33:DD:64:ILE:HG12 | 2.11 | 0.51 |
| 38:DI:6:LEU:HD23 | 38:DI:6:LEU:N | 2.25 | 0.51 |
| 42:DQ:7:MET:O | 42:DQ:10:ARG:NH2 | 2.41 | 0.51 |
| 45:DT:41:ARG:CZ | 45:DT:43:GLN:HB2 | 2.41 | 0.51 |
| 47:DV:18:LEU:O | 47:DV:19:LYS:HB2 | 2.11 | 0.51 |
| 47:DV:62:LEU:CB | 47:DV:98:GLU:HA | 2.38 | 0.51 |
| 50:DY:7:VAL:CB | 50:DY:8:LYS:NZ | 2.73 | 0.51 |
| 1:AA:1418:A:C2 | 1:AA:1483:A:C2 | 2.99 | 0.51 |
| 1:AA:1508:G:H2' | 1:AA:1509:C:C6 | 2.46 | 0.51 |
| 1:AA:20:U:H2' | 1:AA:21:G:O4' | 2.11 | 0.51 |
| 1:AA:327:A:H3' | 1:AA:328:C:H5'' | 1.92 | 0.51 |
| 1:AA:685:G:C2 | 1:AA:686:U:C4 | 2.99 | 0.51 |
| 1:AA:877:C:H5'' | 8:AH:88:LYS:CD | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:20:SER:CB | 3:AC:40:ARG:HH22 | 2.15 | 0.51 |
| 4:AD:108:LEU:HB3 | 4:AD:110:PHE:CD1 | 2.45 | 0.51 |
| 4:AD:14:ARG:HA | 4:AD:39:PRO:HB3 | 1.92 | 0.51 |
| 6:AF:17:SER:O | 6:AF:21:LEU:HD22 | 2.11 | 0.51 |
| 10:AJ:84:GLN:O | 10:AJ:88:LEU:HB2 | 2.11 | 0.51 |
| 18:AR:19:LYS:O | 18:AR:20:ALA:HB2 | 2.10 | 0.51 |
| 23:B1:60:PHE:HZ | 23:B1:90:ILE:HG21 | 1.74 | 0.51 |
| 31:BA:109:G:C4 | 31:BA:110:G:C8 | 2.99 | 0.51 |
| 31:BA:1168:G:C2' | 31:BA:1169:G:H5' | 2.41 | 0.51 |
| 31:BA:1300:U:C3' | 31:BA:1301:A:C5' | 2.89 | 0.51 |
| 31:BA:1505:C:C2' | 31:BA:1506:C:O5' | 2.59 | 0.51 |
| 31:BA:1786:A:H1' | 31:BA:1938:A:N6 | 2.26 | 0.51 |
| 31:BA:2238:G:H4' | 31:BA:2239:G:OP1 | 2.10 | 0.51 |
| 31:BA:2619:C:H2' | 31:BA:2620:C:H6 | 1.76 | 0.51 |
| 31:BA:271(L):U:H4' | 31:BA:271(M):G:N7 | 2.26 | 0.51 |
| 31:BA:2774:C:H2' | 31:BA:2775:A:O4' | 2.10 | 0.51 |
| 31:BA:900:A:H5'' | 31:BA:901:A:OP2 | 2.11 | 0.51 |
| 35:BF:46:ARG:NH1 | 35:BF:46:ARG:CG | 2.61 | 0.51 |
| 39:BN:111:PRO:HA | 39:BN:114:ARG:NH1 | 2.25 | 0.51 |
| 39:BN:56:ASN:N | 39:BN:125:GLY:H | 2.08 | 0.51 |
| 41:BP:115:LEU:HA | 41:BP:134:ALA:CB | 2.33 | 0.51 |
| 41:BP:88:LEU:O | 41:BP:90:ARG:N | 2.41 | 0.51 |
| 42:BQ:29:PHE:HD1 | 42:BQ:29:PHE:N | 2.09 | 0.51 |
| 31:BA:870:A:C5' | 42:BQ:7:MET:HB2 | 2.26 | 0.51 |
| 43:BR:10:LEU:HB3 | 43:BR:17:ARG:CZ | 2.40 | 0.51 |
| 44:BS:74:ALA:HB1 | 44:BS:103:GLU:HB2 | 1.93 | 0.51 |
| 44:BS:97:ARG:HD2 | 44:BS:98:VAL:N | 2.26 | 0.51 |
| 45:BT:57:PHE:C | 45:BT:59:THR:H | 2.13 | 0.51 |
| 47:BV:70:ILE:CB | 47:BV:90:PRO:HB2 | 2.38 | 0.51 |
| 47:BV:18:LEU:CD1 | 47:BV:98:GLU:OE1 | 2.57 | 0.51 |
| 48:BW:92:ARG:O | 48:BW:93:ALA:HB3 | 2.10 | 0.51 |
| 51:BZ:151:HIS:HA | 51:BZ:171:ILE:HD13 | 1.93 | 0.51 |
| 51:BZ:65:GLN:OE1 | 51:BZ:67:LEU:HD11 | 2.11 | 0.51 |
| 1:CA:1068:G:OP2 | 1:CA:1068:G:H8 | 1.94 | 0.51 |
| 1:CA:1148:U:H2' | 1:CA:1149:C:O4' | 2.11 | 0.51 |
| 1:CA:343:U:H2' | 1:CA:346:G:O6 | 2.10 | 0.51 |
| 1:CA:356:A:H1' | 1:CA:368:U:O2' | 2.11 | 0.51 |
| 1:CA:736:C:H2' | 1:CA:737:A:H8 | 1.74 | 0.51 |
| 4:CD:14:ARG:HA | 4:CD:39:PRO:HB3 | 1.92 | 0.51 |
| 4:CD:93:PHE:O | 4:CD:97:LEU:HG | 2.11 | 0.51 |
| 5:CE:105:VAL:O | 5:CE:109:ILE:HG13 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:CG:152:ALA:O | 7:CG:155:ARG:HG3 | 2.10 | 0.51 |
| 10:CJ:51:ARG:HG3 | 10:CJ:61:GLU:N | 2.26 | 0.51 |
| 13:CM:97:PRO:O | 13:CM:98:VAL:HA | 2.11 | 0.51 |
| 18:CR:59:SER:OG | 18:CR:62:GLU:HG3 | 2.10 | 0.51 |
| 18:CR:61:LYS:O | 18:CR:65:ILE:HG13 | 2.11 | 0.51 |
| 20:CT:56:MET:HG3 | 20:CT:88:VAL:HG21 | 1.93 | 0.51 |
| 23:D1:73:LEU:HD13 | 23:D1:90:ILE:HG22 | 1.92 | 0.51 |
| 24:D2:29:LYS:O | 24:D2:33:MET:SD | 2.69 | 0.51 |
| 24:D2:41:ILE:O | 24:D2:44:LEU:N | 2.41 | 0.51 |
| 30:D8:39:LYS:HE2 | 30:D8:42:ARG:NH1 | 2.27 | 0.51 |
| 31:DA:1112:G:C1' | 31:DA:1113:U:OP1 | 2.59 | 0.51 |
| 31:DA:174:C:H3' | 31:DA:175:G:H5'' | 1.90 | 0.51 |
| 31:DA:1970:A:C5' | 31:DA:1972:A:H1' | 2.36 | 0.51 |
| 31:DA:2302:G:C6 | 31:DA:2315:G:C6 | 2.98 | 0.51 |
| 31:DA:2364:C:C2' | 31:DA:2365:G:H5' | 2.41 | 0.51 |
| 30:D8:35:GLN:OE1 | 31:DA:2421:G:OP2 | 2.28 | 0.51 |
| 31:DA:271(G):C:O2 | 31:DA:271(G):C:H2' | 2.11 | 0.51 |
| 31:DA:2864:G:H2' | 31:DA:2865:U:O4' | 2.09 | 0.51 |
| 31:DA:64:A:O2' | 31:DA:65:C:H5' | 2.11 | 0.51 |
| 32:DB:38:C:O4' | 44:DS:95:HIS:NE2 | 2.37 | 0.51 |
| 33:DD:241:PRO:O | 33:DD:243:GLY:N | 2.43 | 0.51 |
| 36:DG:174:GLU:HG3 | 36:DG:180:PHE:CD1 | 2.46 | 0.51 |
| 38:DI:40:THR:CG2 | 38:DI:43:ASN:HD22 | 2.24 | 0.51 |
| 39:DN:87:LEU:O | 39:DN:88:GLU:C | 2.49 | 0.51 |
| 41:DP:71:VAL:HG13 | 41:DP:72:PRO:HD3 | 1.91 | 0.51 |
| 46:DU:104:GLN:HB2 | 47:DV:43:GLU:OE2 | 2.11 | 0.51 |
| 46:DU:92:ARG:HH22 | 47:DV:10:LYS:CB | 2.24 | 0.51 |
| 50:DY:68:HIS:H | 50:DY:71:LYS:HZ1 | 1.58 | 0.51 |
| 1:AA:987:G:N2 | 1:AA:1219:U:C2 | 2.80 | 0.50 |
| 1:AA:1470:G:C2' | 1:AA:1471:G:H5' | 2.41 | 0.50 |
| 1:AA:510:A:H5'' | 1:AA:511:C:OP2 | 2.11 | 0.50 |
| 1:AA:55:A:C4 | 1:AA:56:U:C6 | 2.99 | 0.50 |
| 1:AA:944:G:H5'' | 1:AA:945:G:OP2 | 2.10 | 0.50 |
| 2:AB:153:ARG:O | 2:AB:154:LEU:C | 2.50 | 0.50 |
| 2:AB:189:ASP:OD1 | 2:AB:189:ASP:N | 2.43 | 0.50 |
| 1:AA:1189:C:H5'' | 3:AC:5:ILE:HG21 | 1.92 | 0.50 |
| 2:AB:178:ARG:HH21 | 8:AH:68:ARG:HH22 | 1.58 | 0.50 |
| 13:AM:83:ASP:CG | 13:AM:84:ILE:H | 2.14 | 0.50 |
| 23:B1:89:GLU:O | 23:B1:93:GLU:N | 2.42 | 0.50 |
| 24:B2:14:ARG:NE | 24:B2:57:ILE:HB | 2.27 | 0.50 |
| 27:B5:36:CYS:O | 27:B5:38:ALA:N | 2.43 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:B5:51:TYR:HD2 | 27:B5:52:TYR:CZ | 2.28 | 0.50 |
| 30:B8:10:ALA:HB2 | 30:B8:59:LYS:NZ | 2.26 | 0.50 |
| 31:BA:1112:G:C1' | 31:BA:1113:U:OP1 | 2.59 | 0.50 |
| 31:BA:1412:A:H2' | 31:BA:1413:G:C8 | 2.46 | 0.50 |
| 31:BA:1449:A:H5'' | 31:BA:1449:A:H8 | 1.75 | 0.50 |
| 31:BA:2262:U:H2' | 31:BA:2263:C:H5' | 1.92 | 0.50 |
| 31:BA:2579:C:O3' | 34:BE:131:ALA:HB3 | 2.11 | 0.50 |
| 31:BA:2656:U:C2' | 31:BA:2657:A:H5'' | 2.41 | 0.50 |
| 31:BA:271(D):G:C6 | 31:BA:271(E):U:C4 | 2.99 | 0.50 |
| 31:BA:2762:G:H8 | 31:BA:2762:G:C5' | 2.23 | 0.50 |
| 31:BA:363(A):A:C2 | 31:BA:363(B):G:C8 | 2.99 | 0.50 |
| 31:BA:454:A:H4' | 31:BA:455:C:OP2 | 2.11 | 0.50 |
| 31:BA:836:G:H2' | 31:BA:837:C:C6 | 2.46 | 0.50 |
| 33:BD:27:THR:HG23 | 33:BD:28:GLU:H | 1.70 | 0.50 |
| 33:BD:30:GLU:CD | 33:BD:63:ARG:HE | 2.14 | 0.50 |
| 36:BG:39:ILE:HD12 | 36:BG:40:ASN:N | 2.26 | 0.50 |
| 37:BH:170:ARG:H | 37:BH:170:ARG:HD2 | 1.75 | 0.50 |
| 41:BP:124:LYS:HG2 | 41:BP:143:GLY:HA3 | 1.93 | 0.50 |
| 46:BU:61:TRP:O | 46:BU:62:ILE:C | 2.49 | 0.50 |
| 47:BV:1:MET:H2 | 47:BV:44:LYS:HD2 | 1.76 | 0.50 |
| 49:BX:63:LYS:O | 49:BX:68:ARG:HA | 2.11 | 0.50 |
| 50:BY:7:VAL:HB | 50:BY:8:LYS:HD2 | 1.92 | 0.50 |
| 51:BZ:67:LEU:N | 51:BZ:67:LEU:HD12 | 2.26 | 0.50 |
| 1:CA:1218:C:H2' | 1:CA:1219:U:C6 | 2.46 | 0.50 |
| 1:CA:1530:G:OP1 | 1:CA:1530:G:C4' | 2.58 | 0.50 |
| 1:CA:458:C:H2' | 1:CA:460:G:H8 | 1.76 | 0.50 |
| 1:CA:473:G:N3 | 1:CA:474:G:C8 | 2.79 | 0.50 |
| 1:CA:491:G:H2' | 1:CA:492:G:C8 | 2.46 | 0.50 |
| 1:CA:738:C:C2 | 1:CA:739:C:C5 | 2.99 | 0.50 |
| 1:CA:839:U:OP2 | 1:CA:840:C:H5 | 1.94 | 0.50 |
| 5:CE:139:LEU:HA | 5:CE:142:LEU:CD1 | 2.41 | 0.50 |
| 1:CA:363:A:C2 | 12:CL:31:PRO:HG2 | 2.45 | 0.50 |
| 13:CM:81:LEU:CD1 | 13:CM:88:ARG:HH12 | 2.24 | 0.50 |
| 23:D1:33:LYS:HB3 | 31:DA:2395:C:O2' | 2.11 | 0.50 |
| 25:D3:11:SER:HB3 | 31:DA:988:A:P | 2.51 | 0.50 |
| 30:D8:39:LYS:HD3 | 30:D8:39:LYS:C | 2.31 | 0.50 |
| 31:DA:1948:G:H2' | 31:DA:1949:G:O5' | 2.11 | 0.50 |
| 31:DA:2461:C:H2' | 31:DA:2462:U:H6 | 1.76 | 0.50 |
| 31:DA:2480:C:N4 | 31:DA:2481:G:C6 | 2.79 | 0.50 |
| 31:DA:2863:C:OP1 | 45:DT:93:ARG:NH1 | 2.44 | 0.50 |
| 23:D1:69:LYS:NZ | 31:DA:372:G:OP2 | 2.33 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:620:G:H5' | 31:DA:620:G:N3 | 2.26 | 0.50 |
| 31:DA:790:C:O2' | 31:DA:791:C:C5' | 2.59 | 0.50 |
| 31:DA:916:G:H2' | 31:DA:917:A:H5'' | 1.93 | 0.50 |
| 33:DD:31:LYS:O | 33:DD:32:SER:C | 2.49 | 0.50 |
| 34:DE:66:HIS:CG | 34:DE:66:HIS:O | 2.64 | 0.50 |
| 37:DH:85:LYS:HE2 | 37:DH:145:ALA:HB2 | 1.92 | 0.50 |
| 39:DN:112:LEU:C | 39:DN:112:LEU:HD12 | 2.27 | 0.50 |
| 39:DN:87:LEU:HD22 | 39:DN:91:LEU:HD11 | 1.92 | 0.50 |
| 40:DO:43:VAL:HG23 | 40:DO:56:ASP:O | 2.11 | 0.50 |
| 31:DA:814:C:C5 | 41:DP:27:HIS:CE1 | 2.99 | 0.50 |
| 31:DA:2870:C:C5' | 43:DR:65:LEU:HD21 | 2.40 | 0.50 |
| 43:DR:4:LEU:C | 43:DR:6:SER:H | 2.12 | 0.50 |
| 47:DV:18:LEU:CD1 | 47:DV:98:GLU:OE1 | 2.59 | 0.50 |
| 1:AA:1058:G:C6 | 1:AA:1059:C:N3 | 2.80 | 0.50 |
| 1:AA:1159:U:C4 | 1:AA:1182:G:C4 | 2.99 | 0.50 |
| 1:AA:159:G:H21 | 1:AA:161:A:H3' | 1.73 | 0.50 |
| 1:AA:674:G:O2' | 1:AA:675:A:H5' | 2.11 | 0.50 |
| 9:AI:28:VAL:HA | 9:AI:63:ILE:O | 2.10 | 0.50 |
| 13:AM:94:ARG:HG2 | 19:AS:82:GLY:N | 2.26 | 0.50 |
| 1:AA:1216:G:H5'' | 14:AN:5:ALA:CB | 2.41 | 0.50 |
| 15:AO:63:ARG:HG2 | 15:AO:67:LEU:HD12 | 1.92 | 0.50 |
| 23:B1:85:LEU:HD23 | 23:B1:85:LEU:N | 2.26 | 0.50 |
| 31:BA:1173:G:H3' | 31:BA:1174:A:H5' | 1.92 | 0.50 |
| 31:BA:1495:A:C2 | 31:BA:1496:A:C2 | 3.00 | 0.50 |
| 31:BA:1935:G:H1' | 31:BA:1964:G:N2 | 2.26 | 0.50 |
| 31:BA:2186:G:C2' | 31:BA:2187:G:H5'' | 2.42 | 0.50 |
| 31:BA:2511:U:O4 | 31:BA:2575:C:N3 | 2.45 | 0.50 |
| 31:BA:2624:G:C2' | 31:BA:2625:G:H5' | 2.41 | 0.50 |
| 31:BA:2689:U:H5'' | 31:BA:2690:C:H5' | 1.92 | 0.50 |
| 31:BA:466:A:H1' | 31:BA:683:C:O4' | 2.11 | 0.50 |
| 31:BA:196:A:C4 | 31:BA:805:G:O6 | 2.64 | 0.50 |
| 38:BI:27:ARG:CG | 38:BI:27:ARG:HH11 | 2.24 | 0.50 |
| 45:BT:23:ARG:HB2 | 45:BT:24:PRO:CD | 2.39 | 0.50 |
| 49:BX:40:LYS:C | 49:BX:42:ALA:H | 2.15 | 0.50 |
| 1:CA:1089:G:C6 | 1:CA:1090:U:C4 | 2.99 | 0.50 |
| 1:CA:1108:G:OP1 | 3:CC:175:LEU:HD12 | 2.11 | 0.50 |
| 1:CA:264:U:O2' | 17:CQ:64:PRO:HB2 | 2.11 | 0.50 |
| 6:CF:73:ASN:O | 6:CF:76:ALA:HB3 | 2.11 | 0.50 |
| 3:CC:18:TRP:HD1 | 14:CN:51:GLY:O | 1.94 | 0.50 |
| 20:CT:73:HIS:O | 20:CT:76:ALA:HB3 | 2.11 | 0.50 |
| 27:D5:45:VAL:HA | 27:D5:51:TYR:HE1 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 28:D6:51:GLU:O | 28:D6:52:VAL:HB | 2.09 | 0.50 |
| 30:D8:53:PRO:HA | 30:D8:56:GLU:HB2 | 1.94 | 0.50 |
| 30:D8:60:LEU:C | 30:D8:63:PRO:HD2 | 2.32 | 0.50 |
| 31:DA:1642:G:H2' | 31:DA:1643:G:O4' | 2.12 | 0.50 |
| 31:DA:1826:G:H4' | 33:DD:242:ARG:CZ | 2.41 | 0.50 |
| 31:DA:2308:G:H2' | 31:DA:2309:A:N7 | 2.26 | 0.50 |
| 31:DA:2360:A:O2' | 31:DA:2361:A:H5'' | 2.11 | 0.50 |
| 31:DA:2702:U:O2 | 31:DA:2702:U:OP1 | 2.28 | 0.50 |
| 31:DA:271(L):U:H5'' | 31:DA:271(M):G:C4 | 2.46 | 0.50 |
| 31:DA:322:A:H3' | 35:DF:169:ASN:HD21 | 1.75 | 0.50 |
| 31:DA:414:C:H2' | 31:DA:415:A:C8 | 2.45 | 0.50 |
| 31:DA:675:A:C8 | 31:DA:804:A:C6 | 2.98 | 0.50 |
| 33:DD:221:VAL:HG22 | 33:DD:226:MET:HE2 | 1.93 | 0.50 |
| 33:DD:35:LYS:HA | 33:DD:64:ILE:CG2 | 2.41 | 0.50 |
| 34:DE:137:HIS:HB3 | 34:DE:138:PRO:HD2 | 1.93 | 0.50 |
| 35:DF:110:LEU:HD21 | 35:DF:181:LEU:CD2 | 2.42 | 0.50 |
| 36:DG:29:TRP:C | 36:DG:31:VAL:N | 2.64 | 0.50 |
| 37:DH:89:ILE:HG22 | 37:DH:162:ILE:HG22 | 1.93 | 0.50 |
| 40:DO:26:LYS:HE3 | 40:DO:37:ASP:OD1 | 2.11 | 0.50 |
| 42:DQ:141:GLN:HB3 | 51:DZ:70:LEU:HD13 | 1.93 | 0.50 |
| 46:DU:91:ASP:O | 46:DU:92:ARG:HB3 | 2.10 | 0.50 |
| 47:DV:66:ARG:CD | 47:DV:67:GLY:N | 2.74 | 0.50 |
| 49:DX:73:ARG:N | 49:DX:74:PRO:HD3 | 2.27 | 0.50 |
| 1:AA:1030(A):G:H1' | 1:AA:1031:G:N2 | 2.17 | 0.50 |
| 1:AA:1053:G:C3' | 1:AA:1054:C:H5' | 2.41 | 0.50 |
| 1:AA:125:U:H2' | 1:AA:126:G:C8 | 2.47 | 0.50 |
| 1:AA:1350:A:H2' | 1:AA:1351:U:C6 | 2.47 | 0.50 |
| 1:AA:1442(B):A:OP1 | 1:AA:1442(B):A:H4' | 2.10 | 0.50 |
| 1:AA:189(K):U:H2' | 1:AA:189(L):G:C8 | 2.46 | 0.50 |
| 1:AA:380:G:N2 | 1:AA:384:G:C5 | 2.78 | 0.50 |
| 1:AA:450:G:OP1 | 1:AA:452:A:OP1 | 2.29 | 0.50 |
| 1:AA:654:G:C2 | 1:AA:753:A:C4 | 2.99 | 0.50 |
| 1:AA:687:A:H4' | 11:AK:47:VAL:HG13 | 1.94 | 0.50 |
| 1:AA:820:U:H4' | 1:AA:821:G:OP2 | 2.12 | 0.50 |
| 3:AC:153:VAL:HG12 | 3:AC:154:SER:H | 1.76 | 0.50 |
| 4:AD:148:VAL:HG12 | 4:AD:149:ALA:N | 2.26 | 0.50 |
| 5:AE:33:VAL:HG12 | 5:AE:34:VAL:N | 2.26 | 0.50 |
| 6:AF:3:ARG:HB3 | 6:AF:93:SER:HB2 | 1.93 | 0.50 |
| 10:AJ:16:LEU:HD13 | 10:AJ:16:LEU:O | 2.11 | 0.50 |
| 10:AJ:51:ARG:HG3 | 10:AJ:61:GLU:N | 2.26 | 0.50 |
| 13:AM:14:ARG:NH1 | 13:AM:42:ALA:HA | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:AM:17:VAL:O | 13:AM:20:THR:HB | 2.12 | 0.50 |
| 31:BA:1328:G:H2' | 31:BA:1330:C:C5 | 2.46 | 0.50 |
| 1:AA:1494:G:N2 | 31:BA:1912:A:C2 | 2.79 | 0.50 |
| 31:BA:2712:U:O2' | 31:BA:2712(A):A:P | 2.70 | 0.50 |
| 31:BA:543:C:N3 | 31:BA:551:G:N1 | 2.58 | 0.50 |
| 31:BA:548:A:HO2' | 31:BA:549:G:P | 2.35 | 0.50 |
| 31:BA:588:U:O4 | 31:BA:670:A:H1' | 2.11 | 0.50 |
| 32:BB:35:U:O2' | 32:BB:36:C:H5' | 2.11 | 0.50 |
| 32:BB:43:C:H4' | 36:BG:66:GLN:NE2 | 2.26 | 0.50 |
| 33:BD:35:LYS:HB3 | 33:BD:63:ARG:CA | 2.30 | 0.50 |
| 37:BH:158:HIS:HE1 | 37:BH:168:PRO:O | 1.94 | 0.50 |
| 39:BN:39:ARG:HD3 | 39:BN:41:ASP:HB2 | 1.92 | 0.50 |
| 39:BN:78:TYR:H | 39:BN:79:PRO:CD | 2.25 | 0.50 |
| 31:BA:1190:G:O3' | 41:BP:35:HIS:HB3 | 2.12 | 0.50 |
| 41:BP:50:ARG:O | 41:BP:57:THR:HG23 | 2.11 | 0.50 |
| 43:BR:5:LYS:HD2 | 43:BR:5:LYS:N | 2.27 | 0.50 |
| 50:BY:42:VAL:CG2 | 50:BY:67:LEU:HD13 | 2.41 | 0.50 |
| 1:CA:105:G:H2' | 1:CA:106:C:C6 | 2.47 | 0.50 |
| 1:CA:1252:A:H61 | 1:CA:1285:A:H61 | 1.57 | 0.50 |
| 1:CA:1329:A:N7 | 21:CU:7:ARG:NH2 | 2.56 | 0.50 |
| 1:CA:171:A:H2' | 1:CA:172:A:C8 | 2.45 | 0.50 |
| 1:CA:425:G:N2 | 1:CA:426:G:H1' | 2.26 | 0.50 |
| 1:CA:657:G:C2 | 1:CA:750:G:C5 | 3.00 | 0.50 |
| 1:CA:673:G:H2' | 1:CA:674:G:H8 | 1.73 | 0.50 |
| 4:CD:160:GLN:HA | 4:CD:163:GLU:HB2 | 1.92 | 0.50 |
| 7:CG:85:TYR:HD1 | 7:CG:154:TYR:HE1 | 1.60 | 0.50 |
| 1:CA:963:G:N2 | 10:CJ:55:LYS:HE2 | 2.27 | 0.50 |
| 16:CP:50:LYS:HD3 | 16:CP:51:VAL:N | 2.26 | 0.50 |
| 22:D0:71:ASP:O | 22:D0:72:ARG:HG2 | 2.11 | 0.50 |
| 22:D0:72:ARG:HH21 | 22:D0:75:LEU:HD12 | 1.75 | 0.50 |
| 24:D2:14:ARG:NE | 24:D2:57:ILE:HB | 2.27 | 0.50 |
| 30:D8:18:ALA:HB3 | 31:DA:651:G:H4' | 1.93 | 0.50 |
| 31:DA:1209:G:H21 | 31:DA:1210:A:H62 | 1.58 | 0.50 |
| 23:D1:8:SER:HB3 | 31:DA:1364:G:OP1 | 2.12 | 0.50 |
| 31:DA:2820:A:H2' | 31:DA:2820:A:N3 | 2.26 | 0.50 |
| 31:DA:28:A:C5 | 31:DA:29:U:C5 | 2.99 | 0.50 |
| 31:DA:92:A:H2' | 31:DA:93:G:H8 | 1.76 | 0.50 |
| 31:DA:996:A:H4' | 46:DU:92:ARG:CZ | 2.41 | 0.50 |
| 32:DB:29:A:H2' | 32:DB:30:C:C6 | 2.47 | 0.50 |
| 31:DA:1902:C:OP1 | 33:DD:242:ARG:HD2 | 2.10 | 0.50 |
| 35:DF:199:TRP:CH2 | 35:DF:203:GLN:NE2 | 2.80 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:DH:41:MET:HB3 | 37:DH:43:VAL:HG13 | 1.94 | 0.50 |
| 39:DN:79:PRO:HD2 | 39:DN:81:GLY:H | 1.76 | 0.50 |
| 41:DP:146:VAL:HG22 | 41:DP:147:LEU:H | 1.75 | 0.50 |
| 41:DP:16:ARG:O | 41:DP:18:ARG:N | 2.45 | 0.50 |
| 47:DV:56:SER:O | 47:DV:57:VAL:HB | 2.12 | 0.50 |
| 1:AA:1441:G:H5'' | 1:AA:1442:G:C5' | 2.42 | 0.50 |
| 1:AA:357:G:C2' | 1:AA:358:U:H5' | 2.42 | 0.50 |
| 1:AA:515:G:N2 | 1:AA:537:G:C4 | 2.79 | 0.50 |
| 1:AA:81:U:C4 | 1:AA:83:U:C5 | 3.00 | 0.50 |
| 1:AA:90:U:O2' | 1:AA:91:C:C5 | 2.62 | 0.50 |
| 1:AA:96:U:O2' | 1:AA:97:G:P | 2.70 | 0.50 |
| 2:AB:163:PHE:HA | 2:AB:185:ILE:O | 2.11 | 0.50 |
| 1:AA:1205:U:O2' | 3:AC:195:VAL:HG23 | 2.12 | 0.50 |
| 3:AC:64:VAL:HB | 3:AC:99:VAL:HG12 | 1.94 | 0.50 |
| 7:AG:69:VAL:HG12 | 7:AG:69:VAL:O | 2.12 | 0.50 |
| 12:AL:18:VAL:O | 12:AL:19:ARG:HB3 | 2.10 | 0.50 |
| 27:B5:36:CYS:C | 27:B5:38:ALA:N | 2.65 | 0.50 |
| 31:BA:1245:G:OP1 | 41:BP:16:ARG:HD2 | 2.11 | 0.50 |
| 31:BA:1592:C:C2' | 31:BA:1593:G:C5' | 2.75 | 0.50 |
| 31:BA:1886:C:O5' | 31:BA:1886:C:H6 | 1.94 | 0.50 |
| 31:BA:17:G:H2' | 31:BA:18:C:C6 | 2.46 | 0.50 |
| 31:BA:2723:C:H5'' | 43:BR:2:ARG:CD | 2.38 | 0.50 |
| 31:BA:352:G:O2' | 31:BA:353:G:H3' | 2.11 | 0.50 |
| 24:B2:49:LYS:HE2 | 31:BA:76:C:OP1 | 2.12 | 0.50 |
| 25:B3:11:SER:HB3 | 31:BA:988:A:P | 2.52 | 0.50 |
| 33:BD:125:ILE:HG13 | 33:BD:137:PRO:CD | 2.41 | 0.50 |
| 34:BE:160:TYR:CD2 | 34:BE:161:GLY:N | 2.79 | 0.50 |
| 34:BE:63:LEU:O | 34:BE:64:LYS:C | 2.50 | 0.50 |
| 38:BI:1:MET:CG | 38:BI:23:PRO:HA | 2.35 | 0.50 |
| 39:BN:34:LEU:O | 39:BN:49:GLY:HA3 | 2.11 | 0.50 |
| 31:BA:833:U:H5'' | 41:BP:48:PRO:HB3 | 1.93 | 0.50 |
| 30:B8:25:MET:HG3 | 41:BP:64:LYS:HB2 | 1.93 | 0.50 |
| 43:BR:12:ARG:HG3 | 43:BR:12:ARG:HH11 | 1.76 | 0.50 |
| 44:BS:16:ASN:C | 44:BS:20:ARG:HH21 | 2.15 | 0.50 |
| 45:BT:28:VAL:HB | 45:BT:88:ILE:HG13 | 1.94 | 0.50 |
| 45:BT:34:VAL:O | 45:BT:35:LYS:HB3 | 2.10 | 0.50 |
| 47:BV:18:LEU:O | 47:BV:19:LYS:HB2 | 2.11 | 0.50 |
| 47:BV:72:VAL:CA | 47:BV:88:ARG:HH12 | 2.15 | 0.50 |
| 24:B2:26:ARG:CG | 49:BX:5:TYR:HB3 | 2.41 | 0.50 |
| 1:CA:1206:G:C6 | 1:CA:1207:G:C6 | 2.99 | 0.50 |
| 1:CA:1429:C:H2' | 1:CA:1430:C:H6 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:353:A:C5' | 1:CA:353:A:C8 | 2.88 | 0.50 |
| 1:CA:411:A:C6 | 1:CA:429:U:C4 | 2.99 | 0.50 |
| 1:CA:41:G:H2' | 1:CA:42:G:C8 | 2.46 | 0.50 |
| 1:CA:750:G:C2 | 1:CA:751:U:C6 | 3.00 | 0.50 |
| 1:CA:977:A:H8 | 1:CA:1223:C:N3 | 2.10 | 0.50 |
| 2:CB:106:LYS:HG2 | 2:CB:106:LYS:O | 2.11 | 0.50 |
| 1:CA:1189:C:O3' | 3:CC:5:ILE:HD12 | 2.10 | 0.50 |
| 1:CA:710:G:H5'' | 6:CF:54:LYS:HE3 | 1.94 | 0.50 |
| 6:CF:91:VAL:HG12 | 6:CF:92:LYS:N | 2.27 | 0.50 |
| 8:CH:6:ILE:H | 8:CH:6:ILE:CD1 | 2.22 | 0.50 |
| 11:CK:15:ALA:HA | 11:CK:77:MET:HA | 1.93 | 0.50 |
| 24:D2:57:ILE:HG23 | 24:D2:57:ILE:O | 2.11 | 0.50 |
| 27:D5:29:THR:HG21 | 31:DA:2815:C:H5' | 1.93 | 0.50 |
| 30:D8:50:LEU:HD12 | 30:D8:51:ALA:N | 2.26 | 0.50 |
| 31:DA:1005:C:C2 | 31:DA:1143:A:C5 | 2.99 | 0.50 |
| 31:DA:1446:C:O2 | 31:DA:1447:G:C8 | 2.64 | 0.50 |
| 31:DA:1593:G:H5' | 31:DA:1593:G:H8 | 1.76 | 0.50 |
| 31:DA:2192:G:O2' | 31:DA:2193:G:H5' | 2.11 | 0.50 |
| 31:DA:2846:G:H2' | 31:DA:2847:U:O4' | 2.11 | 0.50 |
| 31:DA:570:G:H2' | 31:DA:2030:A:C5 | 2.46 | 0.50 |
| 31:DA:631:A:OP1 | 41:DP:64:LYS:CE | 2.59 | 0.50 |
| 33:DD:13:ARG:HD2 | 33:DD:16:MET:CE | 2.41 | 0.50 |
| 33:DD:35:LYS:HE2 | 33:DD:104:TYR:CB | 2.36 | 0.50 |
| 35:DF:119:ARG:HG2 | 35:DF:119:ARG:O | 2.12 | 0.50 |
| 35:DF:203:GLN:HA | 35:DF:206:ILE:O | 2.11 | 0.50 |
| 31:DA:1140:C:OP1 | 39:DN:23:LEU:O | 2.29 | 0.50 |
| 41:DP:47:ASP:CB | 41:DP:48:PRO:O | 2.51 | 0.50 |
| 50:DY:45:VAL:CG2 | 50:DY:62:GLU:N | 2.74 | 0.50 |
| 1:AA:131:C:H2' | 1:AA:132:C:H6 | 1.77 | 0.50 |
| 1:AA:373:A:C2 | 1:AA:374:A:C8 | 3.00 | 0.50 |
| 1:AA:738:C:C2 | 1:AA:739:C:C5 | 2.99 | 0.50 |
| 11:AK:124:LYS:HB3 | 11:AK:125:PHE:HD1 | 1.75 | 0.50 |
| 14:AN:24:CYS:HB3 | 14:AN:27:CYS:O | 2.12 | 0.50 |
| 16:AP:36:ILE:HG13 | 16:AP:36:ILE:O | 2.11 | 0.50 |
| 1:AA:192:U:H4' | 20:AT:103:GLY:HA2 | 1.93 | 0.50 |
| 23:B1:10:LYS:HB2 | 23:B1:14:VAL:CA | 2.41 | 0.50 |
| 24:B2:40:SER:OG | 24:B2:41:ILE:N | 2.44 | 0.50 |
| 25:B3:45:GLY:O | 25:B3:48:GLU:HB2 | 2.12 | 0.50 |
| 31:BA:1332:G:H8 | 31:BA:1332:G:H5' | 1.74 | 0.50 |
| 31:BA:1563:G:H2' | 31:BA:1564:C:H6 | 1.76 | 0.50 |
| 31:BA:1593:G:H5' | 31:BA:1593:G:C8 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:1902:C:H2' | 31:BA:1903:G:O5' | 2.12 | 0.50 |
| 31:BA:2001:A:H2' | 31:BA:2002:G:C8 | 2.46 | 0.50 |
| 31:BA:2664:G:C2' | 31:BA:2665:A:O5' | 2.60 | 0.50 |
| 31:BA:363(B):G:N3 | 31:BA:363(B):G:H2' | 2.26 | 0.50 |
| 31:BA:414:C:H2' | 31:BA:415:A:C8 | 2.46 | 0.50 |
| 31:BA:706:A:H2' | 31:BA:707:G:O4' | 2.12 | 0.50 |
| 34:BE:3:GLY:O | 34:BE:4:ILE:HB | 2.12 | 0.50 |
| 34:BE:61:ARG:N | 34:BE:62:PRO:CD | 2.75 | 0.50 |
| 32:BB:42:C:O4' | 36:BG:69:ALA:HB2 | 2.12 | 0.50 |
| 44:BS:39:ILE:O | 44:BS:48:LEU:HD12 | 2.12 | 0.50 |
| 50:BY:14:LEU:HD11 | 50:BY:22:GLY:HA2 | 1.93 | 0.50 |
| 51:BZ:146:ILE:HA | 51:BZ:174:VAL:HG12 | 1.93 | 0.50 |
| 1:CA:509:A:O2' | 1:CA:510:A:O5' | 2.29 | 0.50 |
| 1:CA:668:G:O2' | 1:CA:669:U:H5' | 2.11 | 0.50 |
| 1:CA:682:G:C6 | 1:CA:683:G:N7 | 2.80 | 0.50 |
| 1:CA:73:G:N1 | 1:CA:97:G:C6 | 2.80 | 0.50 |
| 2:CB:12:GLU:HA | 2:CB:16:HIS:HB2 | 1.93 | 0.50 |
| 1:CA:532:A:N6 | 3:CC:193:TYR:HB3 | 2.17 | 0.50 |
| 1:CA:1205:U:O2' | 3:CC:195:VAL:HG23 | 2.12 | 0.50 |
| 3:CC:34:LEU:HD23 | 3:CC:34:LEU:O | 2.12 | 0.50 |
| 5:CE:75:THR:HG23 | 5:CE:76:ILE:N | 2.26 | 0.50 |
| 6:CF:12:PRO:HB2 | 6:CF:57:GLN:HB2 | 1.93 | 0.50 |
| 8:CH:123:GLU:O | 8:CH:127:LEU:HB2 | 2.11 | 0.50 |
| 17:CQ:74:LEU:HD12 | 17:CQ:75:ARG:HG2 | 1.94 | 0.50 |
| 23:D1:46:LEU:H | 23:D1:46:LEU:CD1 | 2.03 | 0.50 |
| 23:D1:90:ILE:O | 23:D1:94:LEU:HB2 | 2.11 | 0.50 |
| 24:D2:34:GLU:OE2 | 24:D2:34:GLU:N | 2.44 | 0.50 |
| 24:D2:44:LEU:O | 24:D2:44:LEU:HD12 | 2.12 | 0.50 |
| 24:D2:46:GLN:NE2 | 24:D2:47:ASN:CA | 2.74 | 0.50 |
| 24:D2:47:ASN:HD22 | 24:D2:47:ASN:N | 2.09 | 0.50 |
| 24:D2:53:LEU:CA | 24:D2:56:GLN:HE22 | 2.23 | 0.50 |
| 31:DA:1165:U:O2' | 31:DA:1166:C:H5' | 2.10 | 0.50 |
| 31:DA:1300:U:H2' | 31:DA:1626:G:C2 | 2.46 | 0.50 |
| 31:DA:1628:G:H2' | 31:DA:1629:U:C6 | 2.47 | 0.50 |
| 31:DA:1932:A:C2 | 31:DA:1969:A:C2 | 3.00 | 0.50 |
| 31:DA:2471:C:C4 | 31:DA:2472:G:C5 | 2.99 | 0.50 |
| 31:DA:2537:U:H2' | 31:DA:2538:C:H6 | 1.76 | 0.50 |
| 31:DA:1783:A:C2 | 31:DA:2587:A:C4 | 2.99 | 0.50 |
| 31:DA:2762:G:C8 | 31:DA:2762:G:C5' | 2.94 | 0.50 |
| 31:DA:442:G:O4' | 35:DF:46:ARG:HD3 | 2.12 | 0.50 |
| 32:DB:21:G:O2' | 32:DB:22:U:OP2 | 2.30 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DE:28:ALA:HB3 | 34:DE:93:VAL:HG22 | 1.92 | 0.50 |
| 35:DF:205:ARG:O | 35:DF:206:ILE:HG13 | 2.12 | 0.50 |
| 36:DG:133:LEU:C | 36:DG:133:LEU:HD12 | 2.32 | 0.50 |
| 38:DI:10:GLU:O | 38:DI:12:LEU:HD23 | 2.10 | 0.50 |
| 39:DN:30:ILE:HG22 | 39:DN:34:LEU:CD2 | 2.42 | 0.50 |
| 45:DT:58:ASN:C | 45:DT:58:ASN:HD22 | 2.14 | 0.50 |
| 51:DZ:165:VAL:HG12 | 51:DZ:166:SER:HG | 1.76 | 0.50 |
| 1:AA:1236:A:O2' | 1:AA:1304:G:H4' | 2.11 | 0.50 |
| 1:AA:624:C:H2' | 1:AA:625:G:C8 | 2.46 | 0.50 |
| 4:AD:194:LEU:N | 4:AD:194:LEU:HD22 | 2.26 | 0.50 |
| 5:AE:34:VAL:O | 5:AE:41:VAL:HA | 2.12 | 0.50 |
| 7:AG:75:VAL:CG2 | 7:AG:144:MET:HB3 | 2.42 | 0.50 |
| 8:AH:54:ASP:O | 8:AH:56:LYS:HG3 | 2.10 | 0.50 |
| 8:AH:82:HIS:CD2 | 8:AH:138:TRP:NE1 | 2.80 | 0.50 |
| 11:AK:21:ILE:HB | 11:AK:84:VAL:HG12 | 1.94 | 0.50 |
| 11:AK:65:ALA:HB3 | 11:AK:97:ALA:HB3 | 1.93 | 0.50 |
| 12:AL:22:SER:C | 12:AL:24:VAL:H | 2.15 | 0.50 |
| 13:AM:24:GLY:C | 13:AM:25:ILE:HD12 | 2.32 | 0.50 |
| 13:AM:71:ARG:O | 13:AM:71:ARG:HG3 | 2.12 | 0.50 |
| 23:B1:11:ARG:HG3 | 23:B1:61:ARG:O | 2.11 | 0.50 |
| 24:B2:35:LEU:HD23 | 24:B2:35:LEU:H | 1.76 | 0.50 |
| 31:BA:1210:A:H5'' | 31:BA:1212:G:O4' | 2.11 | 0.50 |
| 31:BA:1719:G:H2' | 31:BA:1720:U:C5' | 2.42 | 0.50 |
| 31:BA:1742:G:C8 | 31:BA:1742:G:H3' | 2.46 | 0.50 |
| 31:BA:1970:A:C5' | 31:BA:1972:A:H1' | 2.37 | 0.50 |
| 31:BA:2092:U:C5 | 31:BA:2226:C:OP2 | 2.64 | 0.50 |
| 32:BB:49:C:H2' | 32:BB:50:G:C8 | 2.47 | 0.50 |
| 32:BB:94:C:H2' | 32:BB:95:C:H6 | 1.77 | 0.50 |
| 36:BG:121:ASN:OD1 | 36:BG:123:ASN:HB2 | 2.11 | 0.50 |
| 36:BG:33:ARG:HB2 | 36:BG:162:THR:OG1 | 2.12 | 0.50 |
| 37:BH:43:VAL:O | 37:BH:43:VAL:CG2 | 2.55 | 0.50 |
| 39:BN:133:GLN:HG2 | 39:BN:135:PRO:HD3 | 1.93 | 0.50 |
| 39:BN:87:LEU:HD22 | 39:BN:91:LEU:HD11 | 1.94 | 0.50 |
| 49:BX:31:HIS:HD2 | 49:BX:33:LYS:N | 2.09 | 0.50 |
| 1:CA:1053:G:C3' | 1:CA:1054:C:H5' | 2.42 | 0.50 |
| 1:CA:1441:G:H5'' | 1:CA:1442:G:C5' | 2.42 | 0.50 |
| 1:CA:229:U:O2' | 1:CA:230:G:H5' | 2.10 | 0.50 |
| 1:CA:654:G:C2 | 1:CA:753:A:C4 | 3.00 | 0.50 |
| 1:CA:658:G:H2' | 1:CA:659:U:H6 | 1.75 | 0.50 |
| 13:CM:24:GLY:C | 13:CM:25:ILE:HD12 | 2.31 | 0.50 |
| 16:CP:20:VAL:HG23 | 16:CP:35:LYS:HA | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:CS:63:THR:O | 19:CS:66:MET:HG2 | 2.11 | 0.50 |
| 23:D1:89:GLU:O | 23:D1:90:ILE:C | 2.50 | 0.50 |
| 24:D2:26:ARG:O | 24:D2:30:ARG:HD3 | 2.11 | 0.50 |
| 25:D3:13:ILE:N | 25:D3:13:ILE:HD13 | 2.26 | 0.50 |
| 28:D6:14:THR:O | 28:D6:49:HIS:HA | 2.12 | 0.50 |
| 29:D7:35:ARG:HG3 | 29:D7:42:LEU:HD11 | 1.94 | 0.50 |
| 31:DA:1109:C:H5 | 31:DA:1110:G:C8 | 2.29 | 0.50 |
| 31:DA:1839:G:H8 | 31:DA:1839:G:C5' | 2.25 | 0.50 |
| 31:DA:1858:G:O2' | 31:DA:1884:A:N6 | 2.44 | 0.50 |
| 31:DA:2400:G:N3 | 31:DA:2400:G:H2' | 2.26 | 0.50 |
| 31:DA:543:C:N3 | 31:DA:551:G:N1 | 2.60 | 0.50 |
| 31:DA:854:G:H2' | 31:DA:855:G:H8 | 1.76 | 0.50 |
| 34:DE:201:THR:CG2 | 34:DE:202:LYS:N | 2.71 | 0.50 |
| 34:DE:82:ARG:HG3 | 34:DE:83:ASP:N | 2.27 | 0.50 |
| 37:DH:85:LYS:CD | 37:DH:133:VAL:HB | 2.41 | 0.50 |
| 39:DN:95:PRO:C | 39:DN:97:ARG:N | 2.65 | 0.50 |
| 31:DA:1278:A:O2' | 43:DR:34:ILE:HD11 | 2.12 | 0.50 |
| 51:DZ:108:PRO:HA | 51:DZ:142:SER:HA | 1.93 | 0.50 |
| 1:AA:1006:C:H42 | 1:AA:1024:G:H21 | 1.60 | 0.50 |
| 1:AA:119:A:H4' | 1:AA:120:A:O5' | 2.11 | 0.50 |
| 1:AA:166:G:C4 | 1:AA:167:G:C8 | 3.00 | 0.50 |
| 1:AA:189(B):C:O2' | 1:AA:189(C):C:H5' | 2.11 | 0.50 |
| 1:AA:299:G:C6 | 1:AA:300:A:N1 | 2.80 | 0.50 |
| 3:AC:94:LEU:HD12 | 3:AC:95:THR:N | 2.26 | 0.50 |
| 4:AD:160:GLN:HA | 4:AD:163:GLU:HB2 | 1.93 | 0.50 |
| 5:AE:31:LEU:HD22 | 5:AE:43:LEU:HD11 | 1.94 | 0.50 |
| 1:AA:363:A:C5 | 12:AL:31:PRO:HD2 | 2.47 | 0.50 |
| 22:B0:72:ARG:HH21 | 22:B0:75:LEU:HD12 | 1.77 | 0.50 |
| 30:B8:60:LEU:HB3 | 30:B8:63:PRO:HG2 | 1.93 | 0.50 |
| 31:BA:1142(A):A:C4 | 31:BA:1144:G:C8 | 3.00 | 0.50 |
| 31:BA:118:A:C8 | 31:BA:119:A:C8 | 3.00 | 0.50 |
| 31:BA:175:G:H8 | 31:BA:175:G:C5' | 2.24 | 0.50 |
| 31:BA:213:A:H2' | 31:BA:214:G:O4' | 2.12 | 0.50 |
| 31:BA:2192:G:O2' | 31:BA:2193:G:H5' | 2.11 | 0.50 |
| 31:BA:271(G):C:O2 | 31:BA:271(G):C:H2' | 2.11 | 0.50 |
| 31:BA:271(P):C:O2' | 31:BA:271(Q):G:H5' | 2.12 | 0.50 |
| 31:BA:671:C:H2' | 31:BA:672:C:C6 | 2.47 | 0.50 |
| 33:BD:266:SER:O | 33:BD:267:SER:OG | 2.26 | 0.50 |
| 36:BG:120:LEU:O | 36:BG:122:PRO:HD3 | 2.10 | 0.50 |
| 36:BG:152:LEU:O | 36:BG:153:ARG:HB2 | 2.12 | 0.50 |
| 39:BN:40:PRO:C | 46:BU:64:ARG:NH2 | 2.65 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BP:48:PRO:O | 41:BP:49:ARG:C | 2.50 | 0.50 |
| 41:BP:84:ASN:HA | 41:BP:115:LEU:O | 2.12 | 0.50 |
| 42:BQ:133:ARG:O | 42:BQ:134:ARG:HB2 | 2.11 | 0.50 |
| 46:BU:87:GLY:CA | 47:BV:52:VAL:HG13 | 2.32 | 0.50 |
| 50:BY:86:ARG:HG2 | 50:BY:87:LYS:N | 2.25 | 0.50 |
| 1:CA:1409:C:N4 | 1:CA:1491:G:H1 | 2.09 | 0.50 |
| 1:CA:310:G:C5' | 16:CP:31:LYS:HB2 | 2.41 | 0.50 |
| 1:CA:682:G:N1 | 1:CA:683:G:C5 | 2.80 | 0.50 |
| 4:CD:108:LEU:O | 4:CD:110:PHE:HD1 | 1.93 | 0.50 |
| 9:CI:83:ARG:O | 9:CI:86:VAL:HG12 | 2.11 | 0.50 |
| 11:CK:65:ALA:HB3 | 11:CK:97:ALA:HB3 | 1.92 | 0.50 |
| 16:CP:4:ILE:HG13 | 16:CP:21:VAL:CG1 | 2.30 | 0.50 |
| 22:D0:40:GLN:NE2 | 22:D0:43:THR:HA | 2.26 | 0.50 |
| 23:D1:85:LEU:HB3 | 23:D1:87:PRO:HD3 | 1.92 | 0.50 |
| 30:D8:35:GLN:CG | 31:DA:2420:C:OP1 | 2.60 | 0.50 |
| 31:DA:1353:A:H5'' | 33:DD:38:LYS:HZ1 | 1.77 | 0.50 |
| 31:DA:1449:A:H5'' | 31:DA:1449:A:H8 | 1.77 | 0.50 |
| 31:DA:1527:G:C5' | 31:DA:1528:A:OP1 | 2.60 | 0.50 |
| 31:DA:2694:G:C6 | 31:DA:2695:C:C4 | 3.00 | 0.50 |
| 31:DA:2740:A:C6 | 31:DA:2764:A:C8 | 3.00 | 0.50 |
| 31:DA:2821:A:H2' | 31:DA:2822:G:C8 | 2.46 | 0.50 |
| 31:DA:2850:A:C2 | 31:DA:2851:A:C4 | 3.00 | 0.50 |
| 31:DA:693:C:H2' | 31:DA:694:U:H6 | 1.77 | 0.50 |
| 31:DA:876:C:C4 | 31:DA:877:U:C5 | 2.99 | 0.50 |
| 31:DA:892:G:N3 | 31:DA:892:G:H3' | 2.26 | 0.50 |
| 33:DD:224:ALA:O | 33:DD:225:ALA:HB2 | 2.11 | 0.50 |
| 31:DA:2580:U:C4' | 34:DE:131:ALA:H | 2.24 | 0.50 |
| 40:DO:13:ASN:HD21 | 40:DO:97:ARG:N | 2.08 | 0.50 |
| 44:DS:28:VAL:HB | 44:DS:89:ARG:CB | 2.40 | 0.50 |
| 49:DX:21:PHE:HB3 | 49:DX:90:GLU:HG3 | 1.94 | 0.50 |
| 1:AA:1064:G:O5' | 1:AA:1064:G:H8 | 1.95 | 0.50 |
| 1:AA:1125:U:H2' | 1:AA:1126:U:OP2 | 2.10 | 0.50 |
| 1:AA:977:A:H8 | 1:AA:1223:C:N3 | 2.09 | 0.50 |
| 1:AA:41:G:H2' | 1:AA:42:G:H8 | 1.77 | 0.50 |
| 1:AA:657:G:N2 | 1:AA:750:G:C8 | 2.80 | 0.50 |
| 14:AN:40:CYS:SG | 14:AN:42:ILE:HG12 | 2.52 | 0.50 |
| 17:AQ:33:GLY:O | 17:AQ:34:LYS:O | 2.30 | 0.50 |
| 1:AA:277:C:P | 17:AQ:68:ARG:HH12 | 2.35 | 0.50 |
| 23:B1:53:VAL:HG21 | 23:B1:74:VAL:HG21 | 1.93 | 0.50 |
| 23:B1:85:LEU:HB3 | 23:B1:87:PRO:HD3 | 1.94 | 0.50 |
| 31:BA:2233:U:H2' | 31:BA:2234:G:C8 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:BA:485:C:O2' | 31:BA:486:C:H5' | 2.12 | 0.50 |
| 22:B0:27:GLU:HB3 | 31:BA:856:C:H1' | 1.93 | 0.50 |
| 33:BD:69:ARG:NH2 | 33:BD:128:GLY:O | 2.40 | 0.50 |
| 34:BE:70:ALA:O | 34:BE:72:VAL:N | 2.45 | 0.50 |
| 35:BF:203:GLN:HA | 35:BF:206:ILE:O | 2.12 | 0.50 |
| 38:BI:78:THR:O | 38:BI:79:ILE:HD13 | 2.12 | 0.50 |
| 39:BN:102:ALA:O | 39:BN:106:MET:HG3 | 2.12 | 0.50 |
| 31:BA:832:G:OP1 | 41:BP:40:SER:HB3 | 2.11 | 0.50 |
| 46:BU:8:VAL:HG11 | 46:BU:12:ARG:CZ | 2.42 | 0.50 |
| 47:BV:2:PHE:CE1 | 47:BV:13:ARG:CZ | 2.93 | 0.50 |
| 46:BU:104:GLN:HB2 | 47:BV:43:GLU:OE1 | 2.12 | 0.50 |
| 49:BX:34:ALA:O | 49:BX:35:THR:C | 2.51 | 0.50 |
| 49:BX:37:THR:HG23 | 49:BX:54:VAL:HB | 1.93 | 0.50 |
| 1:CA:1058:G:C6 | 1:CA:1059:C:N3 | 2.80 | 0.50 |
| 1:CA:355:C:C2 | 1:CA:356:A:C8 | 2.99 | 0.50 |
| 1:CA:382:A:C2 | 1:CA:383:A:C4 | 2.99 | 0.50 |
| 1:CA:39:G:C6 | 1:CA:40:C:C5 | 3.00 | 0.50 |
| 2:CB:98:LEU:HB2 | 2:CB:101:MET:CE | 2.42 | 0.50 |
| 6:CF:24:GLU:HG2 | 6:CF:28:ARG:CZ | 2.42 | 0.50 |
| 6:CF:8:ILE:HG22 | 6:CF:9:VAL:H | 1.77 | 0.50 |
| 9:CI:16:ARG:O | 9:CI:63:ILE:HA | 2.12 | 0.50 |
| 1:CA:1372:U:OP1 | 9:CI:72:GLY:N | 2.44 | 0.50 |
| 13:CM:94:ARG:HG2 | 19:CS:82:GLY:N | 2.26 | 0.50 |
| 16:CP:22:THR:HG23 | 16:CP:32:TYR:HA | 1.94 | 0.50 |
| 19:CS:36:ARG:HD2 | 19:CS:52:TYR:O | 2.12 | 0.50 |
| 1:CA:191:G:H1' | 20:CT:105:SER:HA | 1.92 | 0.50 |
| 23:D1:67:ILE:HD12 | 23:D1:68:PRO:HD2 | 1.93 | 0.50 |
| 27:D5:57:VAL:CB | 27:D5:58:LEU:HD12 | 2.41 | 0.50 |
| 31:DA:1173:G:H3' | 31:DA:1174:A:H5' | 1.93 | 0.50 |
| 31:DA:1717:G:C2 | 31:DA:1718:G:C8 | 3.00 | 0.50 |
| 31:DA:1887:C:C2' | 31:DA:1888:G:H5' | 2.42 | 0.50 |
| 31:DA:2494:G:C5 | 31:DA:2495:G:N7 | 2.80 | 0.50 |
| 31:DA:2680:C:H5' | 34:DE:189:PRO:HA | 1.94 | 0.50 |
| 31:DA:683:C:O5' | 31:DA:683:C:H6 | 1.95 | 0.50 |
| 38:DI:1:MET:CG | 38:DI:23:PRO:HA | 2.33 | 0.50 |
| 40:DO:9:GLU:O | 40:DO:83:ALA:HA | 2.11 | 0.50 |
| 41:DP:32:THR:O | 41:DP:36:LYS:HB2 | 2.12 | 0.50 |
| 30:D8:25:MET:HG3 | 41:DP:64:LYS:HB2 | 1.92 | 0.50 |
| 1:AA:1203:C:OP1 | 14:AN:3:ARG:HD3 | 2.12 | 0.50 |
| 1:AA:1206:G:C6 | 1:AA:1207:G:C6 | 3.00 | 0.50 |
| 1:AA:414:A:H2' | 1:AA:415:A:H8 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:561:U:O2' | 1:AA:562:C:OP2 | 2.22 | 0.50 |
| 1:AA:609:A:C2' | 1:AA:610:G:H5' | 2.42 | 0.50 |
| 5:AE:36:ASP:O | 5:AE:37:ARG:CB | 2.60 | 0.50 |
| 2:AB:178:ARG:NH2 | 8:AH:68:ARG:HH22 | 2.09 | 0.50 |
| 13:AM:97:PRO:HB2 | 13:AM:101:GLN:NE2 | 2.27 | 0.50 |
| 16:AP:20:VAL:HG23 | 16:AP:35:LYS:HA | 1.93 | 0.50 |
| 19:AS:36:ARG:HD2 | 19:AS:52:TYR:O | 2.11 | 0.50 |
| 24:B2:45:SER:HA | 24:B2:47:ASN:HD21 | 1.76 | 0.50 |
| 31:BA:1050:A:C2 | 31:BA:2751:G:C5 | 3.00 | 0.50 |
| 31:BA:1131:G:H4' | 39:BN:82:LEU:HG | 1.94 | 0.50 |
| 31:BA:2020:A:C2' | 31:BA:2021:C:H5' | 2.41 | 0.50 |
| 31:BA:2019:A:H2' | 31:BA:2020:A:O5' | 2.12 | 0.50 |
| 22:B0:56:ASP:OD1 | 31:BA:2364:C:H5' | 2.12 | 0.50 |
| 31:BA:2518:A:C8 | 31:BA:2518:A:H5' | 2.47 | 0.50 |
| 31:BA:2637:U:O2' | 31:BA:2638:G:H5' | 2.12 | 0.50 |
| 31:BA:271(P):C:C2' | 31:BA:271(Q):G:H5' | 2.41 | 0.50 |
| 31:BA:2728:U:O2' | 31:BA:2729:G:H5' | 2.12 | 0.50 |
| 31:BA:2820:A:H2' | 31:BA:2820:A:N3 | 2.27 | 0.50 |
| 31:BA:2849:U:H5' | 31:BA:2867:G:H21 | 1.77 | 0.50 |
| 31:BA:68:G:H2' | 31:BA:69:C:C6 | 2.47 | 0.50 |
| 31:BA:922:U:H2' | 31:BA:923:C:C6 | 2.46 | 0.50 |
| 39:BN:23:LEU:O | 39:BN:23:LEU:HD23 | 2.12 | 0.50 |
| 41:BP:71:VAL:HG13 | 41:BP:72:PRO:HD3 | 1.92 | 0.50 |
| 44:BS:93:LYS:O | 44:BS:93:LYS:HE3 | 2.12 | 0.50 |
| 45:BT:31:SER:HA | 45:BT:32:TYR:CE2 | 2.47 | 0.50 |
| 45:BT:50:ILE:CD1 | 45:BT:64:ARG:HB3 | 2.42 | 0.50 |
| 47:BV:19:LYS:HE2 | 47:BV:20:LEU:H | 1.77 | 0.50 |
| 1:CA:1142:G:H3' | 1:CA:1143:G:H8 | 1.77 | 0.50 |
| 1:CA:1242:C:H5' | 21:CU:10:ARG:NH1 | 2.27 | 0.50 |
| 1:CA:1478:C:H2' | 1:CA:1479:C:C6 | 2.46 | 0.50 |
| 1:CA:450:G:OP1 | 1:CA:452:A:OP1 | 2.30 | 0.50 |
| 1:CA:93:G:C2' | 1:CA:96:U:H5' | 2.42 | 0.50 |
| 4:CD:92:VAL:O | 4:CD:96:LEU:HD23 | 2.12 | 0.50 |
| 7:CG:22:LEU:HG | 7:CG:62:PHE:HE2 | 1.77 | 0.50 |
| 10:CJ:30:SER:HG | 10:CJ:81:THR:HG22 | 1.76 | 0.50 |
| 15:CO:56:LEU:O | 15:CO:60:VAL:HG23 | 2.12 | 0.50 |
| 18:CR:19:LYS:O | 18:CR:20:ALA:HB2 | 2.11 | 0.50 |
| 23:D1:14:VAL:O | 23:D1:46:LEU:CD2 | 2.58 | 0.50 |
| 31:DA:1161:C:H1' | 47:DV:8:GLY:O | 2.12 | 0.50 |
| 31:DA:1269:A:H2' | 31:DA:1270:C:C6 | 2.46 | 0.50 |
| 31:DA:142:A:H8 | 31:DA:1408:C:H1' | 1.72 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:1688:U:H5' | 31:DA:1689:A:OP1 | 2.12 | 0.50 |
| 31:DA:203:C:H3' | 31:DA:204:A:H5'' | 1.94 | 0.50 |
| 28:D6:23:THR:HG21 | 31:DA:2419:U:H4' | 1.94 | 0.50 |
| 31:DA:2646:C:OP2 | 31:DA:2732:G:O2' | 2.21 | 0.50 |
| 31:DA:2664:G:C2' | 31:DA:2665:A:O5' | 2.60 | 0.50 |
| 31:DA:340:A:H2' | 31:DA:341:G:C5' | 2.41 | 0.50 |
| 31:DA:357:A:C2 | 31:DA:358:U:O2 | 2.65 | 0.50 |
| 31:DA:435:C:C5 | 31:DA:436:C:C5 | 3.00 | 0.50 |
| 31:DA:61:G:H1 | 31:DA:94:C:H42 | 1.58 | 0.50 |
| 31:DA:966:G:C6 | 31:DA:967:C:N4 | 2.80 | 0.50 |
| 32:DB:8:U:H5' | 32:DB:9:G:OP2 | 2.11 | 0.50 |
| 32:DB:93:G:H2' | 32:DB:94:C:C6 | 2.46 | 0.50 |
| 32:DB:93:G:H2' | 32:DB:94:C:H6 | 1.76 | 0.50 |
| 34:DE:179:GLU:O | 34:DE:180:ASN:HB2 | 2.12 | 0.50 |
| 34:DE:27:LEU:HD12 | 34:DE:181:LEU:HD13 | 1.94 | 0.50 |
| 34:DE:75:VAL:C | 34:DE:77:ILE:N | 2.65 | 0.50 |
| 34:DE:48:GLN:CG | 34:DE:78:LEU:HB3 | 2.41 | 0.50 |
| 36:DG:29:TRP:C | 36:DG:31:VAL:H | 2.15 | 0.50 |
| 38:DI:131:LYS:HG2 | 38:DI:132:PRO:HA | 1.92 | 0.50 |
| 42:DQ:16:ARG:CG | 42:DQ:17:LEU:N | 2.75 | 0.50 |
| 43:DR:71:GLN:HE21 | 43:DR:71:GLN:CA | 2.19 | 0.50 |
| 46:DU:101:ARG:O | 46:DU:102:GLU:C | 2.50 | 0.50 |
| 49:DX:44:GLU:HB2 | 49:DX:49:VAL:O | 2.12 | 0.50 |
| 50:DY:45:VAL:CG1 | 50:DY:46:LYS:H | 2.25 | 0.50 |
| 1:AA:1135:U:H4' | 1:AA:1136:U:H5 | 1.76 | 0.49 |
| 1:AA:1442(A):G:C3' | 1:AA:1442(B):A:C5' | 2.87 | 0.49 |
| 1:AA:343:U:O2' | 1:AA:346:G:O6 | 2.24 | 0.49 |
| 1:AA:1189:C:O3' | 3:AC:5:ILE:HD12 | 2.12 | 0.49 |
| 4:AD:172:PRO:O | 4:AD:187:ARG:NH1 | 2.43 | 0.49 |
| 15:AO:87:ILE:HG22 | 15:AO:88:ARG:HG3 | 1.94 | 0.49 |
| 24:B2:53:LEU:CA | 24:B2:56:GLN:HE22 | 2.24 | 0.49 |
| 30:B8:32:LEU:CG | 30:B8:35:GLN:H | 2.24 | 0.49 |
| 31:BA:1331:A:HO2' | 31:BA:1332:G:H8 | 1.60 | 0.49 |
| 31:BA:1357:U:H2' | 31:BA:1358:G:O4' | 2.12 | 0.49 |
| 31:BA:154:G:H2' | 31:BA:154(A):C:O2 | 2.11 | 0.49 |
| 31:BA:1884:A:N1 | 31:BA:1885:A:C5 | 2.80 | 0.49 |
| 31:BA:2756:U:H1' | 31:BA:2757:A:H5'' | 1.94 | 0.49 |
| 31:BA:643:A:H2' | 31:BA:644:A:O5' | 2.12 | 0.49 |
| 31:BA:716:A:H2' | 31:BA:717:G:O5' | 2.12 | 0.49 |
| 31:BA:754:C:H2' | 31:BA:755:C:C6 | 2.47 | 0.49 |
| 31:BA:84:A:H5'' | 50:BY:9:LYS:HD3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 31:BA:876:C:C2 | 31:BA:877:U:C6 | 2.99 | 0.49 |
| 33:BD:231:HIS:ND1 | 33:BD:232:PRO:HD2 | 2.27 | 0.49 |
| 38:BI:98:ALA:HA | 38:BI:109:ILE:CD1 | 2.42 | 0.49 |
| 41:BP:52:GLU:C | 41:BP:54:GLY:H | 2.15 | 0.49 |
| 41:BP:55:ARG:O | 41:BP:56:SER:OG | 2.21 | 0.49 |
| 42:BQ:23:GLY:O | 42:BQ:99:PRO:O | 2.30 | 0.49 |
| 44:BS:34:HIS:CE1 | 44:BS:54:LEU:CB | 2.89 | 0.49 |
| 44:BS:97:ARG:HG3 | 44:BS:97:ARG:O | 2.12 | 0.49 |
| 48:BW:70:TYR:O | 48:BW:107:LEU:HD12 | 2.12 | 0.49 |
| 1:CA:376:G:H2' | 1:CA:377:G:H8 | 1.77 | 0.49 |
| 1:CA:62:U:O2' | 1:CA:379:C:H1' | 2.12 | 0.49 |
| 1:CA:79:G:H4' | 1:CA:80:G:OP1 | 2.11 | 0.49 |
| 2:CB:44:LEU:HD12 | 2:CB:44:LEU:N | 2.24 | 0.49 |
| 3:CC:125:GLU:OE2 | 3:CC:189:ALA:HA | 2.12 | 0.49 |
| 4:CD:50:ARG:HD2 | 4:CD:51:PRO:O | 2.12 | 0.49 |
| 4:CD:3:ARG:HD3 | 4:CD:5:ILE:HG13 | 1.94 | 0.49 |
| 9:CI:79:LEU:HD11 | 9:CI:83:ARG:NH2 | 2.27 | 0.49 |
| 10:CJ:16:LEU:O | 10:CJ:16:LEU:HD13 | 2.12 | 0.49 |
| 1:CA:948:C:OP1 | 13:CM:107:ALA:HA | 2.11 | 0.49 |
| 23:D1:87:PRO:O | 23:D1:91:LYS:N | 2.28 | 0.49 |
| 28:D6:10:LEU:N | 28:D6:10:LEU:CD2 | 2.74 | 0.49 |
| 30:D8:47:LYS:HD2 | 30:D8:48:PHE:O | 2.11 | 0.49 |
| 31:DA:1168:G:C2' | 31:DA:1169:G:H5' | 2.42 | 0.49 |
| 31:DA:1804:C:H2' | 31:DA:1805:U:H6 | 1.77 | 0.49 |
| 31:DA:2503:A:C8 | 55:DA:3330:ERY:H293 | 2.47 | 0.49 |
| 31:DA:2660:A:C5' | 31:DA:2661:G:N2 | 2.72 | 0.49 |
| 31:DA:2712:U:O2' | 31:DA:2712(A):A:OP2 | 2.27 | 0.49 |
| 31:DA:601:C:O2 | 31:DA:605:C:H4' | 2.12 | 0.49 |
| 31:DA:607:U:C2 | 31:DA:621:A:N1 | 2.80 | 0.49 |
| 31:DA:866:A:C6 | 31:DA:914:C:C5 | 3.00 | 0.49 |
| 34:DE:103:ASP:OD2 | 34:DE:168:MET:HE1 | 2.12 | 0.49 |
| 41:DP:144:GLU:N | 41:DP:145:PRO:CD | 2.75 | 0.49 |
| 31:DA:389:G:H22 | 41:DP:72:PRO:HD3 | 1.77 | 0.49 |
| 44:DS:35:ILE:HG22 | 44:DS:53:SER:HB2 | 1.93 | 0.49 |
| 44:DS:98:VAL:CG1 | 44:DS:100:ALA:H | 2.24 | 0.49 |
| 49:DX:18:TYR:O | 49:DX:19:ALA:C | 2.50 | 0.49 |
| 49:DX:25:LYS:CG | 49:DX:26:TYR:N | 2.55 | 0.49 |
| 31:DA:143:G:H1' | 49:DX:38:GLU:HG3 | 1.93 | 0.49 |
| 51:DZ:156:LYS:O | 51:DZ:158:PRO:HD3 | 2.12 | 0.49 |
| 51:DZ:54:HIS:HE1 | 51:DZ:123:ASP:CG | 2.14 | 0.49 |
| 1:AA:1228:C:P | 13:AM:108:ARG:HH22 | 2.35 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:195:A:C5 | 1:AA:196:A:N1 | 2.80 | 0.49 |
| 1:AA:343:U:H2' | 1:AA:346:G:O6 | 2.12 | 0.49 |
| 1:AA:688:G:H2' | 1:AA:689:C:C6 | 2.47 | 0.49 |
| 1:AA:814:A:N7 | 1:AA:816:A:C5 | 2.80 | 0.49 |
| 1:AA:872:A:C2 | 1:AA:874:G:C6 | 3.00 | 0.49 |
| 2:AB:116:GLU:HA | 2:AB:119:GLU:HB2 | 1.93 | 0.49 |
| 2:AB:42:ILE:HD11 | 2:AB:202:PRO:HB2 | 1.93 | 0.49 |
| 5:AE:103:GLY:C | 5:AE:106:PRO:HD2 | 2.32 | 0.49 |
| 6:AF:63:TYR:N | 6:AF:63:TYR:CD2 | 2.80 | 0.49 |
| 6:AF:78:GLU:O | 6:AF:81:ILE:HG13 | 2.11 | 0.49 |
| 9:AI:11:LYS:HG2 | 9:AI:11:LYS:O | 2.12 | 0.49 |
| 17:AQ:99:SER:C | 17:AQ:100:LYS:HD3 | 2.32 | 0.49 |
| 20:AT:63:ILE:HD13 | 20:AT:80:ARG:HB2 | 1.93 | 0.49 |
| 23:B1:73:LEU:HD13 | 23:B1:90:ILE:HG22 | 1.93 | 0.49 |
| 24:B2:23:LYS:HB2 | 49:BX:5:TYR:CE1 | 2.47 | 0.49 |
| 31:BA:1106:A:H2' | 31:BA:1107:G:O5' | 2.10 | 0.49 |
| 31:BA:53:A:H61 | 31:BA:117:G:C2' | 2.25 | 0.49 |
| 31:BA:1859:A:C6 | 31:BA:1884:A:C8 | 2.99 | 0.49 |
| 31:BA:530:G:C5 | 31:BA:2022:U:H5'' | 2.48 | 0.49 |
| 31:BA:2880:C:O2' | 43:BR:90:ARG:HD3 | 2.12 | 0.49 |
| 31:BA:877:U:O2' | 31:BA:878:A:H5'' | 2.11 | 0.49 |
| 33:BD:25:THR:CG2 | 33:BD:82:ILE:N | 2.75 | 0.49 |
| 37:BH:137:ASP:HB3 | 37:BH:140:LYS:H | 1.77 | 0.49 |
| 37:BH:149:ARG:O | 37:BH:152:ARG:O | 2.30 | 0.49 |
| 39:BN:25:ARG:CG | 39:BN:25:ARG:HH11 | 2.22 | 0.49 |
| 41:BP:108:LYS:C | 41:BP:110:TYR:N | 2.66 | 0.49 |
| 31:BA:2820:A:H1' | 43:BR:5:LYS:HZ3 | 1.78 | 0.49 |
| 49:BX:21:PHE:CE1 | 49:BX:26:TYR:CG | 3.00 | 0.49 |
| 50:BY:8:LYS:HE3 | 50:BY:72:VAL:HG23 | 1.94 | 0.49 |
| 51:BZ:92:SER:O | 51:BZ:130:PRO:HG2 | 2.12 | 0.49 |
| 1:CA:1202:G:H2' | 1:CA:1203:C:O4' | 2.12 | 0.49 |
| 1:CA:119:A:H4' | 1:CA:120:A:O5' | 2.12 | 0.49 |
| 1:CA:1404:C:H2' | 1:CA:1405:G:C8 | 2.48 | 0.49 |
| 7:CG:73:MET:HG2 | 7:CG:90:GLU:HA | 1.94 | 0.49 |
| 10:CJ:90:LEU:N | 10:CJ:91:PRO:HD3 | 2.28 | 0.49 |
| 10:CJ:96:ILE:HD13 | 10:CJ:96:ILE:N | 2.27 | 0.49 |
| 12:CL:32:PHE:CE1 | 12:CL:86:ARG:HG3 | 2.45 | 0.49 |
| 12:CL:41:ARG:HG2 | 12:CL:42:THR:H | 1.77 | 0.49 |
| 18:CR:25:THR:CG2 | 18:CR:42:ARG:HH11 | 2.25 | 0.49 |
| 20:CT:97:ALA:O | 20:CT:99:LEU:HG | 2.13 | 0.49 |
| 23:D1:33:LYS:HZ1 | 23:D1:35:THR:HG21 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 24:D2:37:PHE:CD2 | 24:D2:37:PHE:O | 2.65 | 0.49 |
| 24:D2:53:LEU:C | 24:D2:56:GLN:HE22 | 2.15 | 0.49 |
| 31:DA:565:C:H4' | 31:DA:1253:A:C6 | 2.47 | 0.49 |
| 31:DA:1952:A:C6 | 31:DA:1953:A:C6 | 3.00 | 0.49 |
| 31:DA:2075:U:H2' | 31:DA:2238:G:N2 | 2.27 | 0.49 |
| 31:DA:491:G:O2' | 31:DA:492:A:H5' | 2.12 | 0.49 |
| 32:DB:20:C:O2' | 32:DB:21:G:H5'' | 2.12 | 0.49 |
| 34:DE:96:PHE:HA | 34:DE:100:GLU:OE1 | 2.12 | 0.49 |
| 31:DA:252:G:P | 41:DP:50:ARG:HH11 | 2.35 | 0.49 |
| 45:DT:40:THR:O | 45:DT:41:ARG:CB | 2.60 | 0.49 |
| 45:DT:4:GLY:O | 45:DT:7:ILE:HB | 2.11 | 0.49 |
| 47:DV:43:GLU:N | 47:DV:48:GLY:HA2 | 2.26 | 0.49 |
| 31:DA:106:C:H1' | 50:DY:2:ARG:NE | 2.27 | 0.49 |
| 50:DY:39:VAL:O | 50:DY:40:GLU:CD | 2.51 | 0.49 |
| 1:AA:352:C:O2' | 1:AA:354:G:OP1 | 2.25 | 0.49 |
| 1:AA:688:G:H2' | 1:AA:689:C:H6 | 1.77 | 0.49 |
| 4:AD:79:PHE:HZ | 4:AD:204:ILE:HD13 | 1.77 | 0.49 |
| 5:AE:72:GLN:O | 5:AE:75:THR:HG22 | 2.11 | 0.49 |
| 7:AG:66:VAL:O | 7:AG:70:LYS:HG3 | 2.12 | 0.49 |
| 7:AG:85:TYR:HD1 | 7:AG:154:TYR:HE1 | 1.60 | 0.49 |
| 12:AL:38:THR:CG2 | 12:AL:57:LYS:HB2 | 2.42 | 0.49 |
| 3:AC:18:TRP:HD1 | 14:AN:51:GLY:O | 1.95 | 0.49 |
| 20:AT:56:MET:HG3 | 20:AT:88:VAL:HG21 | 1.93 | 0.49 |
| 27:B5:11:THR:HG23 | 31:BA:1263:U:O2' | 2.12 | 0.49 |
| 31:BA:1300:U:H2' | 31:BA:1626:G:C2 | 2.47 | 0.49 |
| 31:BA:2196:C:O2' | 31:BA:2197:U:H5' | 2.12 | 0.49 |
| 31:BA:2282:G:OP1 | 31:BA:2283:C:H1' | 2.13 | 0.49 |
| 31:BA:2287:A:C4 | 31:BA:2289:G:C8 | 2.99 | 0.49 |
| 31:BA:2663:G:C5 | 31:BA:2664:G:C5 | 3.00 | 0.49 |
| 31:BA:2689:U:C4' | 31:BA:2690:C:H5' | 2.42 | 0.49 |
| 31:BA:271(L):U:H5'' | 31:BA:271(M):G:C4 | 2.46 | 0.49 |
| 31:BA:2864:G:H2' | 31:BA:2865:U:O4' | 2.11 | 0.49 |
| 31:BA:2869:G:H2' | 31:BA:2870:C:O4' | 2.12 | 0.49 |
| 31:BA:428:A:H8 | 31:BA:428:A:OP2 | 1.95 | 0.49 |
| 31:BA:966:G:H2' | 31:BA:967:C:H6 | 1.76 | 0.49 |
| 33:BD:30:GLU:HG3 | 33:BD:63:ARG:NH2 | 2.27 | 0.49 |
| 34:BE:111:ARG:HG3 | 43:BR:2:ARG:HG3 | 1.93 | 0.49 |
| 41:BP:81:GLN:NE2 | 41:BP:106:LEU:HA | 2.27 | 0.49 |
| 45:BT:48:ILE:HG22 | 45:BT:50:ILE:HD12 | 1.92 | 0.49 |
| 1:CA:102:G:C6 | 1:CA:103:C:C4 | 3.01 | 0.49 |
| 1:CA:1423:G:H2' | 1:CA:1424:C:H6 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:116:A:H61 | 1:CA:313:A:H1' | 1.78 | 0.49 |
| 1:CA:791:G:C5 | 1:CA:792:A:N7 | 2.81 | 0.49 |
| 2:CB:17:PHE:O | 2:CB:18:GLY:O | 2.30 | 0.49 |
| 2:CB:185:ILE:HA | 2:CB:199:TYR:O | 2.12 | 0.49 |
| 5:CE:101:ILE:HD11 | 5:CE:119:LEU:HA | 1.93 | 0.49 |
| 12:CL:86:ARG:HB2 | 12:CL:101:VAL:CG2 | 2.42 | 0.49 |
| 13:CM:14:ARG:NH1 | 13:CM:42:ALA:HA | 2.27 | 0.49 |
| 17:CQ:65:ILE:H | 17:CQ:65:ILE:HD12 | 1.77 | 0.49 |
| 24:D2:51:ARG:O | 24:D2:52:ASP:HB2 | 2.11 | 0.49 |
| 31:DA:1317:A:H2' | 31:DA:1318:C:C6 | 2.46 | 0.49 |
| 31:DA:2018:G:H2' | 31:DA:2019:A:C8 | 2.48 | 0.49 |
| 31:DA:2196:C:O2' | 31:DA:2197:U:H5' | 2.12 | 0.49 |
| 31:DA:485:C:O2' | 31:DA:486:C:H5' | 2.12 | 0.49 |
| 32:DB:102:A:H8 | 32:DB:102:A:OP2 | 1.95 | 0.49 |
| 33:DD:36:PRO:HA | 33:DD:62:TYR:O | 2.12 | 0.49 |
| 35:DF:24:LEU:CB | 35:DF:25:PRO:HD2 | 2.29 | 0.49 |
| 43:DR:10:LEU:HB3 | 43:DR:17:ARG:CD | 2.41 | 0.49 |
| 45:DT:51:ARG:HG2 | 45:DT:52:ILE:N | 2.26 | 0.49 |
| 31:DA:446:G:OP1 | 46:DU:3:ARG:NH1 | 2.45 | 0.49 |
| 47:DV:83:ARG:O | 47:DV:84:LYS:HD2 | 2.12 | 0.49 |
| 48:DW:64:MET:O | 48:DW:65:LEU:CB | 2.50 | 0.49 |
| 24:D2:26:ARG:CG | 49:DX:5:TYR:HB3 | 2.40 | 0.49 |
| 49:DX:65:ARG:NH2 | 49:DX:66:LEU:H | 2.10 | 0.49 |
| 50:DY:9:LYS:HA | 50:DY:30:VAL:HG21 | 1.95 | 0.49 |
| 51:DZ:146:ILE:HA | 51:DZ:174:VAL:HG12 | 1.93 | 0.49 |
| 1:AA:229:U:O2' | 1:AA:230:G:H5' | 2.12 | 0.49 |
| 1:AA:336:C:O2' | 1:AA:337:C:H5' | 2.13 | 0.49 |
| 1:AA:365:U:H5'' | 1:AA:366:C:OP1 | 2.12 | 0.49 |
| 1:AA:577:G:C8 | 1:AA:816:A:C6 | 3.01 | 0.49 |
| 8:AH:20:TYR:HD1 | 8:AH:65:TYR:CD2 | 2.30 | 0.49 |
| 1:AA:1316:G:H1 | 19:AS:5:LEU:HD21 | 1.78 | 0.49 |
| 20:AT:89:ARG:HD2 | 20:AT:104:LEU:HD21 | 1.93 | 0.49 |
| 30:B8:32:LEU:CA | 30:B8:34:TRP:H | 2.25 | 0.49 |
| 30:B8:34:TRP:HD1 | 31:BA:2391:G:OP1 | 1.95 | 0.49 |
| 30:B8:53:PRO:HA | 30:B8:56:GLU:HB2 | 1.94 | 0.49 |
| 31:BA:1027:A:N6 | 31:BA:1126:A:C4 | 2.81 | 0.49 |
| 31:BA:142:A:H8 | 31:BA:1408:C:H1' | 1.71 | 0.49 |
| 31:BA:1417:C:H2' | 31:BA:1418:G:H5' | 1.94 | 0.49 |
| 31:BA:1494:A:N3 | 31:BA:1494:A:H2' | 2.28 | 0.49 |
| 31:BA:1495:A:H2' | 31:BA:1496:A:N3 | 2.27 | 0.49 |
| 31:BA:1578:U:OP2 | 31:BA:1578:U:H6 | 1.96 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1836:C:C2' | 31:BA:1837:C:H5' | 2.42 | 0.49 |
| 31:BA:1836:C:H2' | 31:BA:1837:C:H6 | 1.76 | 0.49 |
| 31:BA:1893:C:C6 | 31:BA:1894:C:C5 | 3.00 | 0.49 |
| 32:BB:30:C:H2' | 32:BB:31:C:H5' | 1.95 | 0.49 |
| 36:BG:11:TYR:HD2 | 36:BG:12:TYR:CD1 | 2.31 | 0.49 |
| 36:BG:55:LYS:O | 36:BG:59:GLU:HB2 | 2.12 | 0.49 |
| 38:BI:73:GLU:O | 38:BI:73:GLU:HG3 | 2.12 | 0.49 |
| 42:BQ:38:GLU:OE2 | 42:BQ:127:ILE:HG22 | 2.12 | 0.49 |
| 44:BS:89:ARG:O | 44:BS:90:GLY:O | 2.30 | 0.49 |
| 31:BA:1227:G:OP1 | 46:BU:13:LYS:HG2 | 2.12 | 0.49 |
| 31:BA:993:G:N3 | 47:BV:91:TYR:CE1 | 2.80 | 0.49 |
| 50:BY:8:LYS:H | 50:BY:28:LYS:NZ | 2.09 | 0.49 |
| 1:CA:1030(A):G:H1' | 1:CA:1031:G:N2 | 2.16 | 0.49 |
| 1:CA:1158:C:H2' | 1:CA:1158:C:O2 | 2.10 | 0.49 |
| 1:CA:1228:C:P | 13:CM:108:ARG:HH22 | 2.35 | 0.49 |
| 1:CA:409:G:C2' | 1:CA:410:G:H5' | 2.38 | 0.49 |
| 1:CA:538:G:OP2 | 12:CL:115:LYS:HG3 | 2.12 | 0.49 |
| 1:CA:939:G:H5'' | 7:CG:102:ARG:NH2 | 2.28 | 0.49 |
| 4:CD:108:LEU:HB3 | 4:CD:110:PHE:CD1 | 2.46 | 0.49 |
| 5:CE:103:GLY:O | 5:CE:106:PRO:HD2 | 2.13 | 0.49 |
| 5:CE:13:ILE:HG13 | 5:CE:29:GLY:O | 2.12 | 0.49 |
| 9:CI:28:VAL:HG22 | 9:CI:63:ILE:HB | 1.94 | 0.49 |
| 13:CM:3:ARG:HG2 | 13:CM:9:ILE:CG1 | 2.42 | 0.49 |
| 6:CF:96:PRO:HB3 | 18:CR:30:ASP:OD2 | 2.13 | 0.49 |
| 24:D2:40:SER:OG | 24:D2:41:ILE:N | 2.45 | 0.49 |
| 26:D4:11:PRO:C | 26:D4:13:ARG:H | 2.16 | 0.49 |
| 27:D5:36:CYS:HG | 27:D5:49:CYS:HG | 0.50 | 0.49 |
| 31:DA:1495:A:C2 | 31:DA:1496:A:C2 | 3.00 | 0.49 |
| 31:DA:1719:G:H2' | 31:DA:1720:U:C5' | 2.42 | 0.49 |
| 31:DA:1884:A:N1 | 31:DA:1885:A:C5 | 2.80 | 0.49 |
| 31:DA:2469:A:C5 | 31:DA:2470:G:H1' | 2.48 | 0.49 |
| 31:DA:2544:G:H1' | 31:DA:2646:C:H4' | 1.92 | 0.49 |
| 31:DA:26:G:C6 | 31:DA:27:G:N1 | 2.81 | 0.49 |
| 31:DA:27:G:O2' | 31:DA:28:A:OP2 | 2.27 | 0.49 |
| 31:DA:515:A:H1' | 31:DA:581:C:H1' | 1.93 | 0.49 |
| 33:DD:77:ALA:HB2 | 33:DD:97:TYR:CG | 2.46 | 0.49 |
| 34:DE:111:ARG:HG3 | 43:DR:2:ARG:HG3 | 1.95 | 0.49 |
| 35:DF:2:LYS:O | 35:DF:25:PRO:HG2 | 2.13 | 0.49 |
| 40:DO:10:VAL:HG22 | 40:DO:17:ARG:O | 2.13 | 0.49 |
| 41:DP:14:LYS:O | 41:DP:15:ARG:CB | 2.59 | 0.49 |
| 43:DR:41:ALA:O | 43:DR:44:LEU:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:DS:57:LYS:CG | 44:DS:58:LEU:H | 2.26 | 0.49 |
| 50:DY:42:VAL:CG2 | 50:DY:67:LEU:HD13 | 2.43 | 0.49 |
| 50:DY:8:LYS:HE3 | 50:DY:72:VAL:HG23 | 1.93 | 0.49 |
| 51:DZ:118:GLN:O | 51:DZ:120:ILE:N | 2.44 | 0.49 |
| 51:DZ:16:SER:HA | 51:DZ:19:ARG:HD2 | 1.93 | 0.49 |
| 51:DZ:151:HIS:HA | 51:DZ:171:ILE:HD13 | 1.93 | 0.49 |
| 1:AA:1128:C:H1' | 1:AA:1146:A:H61 | 1.76 | 0.49 |
| 1:AA:1365:G:C5 | 1:AA:1366:C:C5 | 3.01 | 0.49 |
| 1:AA:147:G:N2 | 1:AA:148:G:H1' | 2.27 | 0.49 |
| 1:AA:189(B):C:N4 | 1:AA:189(J):G:C6 | 2.81 | 0.49 |
| 1:AA:605:U:H2' | 1:AA:606:G:C8 | 2.48 | 0.49 |
| 1:AA:69:G:N3 | 1:AA:70:G:C8 | 2.81 | 0.49 |
| 2:AB:106:LYS:HG2 | 2:AB:106:LYS:O | 2.13 | 0.49 |
| 2:AB:185:ILE:HA | 2:AB:199:TYR:O | 2.11 | 0.49 |
| 2:AB:44:LEU:HD12 | 2:AB:44:LEU:N | 2.22 | 0.49 |
| 3:AC:188:LEU:O | 3:AC:189:ALA:CB | 2.60 | 0.49 |
| 3:AC:125:GLU:OE2 | 3:AC:189:ALA:HA | 2.12 | 0.49 |
| 8:AH:109:ILE:HG12 | 8:AH:110:ALA:N | 2.27 | 0.49 |
| 9:AI:28:VAL:HG22 | 9:AI:63:ILE:HB | 1.95 | 0.49 |
| 20:AT:97:ALA:O | 20:AT:99:LEU:HG | 2.11 | 0.49 |
| 24:B2:12:GLU:C | 24:B2:12:GLU:CD | 2.72 | 0.49 |
| 31:BA:1185:C:H5'' | 31:BA:1186:G:OP1 | 2.13 | 0.49 |
| 31:BA:1654:A:H2' | 31:BA:1655:A:H8 | 1.77 | 0.49 |
| 31:BA:1802:A:N1 | 31:BA:1822:G:H1' | 2.28 | 0.49 |
| 31:BA:2223:G:H2' | 31:BA:2224:G:C5' | 2.41 | 0.49 |
| 32:BB:20:C:O2' | 32:BB:21:G:H5'' | 2.13 | 0.49 |
| 34:BE:66:HIS:CG | 34:BE:66:HIS:O | 2.64 | 0.49 |
| 35:BF:132:VAL:CG2 | 35:BF:133:ASN:N | 2.76 | 0.49 |
| 36:BG:165:THR:OG1 | 36:BG:168:GLU:HG3 | 2.12 | 0.49 |
| 31:BA:910:A:N7 | 42:BQ:13:GLN:HB2 | 2.27 | 0.49 |
| 44:BS:16:ASN:O | 44:BS:20:ARG:NH2 | 2.46 | 0.49 |
| 44:BS:98:VAL:HG12 | 44:BS:100:ALA:H | 1.78 | 0.49 |
| 49:BX:25:LYS:CG | 49:BX:26:TYR:N | 2.57 | 0.49 |
| 49:BX:60:ARG:CZ | 49:BX:74:PRO:HG2 | 2.42 | 0.49 |
| 50:BY:71:LYS:CB | 50:BY:71:LYS:NZ | 2.70 | 0.49 |
| 1:CA:1160:G:H5' | 2:CB:132:LYS:HE3 | 1.95 | 0.49 |
| 1:CA:200:G:H1 | 1:CA:217:C:N4 | 2.02 | 0.49 |
| 1:CA:38:G:N1 | 1:CA:397:A:C2 | 2.79 | 0.49 |
| 3:CC:108:ASN:ND2 | 3:CC:111:LEU:HD12 | 2.26 | 0.49 |
| 3:CC:29:TYR:OH | 14:CN:54:PRO:HD2 | 2.13 | 0.49 |
| 20:CT:89:ARG:HD2 | 20:CT:104:LEU:HD21 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BP:141:ALA:HB3 | 25:D3:1:MET:HE1 | 1.94 | 0.49 |
| 31:DA:1015:G:C2' | 31:DA:1016:G:H5' | 2.43 | 0.49 |
| 31:DA:1510:G:H2' | 31:DA:1511:C:H5' | 1.93 | 0.49 |
| 31:DA:2563:U:O2 | 31:DA:2565:A:H8 | 1.95 | 0.49 |
| 31:DA:2700:C:O2' | 31:DA:2701:C:H5' | 2.12 | 0.49 |
| 31:DA:2753:A:HO2' | 31:DA:2754:U:H6 | 1.58 | 0.49 |
| 31:DA:2869:G:H2' | 31:DA:2870:C:O4' | 2.12 | 0.49 |
| 31:DA:352:G:O2' | 31:DA:353:G:H3' | 2.12 | 0.49 |
| 31:DA:362:U:H6 | 31:DA:362:U:H3' | 1.77 | 0.49 |
| 31:DA:717:G:H2' | 31:DA:718:A:O4' | 2.12 | 0.49 |
| 31:DA:743:G:H2' | 31:DA:744:G:H5' | 1.94 | 0.49 |
| 31:DA:866:A:C6 | 31:DA:914:C:C6 | 3.00 | 0.49 |
| 32:DB:30:C:H2' | 32:DB:31:C:H5' | 1.93 | 0.49 |
| 34:DE:51:PHE:HB3 | 34:DE:76:ARG:HB3 | 1.94 | 0.49 |
| 36:DG:11:TYR:HD2 | 36:DG:12:TYR:CD1 | 2.30 | 0.49 |
| 38:DI:69:LYS:HG2 | 38:DI:69:LYS:O | 2.13 | 0.49 |
| 39:DN:17:ASP:O | 39:DN:17:ASP:CG | 2.49 | 0.49 |
| 40:DO:90:GLN:O | 40:DO:91:LEU:HB2 | 2.12 | 0.49 |
| 41:DP:96:THR:HG22 | 41:DP:126:VAL:CG2 | 2.42 | 0.49 |
| 43:DR:10:LEU:HB3 | 43:DR:17:ARG:CZ | 2.41 | 0.49 |
| 45:DT:28:VAL:HG11 | 45:DT:46:GLU:OE1 | 2.12 | 0.49 |
| 48:DW:9:TYR:N | 48:DW:102:HIS:CD2 | 2.72 | 0.49 |
| 1:AA:1053:G:N7 | 1:AA:1200:C:H5' | 2.28 | 0.49 |
| 1:AA:427:U:C4 | 1:AA:428:G:C6 | 3.01 | 0.49 |
| 1:AA:586:C:C2' | 1:AA:587:G:H5' | 2.42 | 0.49 |
| 5:AE:12:LEU:HD22 | 5:AE:12:LEU:C | 2.32 | 0.49 |
| 10:AJ:51:ARG:HE | 10:AJ:61:GLU:CB | 2.21 | 0.49 |
| 15:AO:36:ILE:HG22 | 15:AO:37:ASN:HD22 | 1.77 | 0.49 |
| 24:B2:29:LYS:O | 24:B2:33:MET:SD | 2.70 | 0.49 |
| 31:BA:1359:A:H2' | 31:BA:1360:A:H5' | 1.93 | 0.49 |
| 31:BA:1425:G:H2' | 31:BA:1426:G:O4' | 2.13 | 0.49 |
| 31:BA:1945:G:H2' | 31:BA:1946:U:H6 | 1.76 | 0.49 |
| 31:BA:2557:G:H2' | 31:BA:2558:C:C6 | 2.48 | 0.49 |
| 31:BA:309:G:O3' | 50:BY:18:GLY:CA | 2.60 | 0.49 |
| 31:BA:477:A:H2' | 31:BA:478:A:C8 | 2.47 | 0.49 |
| 31:BA:810:U:O2' | 41:BP:33:ARG:CZ | 2.60 | 0.49 |
| 31:BA:892:G:H2' | 31:BA:893:C:O4' | 2.13 | 0.49 |
| 34:BE:201:THR:HG22 | 34:BE:202:LYS:H | 1.73 | 0.49 |
| 35:BF:70:THR:HG22 | 35:BF:72:ARG:H | 1.76 | 0.49 |
| 44:BS:98:VAL:CG1 | 44:BS:100:ALA:H | 2.26 | 0.49 |
| 46:BU:91:ASP:OD2 | 46:BU:96:ALA:N | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:BZ:27:VAL:HG13 | 51:BZ:29:TYR:HD2 | 1.77 | 0.49 |
| 1:CA:136:C:H42 | 1:CA:227:G:H1 | 1.60 | 0.49 |
| 1:CA:69:G:N3 | 1:CA:70:G:C8 | 2.81 | 0.49 |
| 5:CE:72:GLN:O | 5:CE:75:THR:HG22 | 2.12 | 0.49 |
| 6:CF:86:ARG:O | 6:CF:87:ARG:HG2 | 2.13 | 0.49 |
| 1:CA:963:G:H21 | 10:CJ:55:LYS:HD3 | 1.76 | 0.49 |
| 12:CL:119:LYS:O | 12:CL:120:TYR:HB2 | 2.12 | 0.49 |
| 12:CL:55:VAL:HG13 | 12:CL:68:ALA:O | 2.13 | 0.49 |
| 1:CA:177:C:OP1 | 20:CT:65:LYS:HD3 | 2.12 | 0.49 |
| 23:D1:10:LYS:CG | 23:D1:11:ARG:H | 2.25 | 0.49 |
| 30:D8:51:ALA:N | 30:D8:53:PRO:HD2 | 2.27 | 0.49 |
| 31:DA:1130:U:O2 | 31:DA:2025:C:H5'' | 2.13 | 0.49 |
| 31:DA:1505:C:C2' | 31:DA:1506:C:O5' | 2.61 | 0.49 |
| 31:DA:1827:C:C2' | 31:DA:1828:G:H5' | 2.42 | 0.49 |
| 31:DA:2660:A:H5'' | 31:DA:2661:G:H21 | 1.77 | 0.49 |
| 31:DA:271(F):C:C2 | 31:DA:271(G):C:C6 | 3.00 | 0.49 |
| 31:DA:2774:C:H2' | 31:DA:2775:A:O4' | 2.13 | 0.49 |
| 31:DA:300:A:H2' | 31:DA:334:C:H1' | 1.95 | 0.49 |
| 31:DA:358:U:C6 | 31:DA:358:U:H3' | 2.46 | 0.49 |
| 31:DA:373:U:H2' | 31:DA:374:A:H8 | 1.78 | 0.49 |
| 31:DA:804:A:H5'' | 31:DA:805:G:OP1 | 2.13 | 0.49 |
| 34:DE:48:GLN:HE22 | 34:DE:64:LYS:HE2 | 1.78 | 0.49 |
| 35:DF:132:VAL:CG2 | 35:DF:133:ASN:N | 2.75 | 0.49 |
| 36:DG:173:LEU:HB3 | 36:DG:178:PHE:CG | 2.47 | 0.49 |
| 36:DG:61:ALA:HA | 36:DG:64:THR:CG2 | 2.41 | 0.49 |
| 37:DH:93:GLY:O | 37:DH:95:ARG:HG2 | 2.12 | 0.49 |
| 40:DO:69:ILE:O | 40:DO:76:ALA:HA | 2.13 | 0.49 |
| 42:DQ:85:LYS:HG3 | 42:DQ:86:GLY:N | 2.28 | 0.49 |
| 44:DS:98:VAL:HG12 | 44:DS:100:ALA:H | 1.77 | 0.49 |
| 31:DA:814:C:H5'' | 47:DV:86:GLY:HA3 | 1.93 | 0.49 |
| 48:DW:29:LEU:O | 48:DW:33:ARG:HD2 | 2.13 | 0.49 |
| 50:DY:81:LYS:HD3 | 50:DY:97:ARG:HG3 | 1.93 | 0.49 |
| 51:DZ:128:VAL:HG21 | 51:DZ:161:VAL:HG22 | 1.94 | 0.49 |
| 1:AA:1329:A:N7 | 21:AU:7:ARG:NH2 | 2.56 | 0.49 |
| 1:AA:159:G:O2' | 1:AA:160:A:C8 | 2.60 | 0.49 |
| 1:AA:356:A:H1' | 1:AA:368:U:O2' | 2.13 | 0.49 |
| 1:AA:425:G:O2' | 1:AA:426:G:H5' | 2.13 | 0.49 |
| 1:AA:448:A:C2 | 1:AA:449:C:C4 | 3.00 | 0.49 |
| 1:AA:542:G:C2 | 1:AA:543:C:C5 | 3.01 | 0.49 |
| 1:AA:560:U:H5' | 1:AA:566:G:N2 | 2.27 | 0.49 |
| 1:AA:682:G:N1 | 1:AA:683:G:C5 | 2.81 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:963:G:H1 | 1:AA:972:C:H42 | 1.60 | 0.49 |
| 2:AB:21:ARG:CB | 2:AB:39:ILE:HA | 2.43 | 0.49 |
| 4:AD:61:LYS:NZ | 4:AD:62:GLN:NE2 | 2.61 | 0.49 |
| 10:AJ:8:LEU:HG | 10:AJ:96:ILE:HG22 | 1.94 | 0.49 |
| 10:AJ:90:LEU:N | 10:AJ:91:PRO:HD3 | 2.27 | 0.49 |
| 12:AL:32:PHE:CE1 | 12:AL:86:ARG:HG3 | 2.46 | 0.49 |
| 14:AN:22:THR:HB | 14:AN:33:VAL:HG11 | 1.95 | 0.49 |
| 31:BA:142:A:H1' | 31:BA:1408:C:O4' | 2.12 | 0.49 |
| 31:BA:1688:U:H5' | 31:BA:1689:A:OP1 | 2.13 | 0.49 |
| 31:BA:1827:C:C2' | 31:BA:1828:G:H5' | 2.43 | 0.49 |
| 31:BA:2498:C:O2' | 31:BA:2499:C:H5' | 2.13 | 0.49 |
| 31:BA:2658:C:C3' | 31:BA:2659:G:H5'' | 2.41 | 0.49 |
| 31:BA:966:G:C4 | 31:BA:967:C:C5 | 3.01 | 0.49 |
| 32:BB:71:C:O2 | 32:BB:71:C:H2' | 2.11 | 0.49 |
| 33:BD:43:ARG:NH1 | 33:BD:44:ASN:ND2 | 2.60 | 0.49 |
| 34:BE:39:PRO:HA | 34:BE:43:GLY:CA | 2.42 | 0.49 |
| 35:BF:65:TRP:CZ3 | 35:BF:72:ARG:HB3 | 2.48 | 0.49 |
| 36:BG:114:ILE:O | 36:BG:116:ASP:N | 2.45 | 0.49 |
| 36:BG:29:TRP:C | 36:BG:31:VAL:N | 2.66 | 0.49 |
| 37:BH:85:LYS:CE | 37:BH:145:ALA:HB2 | 2.42 | 0.49 |
| 37:BH:93:GLY:O | 37:BH:95:ARG:HG2 | 2.13 | 0.49 |
| 39:BN:131:GLN:CD | 39:BN:134:ARG:HB3 | 2.33 | 0.49 |
| 43:BR:18:LEU:O | 43:BR:19:ALA:C | 2.49 | 0.49 |
| 45:BT:58:ASN:C | 45:BT:58:ASN:HD22 | 2.16 | 0.49 |
| 47:BV:36:PRO:CD | 47:BV:60:GLU:O | 2.61 | 0.49 |
| 49:BX:30:VAL:HG23 | 49:BX:76:ARG:HA | 1.94 | 0.49 |
| 51:BZ:28:MET:CE | 51:BZ:59:LEU:HD12 | 2.42 | 0.49 |
| 1:CA:1133:G:N3 | 1:CA:1142:G:N2 | 2.60 | 0.49 |
| 1:CA:1203:C:OP1 | 14:CN:3:ARG:HD3 | 2.13 | 0.49 |
| 1:CA:189(K):U:H2' | 1:CA:189(L):G:C8 | 2.47 | 0.49 |
| 1:CA:674:G:H2' | 1:CA:675:A:H8 | 1.77 | 0.49 |
| 1:CA:930:C:O2' | 1:CA:931:C:H5' | 2.12 | 0.49 |
| 1:CA:932:C:H4' | 7:CG:4:ARG:NH2 | 2.28 | 0.49 |
| 2:CB:74:LYS:C | 2:CB:78:GLN:HG3 | 2.33 | 0.49 |
| 3:CC:94:LEU:HD12 | 3:CC:95:THR:N | 2.28 | 0.49 |
| 9:CI:79:LEU:HD11 | 9:CI:83:ARG:CZ | 2.42 | 0.49 |
| 11:CK:124:LYS:HB3 | 11:CK:125:PHE:HD1 | 1.77 | 0.49 |
| 12:CL:27:LEU:HD11 | 12:CL:64:TYR:CE1 | 2.47 | 0.49 |
| 12:CL:82:VAL:CG1 | 12:CL:83:VAL:N | 2.76 | 0.49 |
| 16:CP:74:LEU:O | 16:CP:79:VAL:HB | 2.12 | 0.49 |
| 24:D2:37:PHE:CE2 | 24:D2:39:ALA:O | 2.66 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 31:DA:1309:G:H2' | 31:DA:1310:G:H5' | 1.93 | 0.49 |
| 31:DA:1445(A):C:H2' | 31:DA:1446:C:H6 | 1.78 | 0.49 |
| 31:DA:2031:A:OP1 | 31:DA:2031:A:O4' | 2.31 | 0.49 |
| 31:DA:2518:A:H5' | 31:DA:2518:A:H8 | 1.77 | 0.49 |
| 31:DA:2722:G:H2' | 31:DA:2723:C:C6 | 2.47 | 0.49 |
| 31:DA:292:C:O2' | 31:DA:293:U:H5' | 2.12 | 0.49 |
| 31:DA:363(A):A:C2 | 31:DA:363(B):G:C8 | 3.01 | 0.49 |
| 31:DA:910:A:C8 | 42:DQ:13:GLN:HB2 | 2.48 | 0.49 |
| 32:DB:2:C:H2' | 32:DB:3:C:C6 | 2.48 | 0.49 |
| 32:DB:45:A:H2' | 32:DB:46:A:H5' | 1.95 | 0.49 |
| 33:DD:17:THR:CG2 | 33:DD:205:VAL:N | 2.62 | 0.49 |
| 36:DG:165:THR:OG1 | 36:DG:168:GLU:HG3 | 2.13 | 0.49 |
| 31:DA:557:U:O2 | 39:DN:45:ASN:HB2 | 2.13 | 0.49 |
| 39:DN:98:VAL:HG23 | 39:DN:99:LEU:H | 1.77 | 0.49 |
| 40:DO:16:ALA:HB2 | 40:DO:52:VAL:HG11 | 1.95 | 0.49 |
| 44:DS:74:ALA:HB1 | 44:DS:103:GLU:HB2 | 1.94 | 0.49 |
| 44:DS:16:ASN:C | 44:DS:20:ARG:HH21 | 2.15 | 0.49 |
| 46:DU:14:HIS:O | 46:DU:15:LYS:C | 2.51 | 0.49 |
| 50:DY:28:LYS:HD2 | 50:DY:37:VAL:CG1 | 2.43 | 0.49 |
| 51:DZ:14:LYS:HB2 | 51:DZ:17:ALA:CB | 2.42 | 0.49 |
| 51:DZ:56:VAL:HA | 51:DZ:70:LEU:HD23 | 1.93 | 0.49 |
| 1:AA:1084:G:OP1 | 1:AA:1086:U:C4 | 2.66 | 0.49 |
| 1:AA:1293:G:O2' | 1:AA:1294:G:H8 | 1.95 | 0.49 |
| 1:AA:201:C:H42 | 1:AA:203:U:H1' | 1.78 | 0.49 |
| 1:AA:355:C:N3 | 1:AA:356:A:N7 | 2.61 | 0.49 |
| 1:AA:682:G:C6 | 1:AA:683:G:N7 | 2.80 | 0.49 |
| 6:AF:40:VAL:HA | 6:AF:62:TRP:O | 2.12 | 0.49 |
| 1:AA:363:A:C2 | 12:AL:31:PRO:HG2 | 2.47 | 0.49 |
| 17:AQ:22:LEU:HD12 | 17:AQ:23:VAL:H | 1.77 | 0.49 |
| 31:BA:1024:G:C3' | 31:BA:1025:G:H5'' | 2.35 | 0.49 |
| 31:BA:125:G:H4' | 31:BA:126:A:OP2 | 2.13 | 0.49 |
| 31:BA:2327:A:H2' | 31:BA:2328:A:H8 | 1.74 | 0.49 |
| 31:BA:241:A:O4' | 31:BA:243:U:C6 | 2.66 | 0.49 |
| 31:BA:693:C:H2' | 31:BA:694:U:C6 | 2.48 | 0.49 |
| 31:BA:801:G:N7 | 35:BF:53:THR:HG23 | 2.28 | 0.49 |
| 31:BA:1568:G:P | 33:BD:63:ARG:HH22 | 2.36 | 0.49 |
| 34:BE:60:ASN:HD22 | 34:BE:60:ASN:N | 2.09 | 0.49 |
| 36:BG:106:LEU:HD12 | 36:BG:110:ALA:CB | 2.42 | 0.49 |
| 40:BO:42:SER:OG | 40:BO:44:LYS:HE2 | 2.13 | 0.49 |
| 31:BA:2880:C:H1' | 43:BR:92:GLY:O | 2.13 | 0.49 |
| 44:BS:35:ILE:C | 44:BS:36:TYR:CD1 | 2.84 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:B5:25:LEU:HD21 | 48:BW:41:LYS:HE3 | 1.95 | 0.49 |
| 51:BZ:56:VAL:HA | 51:BZ:70:LEU:HD23 | 1.95 | 0.49 |
| 1:CA:976:G:C5' | 1:CA:1358:U:O2' | 2.58 | 0.49 |
| 1:CA:402:G:C6 | 1:CA:403:C:C4 | 3.01 | 0.49 |
| 1:CA:684:A:C6 | 1:CA:685:G:C6 | 3.01 | 0.49 |
| 1:CA:865:A:C2 | 1:CA:918:A:H4' | 2.47 | 0.49 |
| 4:CD:119:GLN:O | 4:CD:123:HIS:HD2 | 1.95 | 0.49 |
| 5:CE:126:ARG:HA | 5:CE:131:ILE:HD11 | 1.94 | 0.49 |
| 8:CH:91:ARG:HG2 | 8:CH:91:ARG:HH11 | 1.77 | 0.49 |
| 9:CI:28:VAL:HA | 9:CI:63:ILE:O | 2.13 | 0.49 |
| 10:CJ:8:LEU:HG | 10:CJ:96:ILE:HG22 | 1.94 | 0.49 |
| 17:CQ:59:ILE:HG22 | 17:CQ:60:ILE:N | 2.28 | 0.49 |
| 22:D0:1:MET:HA | 31:DA:2451:A:H4' | 1.95 | 0.49 |
| 31:DA:1049:C:H1' | 31:DA:1113:U:O2' | 2.13 | 0.49 |
| 31:DA:1171:G:H3' | 31:DA:1173:G:O4' | 2.12 | 0.49 |
| 31:DA:1189:A:N7 | 31:DA:1190:G:C8 | 2.81 | 0.49 |
| 31:DA:1858:G:H1' | 31:DA:1884:A:N6 | 2.28 | 0.49 |
| 31:DA:1893:C:C6 | 31:DA:1894:C:C5 | 3.01 | 0.49 |
| 31:DA:2020:A:C2' | 31:DA:2021:C:H5' | 2.43 | 0.49 |
| 31:DA:2069:G:H2' | 31:DA:2070:G:H5' | 1.94 | 0.49 |
| 31:DA:2228:G:C6 | 31:DA:2229:C:C4 | 3.00 | 0.49 |
| 31:DA:338:G:H2' | 31:DA:339:U:H6 | 1.77 | 0.49 |
| 32:DB:21:G:O2' | 32:DB:22:U:O5' | 2.31 | 0.49 |
| 34:DE:179:GLU:HB3 | 34:DE:181:LEU:CD2 | 2.43 | 0.49 |
| 36:DG:45:GLU:HB2 | 36:DG:47:LYS:CD | 2.42 | 0.49 |
| 38:DI:79:ILE:HG22 | 38:DI:81:VAL:HG23 | 1.95 | 0.49 |
| 41:DP:47:ASP:HB2 | 41:DP:51:PHE:HB2 | 1.95 | 0.49 |
| 42:DQ:17:LEU:HD23 | 42:DQ:17:LEU:N | 2.28 | 0.49 |
| 46:DU:92:ARG:CZ | 47:DV:11:GLN:HG2 | 2.43 | 0.49 |
| 47:DV:80:GLN:HA | 47:DV:82:ARG:H | 1.77 | 0.49 |
| 49:DX:21:PHE:CE1 | 49:DX:26:TYR:CG | 3.00 | 0.49 |
| 31:DA:336:C:H5'' | 50:DY:7:VAL:HG13 | 1.95 | 0.49 |
| 51:DZ:28:MET:CE | 51:DZ:59:LEU:HD12 | 2.43 | 0.49 |
| 1:AA:60:A:C8 | 1:AA:60:A:P | 3.05 | 0.49 |
| 1:AA:920:U:H1' | 1:AA:1080:A:C2 | 2.48 | 0.49 |
| 1:AA:710:G:H5'' | 6:AF:54:LYS:HE3 | 1.95 | 0.49 |
| 8:AH:11:THR:HG23 | 8:AH:14:ARG:NH1 | 2.28 | 0.49 |
| 10:AJ:54:PHE:CZ | 10:AJ:55:LYS:NZ | 2.80 | 0.49 |
| 1:AA:538:G:OP2 | 12:AL:115:LYS:HG3 | 2.13 | 0.49 |
| 12:AL:110:VAL:HG23 | 12:AL:120:TYR:O | 2.13 | 0.49 |
| 12:AL:62:SER:O | 12:AL:64:TYR:N | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:AP:8:ARG:O | 16:AP:9:PHE:CG | 2.66 | 0.49 |
| 30:B8:47:LYS:HD2 | 30:B8:48:PHE:O | 2.12 | 0.49 |
| 31:BA:1162:G:O2' | 47:BV:92:THR:HG23 | 2.12 | 0.49 |
| 31:BA:1354:A:H2' | 31:BA:1355:G:O4' | 2.13 | 0.49 |
| 31:BA:2275:C:H5' | 31:BA:2275:C:H6 | 1.78 | 0.49 |
| 31:BA:2476:A:C2 | 31:BA:2477:C:H5'' | 2.47 | 0.49 |
| 31:BA:2472:G:N1 | 31:BA:2477:C:OP1 | 2.25 | 0.49 |
| 27:B5:7:PRO:HA | 31:BA:2615:U:C2 | 2.48 | 0.49 |
| 31:BA:329:G:OP2 | 50:BY:71:LYS:HE2 | 2.13 | 0.49 |
| 31:BA:721:C:O2 | 31:BA:721:C:H2' | 2.11 | 0.49 |
| 32:BB:41:U:C4 | 36:BG:70:VAL:O | 2.66 | 0.49 |
| 34:BE:57:LYS:HG3 | 34:BE:57:LYS:O | 2.13 | 0.49 |
| 35:BF:195:ASP:CG | 35:BF:197:ASP:HB3 | 2.33 | 0.49 |
| 35:BF:67:GLN:HG3 | 35:BF:67:GLN:O | 2.12 | 0.49 |
| 36:BG:6:ALA:HB3 | 36:BG:104:GLU:OE1 | 2.13 | 0.49 |
| 36:BG:45:GLU:HB2 | 36:BG:47:LYS:CD | 2.43 | 0.49 |
| 37:BH:85:LYS:CD | 37:BH:133:VAL:HB | 2.42 | 0.49 |
| 31:BA:631:A:OP1 | 41:BP:64:LYS:CE | 2.61 | 0.49 |
| 43:BR:117:VAL:O | 43:BR:117:VAL:HG12 | 2.12 | 0.49 |
| 43:BR:51:LEU:HD13 | 43:BR:70:LEU:HD21 | 1.93 | 0.49 |
| 44:BS:61:ASN:ND2 | 44:BS:64:GLU:OE2 | 2.46 | 0.49 |
| 39:BN:2:LYS:NZ | 46:BU:94:ASN:HD21 | 2.11 | 0.49 |
| 47:BV:47:VAL:HG22 | 47:BV:48:GLY:N | 2.28 | 0.49 |
| 47:BV:15:GLU:O | 47:BV:98:GLU:CD | 2.51 | 0.49 |
| 1:CA:189(B):C:O2' | 1:CA:189(C):C:H5' | 2.13 | 0.49 |
| 1:CA:447:G:C6 | 1:CA:485:G:H1' | 2.47 | 0.49 |
| 1:CA:541:G:H2' | 1:CA:542:G:H8 | 1.78 | 0.49 |
| 1:CA:586:C:C2' | 1:CA:587:G:H5' | 2.43 | 0.49 |
| 1:CA:590:C:H2' | 1:CA:591:U:C6 | 2.48 | 0.49 |
| 1:CA:605:U:H2' | 1:CA:606:G:C8 | 2.46 | 0.49 |
| 1:CA:920:U:H1' | 1:CA:1080:A:N3 | 2.27 | 0.49 |
| 1:CA:994:A:N6 | 1:CA:1046:A:H2 | 2.10 | 0.49 |
| 2:CB:153:ARG:O | 2:CB:154:LEU:C | 2.51 | 0.49 |
| 2:CB:97:TRP:CH2 | 2:CB:176:GLU:HG3 | 2.48 | 0.49 |
| 2:CB:42:ILE:HD11 | 2:CB:202:PRO:HB2 | 1.94 | 0.49 |
| 2:CB:67:THR:HG21 | 2:CB:155:LEU:HG | 1.95 | 0.49 |
| 5:CE:139:LEU:HA | 5:CE:142:LEU:HD12 | 1.95 | 0.49 |
| 7:CG:75:VAL:CG2 | 7:CG:144:MET:HB3 | 2.42 | 0.49 |
| 10:CJ:54:PHE:CZ | 10:CJ:55:LYS:NZ | 2.81 | 0.49 |
| 11:CK:48:ILE:HG21 | 11:CK:63:LEU:HD13 | 1.94 | 0.49 |
| 1:CA:363:A:C5 | 12:CL:31:PRO:HD2 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:CM:81:LEU:HB3 | 13:CM:89:GLY:CA | 2.39 | 0.49 |
| 16:CP:20:VAL:HG13 | 16:CP:21:VAL:N | 2.28 | 0.49 |
| 24:D2:12:GLU:C | 24:D2:14:ARG:N | 2.66 | 0.49 |
| 31:DA:1107:G:H2' | 31:DA:1108:U:O4' | 2.13 | 0.49 |
| 31:DA:1185:C:H5'' | 31:DA:1186:G:OP1 | 2.13 | 0.49 |
| 31:DA:1359:A:N7 | 31:DA:1372:U:C4 | 2.80 | 0.49 |
| 31:DA:1512:U:O2' | 31:DA:1513:C:H5' | 2.13 | 0.49 |
| 31:DA:2199:A:OP2 | 31:DA:2200:C:C5 | 2.63 | 0.49 |
| 31:DA:2287:A:C4 | 31:DA:2289:G:C8 | 3.00 | 0.49 |
| 31:DA:2359:C:H2' | 31:DA:2360:A:C5' | 2.30 | 0.49 |
| 31:DA:2660:A:H5'' | 31:DA:2661:G:N2 | 2.28 | 0.49 |
| 31:DA:271(L):U:H4' | 31:DA:271(M):G:N7 | 2.26 | 0.49 |
| 31:DA:300:A:P | 50:DY:84:ARG:NH2 | 2.86 | 0.49 |
| 31:DA:307:G:H22 | 31:DA:310:A:H5' | 1.75 | 0.49 |
| 31:DA:444:C:H4' | 35:DF:49:ALA:HB2 | 1.95 | 0.49 |
| 31:DA:643:A:H2' | 31:DA:644:A:O5' | 2.13 | 0.49 |
| 31:DA:854:G:H2' | 31:DA:855:G:C8 | 2.47 | 0.49 |
| 31:DA:877:U:O2' | 31:DA:878:A:H5'' | 2.12 | 0.49 |
| 33:DD:186:HIS:C | 33:DD:186:HIS:CD2 | 2.87 | 0.49 |
| 31:DA:443:A:H3' | 35:DF:45:ARG:HH21 | 1.78 | 0.49 |
| 37:DH:44:VAL:HG12 | 37:DH:45:VAL:N | 2.19 | 0.49 |
| 50:DY:7:VAL:HB | 50:DY:8:LYS:HD2 | 1.94 | 0.49 |
| 1:AA:1202:G:H2' | 1:AA:1203:C:O4' | 2.13 | 0.49 |
| 1:AA:1313:U:P | 19:AS:6:LYS:HG3 | 2.52 | 0.49 |
| 1:AA:411:A:C6 | 1:AA:429:U:C4 | 3.00 | 0.49 |
| 1:AA:475:G:H2' | 1:AA:476:G:C8 | 2.42 | 0.49 |
| 1:AA:78:G:H22 | 1:AA:91:C:N4 | 2.11 | 0.49 |
| 1:AA:922:G:C2 | 1:AA:923:A:C4 | 3.00 | 0.49 |
| 2:AB:115:LEU:HB2 | 2:AB:145:LEU:HD12 | 1.95 | 0.49 |
| 2:AB:36:ARG:HB2 | 2:AB:41:ILE:HD13 | 1.95 | 0.49 |
| 3:AC:14:ILE:HG23 | 3:AC:15:THR:N | 2.28 | 0.49 |
| 1:AA:1108:G:OP1 | 3:AC:175:LEU:HD12 | 2.12 | 0.49 |
| 4:AD:112:VAL:HG13 | 4:AD:113:SER:N | 2.28 | 0.49 |
| 4:AD:10:ARG:O | 4:AD:13:ARG:HB2 | 2.12 | 0.49 |
| 12:AL:18:VAL:HG23 | 12:AL:19:ARG:N | 2.26 | 0.49 |
| 12:AL:20:LYS:H | 12:AL:20:LYS:HD3 | 1.78 | 0.49 |
| 12:AL:55:VAL:CG1 | 12:AL:56:ALA:N | 2.75 | 0.49 |
| 30:B8:51:ALA:N | 30:B8:53:PRO:HD2 | 2.28 | 0.49 |
| 31:BA:1048:A:OP2 | 31:BA:1110:G:N1 | 2.46 | 0.49 |
| 31:BA:1439:A:C2 | 31:BA:1553:A:C5 | 3.01 | 0.49 |
| 31:BA:1494:A:N3 | 31:BA:1494:A:C2' | 2.75 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:1510:G:H2' | 31:BA:1511:C:H5' | 1.94 | 0.49 |
| 31:BA:1525:G:H2' | 31:BA:1526:G:C8 | 2.48 | 0.49 |
| 31:BA:2480:C:N4 | 31:BA:2481:G:C6 | 2.81 | 0.49 |
| 31:BA:2632:A:H1' | 34:BE:61:ARG:CZ | 2.43 | 0.49 |
| 31:BA:2661:G:HO2' | 31:BA:2662:A:P | 2.33 | 0.49 |
| 31:BA:271(F):C:C2 | 31:BA:271(G):C:C6 | 3.00 | 0.49 |
| 31:BA:2752:C:H2' | 31:BA:2753:A:H5' | 1.94 | 0.49 |
| 31:BA:824:A:C2' | 31:BA:825:C:H5' | 2.42 | 0.49 |
| 32:BB:21:G:O2' | 32:BB:22:U:O5' | 2.29 | 0.49 |
| 33:BD:173:VAL:HG23 | 33:BD:174:ILE:H | 1.78 | 0.49 |
| 33:BD:267:SER:O | 33:BD:268:ARG:CB | 2.61 | 0.49 |
| 42:BQ:16:ARG:C | 42:BQ:17:LEU:HD23 | 2.33 | 0.49 |
| 44:BS:16:ASN:HB3 | 44:BS:20:ARG:NH2 | 2.28 | 0.49 |
| 45:BT:41:ARG:CZ | 45:BT:43:GLN:HB2 | 2.42 | 0.49 |
| 46:BU:102:GLU:HG3 | 47:BV:2:PHE:CE2 | 2.47 | 0.49 |
| 46:BU:60:LEU:O | 46:BU:64:ARG:HG2 | 2.13 | 0.49 |
| 47:BV:79:VAL:HG23 | 47:BV:82:ARG:CD | 2.43 | 0.49 |
| 49:BX:77:LYS:HD3 | 49:BX:78:LYS:HD2 | 1.95 | 0.49 |
| 50:BY:28:LYS:CE | 50:BY:37:VAL:HG12 | 2.42 | 0.49 |
| 1:CA:1054:C:O2 | 1:CA:1054:C:H3' | 2.12 | 0.49 |
| 1:CA:1086:U:H2' | 1:CA:1087:G:H8 | 1.78 | 0.49 |
| 1:CA:1068:G:N3 | 1:CA:1191:A:H2 | 2.09 | 0.49 |
| 1:CA:1238:A:N6 | 1:CA:1299:A:H62 | 2.08 | 0.49 |
| 1:CA:20:U:O2' | 1:CA:21:G:H5' | 2.13 | 0.49 |
| 1:CA:435:C:N4 | 1:CA:436:C:H41 | 2.11 | 0.49 |
| 1:CA:731:G:H5' | 1:CA:766:A:H4' | 1.95 | 0.49 |
| 1:CA:834:C:H2' | 1:CA:835:U:C6 | 2.47 | 0.49 |
| 1:CA:963:G:H1 | 1:CA:972:C:H42 | 1.60 | 0.49 |
| 2:CB:204:ASN:HD21 | 2:CB:206:ASP:H | 1.61 | 0.49 |
| 1:CA:410:G:OP2 | 4:CD:25:ARG:HG3 | 2.13 | 0.49 |
| 9:CI:114:TYR:HD2 | 9:CI:114:TYR:N | 2.11 | 0.49 |
| 15:CO:67:LEU:HD22 | 15:CO:78:TYR:CE1 | 2.47 | 0.49 |
| 20:CT:46:GLU:HG2 | 20:CT:48:LYS:HE2 | 1.95 | 0.49 |
| 23:D1:85:LEU:N | 23:D1:85:LEU:HD23 | 2.26 | 0.49 |
| 24:D2:16:LEU:N | 24:D2:18:PRO:HD2 | 2.27 | 0.49 |
| 31:DA:1158:C:O2' | 31:DA:1159:U:OP2 | 2.31 | 0.49 |
| 31:DA:1276:A:O2' | 43:DR:16:HIS:HE1 | 1.96 | 0.49 |
| 31:DA:1327:C:C2' | 31:DA:1328:G:H5' | 2.43 | 0.49 |
| 31:DA:1472:A:H2' | 31:DA:1473:G:H5' | 1.93 | 0.49 |
| 31:DA:2753:A:O2' | 31:DA:2754:U:P | 2.71 | 0.49 |
| 31:DA:2756:U:H1' | 31:DA:2757:A:H5'' | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:526:A:H5'' | 31:DA:527:C:OP1 | 2.12 | 0.49 |
| 31:DA:70:G:H21 | 31:DA:71:A:H62 | 1.61 | 0.49 |
| 31:DA:990:A:OP2 | 31:DA:991:C:OP2 | 2.30 | 0.49 |
| 31:DA:995:C:N3 | 39:DN:4:TYR:HE1 | 2.11 | 0.49 |
| 32:DB:27:C:H5'' | 32:DB:27:C:H6 | 1.76 | 0.49 |
| 33:DD:35:LYS:HB3 | 33:DD:63:ARG:CA | 2.31 | 0.49 |
| 35:DF:157:VAL:HB | 35:DF:194:MET:HB3 | 1.94 | 0.49 |
| 36:DG:46:ALA:H | 36:DG:82:LEU:CD1 | 2.24 | 0.49 |
| 43:DR:41:ALA:O | 43:DR:42:LYS:C | 2.51 | 0.49 |
| 43:DR:8:ARG:HA | 43:DR:8:ARG:NE | 2.28 | 0.49 |
| 45:DT:84:GLN:OE1 | 45:DT:86:ILE:HD12 | 2.13 | 0.49 |
| 49:DX:60:ARG:CZ | 49:DX:74:PRO:HG2 | 2.42 | 0.49 |
| 50:DY:29:GLU:N | 50:DY:29:GLU:OE1 | 2.46 | 0.49 |
| 50:DY:87:LYS:O | 50:DY:88:LYS:HB2 | 2.13 | 0.49 |
| 1:AA:1004:A:C2' | 1:AA:1038:C:O2 | 2.61 | 0.48 |
| 1:AA:1058:G:H8 | 1:AA:1058:G:O5' | 1.96 | 0.48 |
| 1:AA:1142:G:H3' | 1:AA:1143:G:H8 | 1.77 | 0.48 |
| 1:AA:1271:G:H5' | 1:AA:1314:C:H5' | 1.95 | 0.48 |
| 1:AA:1416:G:H2' | 1:AA:1417:G:O4' | 2.13 | 0.48 |
| 1:AA:1418:A:H1' | 31:BA:1959:G:O4' | 2.13 | 0.48 |
| 1:AA:1504:G:OP1 | 1:AA:1507:A:H4' | 2.13 | 0.48 |
| 1:AA:262:A:N6 | 1:AA:263:A:N6 | 2.60 | 0.48 |
| 1:AA:731:G:OP1 | 1:AA:766:A:H1' | 2.13 | 0.48 |
| 3:AC:58:GLU:H | 3:AC:65:ALA:HB3 | 1.78 | 0.48 |
| 6:AF:67:MET:CE | 6:AF:75:LEU:HD12 | 2.43 | 0.48 |
| 10:AJ:54:PHE:CE2 | 10:AJ:55:LYS:HD2 | 2.48 | 0.48 |
| 11:AK:48:ILE:HG22 | 11:AK:49:GLY:H | 1.78 | 0.48 |
| 17:AQ:45:HIS:O | 17:AQ:73:VAL:HG23 | 2.13 | 0.48 |
| 24:B2:34:GLU:O | 24:B2:36:ARG:HB2 | 2.13 | 0.48 |
| 25:B3:1:MET:O | 25:B3:3:ARG:N | 2.46 | 0.48 |
| 27:B5:40:LYS:CE | 27:B5:46:CYS:HB3 | 2.43 | 0.48 |
| 28:B6:24:GLU:OE1 | 28:B6:24:GLU:CA | 2.58 | 0.48 |
| 31:BA:1952:A:C6 | 31:BA:1953:A:C6 | 3.00 | 0.48 |
| 31:BA:997:G:O2' | 31:BA:998:C:H5' | 2.13 | 0.48 |
| 31:BA:2598:A:O5' | 33:BD:236:GLY:HA3 | 2.11 | 0.48 |
| 35:BF:7:TYR:HD2 | 35:BF:16:GLY:HA3 | 1.77 | 0.48 |
| 36:BG:64:THR:CG2 | 36:BG:65:GLY:N | 2.77 | 0.48 |
| 37:BH:32:GLU:C | 37:BH:33:LEU:HD23 | 2.33 | 0.48 |
| 43:BR:44:LEU:HD22 | 43:BR:48:VAL:HG23 | 1.94 | 0.48 |
| 47:BV:1:MET:HA | 47:BV:1:MET:CE | 2.43 | 0.48 |
| 47:BV:22:VAL:O | 47:BV:23:GLU:CB | 2.51 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:BV:47:VAL:CG1 | 47:BV:48:GLY:H | 2.13 | 0.48 |
| 1:CA:1004:A:C2' | 1:CA:1038:C:O2 | 2.60 | 0.48 |
| 1:CA:1313:U:P | 19:CS:6:LYS:HG3 | 2.53 | 0.48 |
| 1:CA:1423:G:H2' | 1:CA:1424:C:C6 | 2.48 | 0.48 |
| 1:CA:189(B):C:N4 | 1:CA:189(J):G:C6 | 2.80 | 0.48 |
| 1:CA:477:A:O2' | 1:CA:479:C:H5' | 2.12 | 0.48 |
| 1:CA:693:G:H1' | 7:CG:82:GLY:CA | 2.43 | 0.48 |
| 1:CA:706:A:C5 | 1:CA:707:C:C5 | 3.02 | 0.48 |
| 1:CA:731:G:OP1 | 1:CA:766:A:H1' | 2.13 | 0.48 |
| 4:CD:60:GLU:HG2 | 4:CD:202:LEU:HB2 | 1.95 | 0.48 |
| 5:CE:36:ASP:O | 5:CE:37:ARG:CB | 2.61 | 0.48 |
| 12:CL:62:SER:HB2 | 12:CL:64:TYR:HD1 | 1.78 | 0.48 |
| 13:CM:81:LEU:HD11 | 13:CM:88:ARG:HH12 | 1.78 | 0.48 |
| 1:CA:1226:C:OP1 | 13:CM:91:ARG:NH1 | 2.46 | 0.48 |
| 1:CA:277:C:P | 17:CQ:68:ARG:HH12 | 2.36 | 0.48 |
| 19:CS:79:THR:O | 19:CS:80:TYR:HB3 | 2.13 | 0.48 |
| 22:D0:84:LEU:N | 22:D0:84:LEU:HD12 | 2.27 | 0.48 |
| 31:DA:1865:G:H8 | 31:DA:1865:G:H5'' | 1.78 | 0.48 |
| 31:DA:2602:A:H4' | 31:DA:2603:G:O5' | 2.13 | 0.48 |
| 31:DA:2807:G:H22 | 31:DA:2892:A:N6 | 2.11 | 0.48 |
| 31:DA:2807:G:H3' | 31:DA:2808:U:H5'' | 1.94 | 0.48 |
| 34:DE:63:LEU:O | 34:DE:64:LYS:C | 2.51 | 0.48 |
| 36:DG:13:GLU:O | 36:DG:14:GLU:HB2 | 2.13 | 0.48 |
| 36:DG:55:LYS:O | 36:DG:59:GLU:HB2 | 2.13 | 0.48 |
| 39:DN:78:TYR:H | 39:DN:79:PRO:CD | 2.26 | 0.48 |
| 42:DQ:45:GLN:H | 42:DQ:45:GLN:CD | 2.15 | 0.48 |
| 51:DZ:73:GLN:HG2 | 51:DZ:87:ASP:OD1 | 2.13 | 0.48 |
| 1:AA:1088:G:C6 | 1:AA:1089:G:C6 | 3.01 | 0.48 |
| 1:AA:1068:G:N3 | 1:AA:1191:A:H2 | 2.11 | 0.48 |
| 1:AA:763:G:O2' | 1:AA:764:C:H5' | 2.13 | 0.48 |
| 1:AA:826:C:H2' | 1:AA:827:U:C6 | 2.48 | 0.48 |
| 1:AA:983:A:H3' | 1:AA:983:A:N3 | 2.28 | 0.48 |
| 2:AB:67:THR:HG21 | 2:AB:155:LEU:HG | 1.96 | 0.48 |
| 3:AC:82:GLU:O | 3:AC:86:VAL:HG13 | 2.13 | 0.48 |
| 6:AF:69:GLU:HG2 | 6:AF:70:ASP:N | 2.28 | 0.48 |
| 6:AF:9:VAL:HB | 6:AF:87:ARG:HB2 | 1.94 | 0.48 |
| 8:AH:92:ARG:HD2 | 8:AH:92:ARG:N | 2.28 | 0.48 |
| 11:AK:20:TYR:C | 11:AK:21:ILE:HD12 | 2.34 | 0.48 |
| 12:AL:102:ARG:HD2 | 12:AL:108:ALA:O | 2.13 | 0.48 |
| 15:AO:56:LEU:O | 15:AO:60:VAL:HG23 | 2.13 | 0.48 |
| 20:AT:64:ASP:OD2 | 20:AT:81:LYS:NZ | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:B5:52:TYR:CG | 27:B5:52:TYR:O | 2.66 | 0.48 |
| 31:BA:1050:A:C2 | 31:BA:2751:G:C4 | 3.01 | 0.48 |
| 31:BA:1174:A:OP1 | 31:BA:1175:U:H5'' | 2.13 | 0.48 |
| 31:BA:1827:C:O2' | 31:BA:1970:A:N3 | 2.37 | 0.48 |
| 31:BA:2228:G:OP1 | 33:BD:261:LYS:NZ | 2.46 | 0.48 |
| 31:BA:2802:G:H3' | 31:BA:2802:G:P | 2.53 | 0.48 |
| 31:BA:547:A:C8 | 31:BA:549:G:O6 | 2.66 | 0.48 |
| 31:BA:954:G:C5 | 31:BA:955:C:C5 | 3.01 | 0.48 |
| 33:BD:101:GLU:OE1 | 33:BD:103:ARG:HD3 | 2.13 | 0.48 |
| 33:BD:79:VAL:HG21 | 33:BD:111:LEU:CD1 | 2.42 | 0.48 |
| 35:BF:164:ARG:HG2 | 35:BF:164:ARG:NH1 | 2.24 | 0.48 |
| 37:BH:54:ARG:HB3 | 37:BH:65:HIS:CD2 | 2.48 | 0.48 |
| 38:BI:37:VAL:HG12 | 38:BI:38:LEU:N | 2.28 | 0.48 |
| 42:BQ:16:ARG:HG3 | 42:BQ:17:LEU:H | 1.78 | 0.48 |
| 45:BT:109:GLU:HA | 45:BT:112:ARG:CG | 2.43 | 0.48 |
| 47:BV:32:THR:HB | 47:BV:64:HIS:HE1 | 1.79 | 0.48 |
| 49:BX:34:ALA:C | 49:BX:36:LYS:N | 2.65 | 0.48 |
| 49:BX:62:LYS:CB | 49:BX:69:TYR:H | 2.19 | 0.48 |
| 51:BZ:108:PRO:HA | 51:BZ:142:SER:HA | 1.95 | 0.48 |
| 1:CA:189(B):C:N4 | 1:CA:189(I):G:H1 | 2.11 | 0.48 |
| 1:CA:561:U:HO2' | 1:CA:562:C:P | 2.33 | 0.48 |
| 2:CB:188:ALA:HB1 | 2:CB:192:SER:CB | 2.42 | 0.48 |
| 3:CC:113:ALA:HB3 | 3:CC:114:PRO:HD3 | 1.95 | 0.48 |
| 8:CH:87:SER:HB3 | 8:CH:133:LEU:O | 2.12 | 0.48 |
| 1:CA:687:A:H4' | 11:CK:47:VAL:HG13 | 1.95 | 0.48 |
| 12:CL:22:SER:C | 12:CL:24:VAL:H | 2.16 | 0.48 |
| 24:D2:32:LEU:HD21 | 31:DA:61:G:O2' | 2.13 | 0.48 |
| 29:D7:5:TRP:CH2 | 31:DA:686:G:N7 | 2.81 | 0.48 |
| 31:DA:1225:G:O5' | 31:DA:1225:G:H8 | 1.96 | 0.48 |
| 31:DA:1444:G:N2 | 31:DA:1548:C:C2 | 2.81 | 0.48 |
| 31:DA:1563:G:C5 | 31:DA:1564:C:C5 | 3.02 | 0.48 |
| 31:DA:1667:G:H22 | 31:DA:1992:G:H5'' | 1.78 | 0.48 |
| 31:DA:1685:C:H2' | 31:DA:1686:C:H6 | 1.78 | 0.48 |
| 31:DA:1799:G:N7 | 33:DD:179:SER:OG | 2.44 | 0.48 |
| 31:DA:1803:A:H2 | 31:DA:1822:G:N3 | 2.11 | 0.48 |
| 31:DA:2186:G:C2' | 31:DA:2187:G:H5'' | 2.43 | 0.48 |
| 31:DA:284:U:H2' | 31:DA:285:C:C6 | 2.48 | 0.48 |
| 31:DA:28:A:O2' | 31:DA:583:G:H5' | 2.13 | 0.48 |
| 31:DA:1902:C:C4' | 33:DD:244:ARG:HB2 | 2.42 | 0.48 |
| 34:DE:70:ALA:O | 34:DE:72:VAL:N | 2.45 | 0.48 |
| 38:DI:78:THR:O | 38:DI:79:ILE:HD13 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DN:78:TYR:CD1 | 39:DN:79:PRO:HD3 | 2.47 | 0.48 |
| 43:DR:53:HIS:O | 43:DR:56:LYS:HB3 | 2.13 | 0.48 |
| 46:DU:95:LEU:HD12 | 47:DV:11:GLN:HG3 | 1.95 | 0.48 |
| 48:DW:71:VAL:HA | 48:DW:107:LEU:HD12 | 1.94 | 0.48 |
| 1:AA:1368:G:OP2 | 9:AI:112:LYS:HD3 | 2.14 | 0.48 |
| 1:AA:1407:C:O5' | 1:AA:1407:C:H6 | 1.96 | 0.48 |
| 1:AA:359:U:H2' | 1:AA:360:A:C8 | 2.48 | 0.48 |
| 1:AA:706:A:C5 | 1:AA:707:C:C5 | 3.01 | 0.48 |
| 2:AB:188:ALA:HB1 | 2:AB:192:SER:CB | 2.43 | 0.48 |
| 4:AD:170:VAL:HG13 | 4:AD:171:GLY:N | 2.27 | 0.48 |
| 4:AD:60:GLU:HG2 | 4:AD:202:LEU:HB2 | 1.96 | 0.48 |
| 5:AE:122:GLU:OE1 | 5:AE:131:ILE:HG13 | 2.13 | 0.48 |
| 8:AH:97:VAL:O | 8:AH:100:ILE:HG13 | 2.13 | 0.48 |
| 9:AI:105:ASP:CG | 9:AI:107:ARG:HD3 | 2.33 | 0.48 |
| 7:AG:37:ASN:HD21 | 9:AI:40:LEU:CD2 | 2.26 | 0.48 |
| 13:AM:94:ARG:O | 13:AM:96:LEU:HG | 2.13 | 0.48 |
| 27:B5:57:VAL:CG2 | 27:B5:58:LEU:N | 2.76 | 0.48 |
| 31:BA:1642:G:C2' | 31:BA:1643:G:H5' | 2.44 | 0.48 |
| 31:BA:272(G):C:H42 | 31:BA:363(C):G:H1 | 1.61 | 0.48 |
| 31:BA:547:A:O2' | 31:BA:548:A:OP2 | 2.28 | 0.48 |
| 31:BA:610:G:H2' | 31:BA:611:C:C6 | 2.49 | 0.48 |
| 31:BA:662:G:O2' | 31:BA:663:G:H5' | 2.13 | 0.48 |
| 31:BA:855:G:C5 | 31:BA:856:C:C5 | 3.00 | 0.48 |
| 32:BB:13:A:O2' | 32:BB:15:A:O5' | 2.32 | 0.48 |
| 32:BB:45:A:C2 | 32:BB:46:A:C1' | 2.96 | 0.48 |
| 36:BG:13:GLU:O | 36:BG:14:GLU:HB2 | 2.12 | 0.48 |
| 37:BH:54:ARG:HG2 | 37:BH:65:HIS:HD2 | 1.79 | 0.48 |
| 38:BI:109:ILE:HG22 | 38:BI:130:TYR:CZ | 2.48 | 0.48 |
| 39:BN:58:ASP:OD1 | 39:BN:124:ALA:HB1 | 2.13 | 0.48 |
| 41:BP:83:VAL:CG1 | 41:BP:112:LEU:HD21 | 2.44 | 0.48 |
| 44:BS:17:ARG:O | 44:BS:18:ILE:HB | 2.12 | 0.48 |
| 44:BS:57:LYS:HG2 | 44:BS:58:LEU:N | 2.28 | 0.48 |
| 49:BX:65:ARG:NE | 49:BX:65:ARG:HA | 2.28 | 0.48 |
| 51:BZ:156:LYS:O | 51:BZ:158:PRO:HD3 | 2.13 | 0.48 |
| 1:CA:1058:G:O5' | 1:CA:1058:G:H8 | 1.97 | 0.48 |
| 1:CA:106:C:H2' | 1:CA:107:G:H8 | 1.79 | 0.48 |
| 1:CA:738:C:N3 | 1:CA:739:C:C5 | 2.82 | 0.48 |
| 1:CA:781:A:C3' | 1:CA:782:A:H5' | 2.43 | 0.48 |
| 1:CA:84:U:C5 | 1:CA:88:A:C8 | 3.01 | 0.48 |
| 3:CC:111:LEU:HD21 | 3:CC:145:GLY:O | 2.12 | 0.48 |
| 7:CG:66:VAL:HG12 | 7:CG:70:LYS:HE3 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:CL:38:THR:CG2 | 12:CL:57:LYS:HB2 | 2.44 | 0.48 |
| 19:CS:65:ASN:HB2 | 19:CS:66:MET:HE3 | 1.94 | 0.48 |
| 27:D5:41:PRO:O | 27:D5:44:THR:OG1 | 2.31 | 0.48 |
| 28:D6:48:VAL:O | 28:D6:49:HIS:O | 2.31 | 0.48 |
| 29:D7:19:ARG:HG2 | 29:D7:19:ARG:HH11 | 1.78 | 0.48 |
| 30:D8:30:ARG:NH2 | 41:DP:62:LEU:HB2 | 2.29 | 0.48 |
| 31:DA:1047:G:N2 | 31:DA:1111:A:N6 | 2.59 | 0.48 |
| 31:DA:107:C:C4 | 31:DA:108:U:C5 | 3.01 | 0.48 |
| 31:DA:1195:G:C2' | 31:DA:1196:C:H5' | 2.43 | 0.48 |
| 31:DA:1416:G:O2' | 31:DA:1417:C:P | 2.71 | 0.48 |
| 31:DA:1497:U:H2' | 31:DA:1498:C:OP1 | 2.13 | 0.48 |
| 31:DA:1478:G:O2' | 31:DA:1558:A:H2 | 1.97 | 0.48 |
| 31:DA:1925:C:O2' | 31:DA:1926:U:H5' | 2.13 | 0.48 |
| 31:DA:2311:A:O2' | 31:DA:2312:U:O4' | 2.27 | 0.48 |
| 22:D0:43:THR:N | 31:DA:2331:G:H4' | 2.24 | 0.48 |
| 22:D0:36:ILE:HG23 | 31:DA:2354:G:O2' | 2.13 | 0.48 |
| 31:DA:2619:C:O2' | 31:DA:2620:C:H5' | 2.13 | 0.48 |
| 31:DA:363(B):G:N3 | 31:DA:363(B):G:H2' | 2.29 | 0.48 |
| 31:DA:524:U:H2' | 31:DA:525:U:C6 | 2.49 | 0.48 |
| 31:DA:795:C:H2' | 31:DA:796:C:H6 | 1.78 | 0.48 |
| 37:DH:170:ARG:H | 37:DH:170:ARG:HD2 | 1.77 | 0.48 |
| 39:DN:133:GLN:HG2 | 39:DN:135:PRO:HD3 | 1.95 | 0.48 |
| 41:DP:35:HIS:O | 41:DP:36:LYS:HG3 | 2.13 | 0.48 |
| 44:DS:95:HIS:O | 44:DS:96:GLY:C | 2.52 | 0.48 |
| 45:DT:56:GLY:O | 45:DT:59:THR:CG2 | 2.61 | 0.48 |
| 46:DU:92:ARG:NH2 | 47:DV:10:LYS:CA | 2.76 | 0.48 |
| 47:DV:70:ILE:HB | 47:DV:90:PRO:CB | 2.40 | 0.48 |
| 1:AA:1133:G:N3 | 1:AA:1142:G:N2 | 2.60 | 0.48 |
| 1:AA:300:A:O5' | 1:AA:300:A:H8 | 1.96 | 0.48 |
| 1:AA:46:G:O2' | 1:AA:365:U:H1' | 2.13 | 0.48 |
| 1:AA:439:A:C4 | 1:AA:496:A:C2 | 3.01 | 0.48 |
| 1:AA:542:G:H2' | 1:AA:543:C:C6 | 2.46 | 0.48 |
| 2:AB:139:LYS:O | 2:AB:143:GLU:HG2 | 2.13 | 0.48 |
| 4:AD:106:TYR:CE1 | 4:AD:112:VAL:O | 2.67 | 0.48 |
| 4:AD:146:ILE:HD12 | 4:AD:146:ILE:H | 1.79 | 0.48 |
| 5:AE:101:ILE:HD11 | 5:AE:119:LEU:HA | 1.94 | 0.48 |
| 6:AF:12:PRO:HB2 | 6:AF:57:GLN:HB2 | 1.94 | 0.48 |
| 9:AI:4:TYR:CD1 | 9:AI:4:TYR:N | 2.81 | 0.48 |
| 10:AJ:94:VAL:HG12 | 10:AJ:95:GLU:N | 2.29 | 0.48 |
| 15:AO:56:LEU:HD21 | 31:BA:715:G:C2 | 2.48 | 0.48 |
| 18:AR:62:GLU:O | 18:AR:65:ILE:HD12 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:AR:85:LEU:HD12 | 18:AR:86:VAL:H | 1.78 | 0.48 |
| 28:B6:24:GLU:HA | 28:B6:24:GLU:OE1 | 2.13 | 0.48 |
| 30:B8:29:LYS:O | 30:B8:31:HIS:N | 2.46 | 0.48 |
| 30:B8:62:LEU:N | 30:B8:63:PRO:CD | 2.76 | 0.48 |
| 31:BA:1266:G:O5' | 48:BW:15:ARG:NH2 | 2.47 | 0.48 |
| 31:BA:1436:G:H3' | 31:BA:1437:C:H5'' | 1.96 | 0.48 |
| 31:BA:478:A:N1 | 31:BA:500:G:H4' | 2.28 | 0.48 |
| 31:BA:691:C:O2' | 31:BA:692:C:H5' | 2.13 | 0.48 |
| 31:BA:795:C:H2' | 31:BA:796:C:H6 | 1.79 | 0.48 |
| 32:BB:79:C:H2' | 32:BB:80:U:O4' | 2.13 | 0.48 |
| 34:BE:134:ILE:H | 34:BE:134:ILE:CD1 | 2.26 | 0.48 |
| 34:BE:47:VAL:HB | 34:BE:49:LEU:HD22 | 1.96 | 0.48 |
| 35:BF:22:ALA:CA | 35:BF:26:ALA:HB2 | 2.43 | 0.48 |
| 32:BB:41:U:O4 | 36:BG:70:VAL:O | 2.31 | 0.48 |
| 37:BH:44:VAL:HG12 | 37:BH:45:VAL:N | 2.22 | 0.48 |
| 38:BI:94:ALA:HB1 | 38:BI:114:LEU:HD12 | 1.94 | 0.48 |
| 31:BA:832:G:H21 | 41:BP:53:GLY:HA3 | 1.78 | 0.48 |
| 44:BS:16:ASN:HB3 | 44:BS:20:ARG:HH21 | 1.78 | 0.48 |
| 44:BS:28:VAL:HB | 44:BS:89:ARG:CB | 2.41 | 0.48 |
| 45:BT:87:ASP:OD1 | 45:BT:87:ASP:N | 2.45 | 0.48 |
| 31:BA:310:A:OP1 | 50:BY:17:SER:O | 2.31 | 0.48 |
| 51:BZ:10:ARG:HH21 | 51:BZ:26:GLY:H | 1.60 | 0.48 |
| 1:CA:109:A:H2' | 1:CA:326:G:N2 | 2.28 | 0.48 |
| 1:CA:339:C:H2' | 1:CA:340:U:C6 | 2.48 | 0.48 |
| 1:CA:523:A:N6 | 12:CL:53:ARG:HH12 | 2.11 | 0.48 |
| 1:CA:820:U:H4' | 1:CA:821:G:OP2 | 2.13 | 0.48 |
| 3:CC:119:ARG:HH21 | 3:CC:140:ARG:CZ | 2.26 | 0.48 |
| 4:CD:62:GLN:HA | 4:CD:62:GLN:HE21 | 1.78 | 0.48 |
| 6:CF:5:GLU:HB3 | 6:CF:62:TRP:NE1 | 2.27 | 0.48 |
| 6:CF:63:TYR:N | 6:CF:63:TYR:CD2 | 2.81 | 0.48 |
| 10:CJ:22:LYS:NZ | 10:CJ:88:LEU:HD23 | 2.28 | 0.48 |
| 13:CM:97:PRO:HB2 | 13:CM:101:GLN:NE2 | 2.28 | 0.48 |
| 17:CQ:99:SER:O | 17:CQ:100:LYS:HD3 | 2.14 | 0.48 |
| 19:CS:6:LYS:HG2 | 19:CS:7:LYS:HD3 | 1.95 | 0.48 |
| 20:CT:64:ASP:OD2 | 20:CT:81:LYS:NZ | 2.46 | 0.48 |
| 24:D2:41:ILE:CG1 | 31:DA:94(A):G:H22 | 2.26 | 0.48 |
| 30:D8:29:LYS:O | 30:D8:32:LEU:N | 2.47 | 0.48 |
| 31:DA:78:A:C6 | 31:DA:109:G:C6 | 3.00 | 0.48 |
| 31:DA:2276:G:O2' | 31:DA:2277:G:H5' | 2.12 | 0.48 |
| 31:DA:2313:C:H2' | 31:DA:2314:C:C6 | 2.47 | 0.48 |
| 31:DA:2580:U:C5' | 34:DE:131:ALA:HB2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:2593:U:H2' | 31:DA:2594:C:C6 | 2.48 | 0.48 |
| 31:DA:817:C:C2 | 31:DA:818:G:C8 | 3.01 | 0.48 |
| 31:DA:848:G:C4 | 31:DA:933:A:H8 | 2.32 | 0.48 |
| 32:DB:41:U:C4 | 36:DG:70:VAL:O | 2.67 | 0.48 |
| 33:DD:101:GLU:OE1 | 33:DD:103:ARG:HD3 | 2.13 | 0.48 |
| 33:DD:231:HIS:HB3 | 33:DD:233:HIS:O | 2.14 | 0.48 |
| 31:DA:1568:G:P | 33:DD:63:ARG:HH22 | 2.36 | 0.48 |
| 34:DE:179:GLU:HB3 | 34:DE:181:LEU:HD22 | 1.95 | 0.48 |
| 38:DI:76:THR:CG2 | 38:DI:139:GLN:HB3 | 2.43 | 0.48 |
| 30:D8:59:LYS:CD | 41:DP:50:ARG:HB3 | 2.41 | 0.48 |
| 44:DS:17:ARG:C | 44:DS:19:LYS:N | 2.67 | 0.48 |
| 45:DT:28:VAL:O | 45:DT:29:ARG:HD2 | 2.13 | 0.48 |
| 47:DV:19:LYS:CD | 47:DV:20:LEU:H | 2.24 | 0.48 |
| 49:DX:65:ARG:NE | 49:DX:66:LEU:N | 2.61 | 0.48 |
| 50:DY:54:LYS:O | 50:DY:55:TYR:O | 2.30 | 0.48 |
| 1:AA:678:U:H2' | 1:AA:679:C:C6 | 2.48 | 0.48 |
| 1:AA:963:G:H21 | 10:AJ:55:LYS:HD3 | 1.77 | 0.48 |
| 8:AH:48:TYR:HA | 8:AH:60:ARG:O | 2.13 | 0.48 |
| 14:AN:21:TYR:OH | 14:AN:23:ARG:NH2 | 2.47 | 0.48 |
| 14:AN:41:ARG:HG3 | 14:AN:42:ILE:HD13 | 1.95 | 0.48 |
| 16:AP:39:TYR:CD2 | 16:AP:73:LEU:HD13 | 2.49 | 0.48 |
| 23:B1:8:SER:HB3 | 31:BA:1364:G:OP1 | 2.14 | 0.48 |
| 24:B2:51:ARG:O | 24:B2:52:ASP:HB2 | 2.14 | 0.48 |
| 24:B2:57:ILE:O | 24:B2:57:ILE:HG23 | 2.12 | 0.48 |
| 28:B6:39:TYR:HB3 | 28:B6:49:HIS:ND1 | 2.28 | 0.48 |
| 31:BA:1188:U:O2' | 31:BA:1189:A:H5' | 2.14 | 0.48 |
| 31:BA:1628:G:H2' | 31:BA:1629:U:C6 | 2.48 | 0.48 |
| 31:BA:2364:C:O2' | 31:BA:2365:G:H5' | 2.14 | 0.48 |
| 31:BA:2865:U:C4 | 31:BA:2866:U:C4 | 3.01 | 0.48 |
| 31:BA:614:U:H5' | 31:BA:614(C):A:N6 | 2.27 | 0.48 |
| 31:BA:634:C:H2' | 31:BA:635:C:C6 | 2.48 | 0.48 |
| 31:BA:848:G:N3 | 31:BA:933:A:H1' | 2.28 | 0.48 |
| 31:BA:971:C:C2' | 31:BA:972:G:H5' | 2.44 | 0.48 |
| 32:BB:73:A:H3' | 32:BB:74:U:H6 | 1.77 | 0.48 |
| 32:BB:82:G:O2' | 32:BB:83:G:H5' | 2.12 | 0.48 |
| 31:BA:2680:C:H5' | 34:BE:189:PRO:HA | 1.96 | 0.48 |
| 34:BE:167:VAL:CG1 | 34:BE:189:PRO:HD3 | 2.43 | 0.48 |
| 36:BG:57:ALA:CB | 36:BG:90:LEU:HD21 | 2.43 | 0.48 |
| 37:BH:138:LYS:C | 37:BH:140:LYS:N | 2.66 | 0.48 |
| 38:BI:136:VAL:O | 38:BI:136:VAL:HG22 | 2.13 | 0.48 |
| 38:BI:8:PRO:HA | 38:BI:13:GLY:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BN:2:LYS:HZ2 | 46:BU:94:ASN:HD21 | 1.62 | 0.48 |
| 41:BP:71:VAL:CG1 | 41:BP:72:PRO:CD | 2.90 | 0.48 |
| 42:BQ:58:PHE:CD1 | 42:BQ:58:PHE:O | 2.62 | 0.48 |
| 47:BV:64:HIS:HB3 | 47:BV:96:ILE:HG12 | 1.95 | 0.48 |
| 1:CA:131:C:H2' | 1:CA:132:C:C6 | 2.48 | 0.48 |
| 1:CA:394:G:H2' | 1:CA:395:C:H6 | 1.78 | 0.48 |
| 1:CA:719:C:C5 | 1:CA:720:C:C4 | 3.02 | 0.48 |
| 1:CA:814:A:N7 | 1:CA:816:A:C5 | 2.81 | 0.48 |
| 2:CB:161:ALA:HB1 | 2:CB:185:ILE:CD1 | 2.44 | 0.48 |
| 3:CC:188:LEU:O | 3:CC:189:ALA:CB | 2.61 | 0.48 |
| 4:CD:107:ARG:CD | 4:CD:173:TRP:HZ2 | 2.27 | 0.48 |
| 5:CE:36:ASP:O | 5:CE:37:ARG:HB2 | 2.13 | 0.48 |
| 7:CG:69:VAL:O | 7:CG:69:VAL:HG12 | 2.13 | 0.48 |
| 9:CI:61:ALA:HB1 | 9:CI:63:ILE:HD11 | 1.96 | 0.48 |
| 11:CK:21:ILE:HB | 11:CK:84:VAL:HG12 | 1.95 | 0.48 |
| 11:CK:111:ASP:HA | 18:CR:84:LYS:HE2 | 1.95 | 0.48 |
| 30:D8:10:ALA:HB2 | 30:D8:59:LYS:NZ | 2.28 | 0.48 |
| 31:DA:118:A:C8 | 31:DA:119:A:C8 | 3.02 | 0.48 |
| 31:DA:1509(A):A:C5 | 31:DA:1509(B):A:N7 | 2.82 | 0.48 |
| 31:DA:1572:A:O5' | 31:DA:1572:A:H8 | 1.96 | 0.48 |
| 31:DA:175:G:H5' | 31:DA:175:G:C8 | 2.48 | 0.48 |
| 31:DA:1836:C:C2' | 31:DA:1837:C:H5' | 2.44 | 0.48 |
| 31:DA:2321:G:H5'' | 31:DA:2322:A:OP2 | 2.13 | 0.48 |
| 31:DA:257:A:C2' | 31:DA:258:G:H5' | 2.43 | 0.48 |
| 31:DA:2694:G:C5 | 31:DA:2695:C:C5 | 3.02 | 0.48 |
| 31:DA:2773:C:O2' | 31:DA:2774:C:H5' | 2.14 | 0.48 |
| 31:DA:2887:U:H2' | 31:DA:2888:C:C6 | 2.48 | 0.48 |
| 31:DA:247:G:H4' | 31:DA:386:G:C6 | 2.49 | 0.48 |
| 31:DA:810:U:O2' | 41:DP:33:ARG:CZ | 2.61 | 0.48 |
| 31:DA:825:C:C6 | 31:DA:825:C:H3' | 2.48 | 0.48 |
| 33:DD:25:THR:O | 33:DD:25:THR:CG2 | 2.59 | 0.48 |
| 33:DD:34:VAL:C | 33:DD:35:LYS:O | 2.50 | 0.48 |
| 34:DE:201:THR:HG22 | 34:DE:202:LYS:H | 1.76 | 0.48 |
| 34:DE:2:LYS:NZ | 34:DE:95:ILE:O | 2.47 | 0.48 |
| 35:DF:203:GLN:O | 35:DF:206:ILE:C | 2.51 | 0.48 |
| 35:DF:41:LEU:O | 35:DF:44:ARG:HG2 | 2.14 | 0.48 |
| 36:DG:64:THR:HG23 | 36:DG:66:GLN:N | 2.27 | 0.48 |
| 39:DN:128:HIS:O | 39:DN:128:HIS:CD2 | 2.66 | 0.48 |
| 41:DP:52:GLU:C | 41:DP:54:GLY:H | 2.15 | 0.48 |
| 41:DP:95:VAL:HG13 | 41:DP:123:LEU:HD11 | 1.94 | 0.48 |
| 42:DQ:72:LYS:HB3 | 42:DQ:94:VAL:HG23 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:1279:G:H5' | 43:DR:34:ILE:CD1 | 2.44 | 0.48 |
| 44:DS:16:ASN:ND2 | 44:DS:92:TYR:CZ | 2.82 | 0.48 |
| 45:DT:27:THR:O | 45:DT:28:VAL:CG2 | 2.61 | 0.48 |
| 49:DX:53:LYS:N | 49:DX:80:ILE:HG22 | 2.25 | 0.48 |
| 1:AA:994:A:N6 | 1:AA:1046:A:H2 | 2.10 | 0.48 |
| 1:AA:1132:C:H2' | 1:AA:1133:G:O4' | 2.13 | 0.48 |
| 1:AA:1092:A:C2 | 1:AA:1183:A:C2 | 3.02 | 0.48 |
| 1:AA:1226:C:C5 | 13:AM:104:ARG:HB2 | 2.49 | 0.48 |
| 1:AA:1372:U:H2' | 1:AA:1373:G:O4' | 2.13 | 0.48 |
| 1:AA:510:A:H5'' | 1:AA:511:C:P | 2.53 | 0.48 |
| 1:AA:66:G:C6 | 1:AA:67:C:C5 | 3.01 | 0.48 |
| 1:AA:674:G:H2' | 1:AA:675:A:H8 | 1.78 | 0.48 |
| 1:AA:779:C:H2' | 1:AA:780:A:O4' | 2.14 | 0.48 |
| 3:AC:119:ARG:HH21 | 3:AC:140:ARG:CZ | 2.26 | 0.48 |
| 4:AD:119:GLN:O | 4:AD:123:HIS:HD2 | 1.94 | 0.48 |
| 5:AE:100:VAL:O | 5:AE:107:ARG:NH2 | 2.47 | 0.48 |
| 8:AH:91:ARG:HG2 | 8:AH:91:ARG:HH11 | 1.77 | 0.48 |
| 9:AI:16:ARG:O | 9:AI:63:ILE:HA | 2.13 | 0.48 |
| 10:AJ:24:VAL:HG21 | 10:AJ:37:PRO:HD3 | 1.94 | 0.48 |
| 1:AA:963:G:N2 | 10:AJ:55:LYS:HE2 | 2.28 | 0.48 |
| 11:AK:41:THR:CG2 | 11:AK:42:TRP:H | 2.25 | 0.48 |
| 22:B0:41:ARG:HB3 | 31:BA:2330:G:H1' | 1.95 | 0.48 |
| 29:B7:15:THR:HG22 | 29:B7:16:HIS:ND1 | 2.26 | 0.48 |
| 30:B8:35:GLN:HA | 31:BA:2420:C:P | 2.54 | 0.48 |
| 31:BA:1106:A:C2' | 31:BA:1107:G:C8 | 2.96 | 0.48 |
| 31:BA:1040:C:N4 | 31:BA:1115:G:H1 | 2.12 | 0.48 |
| 31:BA:1579:A:H2' | 31:BA:1580:A:C8 | 2.49 | 0.48 |
| 31:BA:2416:C:H6 | 31:BA:2416:C:O5' | 1.97 | 0.48 |
| 31:BA:2659:G:C5' | 31:BA:2659:G:H8 | 2.27 | 0.48 |
| 31:BA:271(O):C:O2' | 31:BA:271(P):C:C5 | 2.67 | 0.48 |
| 31:BA:2846:G:H2' | 31:BA:2847:U:O4' | 2.14 | 0.48 |
| 31:BA:528:A:H2' | 31:BA:529:A:H5' | 1.95 | 0.48 |
| 32:BB:20:C:C2' | 32:BB:21:G:H5'' | 2.43 | 0.48 |
| 31:BA:2580:U:C5' | 34:BE:131:ALA:HB2 | 2.44 | 0.48 |
| 34:BE:4:ILE:O | 34:BE:4:ILE:HG23 | 2.13 | 0.48 |
| 34:BE:52:LEU:O | 34:BE:74:PRO:CA | 2.62 | 0.48 |
| 35:BF:4:VAL:HG12 | 35:BF:4:VAL:O | 2.13 | 0.48 |
| 37:BH:85:LYS:NZ | 37:BH:145:ALA:HA | 2.29 | 0.48 |
| 37:BH:153:LYS:HB2 | 37:BH:154:PRO:HD3 | 1.95 | 0.48 |
| 37:BH:41:MET:HE2 | 37:BH:41:MET:CA | 2.37 | 0.48 |
| 43:BR:71:GLN:NE2 | 43:BR:71:GLN:HA | 2.19 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:BR:75:LEU:O | 43:BR:75:LEU:HD13 | 2.14 | 0.48 |
| 47:BV:73:SER:HG | 47:BV:74:LYS:N | 2.12 | 0.48 |
| 48:BW:111:HIS:CD2 | 48:BW:112:GLY:H | 2.30 | 0.48 |
| 49:BX:3:THR:HA | 49:BX:6:ASP:OD2 | 2.14 | 0.48 |
| 50:BY:95:LYS:CD | 50:BY:100:ALA:HB1 | 2.15 | 0.48 |
| 51:BZ:16:SER:HA | 51:BZ:19:ARG:HD2 | 1.95 | 0.48 |
| 1:CA:1316:G:H1 | 19:CS:5:LEU:HD21 | 1.78 | 0.48 |
| 1:CA:1504:G:H4' | 1:CA:1505:G:O4' | 2.13 | 0.48 |
| 1:CA:233:C:H2' | 1:CA:234:C:H6 | 1.79 | 0.48 |
| 1:CA:520:A:H2 | 1:CA:536:C:O2 | 1.96 | 0.48 |
| 1:CA:645:C:O2' | 1:CA:646:U:H5' | 2.14 | 0.48 |
| 3:CC:24:ALA:HB1 | 3:CC:28:GLN:O | 2.14 | 0.48 |
| 4:CD:79:PHE:HZ | 4:CD:204:ILE:HD13 | 1.78 | 0.48 |
| 7:CG:12:LEU:HD13 | 7:CG:24:THR:OG1 | 2.14 | 0.48 |
| 9:CI:4:TYR:CD1 | 9:CI:4:TYR:N | 2.82 | 0.48 |
| 10:CJ:94:VAL:HG12 | 10:CJ:95:GLU:N | 2.28 | 0.48 |
| 1:CA:192:U:C1' | 20:CT:103:GLY:HA2 | 2.43 | 0.48 |
| 22:D0:13:GLY:O | 22:D0:14:ARG:CB | 2.38 | 0.48 |
| 24:D2:35:LEU:HD23 | 24:D2:35:LEU:H | 1.79 | 0.48 |
| 25:D3:39:ASP:OD1 | 25:D3:44:ARG:HG3 | 2.14 | 0.48 |
| 25:D3:1:MET:O | 25:D3:3:ARG:N | 2.47 | 0.48 |
| 31:DA:1331:A:O2' | 31:DA:1332:G:H8 | 1.96 | 0.48 |
| 31:DA:2006:C:H6 | 31:DA:2006:C:O5' | 1.97 | 0.48 |
| 31:DA:2184:G:O5' | 31:DA:2184:G:H8 | 1.97 | 0.48 |
| 31:DA:2702:U:OP1 | 31:DA:2702:U:O4' | 2.31 | 0.48 |
| 1:CA:1442(A):G:C6 | 31:DA:2863:C:H4' | 2.49 | 0.48 |
| 31:DA:51:G:N3 | 31:DA:119:A:C2 | 2.81 | 0.48 |
| 31:DA:892:G:H2' | 31:DA:893:C:O4' | 2.13 | 0.48 |
| 32:DB:44:G:C5' | 32:DB:45:A:OP1 | 2.55 | 0.48 |
| 33:DD:127:VAL:HA | 33:DD:193:VAL:HG22 | 1.94 | 0.48 |
| 33:DD:17:THR:O | 33:DD:17:THR:CG2 | 2.61 | 0.48 |
| 34:DE:39:PRO:HA | 34:DE:43:GLY:CA | 2.44 | 0.48 |
| 34:DE:61:ARG:N | 34:DE:62:PRO:CD | 2.76 | 0.48 |
| 35:DF:178:PRO:HG2 | 35:DF:179:GLU:OE1 | 2.14 | 0.48 |
| 42:DQ:27:VAL:HA | 42:DQ:105:GLU:OE1 | 2.14 | 0.48 |
| 42:DQ:78:PRO:O | 42:DQ:79:LEU:CB | 2.62 | 0.48 |
| 43:DR:24:GLN:HE22 | 43:DR:36:THR:HG21 | 1.78 | 0.48 |
| 44:DS:39:ILE:O | 44:DS:48:LEU:HD12 | 2.14 | 0.48 |
| 48:DW:28:SER:OG | 48:DW:31:GLU:HB2 | 2.14 | 0.48 |
| 49:DX:59:VAL:O | 49:DX:60:ARG:O | 2.31 | 0.48 |
| 50:DY:28:LYS:HE3 | 50:DY:37:VAL:HG12 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:DZ:52:SER:OG | 51:DZ:53:ILE:N | 2.45 | 0.48 |
| 1:AA:105:G:H2' | 1:AA:106:C:C6 | 2.48 | 0.48 |
| 1:AA:1081:G:N2 | 1:AA:1082:G:H1' | 2.27 | 0.48 |
| 1:AA:1086:U:H2' | 1:AA:1087:G:H8 | 1.79 | 0.48 |
| 1:AA:1098:C:C4 | 1:AA:1099:G:C8 | 3.02 | 0.48 |
| 1:AA:1332:A:O5' | 1:AA:1332:A:H8 | 1.97 | 0.48 |
| 1:AA:1410:G:N2 | 1:AA:1411:C:C2 | 2.81 | 0.48 |
| 1:AA:1446:U:HO2' | 1:AA:1447:A:H8 | 1.50 | 0.48 |
| 1:AA:243:A:C2 | 1:AA:246:A:C8 | 3.02 | 0.48 |
| 1:AA:273:A:C2' | 1:AA:274:A:H5' | 2.44 | 0.48 |
| 1:AA:541:G:H2' | 1:AA:542:G:H8 | 1.79 | 0.48 |
| 1:AA:93:G:C2' | 1:AA:96:U:H5' | 2.42 | 0.48 |
| 5:AE:13:ILE:HG13 | 5:AE:29:GLY:O | 2.14 | 0.48 |
| 8:AH:20:TYR:HA | 8:AH:65:TYR:CE2 | 2.49 | 0.48 |
| 8:AH:53:VAL:O | 8:AH:54:ASP:CB | 2.62 | 0.48 |
| 15:AO:78:TYR:O | 15:AO:82:ILE:HG22 | 2.14 | 0.48 |
| 18:AR:25:THR:CG2 | 18:AR:42:ARG:HH11 | 2.26 | 0.48 |
| 13:AM:86:CYS:HB2 | 19:AS:73:GLU:OE1 | 2.14 | 0.48 |
| 24:B2:16:LEU:N | 24:B2:18:PRO:HD2 | 2.29 | 0.48 |
| 27:B5:29:THR:HG21 | 31:BA:2815:C:H5' | 1.95 | 0.48 |
| 27:B5:32:PRO:O | 27:B5:33:CYS:CB | 2.60 | 0.48 |
| 29:B7:15:THR:HG22 | 29:B7:16:HIS:CE1 | 2.49 | 0.48 |
| 30:B8:39:LYS:HE2 | 30:B8:39:LYS:O | 2.14 | 0.48 |
| 30:B8:58:ILE:O | 30:B8:61:LEU:HG | 2.14 | 0.48 |
| 31:BA:1885:A:H2' | 31:BA:1886:C:O4' | 2.13 | 0.48 |
| 31:BA:1925:C:O2' | 31:BA:1926:U:H5' | 2.13 | 0.48 |
| 31:BA:1932:A:C2 | 31:BA:1969:A:C2 | 3.02 | 0.48 |
| 31:BA:2448:A:H4' | 31:BA:2449:U:OP2 | 2.13 | 0.48 |
| 31:BA:2602:A:H4' | 31:BA:2603:G:O5' | 2.14 | 0.48 |
| 31:BA:2849:U:H5' | 31:BA:2867:G:N2 | 2.27 | 0.48 |
| 31:BA:61:G:H1 | 31:BA:94:C:N4 | 2.11 | 0.48 |
| 31:BA:664:C:H4' | 31:BA:941:A:OP1 | 2.13 | 0.48 |
| 31:BA:740:U:H2' | 31:BA:741:G:C8 | 2.49 | 0.48 |
| 31:BA:92:A:H2' | 31:BA:93:G:C8 | 2.49 | 0.48 |
| 33:BD:167:GLY:O | 33:BD:168:ARG:HG2 | 2.14 | 0.48 |
| 33:BD:35:LYS:CA | 33:BD:64:ILE:CG2 | 2.91 | 0.48 |
| 34:BE:28:ALA:HB3 | 34:BE:93:VAL:HG22 | 1.93 | 0.48 |
| 35:BF:205:ARG:O | 35:BF:206:ILE:HG13 | 2.13 | 0.48 |
| 39:BN:130:HIS:CD2 | 39:BN:130:HIS:O | 2.66 | 0.48 |
| 43:BR:4:LEU:C | 43:BR:6:SER:H | 2.15 | 0.48 |
| 39:BN:39:ARG:O | 46:BU:64:ARG:NH1 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:BV:51:VAL:CG1 | 47:BV:52:VAL:N | 2.77 | 0.48 |
| 47:BV:6:LYS:HG3 | 47:BV:6:LYS:O | 2.14 | 0.48 |
| 47:BV:73:SER:O | 47:BV:74:LYS:HB2 | 2.13 | 0.48 |
| 46:BU:50:ARG:NH2 | 47:BV:75:PHE:CE2 | 2.81 | 0.48 |
| 1:CA:1081:G:N2 | 1:CA:1082:G:H1' | 2.29 | 0.48 |
| 1:CA:1365:G:C5 | 1:CA:1366:C:C5 | 3.02 | 0.48 |
| 1:CA:373:A:C2 | 1:CA:374:A:C8 | 3.01 | 0.48 |
| 1:CA:90:U:O2' | 1:CA:91:C:C5 | 2.63 | 0.48 |
| 2:CB:163:PHE:HA | 2:CB:185:ILE:O | 2.13 | 0.48 |
| 2:CB:97:TRP:HH2 | 2:CB:176:GLU:CD | 2.17 | 0.48 |
| 2:CB:36:ARG:HB2 | 2:CB:41:ILE:HD13 | 1.95 | 0.48 |
| 4:CD:126:ILE:CG2 | 4:CD:127:THR:H | 2.20 | 0.48 |
| 6:CF:45:LEU:HG | 6:CF:46:ARG:N | 2.29 | 0.48 |
| 8:CH:20:TYR:HD1 | 8:CH:65:TYR:CD2 | 2.31 | 0.48 |
| 18:CR:85:LEU:HD12 | 18:CR:86:VAL:H | 1.78 | 0.48 |
| 20:CT:56:MET:O | 20:CT:59:ALA:HB3 | 2.13 | 0.48 |
| 24:D2:41:ILE:O | 24:D2:42:GLY:O | 2.32 | 0.48 |
| 26:D4:19:GLY:C | 26:D4:21:VAL:N | 2.66 | 0.48 |
| 27:D5:32:PRO:O | 27:D5:33:CYS:CB | 2.61 | 0.48 |
| 30:D8:39:LYS:CD | 30:D8:39:LYS:C | 2.81 | 0.48 |
| 31:DA:1174:A:OP1 | 31:DA:1175:U:H5'' | 2.14 | 0.48 |
| 31:DA:1342:A:H5' | 31:DA:1398:C:OP1 | 2.14 | 0.48 |
| 31:DA:1669:A:H5'' | 31:DA:2550:G:OP1 | 2.14 | 0.48 |
| 31:DA:1696:G:C6 | 31:DA:1697:G:C5 | 3.02 | 0.48 |
| 31:DA:1742:G:H3' | 31:DA:1742:G:C8 | 2.49 | 0.48 |
| 31:DA:303:U:H2' | 31:DA:304:G:C8 | 2.49 | 0.48 |
| 31:DA:478:A:C6 | 31:DA:480:A:C6 | 3.01 | 0.48 |
| 32:DB:28:C:H2' | 32:DB:29:A:O4' | 2.14 | 0.48 |
| 32:DB:45:A:H2' | 32:DB:45:A:N3 | 2.28 | 0.48 |
| 32:DB:79:C:H2' | 32:DB:80:U:O4' | 2.13 | 0.48 |
| 35:DF:7:TYR:HD1 | 35:DF:8:GLN:H | 1.58 | 0.48 |
| 37:DH:41:MET:HE1 | 37:DH:55:PRO:HD3 | 1.95 | 0.48 |
| 44:DS:66:ALA:HA | 44:DS:69:VAL:HG12 | 1.96 | 0.48 |
| 45:DT:30:VAL:HG21 | 45:DT:83:ILE:HG12 | 1.96 | 0.48 |
| 46:DU:75:ASN:HB3 | 46:DU:77:SER:OG | 2.14 | 0.48 |
| 1:AA:175:C:C2 | 1:AA:176:C:C5 | 3.02 | 0.48 |
| 1:AA:295:C:H2' | 1:AA:296:U:O4' | 2.13 | 0.48 |
| 1:AA:738:C:N3 | 1:AA:739:C:C5 | 2.82 | 0.48 |
| 1:AA:985:C:H6 | 1:AA:985:C:O5' | 1.96 | 0.48 |
| 2:AB:68:ILE:HG22 | 2:AB:70:PHE:CE1 | 2.49 | 0.48 |
| 4:AD:93:PHE:O | 4:AD:97:LEU:HG | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:79:LEU:HD11 | 9:AI:83:ARG:CZ | 2.44 | 0.48 |
| 12:AL:22:SER:O | 12:AL:24:VAL:N | 2.47 | 0.48 |
| 20:AT:46:GLU:CG | 20:AT:48:LYS:HE2 | 2.44 | 0.48 |
| 22:B0:55:ARG:HB3 | 22:B0:55:ARG:HE | 1.27 | 0.48 |
| 30:B8:35:GLN:HB3 | 30:B8:36:LYS:H | 1.40 | 0.48 |
| 31:BA:1044:G:C2 | 31:BA:1112:G:O6 | 2.67 | 0.48 |
| 31:BA:1481:U:H5' | 31:BA:1482:G:P | 2.54 | 0.48 |
| 31:BA:1563:G:C5 | 31:BA:1564:C:C5 | 3.01 | 0.48 |
| 31:BA:1668:A:H4' | 31:BA:1669:A:O5' | 2.13 | 0.48 |
| 31:BA:1722:A:N6 | 31:BA:1741:A:H2 | 2.11 | 0.48 |
| 31:BA:2184:G:H8 | 31:BA:2184:G:O5' | 1.96 | 0.48 |
| 31:BA:2092:U:C4 | 31:BA:2226:C:OP2 | 2.67 | 0.48 |
| 31:BA:2518:A:H8 | 31:BA:2518:A:H5' | 1.79 | 0.48 |
| 31:BA:2820:A:O4' | 43:BR:5:LYS:HG3 | 2.13 | 0.48 |
| 31:BA:960:A:H5'' | 31:BA:961:C:OP2 | 2.13 | 0.48 |
| 34:BE:36:ARG:NH1 | 34:BE:85:ASN:ND2 | 2.62 | 0.48 |
| 35:BF:129:PHE:CD2 | 35:BF:163:VAL:HG21 | 2.48 | 0.48 |
| 40:BO:13:ASN:HD22 | 40:BO:13:ASN:H | 1.60 | 0.48 |
| 40:BO:50:GLY:C | 40:BO:52:VAL:N | 2.67 | 0.48 |
| 41:BP:59:LEU:CA | 41:BP:61:ARG:NH1 | 2.59 | 0.48 |
| 42:BQ:20:ALA:CB | 42:BQ:99:PRO:HG2 | 2.43 | 0.48 |
| 44:BS:95:HIS:CG | 44:BS:96:GLY:N | 2.74 | 0.48 |
| 45:BT:40:THR:O | 45:BT:41:ARG:CB | 2.62 | 0.48 |
| 50:BY:45:VAL:HG22 | 50:BY:62:GLU:CA | 2.43 | 0.48 |
| 50:BY:45:VAL:HG21 | 50:BY:62:GLU:H | 1.79 | 0.48 |
| 51:BZ:14:LYS:HB2 | 51:BZ:17:ALA:CB | 2.44 | 0.48 |
| 1:CA:1085:U:C6 | 1:CA:1094:G:N1 | 2.82 | 0.48 |
| 1:CA:1410:G:N2 | 1:CA:1411:C:C2 | 2.82 | 0.48 |
| 1:CA:563:A:N7 | 1:CA:567:G:H1' | 2.28 | 0.48 |
| 1:CA:582:U:C2 | 1:CA:760:G:C6 | 3.02 | 0.48 |
| 1:CA:985:C:H6 | 1:CA:985:C:O5' | 1.97 | 0.48 |
| 2:CB:20:GLU:HG3 | 2:CB:191:ASP:HB2 | 1.96 | 0.48 |
| 2:CB:61:LEU:CD2 | 2:CB:68:ILE:HD11 | 2.44 | 0.48 |
| 4:CD:14:ARG:HA | 4:CD:39:PRO:HG3 | 1.94 | 0.48 |
| 4:CD:13:ARG:HD2 | 4:CD:38:TYR:O | 2.14 | 0.48 |
| 7:CG:27:ILE:HD11 | 7:CG:43:PHE:CD2 | 2.49 | 0.48 |
| 16:CP:79:VAL:HG12 | 16:CP:80:PHE:CG | 2.49 | 0.48 |
| 22:D0:56:ASP:OD1 | 31:DA:2364:C:H5' | 2.14 | 0.48 |
| 27:D5:5:PRO:O | 27:D5:6:VAL:HG23 | 2.14 | 0.48 |
| 31:DA:1158:C:H6 | 31:DA:1158:C:O5' | 1.96 | 0.48 |
| 31:DA:1386:C:OP2 | 31:DA:1396:U:H5 | 1.97 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:1550:C:O2' | 31:DA:1551:C:H5' | 2.13 | 0.48 |
| 31:DA:2243:U:H2' | 31:DA:2244:U:C6 | 2.49 | 0.48 |
| 31:DA:2273:A:O2' | 31:DA:2274:A:H5' | 2.13 | 0.48 |
| 31:DA:2319:G:OP2 | 31:DA:2319:G:H4' | 2.13 | 0.48 |
| 31:DA:2476:A:C6 | 31:DA:2477:C:C5 | 3.02 | 0.48 |
| 31:DA:2521:C:H42 | 31:DA:2544:G:H1 | 1.61 | 0.48 |
| 31:DA:481:G:O2' | 31:DA:482:A:P | 2.71 | 0.48 |
| 33:DD:33:LEU:HB3 | 33:DD:34:VAL:H | 1.35 | 0.48 |
| 34:DE:101:ARG:HG3 | 34:DE:169:ASN:HD21 | 1.78 | 0.48 |
| 41:DP:10:PRO:CD | 41:DP:11:GLY:N | 2.75 | 0.48 |
| 41:DP:85:LEU:HA | 41:DP:88:LEU:HB2 | 1.95 | 0.48 |
| 45:DT:30:VAL:HG21 | 45:DT:83:ILE:N | 2.28 | 0.48 |
| 47:DV:79:VAL:HG23 | 47:DV:82:ARG:CD | 2.43 | 0.48 |
| 31:DA:494:G:O2' | 48:DW:5:ALA:O | 2.27 | 0.48 |
| 31:DA:1341:U:N3 | 49:DX:77:LYS:HE2 | 2.28 | 0.48 |
| 51:DZ:96:VAL:N | 51:DZ:128:VAL:O | 2.47 | 0.48 |
| 1:AA:1456:G:H2' | 1:AA:1457:G:O4' | 2.14 | 0.48 |
| 1:AA:357:G:H2' | 1:AA:358:U:H5' | 1.95 | 0.48 |
| 1:AA:684:A:C6 | 1:AA:685:G:C6 | 3.02 | 0.48 |
| 1:AA:719:C:C5 | 1:AA:720:C:C4 | 3.01 | 0.48 |
| 1:AA:930:C:C2' | 1:AA:931:C:H5' | 2.44 | 0.48 |
| 2:AB:142:LEU:HD23 | 2:AB:142:LEU:C | 2.35 | 0.48 |
| 2:AB:97:TRP:CH2 | 2:AB:176:GLU:HG3 | 2.49 | 0.48 |
| 4:AD:128:VAL:O | 4:AD:130:GLY:N | 2.46 | 0.48 |
| 5:AE:75:THR:HG23 | 5:AE:76:ILE:N | 2.28 | 0.48 |
| 1:AA:710:G:OP1 | 6:AF:54:LYS:HE3 | 2.14 | 0.48 |
| 8:AH:82:HIS:HD2 | 8:AH:138:TRP:NE1 | 2.11 | 0.48 |
| 10:AJ:22:LYS:NZ | 10:AJ:88:LEU:HD23 | 2.29 | 0.48 |
| 1:AA:522:C:H41 | 12:AL:53:ARG:HH22 | 1.61 | 0.48 |
| 20:AT:53:LEU:HA | 20:AT:56:MET:HB2 | 1.96 | 0.48 |
| 20:AT:75:ASN:HD22 | 20:AT:75:ASN:H | 1.62 | 0.48 |
| 23:B1:9:GLY:O | 23:B1:10:LYS:CB | 2.60 | 0.48 |
| 24:B2:46:GLN:NE2 | 24:B2:47:ASN:CA | 2.75 | 0.48 |
| 29:B7:5:TRP:CH2 | 31:BA:686:G:N7 | 2.81 | 0.48 |
| 30:B8:39:LYS:HE2 | 30:B8:42:ARG:NH1 | 2.29 | 0.48 |
| 31:BA:1327:C:C2' | 31:BA:1328:G:H5' | 2.44 | 0.48 |
| 31:BA:1353:A:H5'' | 33:BD:38:LYS:HZ1 | 1.79 | 0.48 |
| 31:BA:1783:A:C2 | 31:BA:2587:A:C5 | 3.02 | 0.48 |
| 31:BA:1948:G:H2' | 31:BA:1949:G:O5' | 2.14 | 0.48 |
| 31:BA:2070:G:H2' | 31:BA:2071:A:H8 | 1.79 | 0.48 |
| 31:BA:2335:A:N7 | 31:BA:2337:G:C5 | 2.82 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:BA:363(C):G:C4 | 31:BA:363(D):G:C8 | 3.02 | 0.48 |
| 31:BA:49:A:H5'' | 31:BA:51:G:O4' | 2.14 | 0.48 |
| 31:BA:708:C:H42 | 31:BA:723:G:H1 | 1.60 | 0.48 |
| 32:BB:29:A:H2' | 32:BB:30:C:C6 | 2.48 | 0.48 |
| 32:BB:66:A:C5 | 32:BB:109:C:C5 | 3.02 | 0.48 |
| 34:BE:120:TRP:O | 34:BE:121:ASN:HB2 | 2.14 | 0.48 |
| 34:BE:27:LEU:HD12 | 34:BE:181:LEU:HD13 | 1.96 | 0.48 |
| 31:BA:271(P):C:O3' | 38:BI:42:SER:OG | 2.31 | 0.48 |
| 39:BN:128:HIS:O | 39:BN:128:HIS:CD2 | 2.66 | 0.48 |
| 39:BN:1:MET:HB3 | 47:BV:20:LEU:CD2 | 2.27 | 0.48 |
| 44:BS:95:HIS:O | 44:BS:97:ARG:O | 2.32 | 0.48 |
| 45:BT:51:ARG:HD2 | 45:BT:62:THR:HG23 | 1.95 | 0.48 |
| 50:BY:54:LYS:O | 50:BY:55:TYR:O | 2.32 | 0.48 |
| 50:BY:89:PHE:O | 50:BY:90:LEU:HB3 | 2.14 | 0.48 |
| 51:BZ:128:VAL:HG21 | 51:BZ:161:VAL:HG22 | 1.96 | 0.48 |
| 51:BZ:7:ALA:O | 51:BZ:38:TYR:O | 2.31 | 0.48 |
| 1:CA:1064:G:O5' | 1:CA:1064:G:H8 | 1.97 | 0.48 |
| 1:CA:129:U:H5' | 17:CQ:3:LYS:NZ | 2.28 | 0.48 |
| 1:CA:27:G:O2' | 1:CA:28:G:H5' | 2.13 | 0.48 |
| 1:CA:764:C:C2 | 1:CA:765:G:C8 | 3.02 | 0.48 |
| 1:CA:983:A:H3' | 1:CA:983:A:N3 | 2.29 | 0.48 |
| 2:CB:21:ARG:CB | 2:CB:39:ILE:HA | 2.44 | 0.48 |
| 3:CC:148:GLY:HA3 | 3:CC:172:ARG:O | 2.14 | 0.48 |
| 9:CI:55:ALA:HB1 | 9:CI:58:ARG:HD2 | 1.96 | 0.48 |
| 11:CK:20:TYR:O | 11:CK:30:VAL:HA | 2.14 | 0.48 |
| 13:CM:20:THR:C | 13:CM:22:ILE:H | 2.18 | 0.48 |
| 13:CM:17:VAL:O | 13:CM:20:THR:HB | 2.13 | 0.48 |
| 18:CR:44:LEU:O | 18:CR:45:SER:O | 2.32 | 0.48 |
| 24:D2:43:GLN:O | 24:D2:46:GLN:CB | 2.62 | 0.48 |
| 29:D7:8:ASN:HD21 | 29:D7:11:LYS:N | 2.07 | 0.48 |
| 30:D8:36:LYS:O | 30:D8:37:SER:O | 2.32 | 0.48 |
| 31:DA:1000:A:C6 | 31:DA:1001:A:C6 | 3.02 | 0.48 |
| 31:DA:1436:G:H3' | 31:DA:1437:C:H5'' | 1.96 | 0.48 |
| 31:DA:1642:G:O2' | 31:DA:1643:G:H5' | 2.14 | 0.48 |
| 31:DA:1747(A):G:O2' | 31:DA:1748:G:H5' | 2.14 | 0.48 |
| 31:DA:1992:G:O2' | 31:DA:1993:U:OP2 | 2.25 | 0.48 |
| 31:DA:2030:A:C5' | 31:DA:2031:A:OP1 | 2.58 | 0.48 |
| 31:DA:2063:C:O2 | 31:DA:2450:A:N1 | 2.47 | 0.48 |
| 31:DA:319:C:H2' | 31:DA:320:A:O4' | 2.14 | 0.48 |
| 31:DA:51:G:H4' | 31:DA:52:A:H5' | 1.96 | 0.48 |
| 31:DA:588:U:H2' | 31:DA:589:C:H6 | 1.72 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:D2:40:SER:HB2 | 31:DA:61:G:H1' | 1.96 | 0.48 |
| 31:DA:92:A:C2' | 31:DA:93:G:O4' | 2.59 | 0.48 |
| 32:DB:20:C:C2' | 32:DB:21:G:H5'' | 2.43 | 0.48 |
| 34:DE:14:ILE:HG23 | 34:DE:23:VAL:HG21 | 1.96 | 0.48 |
| 39:DN:43:THR:N | 39:DN:48:MET:HE3 | 2.29 | 0.48 |
| 39:DN:57:ALA:O | 39:DN:58:ASP:O | 2.31 | 0.48 |
| 44:DS:24:LEU:HB3 | 44:DS:85:VAL:HG12 | 1.95 | 0.48 |
| 46:DU:12:ARG:O | 46:DU:15:LYS:HG3 | 2.14 | 0.48 |
| 31:DA:751:A:C5' | 48:DW:90:ARG:HA | 2.35 | 0.48 |
| 49:DX:87:GLN:HB2 | 49:DX:88:LYS:HD2 | 1.96 | 0.48 |
| 1:AA:1089:G:C6 | 1:AA:1090:U:C4 | 3.02 | 0.48 |
| 1:AA:1158:C:H2' | 1:AA:1158:C:O2 | 2.12 | 0.48 |
| 1:AA:977:A:H8 | 1:AA:1223:C:C4 | 2.31 | 0.48 |
| 1:AA:1423:G:H2' | 1:AA:1424:C:O4' | 2.13 | 0.48 |
| 1:AA:1452:C:H5' | 1:AA:1456:G:C5 | 2.49 | 0.48 |
| 1:AA:16:A:C2' | 1:AA:17:U:H5' | 2.44 | 0.48 |
| 1:AA:308:C:H2' | 1:AA:309:G:C8 | 2.49 | 0.48 |
| 1:AA:498:U:O2 | 1:AA:498:U:H2' | 2.14 | 0.48 |
| 7:AG:36:LYS:NZ | 7:AG:36:LYS:HB2 | 2.29 | 0.48 |
| 12:AL:64:TYR:HB3 | 12:AL:65:GLU:H | 1.47 | 0.48 |
| 19:AS:79:THR:O | 19:AS:80:TYR:HB3 | 2.13 | 0.48 |
| 1:AA:323:U:O3' | 20:AT:22:ARG:HD3 | 2.14 | 0.48 |
| 21:AU:12:LYS:HB3 | 21:AU:22:ARG:HD2 | 1.96 | 0.48 |
| 23:B1:25:LYS:O | 23:B1:26:ARG:CG | 2.61 | 0.48 |
| 23:B1:89:GLU:O | 23:B1:90:ILE:C | 2.51 | 0.48 |
| 31:BA:1049:C:O2 | 31:BA:1049:C:H2' | 2.14 | 0.48 |
| 31:BA:107:C:C2 | 31:BA:108:U:C5 | 3.02 | 0.48 |
| 31:BA:1107:G:H2' | 31:BA:1108:U:O4' | 2.14 | 0.48 |
| 31:BA:1022:G:C6 | 31:BA:1140:C:C4 | 3.02 | 0.48 |
| 31:BA:1225:G:H8 | 31:BA:1225:G:O5' | 1.97 | 0.48 |
| 31:BA:1386:C:OP2 | 31:BA:1396:U:H5 | 1.95 | 0.48 |
| 31:BA:1434:A:H2' | 31:BA:1435:G:H8 | 1.77 | 0.48 |
| 31:BA:1865:G:H5' | 31:BA:1866:C:OP2 | 2.14 | 0.48 |
| 31:BA:2313:C:H2' | 31:BA:2314:C:C6 | 2.46 | 0.48 |
| 31:BA:754:C:O4' | 31:BA:1618:A:H2 | 1.97 | 0.48 |
| 34:BE:108:SER:HB3 | 34:BE:165:VAL:HG21 | 1.96 | 0.48 |
| 35:BF:123:LEU:HD12 | 35:BF:124:LEU:N | 2.29 | 0.48 |
| 36:BG:37:VAL:HG23 | 36:BG:99:MET:HG3 | 1.96 | 0.48 |
| 41:BP:38:GLN:CG | 41:BP:39:LYS:H | 2.16 | 0.48 |
| 42:BQ:133:ARG:O | 42:BQ:134:ARG:CB | 2.62 | 0.48 |
| 31:BA:996:A:H4' | 46:BU:92:ARG:CZ | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:BY:15:VAL:HG12 | 50:BY:16:ALA:N | 2.29 | 0.48 |
| 50:BY:35:TYR:CD2 | 50:BY:69:ALA:HB3 | 2.48 | 0.48 |
| 50:BY:76:CYS:O | 50:BY:96:ILE:HD12 | 2.14 | 0.48 |
| 1:CA:1159:U:C4 | 1:CA:1182:G:C4 | 3.02 | 0.48 |
| 1:CA:1332:A:O5' | 1:CA:1332:A:H8 | 1.97 | 0.48 |
| 1:CA:927:G:OP2 | 1:CA:1503:A:C5 | 2.67 | 0.48 |
| 1:CA:1513:A:H2' | 1:CA:1514:C:C6 | 2.49 | 0.48 |
| 1:CA:407:G:O2' | 4:CD:116:GLN:HG3 | 2.14 | 0.48 |
| 1:CA:425:G:O2' | 1:CA:426:G:H5' | 2.14 | 0.48 |
| 1:CA:649:G:H2' | 1:CA:650:G:H8 | 1.78 | 0.48 |
| 4:CD:10:ARG:O | 4:CD:13:ARG:HB2 | 2.14 | 0.48 |
| 12:CL:10:LEU:HD21 | 12:CL:15:ARG:HE | 1.78 | 0.48 |
| 12:CL:62:SER:O | 12:CL:64:TYR:N | 2.47 | 0.48 |
| 13:CM:44:ARG:CB | 13:CM:46:LYS:HG2 | 2.44 | 0.48 |
| 13:CM:68:GLY:HA2 | 13:CM:71:ARG:HB3 | 1.95 | 0.48 |
| 24:D2:12:GLU:C | 24:D2:12:GLU:CD | 2.72 | 0.48 |
| 27:D5:51:TYR:HB2 | 27:D5:54:GLY:HA3 | 1.95 | 0.48 |
| 30:D8:8:LYS:HB3 | 30:D8:12:LYS:HE3 | 1.96 | 0.48 |
| 31:DA:1357:U:H2' | 31:DA:1358:G:O4' | 2.14 | 0.48 |
| 31:DA:1494:A:N3 | 31:DA:1494:A:C2' | 2.77 | 0.48 |
| 31:DA:1589:C:H2' | 31:DA:1590:U:C6 | 2.49 | 0.48 |
| 31:DA:1688:U:O2 | 31:DA:1700:A:H8 | 1.97 | 0.48 |
| 31:DA:1812:A:C2 | 31:DA:1813:G:C4 | 3.02 | 0.48 |
| 31:DA:2097:C:H2' | 31:DA:2098:U:O4' | 2.13 | 0.48 |
| 31:DA:2323:G:H2' | 31:DA:2324:C:O4' | 2.14 | 0.48 |
| 31:DA:2328:A:H2' | 31:DA:2329:G:H8 | 1.79 | 0.48 |
| 31:DA:662:G:O2' | 31:DA:663:G:H5' | 2.14 | 0.48 |
| 31:DA:801:G:N7 | 35:DF:53:THR:HG23 | 2.28 | 0.48 |
| 31:DA:922:U:H2' | 31:DA:923:C:C6 | 2.48 | 0.48 |
| 31:DA:848:G:N3 | 31:DA:933:A:H1' | 2.29 | 0.48 |
| 33:DD:143:HIS:HD2 | 33:DD:144:ALA:HB2 | 1.77 | 0.48 |
| 33:DD:267:SER:O | 33:DD:268:ARG:HB2 | 2.14 | 0.48 |
| 33:DD:43:ARG:HH11 | 33:DD:44:ASN:ND2 | 2.12 | 0.48 |
| 31:DA:322:A:H3' | 35:DF:169:ASN:ND2 | 2.28 | 0.48 |
| 36:DG:131:TYR:O | 36:DG:159:VAL:HG12 | 2.13 | 0.48 |
| 37:DH:149:ARG:O | 37:DH:152:ARG:O | 2.32 | 0.48 |
| 38:DI:124:GLY:H | 38:DI:142:VAL:HG23 | 1.78 | 0.48 |
| 39:DN:128:HIS:NE2 | 39:DN:131:GLN:HB2 | 2.28 | 0.48 |
| 39:DN:23:LEU:O | 39:DN:23:LEU:HD23 | 2.13 | 0.48 |
| 42:DQ:20:ALA:C | 42:DQ:22:LYS:N | 2.68 | 0.48 |
| 44:DS:67:ARG:H | 44:DS:69:VAL:CG1 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:DS:97:ARG:HG3 | 44:DS:97:ARG:O | 2.14 | 0.48 |
| 46:DU:69:CYS:HB3 | 46:DU:106:PHE:CE2 | 2.48 | 0.48 |
| 48:DW:57:ASN:O | 48:DW:58:ALA:C | 2.52 | 0.48 |
| 50:DY:27:VAL:C | 50:DY:29:GLU:OE1 | 2.52 | 0.48 |
| 1:AA:101:A:H2' | 1:AA:102:G:H5' | 1.95 | 0.47 |
| 1:AA:1085:U:C6 | 1:AA:1094:G:N1 | 2.81 | 0.47 |
| 1:AA:39:G:C6 | 1:AA:40:C:C5 | 3.02 | 0.47 |
| 1:AA:817:C:H4' | 1:AA:818:G:OP1 | 2.13 | 0.47 |
| 2:AB:42:ILE:CD1 | 2:AB:202:PRO:HB2 | 2.43 | 0.47 |
| 2:AB:44:LEU:CD1 | 2:AB:44:LEU:H | 2.23 | 0.47 |
| 3:AC:113:ALA:HB3 | 3:AC:114:PRO:HD3 | 1.95 | 0.47 |
| 3:AC:148:GLY:HA3 | 3:AC:172:ARG:O | 2.13 | 0.47 |
| 4:AD:108:LEU:O | 4:AD:110:PHE:HD1 | 1.96 | 0.47 |
| 7:AG:106:GLN:O | 7:AG:110:GLN:HG3 | 2.14 | 0.47 |
| 1:AA:932:C:H4' | 7:AG:4:ARG:NH2 | 2.29 | 0.47 |
| 26:B4:11:PRO:C | 26:B4:13:ARG:H | 2.16 | 0.47 |
| 29:B7:35:ARG:HD3 | 31:BA:54:G:O2' | 2.13 | 0.47 |
| 31:BA:1411:C:O2' | 31:BA:1412:A:H5' | 2.13 | 0.47 |
| 31:BA:1497:U:H2' | 31:BA:1498:C:OP1 | 2.12 | 0.47 |
| 31:BA:1685:C:H2' | 31:BA:1686:C:H6 | 1.79 | 0.47 |
| 31:BA:2199:A:H5'' | 31:BA:2200:C:OP2 | 2.14 | 0.47 |
| 31:BA:2273:A:O2' | 31:BA:2274:A:H5' | 2.14 | 0.47 |
| 31:BA:2281:C:O2' | 31:BA:2282:G:H5' | 2.14 | 0.47 |
| 31:BA:2473:U:C2 | 31:BA:2474:C:C6 | 3.02 | 0.47 |
| 31:BA:2507:C:H5'' | 31:BA:2573:C:N4 | 2.29 | 0.47 |
| 31:BA:467:G:H2' | 31:BA:468:G:H5' | 1.93 | 0.47 |
| 31:BA:814:C:H5'' | 47:BV:86:GLY:HA3 | 1.94 | 0.47 |
| 32:BB:28:C:H2' | 32:BB:29:A:C8 | 2.48 | 0.47 |
| 33:BD:79:VAL:CG2 | 33:BD:111:LEU:HD11 | 2.44 | 0.47 |
| 34:BE:15:PHE:HA | 34:BE:19:ARG:O | 2.13 | 0.47 |
| 37:BH:156:ALA:O | 37:BH:157:TYR:C | 2.53 | 0.47 |
| 38:BI:131:LYS:HG2 | 38:BI:132:PRO:HA | 1.94 | 0.47 |
| 39:BN:46:VAL:O | 39:BN:47:ALA:HB3 | 2.14 | 0.47 |
| 41:BP:148:LEU:N | 41:BP:148:LEU:HD13 | 2.29 | 0.47 |
| 1:AA:1442(A):G:N7 | 45:BT:118:ARG:HD2 | 2.29 | 0.47 |
| 45:BT:28:VAL:O | 45:BT:29:ARG:CD | 2.62 | 0.47 |
| 45:BT:92:GLY:HA2 | 45:BT:114:LEU:HB3 | 1.95 | 0.47 |
| 50:BY:79:CYS:SG | 50:BY:80:GLY:N | 2.87 | 0.47 |
| 50:BY:87:LYS:HG3 | 50:BY:88:LYS:N | 2.28 | 0.47 |
| 1:CA:999:C:H2' | 1:CA:1000:U:C6 | 2.49 | 0.47 |
| 1:CA:1217:C:H2' | 1:CA:1218:C:O4' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1423:G:H2' | 1:CA:1424:C:O4' | 2.14 | 0.47 |
| 1:CA:382:A:C2 | 1:CA:383:A:C5 | 3.02 | 0.47 |
| 1:CA:457:C:C2 | 1:CA:458:C:C5 | 3.01 | 0.47 |
| 1:CA:46:G:O2' | 1:CA:365:U:H1' | 2.14 | 0.47 |
| 1:CA:684:A:H2' | 1:CA:685:G:H8 | 1.79 | 0.47 |
| 1:CA:705:U:C5 | 1:CA:706:A:C5 | 3.01 | 0.47 |
| 1:CA:84:U:H5 | 1:CA:88:A:N7 | 2.12 | 0.47 |
| 1:CA:1226:C:C5 | 13:CM:104:ARG:HB2 | 2.49 | 0.47 |
| 15:CO:51:HIS:O | 15:CO:54:ARG:HB3 | 2.13 | 0.47 |
| 23:D1:33:LYS:NZ | 23:D1:35:THR:HG21 | 2.28 | 0.47 |
| 23:D1:87:PRO:CD | 23:D1:88:LYS:N | 2.77 | 0.47 |
| 28:D6:20:ASN:CG | 28:D6:21:TYR:N | 2.68 | 0.47 |
| 31:DA:1021:A:C8 | 31:DA:1021:A:C3' | 2.90 | 0.47 |
| 31:DA:1319:G:C6 | 31:DA:1320:C:N4 | 2.82 | 0.47 |
| 31:DA:1439:A:C2 | 31:DA:1553:A:C4 | 3.02 | 0.47 |
| 31:DA:1300:U:H2' | 31:DA:1626:G:N2 | 2.29 | 0.47 |
| 31:DA:1820:U:H4' | 31:DA:1821:A:OP2 | 2.14 | 0.47 |
| 31:DA:2464:C:O2' | 31:DA:2465:C:P | 2.72 | 0.47 |
| 31:DA:2475:C:H5'' | 31:DA:2475:C:C6 | 2.46 | 0.47 |
| 31:DA:2663:G:C5 | 31:DA:2664:G:C5 | 3.02 | 0.47 |
| 31:DA:2698:U:H2' | 31:DA:2699:C:C6 | 2.48 | 0.47 |
| 31:DA:917:A:H8 | 31:DA:917:A:H5' | 1.79 | 0.47 |
| 33:DD:12:SER:O | 33:DD:16:MET:HB2 | 2.14 | 0.47 |
| 36:DG:88:ILE:CG2 | 36:DG:89:GLY:N | 2.77 | 0.47 |
| 38:DI:77:LEU:CD1 | 38:DI:101:LEU:HD22 | 2.43 | 0.47 |
| 42:DQ:16:ARG:C | 42:DQ:17:LEU:HD23 | 2.34 | 0.47 |
| 42:DQ:20:ALA:CB | 42:DQ:99:PRO:HG2 | 2.44 | 0.47 |
| 34:DE:27:LEU:HD22 | 45:DT:1:MET:HE2 | 1.95 | 0.47 |
| 39:DN:40:PRO:C | 46:DU:64:ARG:NH2 | 2.67 | 0.47 |
| 48:DW:18:ARG:NH1 | 48:DW:18:ARG:CG | 2.74 | 0.47 |
| 49:DX:70:LEU:O | 49:DX:71:GLY:C | 2.51 | 0.47 |
| 1:AA:1226:C:OP1 | 13:AM:91:ARG:NH1 | 2.46 | 0.47 |
| 1:AA:651:C:O2' | 1:AA:652:U:H5' | 2.13 | 0.47 |
| 1:AA:66:G:C2 | 1:AA:67:C:C6 | 3.02 | 0.47 |
| 1:AA:966:G:H21 | 9:AI:127:LYS:HE3 | 1.79 | 0.47 |
| 2:AB:204:ASN:HD21 | 2:AB:206:ASP:H | 1.61 | 0.47 |
| 4:AD:64:LEU:HD12 | 4:AD:64:LEU:O | 2.14 | 0.47 |
| 5:AE:80:ILE:HG22 | 8:AH:104:ARG:NH2 | 2.29 | 0.47 |
| 8:AH:87:SER:HB3 | 8:AH:133:LEU:O | 2.13 | 0.47 |
| 9:AI:45:ALA:O | 9:AI:78:LYS:HE3 | 2.14 | 0.47 |
| 16:AP:21:VAL:HG22 | 16:AP:34:GLU:O | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:376:G:O3' | 16:AP:5:ARG:HD2 | 2.13 | 0.47 |
| 23:B1:90:ILE:O | 23:B1:94:LEU:HB2 | 2.14 | 0.47 |
| 31:BA:1173:G:H5' | 31:BA:1174:A:OP2 | 2.14 | 0.47 |
| 27:B5:10:LYS:HE3 | 31:BA:1262:A:N3 | 2.29 | 0.47 |
| 31:BA:154:G:N1 | 31:BA:154(A):C:N4 | 2.62 | 0.47 |
| 31:BA:1902:C:C4' | 33:BD:244:ARG:HB2 | 2.44 | 0.47 |
| 31:BA:1649:G:C6 | 31:BA:2009:G:C6 | 3.02 | 0.47 |
| 31:BA:2031:A:C6 | 31:BA:2498:C:H1' | 2.49 | 0.47 |
| 31:BA:2789:C:H2' | 31:BA:2790:A:OP2 | 2.13 | 0.47 |
| 31:BA:292:C:O2' | 31:BA:293:U:H5' | 2.15 | 0.47 |
| 31:BA:661:C:H2' | 31:BA:662:G:H8 | 1.79 | 0.47 |
| 31:BA:717:G:H2' | 31:BA:718:A:O4' | 2.13 | 0.47 |
| 31:BA:8:A:H2' | 31:BA:9:U:H5 | 1.76 | 0.47 |
| 31:BA:992:C:O2' | 31:BA:993:G:H5' | 2.15 | 0.47 |
| 33:BD:83:GLU:OE1 | 33:BD:104:TYR:OH | 2.27 | 0.47 |
| 34:BE:75:VAL:C | 34:BE:77:ILE:N | 2.67 | 0.47 |
| 40:BO:13:ASN:ND2 | 40:BO:96:THR:H | 2.07 | 0.47 |
| 41:BP:85:LEU:HB3 | 41:BP:114:ILE:HD12 | 1.95 | 0.47 |
| 44:BS:11:LYS:N | 44:BS:11:LYS:HD2 | 2.29 | 0.47 |
| 44:BS:42:ASP:C | 44:BS:44:LYS:N | 2.68 | 0.47 |
| 49:BX:35:THR:O | 49:BX:39:ILE:CG2 | 2.62 | 0.47 |
| 49:BX:93:GLU:HG3 | 49:BX:93:GLU:O | 2.15 | 0.47 |
| 1:CA:101:A:H2' | 1:CA:102:G:H5' | 1.95 | 0.47 |
| 1:CA:1074:G:C2 | 1:CA:1102:A:C2 | 3.02 | 0.47 |
| 1:CA:1132:C:H2' | 1:CA:1133:G:O4' | 2.14 | 0.47 |
| 1:CA:246:A:C4 | 1:CA:282:A:N6 | 2.82 | 0.47 |
| 1:CA:316:G:OP2 | 1:CA:351:G:O2' | 2.32 | 0.47 |
| 1:CA:651:C:O2' | 1:CA:652:U:H5' | 2.14 | 0.47 |
| 1:CA:829:G:O2' | 1:CA:830:G:H5' | 2.14 | 0.47 |
| 4:CD:33:MET:HE2 | 4:CD:37:PRO:HA | 1.95 | 0.47 |
| 5:CE:31:LEU:HD22 | 5:CE:43:LEU:HD11 | 1.95 | 0.47 |
| 7:CG:92:SER:HB3 | 7:CG:94:ARG:HH21 | 1.78 | 0.47 |
| 9:CI:45:ALA:O | 9:CI:78:LYS:HE3 | 2.14 | 0.47 |
| 10:CJ:54:PHE:CE2 | 10:CJ:55:LYS:HD2 | 2.49 | 0.47 |
| 11:CK:48:ILE:HG22 | 11:CK:49:GLY:H | 1.79 | 0.47 |
| 13:CM:82:MET:HB2 | 13:CM:93:ARG:NH1 | 2.29 | 0.47 |
| 15:CO:81:LEU:HD11 | 15:CO:85:LEU:HD12 | 1.94 | 0.47 |
| 20:CT:14:LYS:HA | 20:CT:17:ARG:HE | 1.79 | 0.47 |
| 24:D2:34:GLU:O | 24:D2:34:GLU:HG2 | 2.14 | 0.47 |
| 41:BP:121:LYS:CE | 25:D3:2:PRO:HD3 | 2.44 | 0.47 |
| 31:DA:1106:A:C2' | 31:DA:1107:G:C8 | 2.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:117:G:H5'' | 31:DA:118:A:OP2 | 2.14 | 0.47 |
| 31:DA:1425:G:H2' | 31:DA:1426:G:O4' | 2.15 | 0.47 |
| 31:DA:1497:U:O2 | 31:DA:1497:U:C2' | 2.61 | 0.47 |
| 31:DA:2070:G:C2 | 31:DA:2442:C:C2 | 3.02 | 0.47 |
| 31:DA:2810:A:H2' | 34:DE:61:ARG:HH21 | 1.75 | 0.47 |
| 31:DA:34:C:H2' | 31:DA:35:G:OP1 | 2.14 | 0.47 |
| 29:D7:39:ARG:NH2 | 31:DA:468:G:N7 | 2.59 | 0.47 |
| 31:DA:774:A:H2 | 31:DA:787:U:HO2' | 1.53 | 0.47 |
| 31:DA:82:G:O2' | 31:DA:83:G:H5' | 2.14 | 0.47 |
| 31:DA:966:G:H2' | 31:DA:967:C:C6 | 2.48 | 0.47 |
| 34:DE:137:HIS:HB3 | 34:DE:138:PRO:CD | 2.44 | 0.47 |
| 35:DF:123:LEU:HD12 | 35:DF:124:LEU:N | 2.28 | 0.47 |
| 37:DH:44:VAL:O | 37:DH:46:GLU:OE2 | 2.32 | 0.47 |
| 38:DI:62:LYS:HE2 | 38:DI:134:PRO:HG3 | 1.95 | 0.47 |
| 42:DQ:30:GLY:CA | 42:DQ:107:ALA:HB2 | 2.43 | 0.47 |
| 45:DT:109:GLU:HA | 45:DT:112:ARG:CG | 2.43 | 0.47 |
| 45:DT:33:LYS:N | 45:DT:33:LYS:HZ3 | 2.12 | 0.47 |
| 31:DA:535:C:O3' | 46:DU:53:ARG:NH1 | 2.47 | 0.47 |
| 46:DU:92:ARG:NE | 47:DV:11:GLN:HG2 | 2.28 | 0.47 |
| 47:DV:72:VAL:O | 47:DV:89:GLN:O | 2.32 | 0.47 |
| 48:DW:18:ARG:HG2 | 48:DW:18:ARG:NH1 | 2.24 | 0.47 |
| 51:DZ:108:PRO:HG3 | 51:DZ:141:VAL:HG22 | 1.96 | 0.47 |
| 1:AA:1242:C:H5'' | 21:AU:10:ARG:NH1 | 2.29 | 0.47 |
| 1:AA:1431:C:H2' | 1:AA:1432:G:O4' | 2.14 | 0.47 |
| 1:AA:171:A:H2' | 1:AA:172:A:C8 | 2.49 | 0.47 |
| 1:AA:373:A:N3 | 1:AA:374:A:C8 | 2.82 | 0.47 |
| 1:AA:375:U:N3 | 1:AA:376:G:N7 | 2.62 | 0.47 |
| 1:AA:839:U:OP2 | 1:AA:840:C:H5 | 1.97 | 0.47 |
| 2:AB:16:HIS:HA | 2:AB:210:SER:HB2 | 1.96 | 0.47 |
| 3:AC:154:SER:O | 3:AC:165:THR:HA | 2.14 | 0.47 |
| 5:AE:75:THR:HG23 | 5:AE:76:ILE:H | 1.78 | 0.47 |
| 9:AI:61:ALA:HB1 | 9:AI:63:ILE:HD11 | 1.95 | 0.47 |
| 9:AI:79:LEU:HD11 | 9:AI:83:ARG:NH2 | 2.29 | 0.47 |
| 29:B7:40:TRP:CD2 | 31:BA:459:U:H5'' | 2.49 | 0.47 |
| 30:B8:29:LYS:O | 30:B8:30:ARG:C | 2.51 | 0.47 |
| 31:BA:2097:C:H2' | 31:BA:2098:U:O4' | 2.15 | 0.47 |
| 31:BA:287:C:N4 | 31:BA:354:G:H1 | 2.05 | 0.47 |
| 31:BA:861:A:C2 | 31:BA:917:A:C4 | 3.01 | 0.47 |
| 31:BA:985:C:H2' | 31:BA:986:C:C6 | 2.50 | 0.47 |
| 32:BB:38:C:O4' | 44:BS:95:HIS:NE2 | 2.37 | 0.47 |
| 35:BF:84:VAL:O | 35:BF:85:GLY:C | 2.51 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BO:13:ASN:ND2 | 40:BO:97:ARG:N | 2.60 | 0.47 |
| 46:BU:75:ASN:HB3 | 46:BU:77:SER:OG | 2.14 | 0.47 |
| 46:BU:76:TYR:CZ | 46:BU:80:ILE:HG13 | 2.49 | 0.47 |
| 47:BV:66:ARG:HG3 | 47:BV:66:ARG:HH11 | 1.79 | 0.47 |
| 50:BY:90:LEU:CD1 | 50:BY:91:GLU:HG2 | 2.43 | 0.47 |
| 1:CA:357:G:C2 | 1:CA:358:U:C6 | 3.02 | 0.47 |
| 1:CA:484:G:H4' | 1:CA:485:G:OP1 | 2.15 | 0.47 |
| 1:CA:577:G:H2' | 1:CA:578:C:H6 | 1.79 | 0.47 |
| 1:CA:84:U:H5 | 1:CA:88:A:C8 | 2.32 | 0.47 |
| 2:CB:42:ILE:CD1 | 2:CB:202:PRO:HB2 | 2.45 | 0.47 |
| 11:CK:105:VAL:HG23 | 11:CK:105:VAL:O | 2.14 | 0.47 |
| 12:CL:70:ILE:N | 12:CL:70:ILE:HD12 | 2.29 | 0.47 |
| 1:CA:626:U:H4' | 16:CP:38:TYR:CZ | 2.49 | 0.47 |
| 16:CP:8:ARG:O | 16:CP:9:PHE:CG | 2.68 | 0.47 |
| 28:D6:39:TYR:HB3 | 28:D6:49:HIS:ND1 | 2.29 | 0.47 |
| 29:D7:24:THR:O | 29:D7:28:ARG:HG3 | 2.14 | 0.47 |
| 31:DA:1040:C:N4 | 31:DA:1115:G:H1 | 2.12 | 0.47 |
| 31:DA:1138:G:O2' | 39:DN:105:GLY:HA3 | 2.14 | 0.47 |
| 31:DA:1635:G:H2' | 31:DA:1636:C:H6 | 1.79 | 0.47 |
| 31:DA:241:A:H5' | 31:DA:243:U:O4' | 2.14 | 0.47 |
| 31:DA:271(O):C:O2' | 31:DA:271(P):C:C5 | 2.67 | 0.47 |
| 31:DA:491:G:H2' | 31:DA:492:A:H8 | 1.79 | 0.47 |
| 31:DA:723:G:H2' | 31:DA:724:U:O4' | 2.15 | 0.47 |
| 31:DA:884:C:O2' | 31:DA:892:G:C8 | 2.51 | 0.47 |
| 31:DA:900:A:H5'' | 31:DA:901:A:OP2 | 2.14 | 0.47 |
| 33:DD:221:VAL:HG22 | 33:DD:226:MET:CE | 2.43 | 0.47 |
| 35:DF:164:ARG:HG2 | 35:DF:164:ARG:NH1 | 2.23 | 0.47 |
| 35:DF:195:ASP:CG | 35:DF:197:ASP:HB3 | 2.35 | 0.47 |
| 35:DF:3:GLU:HB2 | 35:DF:20:LEU:H | 1.78 | 0.47 |
| 31:DA:2393:A:OP1 | 41:DP:62:LEU:HD12 | 2.14 | 0.47 |
| 44:DS:17:ARG:NE | 44:DS:89:ARG:HH21 | 2.12 | 0.47 |
| 47:DV:2:PHE:CE1 | 47:DV:13:ARG:CZ | 2.97 | 0.47 |
| 47:DV:32:THR:HB | 47:DV:64:HIS:HE1 | 1.78 | 0.47 |
| 48:DW:111:HIS:CD2 | 48:DW:112:GLY:H | 2.32 | 0.47 |
| 49:DX:12:VAL:HG13 | 49:DX:27:THR:O | 2.15 | 0.47 |
| 49:DX:63:LYS:HD2 | 49:DX:70:LEU:HD13 | 1.95 | 0.47 |
| 1:AA:1068:G:H8 | 1:AA:1068:G:OP2 | 1.97 | 0.47 |
| 1:AA:106:C:H2' | 1:AA:107:G:H8 | 1.80 | 0.47 |
| 1:AA:116:A:OP2 | 1:AA:116:A:C8 | 2.67 | 0.47 |
| 1:AA:1313:U:OP2 | 19:AS:6:LYS:HB3 | 2.14 | 0.47 |
| 1:AA:542:G:H5' | 4:AD:41:GLY:CA | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:781:A:H5' | 1:AA:782:A:OP2 | 2.14 | 0.47 |
| 1:AA:914:A:C2' | 1:AA:915:A:H5' | 2.44 | 0.47 |
| 4:AD:121:VAL:O | 4:AD:134:ASP:HA | 2.15 | 0.47 |
| 6:AF:45:LEU:HG | 6:AF:46:ARG:N | 2.28 | 0.47 |
| 6:AF:19:LEU:HD11 | 6:AF:59:TYR:CG | 2.50 | 0.47 |
| 7:AG:66:VAL:HG12 | 7:AG:70:LYS:HE3 | 1.96 | 0.47 |
| 10:AJ:49:VAL:HG11 | 14:AN:41:ARG:O | 2.15 | 0.47 |
| 12:AL:119:LYS:HB2 | 12:AL:120:TYR:CD1 | 2.49 | 0.47 |
| 13:AM:75:ALA:O | 13:AM:79:LYS:HG3 | 2.14 | 0.47 |
| 19:AS:16:LEU:O | 19:AS:20:LEU:HB2 | 2.15 | 0.47 |
| 23:B1:26:ARG:HB2 | 23:B1:34:THR:HB | 1.97 | 0.47 |
| 23:B1:33:LYS:NZ | 23:B1:35:THR:CG2 | 2.77 | 0.47 |
| 31:BA:157:U:H6 | 31:BA:157:U:OP2 | 1.97 | 0.47 |
| 31:BA:2199:A:N3 | 31:BA:2199:A:H2' | 2.29 | 0.47 |
| 31:BA:27:G:C4 | 31:BA:512:G:N2 | 2.83 | 0.47 |
| 31:BA:280:C:C2' | 31:BA:281:G:O5' | 2.63 | 0.47 |
| 31:BA:2836:U:C4 | 31:BA:2883:A:N6 | 2.82 | 0.47 |
| 31:BA:329:G:H22 | 50:BY:19:LYS:NZ | 2.13 | 0.47 |
| 31:BA:543:C:H5 | 31:BA:547:A:H62 | 1.62 | 0.47 |
| 31:BA:784:A:C8 | 31:BA:792:G:C5 | 3.03 | 0.47 |
| 31:BA:84:A:H5'' | 50:BY:9:LYS:CD | 2.44 | 0.47 |
| 32:BB:110:G:N1 | 32:BB:111:G:C5 | 2.83 | 0.47 |
| 32:BB:28:C:H2' | 32:BB:29:A:H8 | 1.80 | 0.47 |
| 33:BD:131:LEU:HB2 | 33:BD:136:ILE:CD1 | 2.42 | 0.47 |
| 33:BD:35:LYS:HG2 | 33:BD:64:ILE:H | 1.79 | 0.47 |
| 35:BF:68:LYS:O | 35:BF:68:LYS:HG2 | 2.15 | 0.47 |
| 36:BG:61:ALA:HA | 36:BG:64:THR:CG2 | 2.44 | 0.47 |
| 37:BH:94:TYR:HA | 37:BH:106:THR:O | 2.15 | 0.47 |
| 37:BH:94:TYR:CD1 | 37:BH:94:TYR:N | 2.83 | 0.47 |
| 38:BI:77:LEU:CD1 | 38:BI:101:LEU:HD22 | 2.44 | 0.47 |
| 47:BV:80:GLN:HA | 47:BV:82:ARG:H | 1.79 | 0.47 |
| 49:BX:59:VAL:O | 49:BX:60:ARG:O | 2.32 | 0.47 |
| 51:BZ:135:GLU:O | 51:BZ:136:PHE:HB3 | 2.14 | 0.47 |
| 51:BZ:73:GLN:HG2 | 51:BZ:87:ASP:CG | 2.34 | 0.47 |
| 1:CA:1125:U:O4 | 10:CJ:73:ASP:OD2 | 2.32 | 0.47 |
| 1:CA:308:C:H2' | 1:CA:309:G:C8 | 2.48 | 0.47 |
| 1:CA:355:C:O2' | 1:CA:356:A:H5' | 2.14 | 0.47 |
| 1:CA:451:A:N7 | 1:CA:481:G:C6 | 2.82 | 0.47 |
| 1:CA:78:G:H22 | 1:CA:91:C:N4 | 2.12 | 0.47 |
| 3:CC:155:GLY:O | 3:CC:156:ARG:CB | 2.63 | 0.47 |
| 3:CC:154:SER:O | 3:CC:165:THR:HA | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:CD:148:VAL:CG1 | 4:CD:149:ALA:N | 2.77 | 0.47 |
| 7:CG:106:GLN:O | 7:CG:110:GLN:HG3 | 2.14 | 0.47 |
| 9:CI:105:ASP:CG | 9:CI:107:ARG:HD3 | 2.35 | 0.47 |
| 9:CI:21:PRO:HA | 9:CI:58:ARG:O | 2.14 | 0.47 |
| 1:CA:963:G:H21 | 10:CJ:55:LYS:CD | 2.27 | 0.47 |
| 13:CM:86:CYS:HB2 | 19:CS:73:GLU:OE1 | 2.15 | 0.47 |
| 20:CT:84:LEU:O | 20:CT:88:VAL:HG23 | 2.14 | 0.47 |
| 23:D1:10:LYS:HB2 | 23:D1:14:VAL:CA | 2.43 | 0.47 |
| 27:D5:2:ALA:N | 31:DA:2015:A:N3 | 2.63 | 0.47 |
| 30:D8:29:LYS:O | 30:D8:31:HIS:N | 2.48 | 0.47 |
| 31:DA:1173:G:H5' | 31:DA:1174:A:OP2 | 2.14 | 0.47 |
| 31:DA:1241:A:C2' | 31:DA:1242:A:O5' | 2.62 | 0.47 |
| 31:DA:1384:A:H1' | 31:DA:1405:U:O4' | 2.14 | 0.47 |
| 31:DA:1689:A:N6 | 31:DA:1698:A:H2 | 2.09 | 0.47 |
| 31:DA:1783:A:N1 | 31:DA:2587:A:C4 | 2.83 | 0.47 |
| 31:DA:1803:A:H4' | 33:DD:259:THR:CG2 | 2.45 | 0.47 |
| 31:DA:2274:A:O5' | 31:DA:2275:C:OP2 | 2.32 | 0.47 |
| 31:DA:2299:G:N1 | 31:DA:2318:G:C8 | 2.83 | 0.47 |
| 31:DA:2416:C:H6 | 31:DA:2416:C:O5' | 1.98 | 0.47 |
| 31:DA:280:C:C2' | 31:DA:281:G:O5' | 2.62 | 0.47 |
| 31:DA:287:C:N4 | 31:DA:354:G:H1 | 2.05 | 0.47 |
| 31:DA:670:A:H4' | 31:DA:671:C:O5' | 2.14 | 0.47 |
| 32:DB:21:G:O6 | 32:DB:63:G:C4 | 2.68 | 0.47 |
| 33:DD:125:ILE:HG13 | 33:DD:137:PRO:CD | 2.45 | 0.47 |
| 33:DD:35:LYS:CA | 33:DD:64:ILE:CG2 | 2.93 | 0.47 |
| 34:DE:101:ARG:CG | 34:DE:169:ASN:ND2 | 2.77 | 0.47 |
| 32:DB:42:C:O2 | 36:DG:93:THR:N | 2.48 | 0.47 |
| 37:DH:158:HIS:CE1 | 37:DH:168:PRO:C | 2.87 | 0.47 |
| 37:DH:54:ARG:HG2 | 37:DH:65:HIS:HD2 | 1.80 | 0.47 |
| 38:DI:44:LEU:O | 38:DI:47:LEU:HB3 | 2.14 | 0.47 |
| 39:DN:39:ARG:O | 46:DU:64:ARG:NH1 | 2.47 | 0.47 |
| 39:DN:78:TYR:HD1 | 39:DN:79:PRO:CG | 2.27 | 0.47 |
| 44:DS:88:ASP:O | 44:DS:89:ARG:O | 2.31 | 0.47 |
| 31:DA:1225:G:OP1 | 47:DV:88:ARG:HB3 | 2.14 | 0.47 |
| 31:DA:329:G:H22 | 50:DY:19:LYS:NZ | 2.12 | 0.47 |
| 1:AA:411:A:OP1 | 4:AD:30:LYS:NZ | 2.45 | 0.47 |
| 1:AA:96:U:O2' | 1:AA:97:G:H8 | 1.97 | 0.47 |
| 2:AB:15:VAL:HG23 | 2:AB:16:HIS:CE1 | 2.49 | 0.47 |
| 4:AD:12:CYS:SG | 4:AD:19:LEU:O | 2.72 | 0.47 |
| 8:AH:77:GLU:HG2 | 8:AH:78:GLN:H | 1.79 | 0.47 |
| 12:AL:10:LEU:HD21 | 12:AL:15:ARG:HE | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:AL:62:SER:HB2 | 12:AL:64:TYR:HD1 | 1.80 | 0.47 |
| 1:AA:450:G:C5' | 16:AP:41:PRO:O | 2.57 | 0.47 |
| 18:AR:66:LEU:HD11 | 18:AR:70:ILE:HD11 | 1.96 | 0.47 |
| 22:B0:13:GLY:O | 22:B0:14:ARG:CB | 2.40 | 0.47 |
| 31:BA:1321:A:H2' | 31:BA:1322:A:O4' | 2.15 | 0.47 |
| 31:BA:1490:A:H5' | 31:BA:1491:G:OP2 | 2.15 | 0.47 |
| 31:BA:1507:A:C2 | 31:BA:1508:A:H1' | 2.50 | 0.47 |
| 31:BA:1659:U:C4 | 31:BA:1660:C:C5 | 3.03 | 0.47 |
| 31:BA:1777:U:O2' | 31:BA:1778:U:H5' | 2.15 | 0.47 |
| 31:BA:2199:A:C5' | 31:BA:2200:C:OP2 | 2.63 | 0.47 |
| 31:BA:2526:G:H5' | 31:BA:2742:C:O2' | 2.15 | 0.47 |
| 31:BA:2884:U:C2' | 31:BA:2885:C:H5' | 2.45 | 0.47 |
| 31:BA:303:U:H2' | 31:BA:304:G:C8 | 2.49 | 0.47 |
| 31:BA:528:A:O2' | 31:BA:529:A:H5' | 2.15 | 0.47 |
| 31:BA:753:C:O5' | 31:BA:753:C:H6 | 1.97 | 0.47 |
| 31:BA:83:G:H22 | 31:BA:102:G:HO2' | 1.61 | 0.47 |
| 31:BA:900:A:C5' | 31:BA:901:A:OP2 | 2.62 | 0.47 |
| 32:BB:78:A:C2 | 32:BB:100:A:C4 | 3.02 | 0.47 |
| 33:BD:89:SER:HB2 | 33:BD:159:ALA:HB2 | 1.95 | 0.47 |
| 36:BG:174:GLU:HG3 | 36:BG:180:PHE:CD1 | 2.49 | 0.47 |
| 37:BH:117:PRO:HA | 37:BH:123:PHE:HE1 | 1.79 | 0.47 |
| 37:BH:90:LYS:CB | 37:BH:159:GLU:O | 2.63 | 0.47 |
| 38:BI:114:LEU:HD23 | 38:BI:114:LEU:HA | 1.69 | 0.47 |
| 41:BP:146:VAL:CG2 | 41:BP:147:LEU:N | 2.71 | 0.47 |
| 41:BP:14:LYS:O | 41:BP:15:ARG:CB | 2.62 | 0.47 |
| 43:BR:10:LEU:HB3 | 43:BR:17:ARG:CD | 2.45 | 0.47 |
| 43:BR:50:HIS:O | 43:BR:54:LEU:HD22 | 2.14 | 0.47 |
| 44:BS:16:ASN:ND2 | 44:BS:92:TYR:CZ | 2.82 | 0.47 |
| 44:BS:63:THR:O | 44:BS:66:ALA:O | 2.32 | 0.47 |
| 50:BY:87:LYS:O | 50:BY:88:LYS:HB2 | 2.15 | 0.47 |
| 51:BZ:167:PRO:O | 51:BZ:168:GLU:HB2 | 2.15 | 0.47 |
| 1:CA:1098:C:C4 | 1:CA:1099:G:C8 | 3.02 | 0.47 |
| 1:CA:1338:G:O2' | 1:CA:1339:A:H5' | 2.14 | 0.47 |
| 1:CA:255:G:H2' | 1:CA:256:U:C6 | 2.50 | 0.47 |
| 1:CA:448:A:C2 | 1:CA:449:C:C4 | 3.02 | 0.47 |
| 1:CA:524:G:O5' | 1:CA:524:G:H8 | 1.97 | 0.47 |
| 2:CB:53:ARG:HA | 2:CB:56:ARG:HB2 | 1.96 | 0.47 |
| 5:CE:80:ILE:HG22 | 8:CH:104:ARG:NH2 | 2.29 | 0.47 |
| 8:CH:53:VAL:O | 8:CH:54:ASP:CB | 2.60 | 0.47 |
| 8:CH:77:GLU:HG2 | 8:CH:78:GLN:H | 1.79 | 0.47 |
| 11:CK:91:ARG:O | 11:CK:95:ILE:HG12 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:CT:53:LEU:HA | 20:CT:56:MET:HB2 | 1.96 | 0.47 |
| 30:D8:35:GLN:HE21 | 30:D8:36:LYS:NZ | 2.12 | 0.47 |
| 31:DA:1022:G:C5 | 31:DA:1140:C:N4 | 2.82 | 0.47 |
| 31:DA:1525:G:H2' | 31:DA:1526:G:C8 | 2.49 | 0.47 |
| 31:DA:1662:C:O2' | 31:DA:1663:C:H5' | 2.15 | 0.47 |
| 31:DA:1948:G:H2' | 31:DA:1949:G:C5' | 2.45 | 0.47 |
| 31:DA:2298:A:H2' | 31:DA:2299:G:O4' | 2.14 | 0.47 |
| 27:D5:7:PRO:HA | 31:DA:2615:U:N1 | 2.29 | 0.47 |
| 31:DA:2802:G:H3' | 31:DA:2802:G:P | 2.54 | 0.47 |
| 31:DA:2859:G:H4' | 31:DA:2860:A:OP1 | 2.15 | 0.47 |
| 32:DB:73:A:C4 | 32:DB:105:A:C2 | 3.02 | 0.47 |
| 31:DA:2598:A:O5' | 33:DD:236:GLY:HA3 | 2.13 | 0.47 |
| 31:DA:2228:G:OP1 | 33:DD:261:LYS:NZ | 2.47 | 0.47 |
| 34:DE:61:ARG:H | 34:DE:62:PRO:CD | 2.24 | 0.47 |
| 35:DF:46:ARG:CG | 35:DF:46:ARG:NH1 | 2.63 | 0.47 |
| 37:DH:94:TYR:HA | 37:DH:106:THR:O | 2.15 | 0.47 |
| 43:DR:77:ARG:O | 43:DR:78:LYS:C | 2.52 | 0.47 |
| 45:DT:106:SER:O | 45:DT:107:ASP:HB3 | 2.15 | 0.47 |
| 48:DW:29:LEU:HG | 48:DW:33:ARG:HD2 | 1.96 | 0.47 |
| 1:AA:1067:A:O2' | 1:AA:1093:A:O2' | 2.27 | 0.47 |
| 1:AA:1270:C:H2' | 1:AA:1271:G:O4' | 2.14 | 0.47 |
| 1:AA:154:C:H2' | 1:AA:155:C:H6 | 1.80 | 0.47 |
| 1:AA:189(B):C:N4 | 1:AA:189(I):G:H1 | 2.13 | 0.47 |
| 1:AA:338:A:C6 | 1:AA:339:C:C4 | 3.02 | 0.47 |
| 1:AA:473:G:N3 | 1:AA:474:G:C8 | 2.81 | 0.47 |
| 1:AA:451:A:N7 | 1:AA:481:G:C6 | 2.83 | 0.47 |
| 1:AA:696:A:O5' | 1:AA:696:A:H8 | 1.98 | 0.47 |
| 1:AA:84:U:C5 | 1:AA:88:A:C8 | 3.02 | 0.47 |
| 1:AA:999:C:H2' | 1:AA:1000:U:C6 | 2.50 | 0.47 |
| 2:AB:12:GLU:HA | 2:AB:16:HIS:HB2 | 1.96 | 0.47 |
| 3:AC:155:GLY:O | 3:AC:156:ARG:CB | 2.60 | 0.47 |
| 3:AC:29:TYR:OH | 14:AN:54:PRO:HD2 | 2.15 | 0.47 |
| 4:AD:92:VAL:O | 4:AD:96:LEU:HD23 | 2.14 | 0.47 |
| 16:AP:20:VAL:HG13 | 16:AP:21:VAL:N | 2.28 | 0.47 |
| 30:B8:35:GLN:O | 30:B8:37:SER:N | 2.48 | 0.47 |
| 31:BA:1015:G:H2' | 31:BA:1016:G:H5' | 1.97 | 0.47 |
| 31:BA:1025:G:OP1 | 31:BA:1025:G:H8 | 1.97 | 0.47 |
| 31:BA:1040:C:H42 | 31:BA:1115:G:H1 | 1.62 | 0.47 |
| 31:BA:1719:G:O2' | 31:BA:1720:U:H5' | 2.15 | 0.47 |
| 31:BA:2564:A:C6 | 31:BA:2565:A:C6 | 3.03 | 0.47 |
| 31:BA:616:G:H2' | 31:BA:618:C:O4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:BA:825:C:C6 | 31:BA:825:C:H3' | 2.50 | 0.47 |
| 33:BD:35:LYS:HD3 | 33:BD:64:ILE:N | 2.29 | 0.47 |
| 33:BD:34:VAL:C | 33:BD:35:LYS:O | 2.52 | 0.47 |
| 33:BD:85:ASP:OD1 | 33:BD:86:PRO:HD2 | 2.14 | 0.47 |
| 34:BE:2:LYS:NZ | 34:BE:95:ILE:O | 2.46 | 0.47 |
| 36:BG:88:ILE:CG2 | 36:BG:89:GLY:N | 2.78 | 0.47 |
| 37:BH:137:ASP:HB2 | 37:BH:140:LYS:HB2 | 1.94 | 0.47 |
| 38:BI:27:ARG:HG2 | 38:BI:27:ARG:HH11 | 1.80 | 0.47 |
| 38:BI:29:TYR:O | 38:BI:32:PRO:HD2 | 2.14 | 0.47 |
| 39:BN:128:HIS:NE2 | 39:BN:131:GLN:HB2 | 2.29 | 0.47 |
| 40:BO:87:ILE:CG2 | 40:BO:88:ASN:N | 2.77 | 0.47 |
| 41:BP:107:LYS:C | 41:BP:109:GLY:N | 2.66 | 0.47 |
| 42:BQ:42:ILE:HD13 | 42:BQ:97:VAL:CG2 | 2.43 | 0.47 |
| 43:BR:8:ARG:NE | 43:BR:8:ARG:HA | 2.29 | 0.47 |
| 46:BU:93:LYS:H | 46:BU:93:LYS:CD | 2.23 | 0.47 |
| 47:BV:36:PRO:HD2 | 47:BV:60:GLU:O | 2.14 | 0.47 |
| 49:BX:18:TYR:O | 49:BX:19:ALA:C | 2.52 | 0.47 |
| 50:BY:27:VAL:C | 50:BY:29:GLU:OE1 | 2.53 | 0.47 |
| 1:CA:1053:G:N7 | 1:CA:1200:C:H5' | 2.29 | 0.47 |
| 1:CA:977:A:H8 | 1:CA:1223:C:C4 | 2.33 | 0.47 |
| 1:CA:1238:A:N6 | 1:CA:1299:A:N6 | 2.61 | 0.47 |
| 1:CA:154:C:H2' | 1:CA:155:C:H6 | 1.80 | 0.47 |
| 1:CA:343:U:C2' | 1:CA:346:G:O6 | 2.63 | 0.47 |
| 2:CB:8:LYS:HZ2 | 2:CB:217:ARG:HH11 | 1.61 | 0.47 |
| 3:CC:107:GLN:O | 3:CC:108:ASN:HB2 | 2.14 | 0.47 |
| 4:CD:74:GLN:O | 4:CD:78:LEU:HG | 2.14 | 0.47 |
| 4:CD:82:ALA:O | 4:CD:83:SER:C | 2.53 | 0.47 |
| 10:CJ:75:ILE:HG13 | 10:CJ:76:ASN:N | 2.29 | 0.47 |
| 12:CL:25:PRO:O | 12:CL:27:LEU:HD22 | 2.14 | 0.47 |
| 1:CA:750:G:H21 | 15:CO:24:SER:H | 1.61 | 0.47 |
| 15:CO:17:ARG:HG2 | 15:CO:26:GLU:HG3 | 1.97 | 0.47 |
| 16:CP:48:TRP:CD1 | 16:CP:48:TRP:N | 2.75 | 0.47 |
| 31:DA:1900:A:N1 | 31:DA:1970:A:C6 | 2.83 | 0.47 |
| 31:DA:2287:A:O2' | 31:DA:2288:A:H3' | 2.14 | 0.47 |
| 31:DA:2645:G:H3' | 31:DA:2646:C:H5' | 1.95 | 0.47 |
| 31:DA:2703:C:H2' | 31:DA:2704:C:C6 | 2.48 | 0.47 |
| 31:DA:352:G:HO2' | 31:DA:353:G:P | 2.38 | 0.47 |
| 31:DA:543:C:H5 | 31:DA:547:A:H62 | 1.62 | 0.47 |
| 31:DA:910:A:N7 | 42:DQ:13:GLN:HB2 | 2.30 | 0.47 |
| 31:DA:92:A:H2' | 31:DA:93:G:C8 | 2.50 | 0.47 |
| 34:DE:120:TRP:CD2 | 34:DE:155:LYS:HD3 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:D4:14:ILE:CB | 36:DG:5:VAL:HG13 | 2.45 | 0.47 |
| 37:DH:85:LYS:NZ | 37:DH:145:ALA:HA | 2.29 | 0.47 |
| 39:DN:22:THR:HA | 39:DN:61:ARG:O | 2.15 | 0.47 |
| 41:DP:78:PRO:HB2 | 41:DP:111:ARG:HE | 1.80 | 0.47 |
| 43:DR:74:LYS:O | 43:DR:77:ARG:HB2 | 2.15 | 0.47 |
| 44:DS:53:SER:O | 44:DS:55:ALA:N | 2.48 | 0.47 |
| 45:DT:16:ARG:HD3 | 45:DT:16:ARG:HA | 1.54 | 0.47 |
| 45:DT:51:ARG:HD2 | 45:DT:62:THR:HG23 | 1.96 | 0.47 |
| 47:DV:73:SER:O | 47:DV:74:LYS:HB2 | 2.14 | 0.47 |
| 47:DV:79:VAL:O | 47:DV:80:GLN:CG | 2.62 | 0.47 |
| 47:DV:25:LEU:HD12 | 47:DV:94:LEU:HD22 | 1.97 | 0.47 |
| 49:DX:55:ASN:HB2 | 49:DX:78:LYS:HD2 | 1.96 | 0.47 |
| 51:DZ:117:LEU:HA | 51:DZ:174:VAL:HA | 1.95 | 0.47 |
| 1:AA:1316:G:O3' | 14:AN:18:VAL:HG22 | 2.14 | 0.47 |
| 1:AA:134:A:H1' | 1:AA:325:A:C5 | 2.49 | 0.47 |
| 1:AA:20:U:O2' | 1:AA:21:G:H5' | 2.15 | 0.47 |
| 1:AA:51:A:C4 | 1:AA:353:A:C6 | 3.03 | 0.47 |
| 3:AC:24:ALA:HB1 | 3:AC:28:GLN:O | 2.14 | 0.47 |
| 4:AD:3:ARG:HD3 | 4:AD:5:ILE:HG13 | 1.95 | 0.47 |
| 11:AK:20:TYR:O | 11:AK:30:VAL:HA | 2.15 | 0.47 |
| 13:AM:78:ILE:HG22 | 13:AM:93:ARG:HH22 | 1.79 | 0.47 |
| 13:AM:91:ARG:HB2 | 13:AM:98:VAL:CG2 | 2.45 | 0.47 |
| 15:AO:25:THR:O | 15:AO:29:VAL:HG23 | 2.15 | 0.47 |
| 15:AO:66:LEU:O | 15:AO:69:TYR:HB3 | 2.15 | 0.47 |
| 16:AP:14:ASN:N | 16:AP:15:PRO:HD3 | 2.29 | 0.47 |
| 20:AT:29:LYS:O | 20:AT:33:ILE:HG12 | 2.14 | 0.47 |
| 22:B0:56:ASP:O | 22:B0:57:PHE:HB2 | 2.15 | 0.47 |
| 24:B2:26:ARG:O | 24:B2:30:ARG:HD3 | 2.15 | 0.47 |
| 24:B2:43:GLN:O | 24:B2:46:GLN:CB | 2.62 | 0.47 |
| 31:BA:1359:A:N7 | 31:BA:1372:U:C4 | 2.81 | 0.47 |
| 31:BA:1487:G:C2 | 31:BA:1488:G:C4 | 3.03 | 0.47 |
| 31:BA:1803:A:H4' | 33:BD:259:THR:CG2 | 2.45 | 0.47 |
| 31:BA:2232:U:O2' | 31:BA:2233:U:H5' | 2.15 | 0.47 |
| 31:BA:2287:A:C5 | 31:BA:2289:G:C5 | 3.02 | 0.47 |
| 31:BA:2524:G:H8 | 31:BA:2524:G:C5' | 2.17 | 0.47 |
| 31:BA:2674:G:H2' | 31:BA:2675:A:O4' | 2.14 | 0.47 |
| 31:BA:302:C:O2' | 31:BA:303:U:H5' | 2.14 | 0.47 |
| 31:BA:455:C:N3 | 31:BA:473:G:H5' | 2.29 | 0.47 |
| 31:BA:661:C:H2' | 31:BA:662:G:C8 | 2.49 | 0.47 |
| 31:BA:975:C:O2 | 31:BA:975:C:H2' | 2.15 | 0.47 |
| 31:BA:9:U:HO2' | 31:BA:10:G:P | 2.38 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BD:115:GLN:HG2 | 33:BD:116:GLN:O | 2.14 | 0.47 |
| 33:BD:267:SER:HA | 33:BD:270:ILE:HG13 | 1.96 | 0.47 |
| 34:BE:77:ILE:HG23 | 34:BE:78:LEU:N | 2.29 | 0.47 |
| 36:BG:29:TRP:C | 36:BG:31:VAL:H | 2.17 | 0.47 |
| 36:BG:67:LYS:H | 36:BG:67:LYS:HD2 | 1.78 | 0.47 |
| 36:BG:86:MET:HB2 | 36:BG:87:PRO:HD2 | 1.97 | 0.47 |
| 37:BH:89:ILE:HG13 | 37:BH:129:THR:O | 2.15 | 0.47 |
| 37:BH:85:LYS:HZ3 | 37:BH:145:ALA:HB2 | 1.80 | 0.47 |
| 39:BN:36:GLY:H | 39:BN:42:TRP:HZ3 | 1.60 | 0.47 |
| 31:BA:557:U:O2 | 39:BN:45:ASN:HB2 | 2.15 | 0.47 |
| 41:BP:85:LEU:HD13 | 41:BP:114:ILE:HD11 | 1.97 | 0.47 |
| 42:BQ:63:LYS:HG2 | 42:BQ:65:PHE:CZ | 2.50 | 0.47 |
| 46:BU:112:ARG:HH11 | 46:BU:112:ARG:HG2 | 1.80 | 0.47 |
| 46:BU:83:LEU:C | 46:BU:88:ILE:HD11 | 2.35 | 0.47 |
| 47:BV:2:PHE:O | 47:BV:3:ALA:HB3 | 2.14 | 0.47 |
| 47:BV:50:PRO:C | 47:BV:51:VAL:HG23 | 2.35 | 0.47 |
| 50:BY:45:VAL:HG22 | 50:BY:62:GLU:N | 2.29 | 0.47 |
| 51:BZ:117:LEU:HA | 51:BZ:174:VAL:HA | 1.96 | 0.47 |
| 1:CA:1084:G:OP1 | 1:CA:1086:U:C4 | 2.67 | 0.47 |
| 1:CA:115:G:H4' | 1:CA:116:A:O5' | 2.14 | 0.47 |
| 1:CA:1206:G:O6 | 1:CA:1207:G:C6 | 2.68 | 0.47 |
| 3:CC:82:GLU:O | 3:CC:86:VAL:HG13 | 2.15 | 0.47 |
| 4:CD:100:ARG:NH1 | 4:CD:137:SER:HA | 2.29 | 0.47 |
| 4:CD:31:CYS:SG | 4:CD:31:CYS:O | 2.73 | 0.47 |
| 4:CD:79:PHE:CD1 | 4:CD:207:TYR:HD1 | 2.32 | 0.47 |
| 6:CF:11:ASN:HB3 | 6:CF:14:LEU:CG | 2.38 | 0.47 |
| 10:CJ:22:LYS:HZ2 | 10:CJ:88:LEU:HD23 | 1.79 | 0.47 |
| 1:CA:950:U:H6 | 13:CM:102:ARG:NH1 | 2.12 | 0.47 |
| 16:CP:14:ASN:N | 16:CP:15:PRO:HD3 | 2.30 | 0.47 |
| 23:D1:41:ARG:NH1 | 23:D1:41:ARG:CG | 2.53 | 0.47 |
| 23:D1:94:LEU:O | 23:D1:95:LEU:HG | 2.14 | 0.47 |
| 30:D8:62:LEU:N | 30:D8:63:PRO:HD2 | 2.29 | 0.47 |
| 31:DA:1181:C:C2' | 31:DA:1182:A:H5' | 2.45 | 0.47 |
| 31:DA:1264:G:H3' | 31:DA:1265:A:H5'' | 1.97 | 0.47 |
| 31:DA:125:G:H4' | 31:DA:126:A:OP2 | 2.15 | 0.47 |
| 31:DA:1464:C:O2' | 31:DA:1528:A:H1' | 2.14 | 0.47 |
| 31:DA:1494:A:N3 | 31:DA:1494:A:H2' | 2.29 | 0.47 |
| 31:DA:2299:G:C6 | 31:DA:2318:G:C8 | 3.02 | 0.47 |
| 31:DA:2406:U:C2 | 41:DP:72:PRO:HG2 | 2.50 | 0.47 |
| 31:DA:2543:G:H5' | 31:DA:2543:G:H8 | 1.80 | 0.47 |
| 31:DA:2635:C:H2' | 31:DA:2636:U:O5' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:271(F):C:H2' | 31:DA:271(G):C:C6 | 2.42 | 0.47 |
| 31:DA:2789:C:H2' | 31:DA:2790:A:OP2 | 2.14 | 0.47 |
| 31:DA:481:G:C4 | 31:DA:507:A:C2 | 3.03 | 0.47 |
| 31:DA:49:A:H5'' | 31:DA:51:G:O4' | 2.15 | 0.47 |
| 31:DA:839:U:H2' | 31:DA:840:C:C6 | 2.49 | 0.47 |
| 31:DA:878:A:C6 | 31:DA:900:A:C8 | 3.02 | 0.47 |
| 31:DA:971:C:H2' | 31:DA:972:G:C5' | 2.44 | 0.47 |
| 32:DB:110:G:N1 | 32:DB:111:G:C5 | 2.83 | 0.47 |
| 32:DB:21:G:N3 | 32:DB:21:G:H2' | 2.30 | 0.47 |
| 32:DB:1:U:C5 | 32:DB:2:C:C5 | 3.02 | 0.47 |
| 33:DD:228:PRO:CD | 33:DD:235:GLY:HA3 | 2.38 | 0.47 |
| 34:DE:47:VAL:O | 34:DE:80:GLU:HA | 2.15 | 0.47 |
| 36:DG:135:LEU:HD23 | 36:DG:140:ILE:HD11 | 1.95 | 0.47 |
| 38:DI:56:LYS:HZ2 | 38:DI:57:ARG:N | 2.13 | 0.47 |
| 45:DT:29:ARG:HD2 | 45:DT:29:ARG:HA | 1.51 | 0.47 |
| 31:DA:2876:G:H4' | 45:DT:3:ARG:HD3 | 1.96 | 0.47 |
| 46:DU:104:GLN:HB2 | 47:DV:43:GLU:OE1 | 2.14 | 0.47 |
| 47:DV:19:LYS:HE2 | 47:DV:20:LEU:N | 2.28 | 0.47 |
| 47:DV:64:HIS:HB3 | 47:DV:96:ILE:HG12 | 1.96 | 0.47 |
| 49:DX:80:ILE:HG23 | 49:DX:81:VAL:N | 2.28 | 0.47 |
| 1:AA:1016:A:H2' | 1:AA:1017:G:O4' | 2.15 | 0.47 |
| 1:AA:1077:G:C6 | 1:AA:1081:G:O6 | 2.68 | 0.47 |
| 1:AA:109:A:H2' | 1:AA:326:G:N2 | 2.29 | 0.47 |
| 1:AA:1254:C:OP1 | 10:AJ:45:ARG:HG2 | 2.15 | 0.47 |
| 1:AA:1301:U:H3' | 1:AA:1302:U:C5' | 2.45 | 0.47 |
| 1:AA:976:G:C5' | 1:AA:1358:U:O2' | 2.56 | 0.47 |
| 1:AA:343:U:C2' | 1:AA:346:G:O6 | 2.63 | 0.47 |
| 1:AA:407:G:H4' | 4:AD:115:ARG:O | 2.14 | 0.47 |
| 1:AA:484:G:H4' | 1:AA:485:G:OP1 | 2.15 | 0.47 |
| 1:AA:625:G:C4 | 1:AA:626:U:C5 | 3.03 | 0.47 |
| 1:AA:668:G:O2' | 1:AA:669:U:H5' | 2.15 | 0.47 |
| 1:AA:721:G:N1 | 1:AA:733:A:C2 | 2.82 | 0.47 |
| 2:AB:107:THR:O | 2:AB:110:GLN:HB2 | 2.15 | 0.47 |
| 4:AD:150:GLU:H | 4:AD:150:GLU:CD | 2.17 | 0.47 |
| 8:AH:87:SER:HB2 | 8:AH:93:VAL:HB | 1.95 | 0.47 |
| 16:AP:51:VAL:O | 16:AP:51:VAL:HG12 | 2.14 | 0.47 |
| 19:AS:22:LEU:O | 19:AS:26:GLY:HA2 | 2.15 | 0.47 |
| 20:AT:94:ALA:O | 20:AT:95:ALA:CB | 2.63 | 0.47 |
| 31:BA:1509(A):A:C5 | 31:BA:1509(B):A:N7 | 2.82 | 0.47 |
| 31:BA:2378:A:C2 | 44:BS:20:ARG:NH1 | 2.82 | 0.47 |
| 31:BA:2469:A:C5 | 31:BA:2470:G:H1' | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:795:C:H2' | 31:BA:796:C:C6 | 2.49 | 0.47 |
| 31:BA:855:G:C6 | 31:BA:856:C:C4 | 3.02 | 0.47 |
| 31:BA:911:A:C4 | 42:BQ:9:TYR:OH | 2.66 | 0.47 |
| 35:BF:113:ALA:HB1 | 35:BF:186:ILE:HG21 | 1.97 | 0.47 |
| 36:BG:125:PHE:HE2 | 36:BG:173:LEU:HD12 | 1.80 | 0.47 |
| 38:BI:88:ILE:HG13 | 38:BI:122:GLU:N | 2.30 | 0.47 |
| 38:BI:3:VAL:HG12 | 38:BI:38:LEU:HA | 1.95 | 0.47 |
| 38:BI:40:THR:CG2 | 38:BI:43:ASN:HD22 | 2.27 | 0.47 |
| 40:BO:43:VAL:HG23 | 40:BO:56:ASP:O | 2.14 | 0.47 |
| 41:BP:10:PRO:CD | 41:BP:11:GLY:N | 2.70 | 0.47 |
| 43:BR:37:THR:OG1 | 43:BR:40:LYS:HG3 | 2.15 | 0.47 |
| 45:BT:68:TYR:O | 45:BT:70:VAL:N | 2.47 | 0.47 |
| 49:BX:41:ASN:O | 49:BX:45:THR:CG2 | 2.63 | 0.47 |
| 49:BX:70:LEU:O | 49:BX:71:GLY:C | 2.53 | 0.47 |
| 1:CA:1293:G:O2' | 1:CA:1294:G:H8 | 1.97 | 0.47 |
| 1:CA:1271:G:H5' | 1:CA:1314:C:H5' | 1.96 | 0.47 |
| 1:CA:1429:C:H2' | 1:CA:1430:C:C6 | 2.50 | 0.47 |
| 1:CA:1442(A):G:C3' | 1:CA:1442(B):A:C5' | 2.87 | 0.47 |
| 1:CA:1456:G:H2' | 1:CA:1457:G:O4' | 2.15 | 0.47 |
| 1:CA:273:A:C2' | 1:CA:274:A:H5' | 2.45 | 0.47 |
| 1:CA:540:G:H2' | 1:CA:541:G:O4' | 2.14 | 0.47 |
| 1:CA:764:C:H2' | 1:CA:765:G:O5' | 2.14 | 0.47 |
| 1:CA:73:G:H2' | 1:CA:76:C:O5' | 2.15 | 0.47 |
| 3:CC:47:LEU:HD23 | 3:CC:52:LEU:HD13 | 1.95 | 0.47 |
| 5:CE:122:GLU:OE1 | 5:CE:131:ILE:HG13 | 2.14 | 0.47 |
| 8:CH:82:HIS:CD2 | 8:CH:138:TRP:NE1 | 2.82 | 0.47 |
| 13:CM:3:ARG:HG2 | 13:CM:9:ILE:HD11 | 1.97 | 0.47 |
| 6:CF:50:TYR:CE1 | 18:CR:77:GLY:HA2 | 2.50 | 0.47 |
| 24:D2:56:GLN:CD | 24:D2:56:GLN:N | 2.68 | 0.47 |
| 28:D6:32:ASN:O | 28:D6:33:LYS:CB | 2.62 | 0.47 |
| 28:D6:40:CYS:SG | 28:D6:45:LYS:HD3 | 2.55 | 0.47 |
| 31:DA:1108:U:H2' | 31:DA:1109:C:C5' | 2.41 | 0.47 |
| 31:DA:1507:A:C2 | 31:DA:1508:A:H1' | 2.49 | 0.47 |
| 31:DA:1380:G:N2 | 31:DA:1570:A:C2 | 2.83 | 0.47 |
| 31:DA:2199:A:N3 | 31:DA:2199:A:H2' | 2.30 | 0.47 |
| 31:DA:2287:A:C2 | 31:DA:2346:A:N1 | 2.83 | 0.47 |
| 31:DA:2629:A:N3 | 31:DA:2629:A:H2' | 2.30 | 0.47 |
| 31:DA:2655:G:O2' | 31:DA:2656:U:H5 | 1.97 | 0.47 |
| 31:DA:2772:C:H2' | 31:DA:2773:C:C6 | 2.49 | 0.47 |
| 31:DA:528:A:H8 | 31:DA:528:A:H3' | 1.79 | 0.47 |
| 33:DD:30:GLU:CG | 33:DD:63:ARG:NE | 2.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:DD:62:TYR:CE1 | 33:DD:64:ILE:HA | 2.50 | 0.47 |
| 36:DG:101:ILE:HG23 | 36:DG:102:PHE:N | 2.30 | 0.47 |
| 38:DI:75:LEU:HD11 | 38:DI:105:HIS:CE1 | 2.50 | 0.47 |
| 40:DO:22:ILE:HA | 40:DO:22:ILE:HD13 | 1.54 | 0.47 |
| 42:DQ:141:GLN:C | 51:DZ:70:LEU:HD13 | 2.35 | 0.47 |
| 43:DR:13:HIS:CE1 | 43:DR:15:SER:OG | 2.68 | 0.47 |
| 45:DT:100:TYR:HD2 | 45:DT:103:ARG:NH2 | 2.12 | 0.47 |
| 31:DA:1012:U:OP1 | 46:DU:75:ASN:OD1 | 2.33 | 0.47 |
| 31:DA:996:A:O4' | 46:DU:92:ARG:NH2 | 2.46 | 0.47 |
| 46:DU:92:ARG:HH22 | 47:DV:10:LYS:HG2 | 1.79 | 0.47 |
| 49:DX:65:ARG:O | 49:DX:66:LEU:HB3 | 2.15 | 0.47 |
| 1:AA:1206:G:H4' | 3:AC:192:THR:O | 2.14 | 0.47 |
| 1:AA:1245:A:N1 | 1:AA:1293:G:C6 | 2.83 | 0.47 |
| 1:AA:1338:G:O2' | 1:AA:1339:A:H5' | 2.15 | 0.47 |
| 1:AA:1428:A:H2' | 1:AA:1429:C:C6 | 2.50 | 0.47 |
| 1:AA:1478:C:H2' | 1:AA:1479:C:C6 | 2.50 | 0.47 |
| 1:AA:1483:A:H2 | 31:BA:1959:G:N3 | 2.13 | 0.47 |
| 1:AA:1525:G:OP1 | 11:AK:120:ARG:NH2 | 2.48 | 0.47 |
| 1:AA:284:G:H2' | 1:AA:285:G:H8 | 1.80 | 0.47 |
| 1:AA:376:G:C4 | 1:AA:389:A:C2 | 3.03 | 0.47 |
| 1:AA:834:C:H2' | 1:AA:835:U:C6 | 2.50 | 0.47 |
| 2:AB:161:ALA:HB1 | 2:AB:185:ILE:CD1 | 2.45 | 0.47 |
| 3:AC:108:ASN:HD22 | 3:AC:111:LEU:HD12 | 1.80 | 0.47 |
| 3:AC:15:THR:HG21 | 3:AC:181:ASN:HA | 1.97 | 0.47 |
| 1:AA:407:G:O2' | 4:AD:116:GLN:HG3 | 2.14 | 0.47 |
| 4:AD:107:ARG:CD | 4:AD:173:TRP:HZ2 | 2.25 | 0.47 |
| 1:AA:626:U:H4' | 16:AP:38:TYR:CZ | 2.50 | 0.47 |
| 17:AQ:59:ILE:HG22 | 17:AQ:60:ILE:N | 2.30 | 0.47 |
| 18:AR:22:VAL:HG12 | 18:AR:22:VAL:O | 2.15 | 0.47 |
| 1:AA:719:C:H1' | 18:AR:49:LYS:HB3 | 1.97 | 0.47 |
| 23:B1:79:GLY:O | 23:B1:80:LEU:HG | 2.14 | 0.47 |
| 25:B3:36:VAL:HG23 | 25:B3:36:VAL:O | 2.13 | 0.47 |
| 26:B4:19:GLY:C | 26:B4:21:VAL:N | 2.67 | 0.47 |
| 27:B5:40:LYS:CE | 27:B5:49:CYS:SG | 3.03 | 0.47 |
| 29:B7:19:ARG:NH1 | 29:B7:19:ARG:HG2 | 2.30 | 0.47 |
| 30:B8:50:LEU:HD12 | 30:B8:51:ALA:N | 2.30 | 0.47 |
| 31:BA:1209:G:H21 | 31:BA:1210:A:N6 | 2.12 | 0.47 |
| 31:BA:1528:A:O2' | 31:BA:1528(A):A:P | 2.73 | 0.47 |
| 31:BA:226:G:H21 | 31:BA:228:A:H62 | 1.62 | 0.47 |
| 30:B8:31:HIS:HB3 | 31:BA:2420:C:H41 | 1.80 | 0.47 |
| 31:BA:2722:G:O2' | 43:BR:5:LYS:HB2 | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:362:U:C6 | 31:BA:362:U:H3' | 2.49 | 0.47 |
| 31:BA:363(C):G:H2' | 31:BA:363(D):G:O4' | 2.15 | 0.47 |
| 33:BD:127:VAL:HA | 33:BD:193:VAL:HG22 | 1.97 | 0.47 |
| 36:BG:118:ARG:HB2 | 36:BG:181:ARG:CZ | 2.45 | 0.47 |
| 41:BP:119:GLU:HB3 | 25:D3:1:MET:H2 | 1.80 | 0.47 |
| 44:BS:35:ILE:HG22 | 44:BS:53:SER:HB2 | 1.97 | 0.47 |
| 44:BS:24:LEU:HB3 | 44:BS:85:VAL:HG12 | 1.96 | 0.47 |
| 47:BV:40:LEU:HD12 | 47:BV:40:LEU:C | 2.35 | 0.47 |
| 50:BY:90:LEU:HG | 50:BY:91:GLU:N | 2.29 | 0.47 |
| 1:CA:102:G:C4 | 1:CA:103:C:C6 | 3.03 | 0.47 |
| 1:CA:994:A:H62 | 1:CA:1046:A:H2 | 1.63 | 0.47 |
| 1:CA:1160:G:H2' | 1:CA:1160:G:N3 | 2.29 | 0.47 |
| 1:CA:295:C:H2' | 1:CA:296:U:O4' | 2.14 | 0.47 |
| 1:CA:411:A:C4 | 1:CA:413:G:O4' | 2.68 | 0.47 |
| 1:CA:414:A:H2' | 1:CA:415:A:H8 | 1.80 | 0.47 |
| 1:CA:417:C:H2' | 1:CA:418:C:H5' | 1.95 | 0.47 |
| 1:CA:785:G:C2' | 1:CA:786:G:H5' | 2.45 | 0.47 |
| 1:CA:940:C:H2' | 1:CA:941:G:H8 | 1.80 | 0.47 |
| 2:CB:68:ILE:HG22 | 2:CB:70:PHE:CE1 | 2.50 | 0.47 |
| 3:CC:14:ILE:HG23 | 3:CC:15:THR:N | 2.29 | 0.47 |
| 3:CC:15:THR:HG21 | 3:CC:181:ASN:HA | 1.97 | 0.47 |
| 6:CF:76:ALA:HB1 | 6:CF:80:ARG:NH2 | 2.30 | 0.47 |
| 9:CI:11:LYS:O | 9:CI:11:LYS:HG2 | 2.15 | 0.47 |
| 14:CN:21:TYR:OH | 14:CN:23:ARG:NH2 | 2.48 | 0.47 |
| 19:CS:16:LEU:O | 19:CS:20:LEU:HB2 | 2.15 | 0.47 |
| 23:D1:19:GLN:CD | 23:D1:44:PRO:HG3 | 2.35 | 0.47 |
| 30:D8:48:PHE:CD1 | 30:D8:48:PHE:N | 2.81 | 0.47 |
| 31:DA:1312:U:OP2 | 49:DX:62:LYS:HE3 | 2.14 | 0.47 |
| 31:DA:1655:A:C8 | 31:DA:1656:C:C5 | 3.02 | 0.47 |
| 31:DA:2471:C:O2 | 31:DA:2471:C:H2' | 2.14 | 0.47 |
| 31:DA:2471:C:N4 | 31:DA:2472:G:C6 | 2.82 | 0.47 |
| 31:DA:26:G:H1' | 31:DA:515:A:H61 | 1.80 | 0.47 |
| 31:DA:2804:C:C2' | 31:DA:2805:G:H5' | 2.45 | 0.47 |
| 31:DA:606:U:H4' | 31:DA:658:C:H4' | 1.96 | 0.47 |
| 31:DA:745:G:OP2 | 34:DE:133:LYS:HE3 | 2.15 | 0.47 |
| 31:DA:904:C:H2' | 31:DA:904:C:O2 | 2.15 | 0.47 |
| 31:DA:847:U:OP2 | 31:DA:928:G:O6 | 2.31 | 0.47 |
| 36:DG:139:LEU:C | 36:DG:141:PHE:H | 2.17 | 0.47 |
| 38:DI:109:ILE:HG22 | 38:DI:130:TYR:CZ | 2.50 | 0.47 |
| 38:DI:94:ALA:HB1 | 38:DI:114:LEU:HD12 | 1.96 | 0.47 |
| 39:DN:15:LEU:HD21 | 39:DN:55:VAL:CG2 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:DO:73:ASP:OD2 | 45:DT:32:TYR:HE1 | 1.97 | 0.47 |
| 41:DP:140:ALA:O | 41:DP:141:ALA:HB3 | 2.14 | 0.47 |
| 41:DP:148:LEU:HD13 | 41:DP:148:LEU:N | 2.29 | 0.47 |
| 43:DR:5:LYS:HD2 | 43:DR:5:LYS:N | 2.30 | 0.47 |
| 44:DS:11:LYS:N | 44:DS:11:LYS:HD2 | 2.30 | 0.47 |
| 44:DS:16:ASN:O | 44:DS:20:ARG:NH2 | 2.48 | 0.47 |
| 50:DY:14:LEU:HD11 | 50:DY:22:GLY:HA2 | 1.97 | 0.47 |
| 1:AA:1442(A):G:C8 | 45:BT:118:ARG:HD2 | 2.49 | 0.47 |
| 1:AA:193:C:H2' | 1:AA:194:C:C6 | 2.49 | 0.47 |
| 1:AA:292:G:N7 | 1:AA:293:G:H1' | 2.30 | 0.47 |
| 1:AA:339:C:H2' | 1:AA:340:U:C6 | 2.50 | 0.47 |
| 1:AA:405:U:H5'' | 1:AA:406:G:O4' | 2.14 | 0.47 |
| 1:AA:586:C:H2' | 1:AA:587:G:H5' | 1.96 | 0.47 |
| 1:AA:785:G:C2' | 1:AA:786:G:H5' | 2.44 | 0.47 |
| 1:AA:881:G:P | 12:AL:12:ARG:HH22 | 2.38 | 0.47 |
| 3:AC:19:GLU:O | 3:AC:19:GLU:HG2 | 2.14 | 0.47 |
| 7:AG:27:ILE:HD11 | 7:AG:43:PHE:CD2 | 2.50 | 0.47 |
| 8:AH:113:SER:H | 8:AH:134:ILE:CG1 | 2.27 | 0.47 |
| 11:AK:41:THR:HG22 | 11:AK:42:TRP:H | 1.80 | 0.47 |
| 12:AL:38:THR:HG23 | 12:AL:39:VAL:N | 2.30 | 0.47 |
| 12:AL:87:GLY:H | 12:AL:99:HIS:H | 1.63 | 0.47 |
| 15:AO:37:ASN:ND2 | 15:AO:37:ASN:N | 2.62 | 0.47 |
| 27:B5:51:TYR:HB2 | 27:B5:54:GLY:HA3 | 1.96 | 0.47 |
| 27:B5:57:VAL:C | 27:B5:58:LEU:HD12 | 2.35 | 0.47 |
| 31:BA:132:G:H1 | 31:BA:147:U:H3 | 1.61 | 0.47 |
| 31:BA:1331:A:O2' | 31:BA:1332:G:H8 | 1.98 | 0.47 |
| 31:BA:2070:G:H2' | 31:BA:2071:A:C8 | 2.50 | 0.47 |
| 31:BA:2287:A:O2' | 31:BA:2288:A:H3' | 2.15 | 0.47 |
| 31:BA:2593:U:H2' | 31:BA:2594:C:C6 | 2.50 | 0.47 |
| 31:BA:2659:G:H8 | 31:BA:2659:G:H5'' | 1.80 | 0.47 |
| 31:BA:2821:A:H2' | 31:BA:2822:G:C8 | 2.50 | 0.47 |
| 31:BA:322:A:C5 | 31:BA:340:A:C2 | 3.03 | 0.47 |
| 31:BA:484:C:H2' | 31:BA:485:C:H6 | 1.77 | 0.47 |
| 31:BA:528:A:C8 | 31:BA:528:A:H3' | 2.49 | 0.47 |
| 31:BA:639:U:H2' | 31:BA:640:C:H6 | 1.79 | 0.47 |
| 31:BA:892:G:C5 | 31:BA:893:C:C5 | 3.02 | 0.47 |
| 32:BB:40:U:H3' | 32:BB:41:U:H5'' | 1.96 | 0.47 |
| 36:BG:139:LEU:C | 36:BG:141:PHE:H | 2.18 | 0.47 |
| 40:BO:104:ARG:O | 40:BO:107:ARG:HB3 | 2.15 | 0.47 |
| 41:BP:144:GLU:N | 41:BP:145:PRO:CD | 2.76 | 0.47 |
| 43:BR:75:LEU:C | 43:BR:75:LEU:CD1 | 2.83 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BS:67:ARG:H | 44:BS:69:VAL:CG1 | 2.27 | 0.47 |
| 44:BS:95:HIS:O | 44:BS:98:VAL:CG2 | 2.63 | 0.47 |
| 49:BX:76:ARG:HD2 | 49:BX:77:LYS:HB2 | 1.97 | 0.47 |
| 49:BX:52:VAL:HB | 49:BX:80:ILE:CG2 | 2.45 | 0.47 |
| 50:BY:45:VAL:HG13 | 50:BY:62:GLU:OE2 | 2.14 | 0.47 |
| 51:BZ:143:GLY:C | 51:BZ:144:LEU:HD22 | 2.36 | 0.47 |
| 51:BZ:151:HIS:ND1 | 51:BZ:170:THR:HG22 | 2.30 | 0.47 |
| 51:BZ:117:LEU:CB | 51:BZ:174:VAL:HG22 | 2.45 | 0.47 |
| 1:CA:137:C:H2' | 1:CA:137:C:O2 | 2.14 | 0.47 |
| 1:CA:149:A:O2' | 1:CA:150:C:P | 2.73 | 0.47 |
| 1:CA:373:A:N3 | 1:CA:374:A:C8 | 2.82 | 0.47 |
| 1:CA:407:G:H4' | 4:CD:115:ARG:O | 2.14 | 0.47 |
| 1:CA:427:U:C4 | 1:CA:428:G:C6 | 3.03 | 0.47 |
| 1:CA:444:C:H2' | 1:CA:445:G:H8 | 1.80 | 0.47 |
| 1:CA:790:A:C6 | 1:CA:791:G:C6 | 3.03 | 0.47 |
| 2:CB:238:LEU:O | 2:CB:240:GLN:N | 2.47 | 0.47 |
| 12:CL:64:TYR:HB3 | 12:CL:65:GLU:H | 1.48 | 0.47 |
| 13:CM:14:ARG:CZ | 13:CM:42:ALA:HA | 2.45 | 0.47 |
| 13:CM:75:ALA:O | 13:CM:79:LYS:HG3 | 2.15 | 0.47 |
| 17:CQ:18:THR:OG1 | 17:CQ:69:LYS:NZ | 2.43 | 0.47 |
| 23:D1:25:LYS:O | 23:D1:26:ARG:HG3 | 2.14 | 0.47 |
| 24:D2:26:ARG:HG3 | 24:D2:29:LYS:HZ1 | 1.80 | 0.47 |
| 28:D6:24:GLU:OE1 | 28:D6:24:GLU:CA | 2.62 | 0.47 |
| 28:D6:25:LYS:O | 31:DA:2286:A:H2 | 1.98 | 0.47 |
| 30:D8:52:LYS:N | 30:D8:53:PRO:CD | 2.63 | 0.47 |
| 31:DA:1592:C:C2' | 31:DA:1593:G:C5' | 2.80 | 0.47 |
| 31:DA:1803:A:C2 | 31:DA:1822:G:N3 | 2.83 | 0.47 |
| 31:DA:1865:G:N2 | 31:DA:1877:A:C8 | 2.83 | 0.47 |
| 31:DA:2292:C:C2' | 31:DA:2293:C:H5' | 2.45 | 0.47 |
| 31:DA:2439:A:C5' | 31:DA:2439:A:C8 | 2.98 | 0.47 |
| 31:DA:540:C:H2' | 31:DA:541:C:C6 | 2.50 | 0.47 |
| 31:DA:676:A:H2 | 31:DA:802:A:N6 | 2.11 | 0.47 |
| 31:DA:773:U:C5' | 33:DD:47:GLY:HA2 | 2.45 | 0.47 |
| 31:DA:832:G:H21 | 41:DP:53:GLY:HA3 | 1.80 | 0.47 |
| 31:DA:876:C:C2 | 31:DA:877:U:C6 | 3.02 | 0.47 |
| 31:DA:864:G:N2 | 31:DA:913:U:C2 | 2.83 | 0.47 |
| 32:DB:71:C:H2' | 32:DB:71:C:O2 | 2.15 | 0.47 |
| 31:DA:1353:A:H5'' | 33:DD:38:LYS:NZ | 2.30 | 0.47 |
| 34:DE:201:THR:HG22 | 34:DE:203:LYS:N | 2.30 | 0.47 |
| 34:DE:57:LYS:O | 34:DE:57:LYS:HG3 | 2.15 | 0.47 |
| 36:DG:114:ILE:O | 36:DG:116:ASP:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DG:19:LEU:HG | 36:DG:175:LEU:CD1 | 2.45 | 0.47 |
| 37:DH:153:LYS:HB2 | 37:DH:154:PRO:HD3 | 1.97 | 0.47 |
| 38:DI:29:TYR:O | 38:DI:32:PRO:HD2 | 2.15 | 0.47 |
| 38:DI:5:LEU:HD21 | 38:DI:19:VAL:CG1 | 2.45 | 0.47 |
| 41:DP:81:GLN:NE2 | 41:DP:106:LEU:HA | 2.29 | 0.47 |
| 41:DP:112:LEU:O | 41:DP:128:HIS:HB2 | 2.15 | 0.47 |
| 43:DR:53:HIS:CD2 | 43:DR:94:TYR:OH | 2.64 | 0.47 |
| 44:DS:89:ARG:CA | 44:DS:89:ARG:NE | 2.76 | 0.47 |
| 45:DT:33:LYS:N | 45:DT:33:LYS:HZ2 | 2.12 | 0.47 |
| 50:DY:87:LYS:HG3 | 50:DY:88:LYS:N | 2.30 | 0.47 |
| 50:DY:97:ARG:O | 50:DY:98:VAL:C | 2.53 | 0.47 |
| 42:DQ:134:ARG:NH2 | 51:DZ:122:ARG:HD2 | 2.25 | 0.47 |
| 1:AA:137:C:H2' | 1:AA:137:C:O2 | 2.14 | 0.47 |
| 1:AA:1429:C:H2' | 1:AA:1430:C:H6 | 1.80 | 0.47 |
| 1:AA:1504:G:H4' | 1:AA:1505:G:O4' | 2.15 | 0.47 |
| 1:AA:402:G:C6 | 1:AA:403:C:C4 | 3.03 | 0.47 |
| 1:AA:411:A:C4 | 1:AA:413:G:O4' | 2.68 | 0.47 |
| 1:AA:477:A:O2' | 1:AA:479:C:H5' | 2.14 | 0.47 |
| 1:AA:539:A:OP1 | 12:AL:114:LYS:HE2 | 2.15 | 0.47 |
| 1:AA:563:A:N7 | 1:AA:567:G:H1' | 2.30 | 0.47 |
| 1:AA:665:A:C2 | 1:AA:732:C:C2 | 3.03 | 0.47 |
| 1:AA:946:A:C2 | 1:AA:1236:A:C2 | 3.03 | 0.47 |
| 2:AB:91:PRO:N | 2:AB:154:LEU:HD12 | 2.30 | 0.47 |
| 4:AD:158:ILE:HG23 | 4:AD:162:LEU:HD12 | 1.97 | 0.47 |
| 4:AD:61:LYS:HA | 4:AD:203:VAL:HG22 | 1.97 | 0.47 |
| 4:AD:50:ARG:HD2 | 4:AD:51:PRO:O | 2.15 | 0.47 |
| 4:AD:65:ARG:HG3 | 4:AD:75:PHE:CD1 | 2.48 | 0.47 |
| 9:AI:55:ALA:HB1 | 9:AI:58:ARG:HD2 | 1.96 | 0.47 |
| 11:AK:85:ARG:HA | 11:AK:112:THR:OG1 | 2.15 | 0.47 |
| 13:AM:81:LEU:CD1 | 13:AM:88:ARG:HH12 | 2.28 | 0.47 |
| 17:AQ:63:ARG:HG2 | 17:AQ:64:PRO:HD2 | 1.97 | 0.47 |
| 22:B0:65:GLY:HA2 | 22:B0:84:LEU:CD2 | 2.45 | 0.47 |
| 23:B1:19:GLN:CD | 23:B1:44:PRO:HG3 | 2.35 | 0.47 |
| 29:B7:5:TRP:NE1 | 29:B7:7:PRO:HG3 | 2.30 | 0.47 |
| 30:B8:8:LYS:O | 30:B8:12:LYS:HG3 | 2.15 | 0.47 |
| 30:B8:18:ALA:HB3 | 31:BA:651:G:H4' | 1.97 | 0.47 |
| 31:BA:1224:C:O3' | 47:BV:88:ARG:HB3 | 2.15 | 0.47 |
| 31:BA:128:C:O2' | 31:BA:129:C:O5' | 2.33 | 0.47 |
| 31:BA:1475:G:H5' | 31:BA:1476:C:OP2 | 2.15 | 0.47 |
| 31:BA:1866:C:H2' | 31:BA:1876:A:O4' | 2.14 | 0.47 |
| 31:BA:1992:G:O2' | 31:BA:1993:U:OP2 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:670:A:H4' | 31:BA:671:C:O5' | 2.14 | 0.47 |
| 31:BA:878:A:H2' | 31:BA:879:G:H5' | 1.96 | 0.47 |
| 32:BB:27:C:H5'' | 32:BB:27:C:H6 | 1.79 | 0.47 |
| 32:BB:52:A:O2' | 32:BB:53:A:C8 | 2.61 | 0.47 |
| 33:BD:34:VAL:O | 33:BD:34:VAL:HG13 | 2.15 | 0.47 |
| 33:BD:35:LYS:HG2 | 33:BD:64:ILE:CA | 2.45 | 0.47 |
| 34:BE:12:THR:O | 34:BE:23:VAL:HG23 | 2.14 | 0.47 |
| 35:BF:64:ILE:HD12 | 35:BF:65:TRP:CE2 | 2.50 | 0.47 |
| 37:BH:85:LYS:NZ | 37:BH:145:ALA:CA | 2.78 | 0.47 |
| 38:BI:75:LEU:HD11 | 38:BI:105:HIS:CE1 | 2.49 | 0.47 |
| 38:BI:76:THR:CG2 | 38:BI:139:GLN:HB3 | 2.45 | 0.47 |
| 39:BN:15:LEU:HD22 | 39:BN:16:ILE:H | 1.80 | 0.47 |
| 41:BP:100:LEU:HD12 | 41:BP:100:LEU:HA | 1.77 | 0.47 |
| 42:BQ:20:ALA:HA | 42:BQ:98:LYS:HD3 | 1.97 | 0.47 |
| 45:BT:109:GLU:HA | 45:BT:112:ARG:HG2 | 1.97 | 0.47 |
| 39:BN:2:LYS:HZ3 | 46:BU:94:ASN:ND2 | 2.12 | 0.47 |
| 47:BV:27:ALA:O | 47:BV:28:GLU:C | 2.52 | 0.47 |
| 49:BX:65:ARG:NH2 | 49:BX:66:LEU:H | 2.13 | 0.47 |
| 1:CA:375:U:N3 | 1:CA:376:G:N7 | 2.63 | 0.47 |
| 1:CA:66:G:C2 | 1:CA:67:C:C6 | 3.03 | 0.47 |
| 1:CA:734:G:C5 | 1:CA:735:C:C4 | 3.03 | 0.47 |
| 3:CC:112:SER:HB3 | 3:CC:115:LEU:HD12 | 1.97 | 0.47 |
| 5:CE:100:VAL:O | 5:CE:107:ARG:NH2 | 2.48 | 0.47 |
| 7:CG:37:ASN:HD21 | 9:CI:40:LEU:CD2 | 2.28 | 0.47 |
| 20:CT:30:LYS:HD2 | 20:CT:30:LYS:O | 2.15 | 0.47 |
| 20:CT:75:ASN:ND2 | 20:CT:75:ASN:H | 2.13 | 0.47 |
| 31:DA:1050:A:C2 | 31:DA:2751:G:C5 | 3.03 | 0.47 |
| 31:DA:9:U:HO2' | 31:DA:10:G:P | 2.38 | 0.47 |
| 31:DA:1003:G:N2 | 31:DA:1153:C:C2 | 2.83 | 0.47 |
| 31:DA:1481:U:H5' | 31:DA:1482:G:P | 2.55 | 0.47 |
| 31:DA:1591:G:C5' | 31:DA:1591:G:H8 | 2.27 | 0.47 |
| 31:DA:1901:A:H2' | 31:DA:1902:C:H5' | 1.97 | 0.47 |
| 31:DA:2017:U:H5'' | 31:DA:2018:G:OP2 | 2.14 | 0.47 |
| 31:DA:910:A:H2' | 31:DA:2264:C:O2' | 2.15 | 0.47 |
| 31:DA:2287:A:C5 | 31:DA:2289:G:C5 | 3.03 | 0.47 |
| 28:D6:45:LYS:HB3 | 31:DA:2371:G:H4' | 1.96 | 0.47 |
| 31:DA:2392:A:C8 | 41:DP:60:MET:HG2 | 2.50 | 0.47 |
| 31:DA:2473:U:C2 | 31:DA:2474:C:C6 | 3.03 | 0.47 |
| 31:DA:2524:G:C5' | 31:DA:2524:G:H8 | 2.17 | 0.47 |
| 31:DA:2712:U:O2' | 31:DA:2713:A:H5' | 2.14 | 0.47 |
| 31:DA:2791:C:H4' | 31:DA:2792:G:O5' | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:D0:77:ARG:NH2 | 31:DA:857:C:OP1 | 2.42 | 0.47 |
| 32:DB:20:C:C2' | 32:DB:21:G:H5' | 2.34 | 0.47 |
| 32:DB:1:U:C6 | 32:DB:2:C:C5 | 3.03 | 0.47 |
| 33:DD:35:LYS:HG2 | 33:DD:64:ILE:CG2 | 2.42 | 0.47 |
| 34:DE:3:GLY:O | 34:DE:4:ILE:HB | 2.15 | 0.47 |
| 36:DG:57:ALA:CB | 36:DG:90:LEU:HD21 | 2.45 | 0.47 |
| 39:DN:82:LEU:H | 39:DN:82:LEU:CD1 | 2.22 | 0.47 |
| 42:DQ:16:ARG:NH1 | 42:DQ:16:ARG:CB | 2.78 | 0.47 |
| 43:DR:117:VAL:HG12 | 43:DR:117:VAL:O | 2.15 | 0.47 |
| 50:DY:45:VAL:CG1 | 50:DY:46:LYS:N | 2.78 | 0.47 |
| 1:AA:1054:C:C2' | 1:AA:1055:A:H5'' | 2.45 | 0.46 |
| 1:AA:129:U:H5' | 17:AQ:3:LYS:NZ | 2.30 | 0.46 |
| 1:AA:1404:C:H2' | 1:AA:1405:G:C8 | 2.50 | 0.46 |
| 1:AA:1521:G:H2' | 1:AA:1522:U:C6 | 2.50 | 0.46 |
| 1:AA:553:A:H2' | 1:AA:554:C:C6 | 2.49 | 0.46 |
| 1:AA:621:A:O2' | 1:AA:622:A:H5' | 2.15 | 0.46 |
| 1:AA:736:C:H2' | 1:AA:737:A:H8 | 1.77 | 0.46 |
| 1:AA:73:G:H2' | 1:AA:76:C:O5' | 2.15 | 0.46 |
| 1:AA:872:A:C5 | 1:AA:874:G:C8 | 3.03 | 0.46 |
| 4:AD:135:LEU:O | 4:AD:136:PRO:C | 2.53 | 0.46 |
| 4:AD:79:PHE:CD1 | 4:AD:207:TYR:HD1 | 2.33 | 0.46 |
| 12:AL:126:LYS:HE2 | 12:AL:128:ALA:H | 1.80 | 0.46 |
| 13:AM:14:ARG:CZ | 13:AM:42:ALA:HA | 2.45 | 0.46 |
| 13:AM:82:MET:HB2 | 13:AM:93:ARG:NH1 | 2.29 | 0.46 |
| 13:AM:3:ARG:HG2 | 13:AM:9:ILE:HD11 | 1.98 | 0.46 |
| 15:AO:55:GLY:O | 15:AO:58:MET:N | 2.48 | 0.46 |
| 23:B1:48:LYS:HA | 23:B1:48:LYS:HD3 | 1.35 | 0.46 |
| 27:B5:45:VAL:HA | 27:B5:51:TYR:HE1 | 1.80 | 0.46 |
| 31:BA:1417:C:O2' | 31:BA:1418:G:H5' | 2.15 | 0.46 |
| 31:BA:175:G:H5' | 31:BA:175:G:C8 | 2.50 | 0.46 |
| 31:BA:26:G:C6 | 31:BA:27:G:N1 | 2.83 | 0.46 |
| 31:BA:2876:G:H4' | 45:BT:3:ARG:HE | 1.80 | 0.46 |
| 31:BA:389:G:H22 | 41:BP:72:PRO:HD3 | 1.80 | 0.46 |
| 31:BA:603:A:O2' | 31:BA:604:G:OP2 | 2.17 | 0.46 |
| 31:BA:780:G:C2 | 31:BA:782:A:C2 | 3.03 | 0.46 |
| 31:BA:882:G:H8 | 31:BA:882:G:O5' | 1.98 | 0.46 |
| 34:BE:36:ARG:HH11 | 34:BE:85:ASN:ND2 | 2.12 | 0.46 |
| 35:BF:160:ASN:ND2 | 35:BF:160:ASN:C | 2.66 | 0.46 |
| 36:BG:64:THR:HG23 | 36:BG:66:GLN:N | 2.26 | 0.46 |
| 37:BH:157:TYR:CD1 | 37:BH:171:LEU:N | 2.82 | 0.46 |
| 46:BU:104:GLN:HB2 | 47:BV:43:GLU:CD | 2.35 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BU:112:ARG:O | 46:BU:115:ALA:HB3 | 2.16 | 0.46 |
| 47:BV:52:VAL:HG12 | 47:BV:52:VAL:O | 2.15 | 0.46 |
| 49:BX:83:VAL:O | 49:BX:83:VAL:HG23 | 2.15 | 0.46 |
| 51:BZ:33:LEU:HA | 51:BZ:33:LEU:HD12 | 1.71 | 0.46 |
| 51:BZ:96:VAL:N | 51:BZ:128:VAL:O | 2.45 | 0.46 |
| 1:CA:127:G:C2 | 1:CA:128:G:C8 | 3.04 | 0.46 |
| 1:CA:1422:G:O3' | 40:DO:49:ARG:NH2 | 2.48 | 0.46 |
| 1:CA:175:C:C2 | 1:CA:176:C:C5 | 3.03 | 0.46 |
| 1:CA:322:C:C5 | 1:CA:328:C:C5 | 2.98 | 0.46 |
| 1:CA:355:C:N3 | 1:CA:356:A:N7 | 2.64 | 0.46 |
| 1:CA:575:G:OP1 | 1:CA:575:G:H4' | 2.15 | 0.46 |
| 2:CB:107:THR:O | 2:CB:110:GLN:HB2 | 2.15 | 0.46 |
| 2:CB:168:THR:CG2 | 2:CB:192:SER:HA | 2.46 | 0.46 |
| 2:CB:24:TRP:CZ3 | 2:CB:26:PRO:HA | 2.50 | 0.46 |
| 4:CD:158:ILE:HG23 | 4:CD:162:LEU:HD12 | 1.97 | 0.46 |
| 6:CF:2:ARG:HB2 | 6:CF:4:TYR:CE2 | 2.49 | 0.46 |
| 6:CF:9:VAL:HB | 6:CF:87:ARG:HB2 | 1.96 | 0.46 |
| 20:CT:12:ALA:O | 20:CT:15:ARG:HB2 | 2.15 | 0.46 |
| 20:CT:94:ALA:O | 20:CT:95:ALA:CB | 2.62 | 0.46 |
| 21:CU:12:LYS:HB3 | 21:CU:22:ARG:HD2 | 1.96 | 0.46 |
| 25:D3:12:PRO:HA | 25:D3:15:TYR:HD1 | 1.80 | 0.46 |
| 28:D6:35:GLU:HG3 | 28:D6:35:GLU:O | 2.10 | 0.46 |
| 29:D7:30:VAL:O | 29:D7:34:ARG:HG3 | 2.14 | 0.46 |
| 30:D8:10:ALA:HB2 | 30:D8:59:LYS:HZ2 | 1.79 | 0.46 |
| 31:DA:1048:A:OP2 | 31:DA:1110:G:N1 | 2.46 | 0.46 |
| 31:DA:1234:U:O2' | 31:DA:1235:G:H5' | 2.15 | 0.46 |
| 31:DA:1321:A:H2' | 31:DA:1322:A:O4' | 2.15 | 0.46 |
| 31:DA:1465:G:N1 | 31:DA:1466:G:C5 | 2.83 | 0.46 |
| 31:DA:1649:G:C6 | 31:DA:2009:G:C6 | 3.03 | 0.46 |
| 31:DA:2320:A:N3 | 31:DA:2320:A:H2' | 2.29 | 0.46 |
| 31:DA:2364:C:O2' | 31:DA:2365:G:H5' | 2.15 | 0.46 |
| 31:DA:2684:U:H1' | 40:DO:70:LYS:HD2 | 1.96 | 0.46 |
| 31:DA:518:G:H4' | 48:DW:18:ARG:CZ | 2.44 | 0.46 |
| 31:DA:900:A:C5' | 31:DA:901:A:OP2 | 2.63 | 0.46 |
| 31:DA:921:G:C5 | 31:DA:922:U:C4 | 3.03 | 0.46 |
| 32:DB:40:U:H3' | 32:DB:41:U:H5'' | 1.98 | 0.46 |
| 33:DD:237:GLU:HB3 | 33:DD:238:GLY:H | 1.58 | 0.46 |
| 36:DG:82:LEU:C | 36:DG:83:ARG:HG3 | 2.36 | 0.46 |
| 41:DP:85:LEU:HD21 | 41:DP:116:GLY:O | 2.14 | 0.46 |
| 47:DV:50:PRO:C | 47:DV:51:VAL:HG23 | 2.34 | 0.46 |
| 47:DV:21:ARG:HB3 | 47:DV:93:GLU:HB2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:DZ:48:PHE:HE2 | 51:DZ:71:VAL:HG11 | 1.79 | 0.46 |
| 1:AA:1098:C:N3 | 1:AA:1099:G:C8 | 2.83 | 0.46 |
| 1:AA:189:G:N1 | 1:AA:189(L):G:C6 | 2.83 | 0.46 |
| 1:AA:565:U:H3' | 1:AA:566:G:H2' | 1.96 | 0.46 |
| 1:AA:69:G:H2' | 1:AA:70:G:H8 | 1.79 | 0.46 |
| 1:AA:939:G:C6 | 1:AA:940:C:N4 | 2.83 | 0.46 |
| 1:AA:966:G:H5'' | 1:AA:969:A:N7 | 2.31 | 0.46 |
| 3:AC:19:GLU:HA | 3:AC:54:ARG:NH2 | 2.30 | 0.46 |
| 4:AD:62:GLN:HE21 | 4:AD:62:GLN:HA | 1.81 | 0.46 |
| 7:AG:75:VAL:HG13 | 7:AG:145:ALA:HB2 | 1.98 | 0.46 |
| 20:AT:92:LEU:C | 20:AT:94:ALA:H | 2.19 | 0.46 |
| 23:B1:76:ARG:CB | 23:B1:78:LYS:HE3 | 2.46 | 0.46 |
| 31:BA:1241:A:C2' | 31:BA:1242:A:O5' | 2.63 | 0.46 |
| 31:BA:1531:C:H5' | 31:BA:1532:C:OP2 | 2.15 | 0.46 |
| 31:BA:2103:C:N3 | 31:BA:2187:G:C6 | 2.83 | 0.46 |
| 31:BA:2400:G:H2' | 31:BA:2400:G:N3 | 2.28 | 0.46 |
| 31:BA:2818:G:C2' | 31:BA:2819:G:H5' | 2.44 | 0.46 |
| 31:BA:307:G:H22 | 31:BA:310:A:H5' | 1.78 | 0.46 |
| 31:BA:64:A:C2' | 31:BA:65:C:H5' | 2.45 | 0.46 |
| 31:BA:900:A:C5 | 31:BA:901:A:C8 | 3.04 | 0.46 |
| 32:BB:1:U:C5 | 32:BB:2:C:C5 | 3.03 | 0.46 |
| 31:BA:1902:C:O2' | 33:BD:244:ARG:CB | 2.60 | 0.46 |
| 33:BD:35:LYS:H | 33:BD:64:ILE:HG23 | 1.80 | 0.46 |
| 35:BF:7:TYR:HD1 | 35:BF:8:GLN:H | 1.58 | 0.46 |
| 36:BG:129:GLY:O | 36:BG:130:ASN:CB | 2.63 | 0.46 |
| 36:BG:60:LEU:C | 36:BG:60:LEU:HD13 | 2.35 | 0.46 |
| 36:BG:82:LEU:C | 36:BG:83:ARG:HG3 | 2.35 | 0.46 |
| 37:BH:158:HIS:NE2 | 37:BH:169:VAL:O | 2.48 | 0.46 |
| 39:BN:109:LYS:H | 39:BN:109:LYS:HG2 | 1.59 | 0.46 |
| 39:BN:95:PRO:C | 39:BN:97:ARG:N | 2.65 | 0.46 |
| 41:BP:47:ASP:HB2 | 41:BP:51:PHE:HB2 | 1.96 | 0.46 |
| 41:BP:85:LEU:HA | 41:BP:88:LEU:HB2 | 1.96 | 0.46 |
| 42:BQ:16:ARG:NH1 | 42:BQ:16:ARG:CB | 2.79 | 0.46 |
| 44:BS:106:ARG:HB3 | 44:BS:106:ARG:HE | 1.34 | 0.46 |
| 45:BT:106:SER:O | 45:BT:107:ASP:HB3 | 2.15 | 0.46 |
| 45:BT:84:GLN:OE1 | 45:BT:86:ILE:HD12 | 2.14 | 0.46 |
| 47:BV:19:LYS:HG2 | 47:BV:96:ILE:CB | 2.43 | 0.46 |
| 51:BZ:29:TYR:HA | 51:BZ:33:LEU:O | 2.14 | 0.46 |
| 1:CA:1270:C:H2' | 1:CA:1271:G:O4' | 2.16 | 0.46 |
| 1:CA:1245:A:N1 | 1:CA:1293:G:C6 | 2.84 | 0.46 |
| 1:CA:1386:G:C2 | 1:CA:1387:G:N7 | 2.83 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:926:G:C6 | 1:CA:1505:G:C6 | 3.03 | 0.46 |
| 1:CA:51:A:C4 | 1:CA:353:A:C6 | 3.04 | 0.46 |
| 1:CA:760:G:C2' | 1:CA:761:G:H5' | 2.45 | 0.46 |
| 1:CA:992:U:C1' | 1:CA:993:G:OP2 | 2.57 | 0.46 |
| 2:CB:98:LEU:HB2 | 2:CB:101:MET:HE2 | 1.96 | 0.46 |
| 7:CG:153:HIS:HE1 | 11:CK:57:THR:HG23 | 1.80 | 0.46 |
| 8:CH:54:ASP:O | 8:CH:56:LYS:HG3 | 2.15 | 0.46 |
| 1:CA:966:G:H21 | 9:CI:127:LYS:HE3 | 1.80 | 0.46 |
| 12:CL:18:VAL:HG23 | 12:CL:19:ARG:N | 2.27 | 0.46 |
| 13:CM:78:ILE:HG22 | 13:CM:93:ARG:HH22 | 1.81 | 0.46 |
| 15:CO:17:ARG:CG | 15:CO:26:GLU:HG3 | 2.45 | 0.46 |
| 18:CR:22:VAL:O | 18:CR:22:VAL:HG12 | 2.15 | 0.46 |
| 18:CR:25:THR:HG22 | 18:CR:42:ARG:NH1 | 2.28 | 0.46 |
| 20:CT:73:HIS:O | 20:CT:74:LYS:O | 2.33 | 0.46 |
| 23:D1:79:GLY:O | 23:D1:80:LEU:HG | 2.15 | 0.46 |
| 24:D2:47:ASN:ND2 | 24:D2:48:HIS:N | 2.63 | 0.46 |
| 28:D6:15:GLU:OE2 | 28:D6:43:CYS:CB | 2.63 | 0.46 |
| 31:DA:1044:G:C2 | 31:DA:1112:G:O6 | 2.69 | 0.46 |
| 31:DA:1354:A:H2' | 31:DA:1355:G:O4' | 2.15 | 0.46 |
| 31:DA:1545:A:C2' | 31:DA:1546:C:O5' | 2.64 | 0.46 |
| 31:DA:1558:A:H1' | 31:DA:1559:G:OP2 | 2.14 | 0.46 |
| 31:DA:1658:C:H2' | 31:DA:1659:U:C6 | 2.50 | 0.46 |
| 31:DA:2506:U:H4' | 31:DA:2507:C:OP1 | 2.15 | 0.46 |
| 31:DA:2544:G:O2' | 31:DA:2545:G:H5' | 2.16 | 0.46 |
| 31:DA:1050:A:C2 | 31:DA:2751:G:C4 | 3.04 | 0.46 |
| 32:DB:15:A:O2' | 32:DB:110:G:C8 | 2.65 | 0.46 |
| 32:DB:41:U:O4 | 36:DG:70:VAL:O | 2.32 | 0.46 |
| 33:DD:206:LEU:HD23 | 33:DD:206:LEU:HA | 1.51 | 0.46 |
| 34:DE:167:VAL:CG1 | 34:DE:189:PRO:HD3 | 2.45 | 0.46 |
| 34:DE:47:VAL:HB | 34:DE:49:LEU:HD22 | 1.96 | 0.46 |
| 35:DF:158:THR:HG21 | 35:DF:160:ASN:HB3 | 1.96 | 0.46 |
| 35:DF:7:TYR:HD2 | 35:DF:16:GLY:HA3 | 1.80 | 0.46 |
| 39:DN:102:ALA:O | 39:DN:106:MET:HG3 | 2.14 | 0.46 |
| 43:DR:103:ARG:NH1 | 43:DR:108:GLY:O | 2.45 | 0.46 |
| 43:DR:41:ALA:O | 43:DR:43:GLU:N | 2.48 | 0.46 |
| 43:DR:75:LEU:HD13 | 43:DR:75:LEU:C | 2.35 | 0.46 |
| 44:DS:85:VAL:CG2 | 44:DS:106:ARG:HB2 | 2.26 | 0.46 |
| 46:DU:28:ARG:HG2 | 46:DU:38:THR:OG1 | 2.15 | 0.46 |
| 48:DW:28:SER:C | 48:DW:30:GLU:N | 2.68 | 0.46 |
| 1:AA:1241:G:H2' | 1:AA:1242:C:C6 | 2.50 | 0.46 |
| 1:AA:233:C:H2' | 1:AA:234:C:H6 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:33:A:H2' | 1:AA:34:C:C6 | 2.50 | 0.46 |
| 1:AA:579:G:H2' | 1:AA:580:U:C6 | 2.50 | 0.46 |
| 1:AA:691:G:H1' | 1:AA:696:A:N6 | 2.30 | 0.46 |
| 1:AA:708:C:O2' | 1:AA:709:G:H5' | 2.15 | 0.46 |
| 1:AA:73:G:N1 | 1:AA:97:G:C6 | 2.84 | 0.46 |
| 1:AA:992:U:C1' | 1:AA:993:G:OP2 | 2.56 | 0.46 |
| 3:AC:107:GLN:O | 3:AC:108:ASN:HB2 | 2.14 | 0.46 |
| 4:AD:148:VAL:CG1 | 4:AD:149:ALA:N | 2.78 | 0.46 |
| 4:AD:14:ARG:HA | 4:AD:39:PRO:CB | 2.45 | 0.46 |
| 6:AF:12:PRO:C | 6:AF:14:LEU:H | 2.19 | 0.46 |
| 6:AF:19:LEU:O | 6:AF:23:LYS:HG3 | 2.16 | 0.46 |
| 8:AH:64:LYS:HG2 | 8:AH:79:VAL:HG21 | 1.98 | 0.46 |
| 11:AK:62:GLN:O | 11:AK:63:LEU:C | 2.53 | 0.46 |
| 13:AM:20:THR:C | 13:AM:22:ILE:H | 2.19 | 0.46 |
| 24:B2:53:LEU:C | 24:B2:56:GLN:HE22 | 2.18 | 0.46 |
| 30:B8:34:TRP:CZ3 | 30:B8:41:ILE:HG23 | 2.45 | 0.46 |
| 31:BA:1178:C:H2' | 31:BA:1179:C:H6 | 1.81 | 0.46 |
| 31:BA:1839:G:C5' | 31:BA:1839:G:H8 | 2.29 | 0.46 |
| 31:BA:2094:G:N2 | 31:BA:2196:C:H1' | 2.30 | 0.46 |
| 31:BA:2319:G:H4' | 31:BA:2319:G:OP2 | 2.15 | 0.46 |
| 31:BA:237:C:C2' | 31:BA:238:C:H5' | 2.45 | 0.46 |
| 31:BA:2698:U:H2' | 31:BA:2699:C:C6 | 2.50 | 0.46 |
| 31:BA:272(B):G:O2' | 31:BA:272(C):G:O4' | 2.32 | 0.46 |
| 31:BA:2808:U:H2' | 31:BA:2809:A:O5' | 2.14 | 0.46 |
| 30:B8:61:LEU:CD1 | 31:BA:593:G:O2' | 2.63 | 0.46 |
| 35:BF:132:VAL:CG2 | 35:BF:133:ASN:H | 2.28 | 0.46 |
| 37:BH:85:LYS:HE2 | 37:BH:145:ALA:H | 1.80 | 0.46 |
| 40:BO:2:ILE:N | 40:BO:2:ILE:HD13 | 2.31 | 0.46 |
| 42:BQ:20:ALA:HB2 | 42:BQ:99:PRO:HG2 | 1.98 | 0.46 |
| 43:BR:75:LEU:C | 43:BR:75:LEU:HD13 | 2.36 | 0.46 |
| 45:BT:51:ARG:CG | 45:BT:98:LYS:HE2 | 2.42 | 0.46 |
| 47:BV:79:VAL:O | 47:BV:80:GLN:CG | 2.63 | 0.46 |
| 50:BY:31:LEU:HD22 | 50:BY:31:LEU:N | 2.30 | 0.46 |
| 51:BZ:71:VAL:HG22 | 51:BZ:88:PHE:HE2 | 1.79 | 0.46 |
| 1:CA:1158:C:O2 | 1:CA:1158:C:C2' | 2.63 | 0.46 |
| 1:CA:1242:C:H5'' | 21:CU:10:ARG:HH12 | 1.80 | 0.46 |
| 1:CA:12:U:H4' | 1:CA:526:C:O2' | 2.15 | 0.46 |
| 1:CA:1372:U:H2' | 1:CA:1373:G:O4' | 2.14 | 0.46 |
| 1:CA:327:A:C5 | 1:CA:329:A:C5 | 3.03 | 0.46 |
| 1:CA:376:G:C4 | 1:CA:389:A:C2 | 3.03 | 0.46 |
| 1:CA:612:C:O2 | 1:CA:629:G:N2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:674:G:O2' | 1:CA:675:A:H5' | 2.16 | 0.46 |
| 3:CC:58:GLU:H | 3:CC:65:ALA:HB3 | 1.80 | 0.46 |
| 6:CF:40:VAL:HA | 6:CF:62:TRP:O | 2.15 | 0.46 |
| 12:CL:36:VAL:HG12 | 12:CL:37:CYS:N | 2.30 | 0.46 |
| 13:CM:91:ARG:HB2 | 13:CM:98:VAL:CG2 | 2.45 | 0.46 |
| 22:D0:25:ARG:HB2 | 22:D0:37:LEU:HD23 | 1.98 | 0.46 |
| 24:D2:30:ARG:NH1 | 24:D2:30:ARG:CG | 2.72 | 0.46 |
| 28:D6:10:LEU:HD22 | 28:D6:10:LEU:N | 2.27 | 0.46 |
| 31:DA:1012:U:O4 | 39:DN:25:ARG:HA | 2.15 | 0.46 |
| 31:DA:1648:C:H2' | 31:DA:1649:G:O5' | 2.16 | 0.46 |
| 31:DA:1826:G:C2' | 31:DA:1827:C:O5' | 2.63 | 0.46 |
| 31:DA:2280:G:C2' | 31:DA:2281:C:H5' | 2.45 | 0.46 |
| 31:DA:2636:U:C2' | 31:DA:2637:U:H5' | 2.46 | 0.46 |
| 31:DA:284:U:H2' | 31:DA:285:C:H6 | 1.78 | 0.46 |
| 31:DA:303:U:H2' | 31:DA:304:G:H8 | 1.80 | 0.46 |
| 31:DA:877:U:C2' | 31:DA:878:A:H5'' | 2.45 | 0.46 |
| 31:DA:574:C:N3 | 34:DE:145:LYS:HE2 | 2.30 | 0.46 |
| 34:DE:70:ALA:O | 34:DE:72:VAL:C | 2.54 | 0.46 |
| 38:DI:114:LEU:HA | 38:DI:114:LEU:HD23 | 1.71 | 0.46 |
| 39:DN:56:ASN:N | 39:DN:125:GLY:H | 2.13 | 0.46 |
| 45:DT:50:ILE:HD11 | 45:DT:102:ILE:CD1 | 2.43 | 0.46 |
| 31:DA:993:G:N3 | 47:DV:91:TYR:HE1 | 2.13 | 0.46 |
| 47:DV:69:LYS:HB2 | 47:DV:93:GLU:OE2 | 2.16 | 0.46 |
| 51:DZ:167:PRO:O | 51:DZ:168:GLU:HB2 | 2.15 | 0.46 |
| 1:AA:1129:C:H4' | 1:AA:1130:A:H5' | 1.97 | 0.46 |
| 1:AA:1513:A:H2' | 1:AA:1514:C:C6 | 2.50 | 0.46 |
| 1:AA:143:A:N1 | 1:AA:220:G:O6 | 2.48 | 0.46 |
| 1:AA:509:A:O2' | 1:AA:510:A:O5' | 2.34 | 0.46 |
| 1:AA:523:A:H61 | 12:AL:53:ARG:HH12 | 1.63 | 0.46 |
| 1:AA:582:U:C2 | 1:AA:760:G:C6 | 3.04 | 0.46 |
| 1:AA:66:G:O4' | 1:AA:173:U:C4 | 2.69 | 0.46 |
| 1:AA:735:C:H6 | 1:AA:735:C:O5' | 1.98 | 0.46 |
| 1:AA:760:G:C2' | 1:AA:761:G:H5' | 2.44 | 0.46 |
| 2:AB:61:LEU:CD2 | 2:AB:68:ILE:HD11 | 2.45 | 0.46 |
| 8:AH:114:THR:HB | 8:AH:130:GLY:O | 2.15 | 0.46 |
| 12:AL:34:ARG:O | 12:AL:61:THR:HG23 | 2.16 | 0.46 |
| 13:AM:19:LEU:HB3 | 13:AM:25:ILE:HG21 | 1.98 | 0.46 |
| 16:AP:39:TYR:OH | 16:AP:41:PRO:HB3 | 2.16 | 0.46 |
| 28:B6:11:LEU:HD23 | 28:B6:26:ASN:H | 1.80 | 0.46 |
| 29:B7:8:ASN:ND2 | 29:B7:11:LYS:N | 2.47 | 0.46 |
| 30:B8:29:LYS:O | 30:B8:32:LEU:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:1209:G:H21 | 31:BA:1210:A:H62 | 1.64 | 0.46 |
| 31:BA:1319:G:C6 | 31:BA:1320:C:N4 | 2.84 | 0.46 |
| 31:BA:1502:C:C6 | 31:BA:1502:C:H5'' | 2.51 | 0.46 |
| 31:BA:1444:G:C2 | 31:BA:1548:C:N3 | 2.84 | 0.46 |
| 31:BA:1741:A:C8 | 31:BA:1742:G:C2 | 3.03 | 0.46 |
| 31:BA:2021:C:H4' | 31:BA:2022:U:OP2 | 2.16 | 0.46 |
| 31:BA:2082:A:H2' | 31:BA:2083:G:O4' | 2.15 | 0.46 |
| 31:BA:303:U:H2' | 31:BA:304:G:H8 | 1.80 | 0.46 |
| 31:BA:338:G:H2' | 31:BA:339:U:H6 | 1.80 | 0.46 |
| 31:BA:34:C:H2' | 31:BA:35:G:OP1 | 2.14 | 0.46 |
| 31:BA:729:G:O5' | 33:BD:208:LYS:NZ | 2.41 | 0.46 |
| 32:BB:40:U:C2' | 32:BB:41:U:OP1 | 2.64 | 0.46 |
| 34:BE:24:THR:HG23 | 34:BE:184:VAL:CG2 | 2.45 | 0.46 |
| 34:BE:201:THR:HG22 | 34:BE:203:LYS:H | 1.79 | 0.46 |
| 34:BE:47:VAL:O | 34:BE:80:GLU:HA | 2.15 | 0.46 |
| 34:BE:51:PHE:CG | 34:BE:52:LEU:N | 2.83 | 0.46 |
| 35:BF:89:VAL:CG1 | 35:BF:90:PHE:N | 2.78 | 0.46 |
| 36:BG:173:LEU:HB3 | 36:BG:178:PHE:CG | 2.50 | 0.46 |
| 37:BH:156:ALA:C | 37:BH:158:HIS:H | 2.19 | 0.46 |
| 37:BH:86:GLU:HA | 37:BH:132:ARG:HA | 1.98 | 0.46 |
| 39:BN:78:TYR:HD1 | 39:BN:79:PRO:N | 2.13 | 0.46 |
| 39:BN:79:PRO:HD2 | 39:BN:81:GLY:H | 1.80 | 0.46 |
| 42:BQ:54:MET:HB3 | 42:BQ:64:ILE:HD13 | 1.97 | 0.46 |
| 49:BX:8:ILE:HD12 | 49:BX:8:ILE:N | 2.29 | 0.46 |
| 50:BY:97:ARG:O | 50:BY:98:VAL:C | 2.53 | 0.46 |
| 1:CA:539:A:H2' | 1:CA:540:G:H8 | 1.79 | 0.46 |
| 1:CA:574:A:H5'' | 1:CA:575:G:OP2 | 2.16 | 0.46 |
| 1:CA:609:A:C2' | 1:CA:610:G:H5' | 2.45 | 0.46 |
| 1:CA:625:G:H2' | 1:CA:626:U:H6 | 1.81 | 0.46 |
| 1:CA:830:G:C5 | 1:CA:831:U:C5 | 3.04 | 0.46 |
| 2:CB:15:VAL:HG23 | 2:CB:16:HIS:CE1 | 2.51 | 0.46 |
| 1:CA:1206:G:H4' | 3:CC:192:THR:O | 2.14 | 0.46 |
| 6:CF:12:PRO:C | 6:CF:14:LEU:H | 2.19 | 0.46 |
| 8:CH:109:ILE:HG12 | 8:CH:110:ALA:N | 2.30 | 0.46 |
| 12:CL:126:LYS:HD2 | 12:CL:127:GLU:H | 1.80 | 0.46 |
| 22:D0:53:MET:HA | 22:D0:58:THR:O | 2.16 | 0.46 |
| 23:D1:28:GLY:C | 23:D1:30:VAL:H | 2.18 | 0.46 |
| 28:D6:11:LEU:HD11 | 28:D6:51:GLU:HB2 | 1.97 | 0.46 |
| 31:DA:1464:C:C2' | 31:DA:1528:A:H8 | 2.27 | 0.46 |
| 31:DA:416:C:C2 | 31:DA:417:C:C6 | 3.04 | 0.46 |
| 31:DA:649:G:H2' | 31:DA:650:C:H6 | 1.77 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:D3:24:LYS:HB3 | 31:DA:849:A:H2 | 1.81 | 0.46 |
| 32:DB:35:U:O2' | 32:DB:36:C:H5' | 2.16 | 0.46 |
| 35:DF:70:THR:HG22 | 35:DF:72:ARG:N | 2.29 | 0.46 |
| 36:DG:129:GLY:O | 36:DG:130:ASN:CB | 2.63 | 0.46 |
| 32:DB:45:A:H1' | 36:DG:95:ARG:NH2 | 2.30 | 0.46 |
| 38:DI:37:VAL:HG12 | 38:DI:38:LEU:N | 2.30 | 0.46 |
| 38:DI:38:LEU:O | 38:DI:40:THR:HG23 | 2.16 | 0.46 |
| 39:DN:131:GLN:CD | 39:DN:134:ARG:HB3 | 2.36 | 0.46 |
| 39:DN:1:MET:HB3 | 47:DV:20:LEU:CD2 | 2.27 | 0.46 |
| 41:DP:85:LEU:CD2 | 41:DP:85:LEU:N | 2.70 | 0.46 |
| 43:DR:74:LYS:CD | 43:DR:77:ARG:HH21 | 2.28 | 0.46 |
| 45:DT:50:ILE:CD1 | 45:DT:64:ARG:HB3 | 2.45 | 0.46 |
| 47:DV:36:PRO:HD2 | 47:DV:60:GLU:O | 2.14 | 0.46 |
| 47:DV:1:MET:H2 | 47:DV:44:LYS:HD2 | 1.78 | 0.46 |
| 49:DX:81:VAL:HG12 | 49:DX:81:VAL:O | 2.14 | 0.46 |
| 50:DY:28:LYS:CE | 50:DY:37:VAL:HG12 | 2.46 | 0.46 |
| 51:DZ:127:LYS:HB3 | 51:DZ:162:GLU:HG3 | 1.97 | 0.46 |
| 1:AA:119:A:N7 | 1:AA:288:A:C2 | 2.83 | 0.46 |
| 1:AA:955:U:C1' | 1:AA:1227:A:H61 | 2.21 | 0.46 |
| 1:AA:329:A:C2 | 1:AA:332:G:C4 | 3.03 | 0.46 |
| 1:AA:457:C:C2 | 1:AA:458:C:C5 | 3.03 | 0.46 |
| 1:AA:518:C:H2' | 1:AA:530:G:N3 | 2.30 | 0.46 |
| 1:AA:735:C:O2' | 1:AA:736:C:H5' | 2.15 | 0.46 |
| 1:AA:829:G:O2' | 1:AA:830:G:H5' | 2.15 | 0.46 |
| 1:AA:84:U:H5 | 1:AA:88:A:C8 | 2.33 | 0.46 |
| 2:AB:105:PHE:C | 2:AB:107:THR:H | 2.19 | 0.46 |
| 2:AB:168:THR:CG2 | 2:AB:192:SER:HA | 2.44 | 0.46 |
| 2:AB:7:VAL:HG12 | 2:AB:11:LEU:HD11 | 1.98 | 0.46 |
| 5:AE:103:GLY:O | 5:AE:106:PRO:HD2 | 2.16 | 0.46 |
| 1:AA:673:G:O3' | 6:AF:87:ARG:NH2 | 2.49 | 0.46 |
| 7:AG:73:MET:HG2 | 7:AG:90:GLU:HA | 1.97 | 0.46 |
| 7:AG:92:SER:HB3 | 7:AG:94:ARG:HH21 | 1.80 | 0.46 |
| 12:AL:119:LYS:O | 12:AL:120:TYR:HB2 | 2.15 | 0.46 |
| 19:AS:6:LYS:HG2 | 19:AS:7:LYS:HD3 | 1.97 | 0.46 |
| 20:AT:73:HIS:O | 20:AT:74:LYS:O | 2.34 | 0.46 |
| 27:B5:32:PRO:HD2 | 31:BA:2886:G:O2' | 2.16 | 0.46 |
| 27:B5:56:LYS:O | 27:B5:57:VAL:C | 2.50 | 0.46 |
| 31:BA:1169:G:N2 | 31:BA:1181:C:C2 | 2.84 | 0.46 |
| 31:BA:1288:U:C2 | 31:BA:1327:C:C2 | 3.03 | 0.46 |
| 31:BA:1648:C:H2' | 31:BA:1649:G:O5' | 2.16 | 0.46 |
| 31:BA:2287:A:C2 | 31:BA:2346:A:N1 | 2.84 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:2635:C:H2' | 31:BA:2636:U:O5' | 2.15 | 0.46 |
| 31:BA:2636:U:C2' | 31:BA:2637:U:H5' | 2.45 | 0.46 |
| 31:BA:265:A:H1' | 31:BA:266:G:O4' | 2.16 | 0.46 |
| 31:BA:363(D):G:C6 | 31:BA:363(E):U:O4 | 2.69 | 0.46 |
| 31:BA:783:A:H3' | 31:BA:783:A:C8 | 2.51 | 0.46 |
| 31:BA:94:C:O2 | 31:BA:94:C:H2' | 2.14 | 0.46 |
| 32:BB:27:C:C4 | 32:BB:28:C:C4 | 3.04 | 0.46 |
| 33:BD:35:LYS:CG | 33:BD:64:ILE:H | 2.28 | 0.46 |
| 35:BF:132:VAL:HG22 | 35:BF:133:ASN:H | 1.79 | 0.46 |
| 37:BH:153:LYS:CG | 37:BH:154:PRO:N | 2.77 | 0.46 |
| 39:BN:3:THR:CG2 | 39:BN:4:TYR:N | 2.78 | 0.46 |
| 39:BN:78:TYR:N | 39:BN:79:PRO:HD3 | 2.30 | 0.46 |
| 43:BR:104:ARG:HD2 | 43:BR:111:LEU:HD11 | 1.96 | 0.46 |
| 43:BR:50:HIS:NE2 | 43:BR:54:LEU:HD21 | 2.30 | 0.46 |
| 48:BW:62:HIS:O | 48:BW:63:ASP:C | 2.53 | 0.46 |
| 50:BY:80:GLY:O | 50:BY:81:LYS:CB | 2.64 | 0.46 |
| 1:CA:132:C:O2' | 1:CA:133:U:H5' | 2.16 | 0.46 |
| 1:CA:1387:G:N3 | 1:CA:1387:G:H2' | 2.31 | 0.46 |
| 1:CA:1521:G:H2' | 1:CA:1522:U:C6 | 2.51 | 0.46 |
| 1:CA:359:U:H2' | 1:CA:360:A:C8 | 2.49 | 0.46 |
| 1:CA:565:U:H3' | 1:CA:566:G:H2' | 1.98 | 0.46 |
| 1:CA:625:G:C4 | 1:CA:626:U:C5 | 3.03 | 0.46 |
| 1:CA:66:G:C4' | 1:CA:173:U:C4 | 2.98 | 0.46 |
| 3:CC:19:GLU:HA | 3:CC:54:ARG:NH2 | 2.30 | 0.46 |
| 4:CD:8:VAL:O | 4:CD:10:ARG:N | 2.49 | 0.46 |
| 12:CL:119:LYS:HB2 | 12:CL:120:TYR:CD1 | 2.51 | 0.46 |
| 15:CO:82:ILE:HG12 | 15:CO:87:ILE:CB | 2.43 | 0.46 |
| 16:CP:68:ASP:C | 16:CP:70:ALA:H | 2.19 | 0.46 |
| 17:CQ:33:GLY:O | 17:CQ:34:LYS:C | 2.54 | 0.46 |
| 23:D1:48:LYS:HD3 | 23:D1:48:LYS:HA | 1.41 | 0.46 |
| 31:DA:1525:G:H2' | 31:DA:1526:G:H8 | 1.80 | 0.46 |
| 31:DA:2031:A:OP1 | 31:DA:2031:A:H8 | 1.99 | 0.46 |
| 31:DA:2082:A:H2' | 31:DA:2083:G:O4' | 2.15 | 0.46 |
| 31:DA:2103:C:N3 | 31:DA:2187:G:C6 | 2.83 | 0.46 |
| 31:DA:2282:G:OP1 | 31:DA:2283:C:H1' | 2.15 | 0.46 |
| 31:DA:2662:A:H5' | 31:DA:2663:G:H1' | 1.98 | 0.46 |
| 31:DA:2526:G:H5' | 31:DA:2742:C:O2' | 2.15 | 0.46 |
| 31:DA:272(J):C:H2' | 31:DA:274:G:OP1 | 2.15 | 0.46 |
| 31:DA:2761:G:C3' | 31:DA:2762:G:H5'' | 2.46 | 0.46 |
| 31:DA:2876:G:H4' | 45:DT:3:ARG:HE | 1.80 | 0.46 |
| 31:DA:311:A:N3 | 31:DA:331:A:H3' | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:414:C:H2' | 31:DA:415:A:H8 | 1.81 | 0.46 |
| 31:DA:900:A:C5 | 31:DA:901:A:C8 | 3.02 | 0.46 |
| 46:DU:57:PHE:O | 46:DU:58:ARG:C | 2.53 | 0.46 |
| 49:DX:5:TYR:O | 49:DX:8:ILE:N | 2.48 | 0.46 |
| 1:AA:1217:C:H2' | 1:AA:1218:C:O4' | 2.15 | 0.46 |
| 1:AA:1442(A):G:C8 | 45:BT:118:ARG:NH1 | 2.71 | 0.46 |
| 1:AA:222:U:H2' | 1:AA:223:U:C6 | 2.50 | 0.46 |
| 1:AA:429:U:H4' | 1:AA:430:A:O5' | 2.15 | 0.46 |
| 1:AA:575:G:OP1 | 1:AA:575:G:H4' | 2.16 | 0.46 |
| 1:AA:748:C:C4' | 1:AA:749:C:O5' | 2.57 | 0.46 |
| 2:AB:97:TRP:HZ2 | 2:AB:102:LEU:HD13 | 1.80 | 0.46 |
| 4:AD:190:ASP:O | 4:AD:191:ARG:C | 2.54 | 0.46 |
| 4:AD:67:ILE:HG22 | 4:AD:68:TYR:CD1 | 2.51 | 0.46 |
| 12:AL:27:LEU:HD11 | 12:AL:64:TYR:CE1 | 2.50 | 0.46 |
| 31:BA:1042:G:C5' | 31:BA:1043:C:OP2 | 2.64 | 0.46 |
| 31:BA:1181:C:C2' | 31:BA:1182:A:H5' | 2.46 | 0.46 |
| 31:BA:1525:G:H2' | 31:BA:1526:G:H8 | 1.80 | 0.46 |
| 31:BA:1688:U:O2 | 31:BA:1700:A:H8 | 1.97 | 0.46 |
| 1:AA:702:A:H2 | 31:BA:1846:G:HO2' | 1.63 | 0.46 |
| 31:BA:2408:U:H2' | 31:BA:2409:G:C8 | 2.50 | 0.46 |
| 31:BA:2657:A:C2 | 31:BA:2664:G:N2 | 2.77 | 0.46 |
| 23:B1:76:ARG:NH1 | 31:BA:271(R):G:OP1 | 2.49 | 0.46 |
| 31:BA:271(T):C:C2 | 31:BA:271(U):G:C8 | 3.03 | 0.46 |
| 31:BA:443:A:H3' | 35:BF:45:ARG:HH21 | 1.78 | 0.46 |
| 31:BA:780:G:N2 | 31:BA:783:A:H62 | 2.05 | 0.46 |
| 31:BA:847:U:OP2 | 31:BA:928:G:O6 | 2.34 | 0.46 |
| 31:BA:999:U:O2' | 31:BA:1000:A:H5' | 2.15 | 0.46 |
| 32:BB:21:G:N3 | 32:BB:21:G:H2' | 2.31 | 0.46 |
| 35:BF:20:LEU:O | 35:BF:23:ASP:HB2 | 2.16 | 0.46 |
| 37:BH:158:HIS:HE1 | 37:BH:168:PRO:C | 2.19 | 0.46 |
| 31:BA:1140:C:OP1 | 39:BN:23:LEU:O | 2.33 | 0.46 |
| 45:BT:30:VAL:CG2 | 45:BT:31:SER:H | 2.28 | 0.46 |
| 45:BT:33:LYS:HB3 | 45:BT:41:ARG:HB3 | 1.97 | 0.46 |
| 45:BT:78:LEU:O | 45:BT:79:HIS:CG | 2.68 | 0.46 |
| 51:BZ:19:ARG:HH11 | 51:BZ:19:ARG:HG2 | 1.81 | 0.46 |
| 51:BZ:5:LEU:HD23 | 51:BZ:5:LEU:HA | 1.65 | 0.46 |
| 1:CA:129:U:O2 | 1:CA:131:C:C5 | 2.69 | 0.46 |
| 1:CA:1301:U:H3' | 1:CA:1302:U:C5' | 2.45 | 0.46 |
| 1:CA:1316:G:O3' | 14:CN:18:VAL:HG22 | 2.16 | 0.46 |
| 1:CA:1320:C:H5' | 19:CS:70:LYS:CG | 2.46 | 0.46 |
| 1:CA:942:G:C2 | 1:CA:1342:C:C2 | 3.03 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:22:LYS:HZ3 | 2:CB:40:HIS:HE1 | 1.62 | 0.46 |
| 3:CC:19:GLU:HG2 | 3:CC:19:GLU:O | 2.16 | 0.46 |
| 4:CD:57:ARG:NH2 | 4:CD:205:GLU:OE2 | 2.49 | 0.46 |
| 11:CK:99:GLN:C | 11:CK:101:SER:H | 2.19 | 0.46 |
| 11:CK:23:ALA:HB1 | 11:CK:88:GLY:HA3 | 1.98 | 0.46 |
| 19:CS:48:THR:HG22 | 19:CS:61:TYR:CD1 | 2.51 | 0.46 |
| 23:D1:10:LYS:O | 23:D1:13:ILE:CG2 | 2.63 | 0.46 |
| 27:D5:10:LYS:HE3 | 31:DA:1262:A:N3 | 2.31 | 0.46 |
| 31:DA:1514:U:C2' | 31:DA:1515:G:H5' | 2.46 | 0.46 |
| 31:DA:1668:A:H4' | 31:DA:1669:A:O5' | 2.16 | 0.46 |
| 31:DA:18:C:O2' | 31:DA:19:C:H5' | 2.16 | 0.46 |
| 31:DA:518:G:H2' | 31:DA:519:U:H6 | 1.81 | 0.46 |
| 31:DA:565:C:H4' | 31:DA:1253:A:N6 | 2.31 | 0.46 |
| 31:DA:656:G:H2' | 31:DA:657:U:O5' | 2.16 | 0.46 |
| 32:DB:50:G:O5' | 32:DB:50:G:H8 | 1.97 | 0.46 |
| 33:DD:11:PRO:C | 33:DD:13:ARG:H | 2.19 | 0.46 |
| 33:DD:253:GLN:HB3 | 33:DD:255:LYS:HE2 | 1.98 | 0.46 |
| 36:DG:15:VAL:HG22 | 36:DG:175:LEU:HB3 | 1.98 | 0.46 |
| 36:DG:64:THR:CG2 | 36:DG:65:GLY:N | 2.78 | 0.46 |
| 37:DH:85:LYS:CE | 37:DH:145:ALA:HB2 | 2.46 | 0.46 |
| 37:DH:158:HIS:NE2 | 37:DH:169:VAL:O | 2.49 | 0.46 |
| 39:DN:99:LEU:O | 39:DN:103:VAL:HG23 | 2.16 | 0.46 |
| 42:DQ:20:ALA:HB2 | 42:DQ:99:PRO:HG2 | 1.98 | 0.46 |
| 43:DR:48:VAL:O | 43:DR:52:ILE:HG12 | 2.16 | 0.46 |
| 43:DR:81:ASP:O | 43:DR:85:PRO:HG2 | 2.16 | 0.46 |
| 48:DW:18:ARG:HG3 | 48:DW:76:VAL:HG22 | 1.96 | 0.46 |
| 1:AA:1128:C:H5' | 9:AI:16:ARG:CZ | 2.45 | 0.46 |
| 1:AA:229:U:C2' | 1:AA:230:G:H5' | 2.45 | 0.46 |
| 1:AA:674:G:H2' | 1:AA:675:A:C8 | 2.51 | 0.46 |
| 1:AA:963:G:H21 | 10:AJ:55:LYS:CD | 2.28 | 0.46 |
| 5:AE:72:GLN:O | 5:AE:73:ASN:HB2 | 2.15 | 0.46 |
| 12:AL:91:LYS:CG | 12:AL:91:LYS:O | 2.63 | 0.46 |
| 16:AP:32:TYR:CD2 | 16:AP:32:TYR:O | 2.69 | 0.46 |
| 1:AA:103:C:OP2 | 20:AT:14:LYS:HD3 | 2.16 | 0.46 |
| 23:B1:8:SER:N | 23:B1:46:LEU:CD1 | 2.78 | 0.46 |
| 24:B2:30:ARG:HA | 24:B2:33:MET:SD | 2.56 | 0.46 |
| 27:B5:2:ALA:N | 31:BA:2015:A:N3 | 2.64 | 0.46 |
| 31:BA:1742:G:N7 | 31:BA:1743:C:C2 | 2.84 | 0.46 |
| 31:BA:2298:A:H2' | 31:BA:2299:G:O4' | 2.15 | 0.46 |
| 31:BA:2317:C:C3' | 31:BA:2318:G:C5' | 2.92 | 0.46 |
| 31:BA:2584:U:H6 | 31:BA:2585:U:C5 | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:28:A:C2 | 31:BA:513:A:C8 | 3.04 | 0.46 |
| 31:BA:315:G:H2' | 31:BA:316:C:C6 | 2.50 | 0.46 |
| 31:BA:470:A:C2 | 31:BA:471:A:C4 | 3.04 | 0.46 |
| 31:BA:755:C:H2' | 31:BA:756:C:C6 | 2.51 | 0.46 |
| 31:BA:84:A:H5' | 50:BY:9:LYS:HB3 | 1.97 | 0.46 |
| 32:BB:45:A:N3 | 32:BB:45:A:H2' | 2.31 | 0.46 |
| 32:BB:87:G:H3' | 32:BB:88:C:C5' | 2.43 | 0.46 |
| 34:BE:119:ARG:HG2 | 34:BE:160:TYR:HB2 | 1.98 | 0.46 |
| 34:BE:51:PHE:HD1 | 34:BE:52:LEU:H | 1.57 | 0.46 |
| 40:BO:3:GLN:HG3 | 40:BO:4:PRO:HD2 | 1.98 | 0.46 |
| 45:BT:107:ASP:H | 45:BT:110:ILE:HG13 | 1.80 | 0.46 |
| 47:BV:43:GLU:HA | 47:BV:48:GLY:CA | 2.46 | 0.46 |
| 47:BV:90:PRO:CD | 47:BV:91:TYR:H | 2.29 | 0.46 |
| 48:BW:83:LYS:O | 48:BW:84:ARG:HD3 | 2.16 | 0.46 |
| 49:BX:81:VAL:HG12 | 49:BX:81:VAL:O | 2.15 | 0.46 |
| 51:BZ:100:VAL:O | 51:BZ:101:PRO:O | 2.33 | 0.46 |
| 51:BZ:150:LEU:C | 51:BZ:151:HIS:CD2 | 2.89 | 0.46 |
| 1:CA:1016:A:H2' | 1:CA:1017:G:O4' | 2.15 | 0.46 |
| 1:CA:951:G:C6 | 1:CA:1231:G:C6 | 3.04 | 0.46 |
| 1:CA:66:G:C6 | 1:CA:67:C:C5 | 3.03 | 0.46 |
| 1:CA:781:A:H5' | 1:CA:782:A:OP2 | 2.15 | 0.46 |
| 1:CA:817:C:H4' | 1:CA:818:G:OP1 | 2.16 | 0.46 |
| 2:CB:16:HIS:HA | 2:CB:210:SER:HB2 | 1.97 | 0.46 |
| 3:CC:109:PRO:HA | 3:CC:115:LEU:HD12 | 1.98 | 0.46 |
| 4:CD:159:ARG:O | 4:CD:163:GLU:N | 2.48 | 0.46 |
| 7:CG:75:VAL:HG13 | 7:CG:145:ALA:HB2 | 1.98 | 0.46 |
| 8:CH:82:HIS:HD2 | 8:CH:138:TRP:NE1 | 2.14 | 0.46 |
| 8:CH:48:TYR:HA | 8:CH:60:ARG:O | 2.16 | 0.46 |
| 15:CO:17:ARG:NH1 | 15:CO:17:ARG:CG | 2.62 | 0.46 |
| 16:CP:9:PHE:CE2 | 16:CP:18:ARG:HB2 | 2.51 | 0.46 |
| 17:CQ:76:LEU:HD12 | 17:CQ:77:VAL:H | 1.81 | 0.46 |
| 23:D1:11:ARG:HB3 | 23:D1:12:PRO:CD | 2.45 | 0.46 |
| 27:D5:33:CYS:SG | 27:D5:40:LYS:HE3 | 2.56 | 0.46 |
| 27:D5:56:LYS:O | 27:D5:57:VAL:C | 2.53 | 0.46 |
| 27:D5:57:VAL:CG2 | 27:D5:58:LEU:N | 2.73 | 0.46 |
| 31:DA:1005:C:O2 | 31:DA:1143:A:C6 | 2.69 | 0.46 |
| 31:DA:1324:G:C4 | 31:DA:1328:G:O6 | 2.69 | 0.46 |
| 31:DA:1412:A:H2' | 31:DA:1413:G:H8 | 1.79 | 0.46 |
| 31:DA:1528:A:O2' | 31:DA:1528(A):A:P | 2.74 | 0.46 |
| 31:DA:2287:A:N3 | 31:DA:2289:G:C8 | 2.83 | 0.46 |
| 31:DA:2565:A:C5' | 31:DA:2566:A:OP2 | 2.62 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:358:U:C6 | 31:DA:358:U:C3' | 2.99 | 0.46 |
| 31:DA:465:G:H2' | 31:DA:466:A:C8 | 2.50 | 0.46 |
| 31:DA:541:C:H2' | 31:DA:542:C:C6 | 2.50 | 0.46 |
| 31:DA:952:G:C6 | 31:DA:966:G:C6 | 3.04 | 0.46 |
| 31:DA:1491:G:O2' | 33:DD:101:GLU:HB2 | 2.16 | 0.46 |
| 33:DD:267:SER:HA | 33:DD:270:ILE:HG13 | 1.98 | 0.46 |
| 34:DE:31:CYS:SG | 34:DE:51:PHE:HD2 | 2.39 | 0.46 |
| 36:DG:25:TYR:CZ | 36:DG:32:PRO:HD3 | 2.51 | 0.46 |
| 37:DH:68:THR:O | 37:DH:69:ARG:C | 2.53 | 0.46 |
| 31:DA:587:C:C4 | 41:DP:33:ARG:HG2 | 2.51 | 0.46 |
| 41:DP:71:VAL:HG13 | 41:DP:72:PRO:CD | 2.46 | 0.46 |
| 44:DS:61:ASN:ND2 | 44:DS:64:GLU:OE2 | 2.49 | 0.46 |
| 45:DT:100:TYR:HB3 | 45:DT:103:ARG:HE | 1.80 | 0.46 |
| 45:DT:90:GLN:HG2 | 45:DT:120:ARG:CZ | 2.46 | 0.46 |
| 47:DV:85:LYS:C | 47:DV:87:HIS:H | 2.13 | 0.46 |
| 48:DW:8:ARG:HA | 48:DW:102:HIS:CD2 | 2.50 | 0.46 |
| 49:DX:47:PHE:O | 49:DX:48:LYS:C | 2.54 | 0.46 |
| 49:DX:59:VAL:HG22 | 49:DX:74:PRO:O | 2.16 | 0.46 |
| 50:DY:89:PHE:O | 50:DY:90:LEU:HB3 | 2.15 | 0.46 |
| 51:DZ:67:LEU:N | 51:DZ:67:LEU:HD12 | 2.31 | 0.46 |
| 1:AA:865:A:H5' | 1:AA:1078:U:O4 | 2.16 | 0.46 |
| 1:AA:1160:G:H2' | 1:AA:1160:G:N3 | 2.29 | 0.46 |
| 1:AA:1255:G:N3 | 1:AA:1255:G:H2' | 2.31 | 0.46 |
| 1:AA:417:C:H2' | 1:AA:418:C:H5' | 1.96 | 0.46 |
| 1:AA:452:A:N7 | 1:AA:480:U:O4 | 2.48 | 0.46 |
| 1:AA:645:C:O2' | 1:AA:646:U:H5' | 2.15 | 0.46 |
| 2:AB:166:ASP:CB | 2:AB:169:LYS:HB2 | 2.44 | 0.46 |
| 3:AC:109:PRO:HA | 3:AC:115:LEU:HD12 | 1.97 | 0.46 |
| 4:AD:58:LEU:HD23 | 4:AD:206:PHE:CZ | 2.50 | 0.46 |
| 13:AM:81:LEU:HB3 | 13:AM:89:GLY:CA | 2.39 | 0.46 |
| 16:AP:79:VAL:HG12 | 16:AP:80:PHE:CD1 | 2.50 | 0.46 |
| 19:AS:4:SER:O | 19:AS:5:LEU:HB2 | 2.16 | 0.46 |
| 23:B1:10:LYS:CG | 23:B1:11:ARG:N | 2.79 | 0.46 |
| 26:B4:25:TYR:C | 26:B4:27:THR:N | 2.68 | 0.46 |
| 31:BA:2200:C:O2 | 31:BA:2200:C:H2' | 2.14 | 0.46 |
| 31:BA:231:C:O2' | 31:BA:232:G:H5' | 2.15 | 0.46 |
| 31:BA:2700:C:O2' | 31:BA:2701:C:H5' | 2.15 | 0.46 |
| 31:BA:2784:C:O2' | 31:BA:2785:C:H5' | 2.16 | 0.46 |
| 31:BA:2804:C:C2' | 31:BA:2805:G:H5' | 2.45 | 0.46 |
| 31:BA:319:C:H2' | 31:BA:320:A:O4' | 2.16 | 0.46 |
| 31:BA:335:C:O5' | 31:BA:335:C:H6 | 1.99 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:B7:12:ARG:HG3 | 31:BA:686:G:O6 | 2.15 | 0.46 |
| 31:BA:773:U:C5' | 33:BD:47:GLY:HA2 | 2.45 | 0.46 |
| 24:B2:41:ILE:CG1 | 31:BA:94(A):G:H22 | 2.28 | 0.46 |
| 32:BB:60:C:O2 | 32:BB:61:G:C8 | 2.69 | 0.46 |
| 33:BD:101:GLU:HG3 | 33:BD:102:LYS:N | 2.31 | 0.46 |
| 31:BA:1902:C:OP1 | 33:BD:242:ARG:HD2 | 2.15 | 0.46 |
| 34:BE:65:GLY:HA2 | 34:BE:70:ALA:HB2 | 1.96 | 0.46 |
| 35:BF:70:THR:HG21 | 35:BF:72:ARG:HB2 | 1.98 | 0.46 |
| 39:BN:65:LYS:NZ | 39:BN:66:LYS:H | 2.12 | 0.46 |
| 43:BR:41:ALA:O | 43:BR:42:LYS:C | 2.54 | 0.46 |
| 44:BS:26:LEU:HD22 | 44:BS:87:PHE:CD1 | 2.50 | 0.46 |
| 47:BV:21:ARG:HB3 | 47:BV:93:GLU:HB2 | 1.98 | 0.46 |
| 48:BW:18:ARG:HG3 | 48:BW:76:VAL:HG22 | 1.97 | 0.46 |
| 1:CA:102:G:H2' | 1:CA:103:C:C6 | 2.39 | 0.46 |
| 1:CA:1411:C:O2' | 1:CA:1412:C:H5' | 2.16 | 0.46 |
| 1:CA:149:A:HO2' | 1:CA:150:C:H5 | 1.59 | 0.46 |
| 1:CA:577:G:H1' | 1:CA:816:A:C4 | 2.51 | 0.46 |
| 1:CA:69:G:H2' | 1:CA:70:G:H8 | 1.80 | 0.46 |
| 1:CA:675:A:N6 | 1:CA:715:A:H61 | 2.14 | 0.46 |
| 2:CB:91:PRO:N | 2:CB:154:LEU:HD12 | 2.30 | 0.46 |
| 2:CB:17:PHE:H | 2:CB:17:PHE:HD2 | 1.64 | 0.46 |
| 5:CE:57:LYS:O | 5:CE:61:TYR:CD2 | 2.66 | 0.46 |
| 6:CF:69:GLU:HG2 | 6:CF:70:ASP:N | 2.30 | 0.46 |
| 11:CK:57:THR:CG2 | 11:CK:58:PRO:HD2 | 2.46 | 0.46 |
| 1:CA:539:A:OP1 | 12:CL:114:LYS:HE2 | 2.16 | 0.46 |
| 12:CL:55:VAL:CG1 | 12:CL:56:ALA:N | 2.78 | 0.46 |
| 13:CM:52:GLU:O | 13:CM:56:LEU:HB2 | 2.15 | 0.46 |
| 17:CQ:7:THR:HA | 17:CQ:57:VAL:O | 2.16 | 0.46 |
| 25:D3:46:ASN:O | 25:D3:49:LYS:N | 2.49 | 0.46 |
| 28:D6:19:ARG:CG | 28:D6:20:ASN:H | 2.26 | 0.46 |
| 28:D6:24:GLU:OE1 | 28:D6:24:GLU:HA | 2.15 | 0.46 |
| 31:DA:1040:C:H42 | 31:DA:1115:G:H1 | 1.62 | 0.46 |
| 31:DA:1341:U:O2 | 49:DX:77:LYS:HE2 | 2.14 | 0.46 |
| 31:DA:1478:G:HO2' | 31:DA:1479:G:H5' | 1.80 | 0.46 |
| 31:DA:2317:C:C3' | 31:DA:2318:G:C5' | 2.92 | 0.46 |
| 22:D0:41:ARG:HB3 | 31:DA:2330:G:H1' | 1.97 | 0.46 |
| 31:DA:2700:C:H2' | 31:DA:2701:C:H5' | 1.98 | 0.46 |
| 31:DA:282:A:C4 | 31:DA:359:A:C2 | 3.04 | 0.46 |
| 31:DA:363(C):G:H2' | 31:DA:363(D):G:H8 | 1.81 | 0.46 |
| 31:DA:755:C:H2' | 31:DA:756:C:C6 | 2.51 | 0.46 |
| 34:DE:116:VAL:CG1 | 34:DE:122:PHE:CD2 | 2.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:1675:C:O2 | 34:DE:129:HIS:HA | 2.16 | 0.46 |
| 36:DG:68:PRO:HB2 | 36:DG:90:LEU:HG | 1.98 | 0.46 |
| 39:DN:17:ASP:C | 39:DN:19:GLU:H | 2.17 | 0.46 |
| 41:DP:85:LEU:HD12 | 41:DP:120:ALA:CB | 2.42 | 0.46 |
| 45:DT:28:VAL:HG22 | 45:DT:46:GLU:HA | 1.98 | 0.46 |
| 47:DV:15:GLU:O | 47:DV:98:GLU:OE2 | 2.33 | 0.46 |
| 49:DX:49:VAL:CG1 | 49:DX:87:GLN:HG2 | 2.46 | 0.46 |
| 50:DY:37:VAL:HG22 | 50:DY:67:LEU:HB3 | 1.98 | 0.46 |
| 1:AA:1169:A:C2' | 1:AA:1170:A:H8 | 2.29 | 0.46 |
| 1:AA:149:A:O2' | 1:AA:150:C:P | 2.73 | 0.46 |
| 1:AA:359:U:H2' | 1:AA:360:A:H8 | 1.81 | 0.46 |
| 1:AA:39:G:C2 | 1:AA:40:C:C6 | 3.04 | 0.46 |
| 1:AA:458:C:N4 | 1:AA:474:G:H1 | 2.14 | 0.46 |
| 1:AA:564:C:C2' | 1:AA:565:U:H5' | 2.45 | 0.46 |
| 1:AA:858:G:O6 | 1:AA:869:G:C8 | 2.69 | 0.46 |
| 2:AB:20:GLU:HG3 | 2:AB:191:ASP:HB2 | 1.98 | 0.46 |
| 6:AF:2:ARG:HB2 | 6:AF:4:TYR:CE2 | 2.51 | 0.46 |
| 6:AF:99:ALA:HB3 | 18:AR:29:PHE:CE2 | 2.50 | 0.46 |
| 1:AA:1125:U:O4 | 10:AJ:73:ASP:OD2 | 2.33 | 0.46 |
| 17:AQ:67:LYS:CA | 17:AQ:70:ARG:HH12 | 2.27 | 0.46 |
| 19:AS:10:PHE:HE2 | 19:AS:37:ARG:O | 1.98 | 0.46 |
| 31:BA:1110:G:OP1 | 31:BA:1110:G:H4' | 2.16 | 0.46 |
| 31:BA:1112:G:N2 | 31:BA:1113:U:O2 | 2.49 | 0.46 |
| 31:BA:1165:U:O2' | 31:BA:1166:C:H5' | 2.15 | 0.46 |
| 31:BA:1572:A:H8 | 31:BA:1572:A:O5' | 1.99 | 0.46 |
| 31:BA:1826:G:C2' | 31:BA:1827:C:O5' | 2.64 | 0.46 |
| 31:BA:2018:G:H2' | 31:BA:2019:A:C8 | 2.50 | 0.46 |
| 31:BA:2306:C:OP2 | 31:BA:2307:G:H8 | 1.99 | 0.46 |
| 28:B6:45:LYS:HB3 | 31:BA:2371:G:H4' | 1.97 | 0.46 |
| 31:BA:2564:A:N6 | 31:BA:2565:A:N6 | 2.64 | 0.46 |
| 31:BA:9:U:C4 | 31:BA:2629:A:C6 | 3.04 | 0.46 |
| 31:BA:354:G:H3' | 31:BA:354:G:C8 | 2.51 | 0.46 |
| 31:BA:70:G:H21 | 31:BA:71:A:H62 | 1.64 | 0.46 |
| 31:BA:729:G:C5 | 33:BD:208:LYS:HB2 | 2.51 | 0.46 |
| 31:BA:842:G:N2 | 31:BA:937:U:C2 | 2.84 | 0.46 |
| 32:BB:87:G:C2' | 32:BB:88:C:H5'' | 2.46 | 0.46 |
| 33:BD:35:LYS:CD | 33:BD:64:ILE:N | 2.79 | 0.46 |
| 33:BD:35:LYS:HG2 | 33:BD:64:ILE:CG2 | 2.43 | 0.46 |
| 34:BE:116:VAL:CG1 | 34:BE:122:PHE:CD2 | 2.99 | 0.46 |
| 34:BE:93:VAL:N | 34:BE:95:ILE:HD13 | 2.31 | 0.46 |
| 35:BF:132:VAL:O | 35:BF:134:GLY:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BG:55:LYS:NZ | 36:BG:148:MET:O | 2.49 | 0.46 |
| 36:BG:15:VAL:HG22 | 36:BG:175:LEU:HB3 | 1.97 | 0.46 |
| 44:BS:17:ARG:HE | 44:BS:89:ARG:HH21 | 1.64 | 0.46 |
| 47:BV:40:LEU:CD1 | 47:BV:40:LEU:C | 2.84 | 0.46 |
| 1:CA:1128:C:H5' | 9:CI:16:ARG:CZ | 2.45 | 0.46 |
| 1:CA:1241:G:H2' | 1:CA:1242:C:C6 | 2.50 | 0.46 |
| 1:CA:1255:G:H2' | 1:CA:1255:G:N3 | 2.31 | 0.46 |
| 1:CA:1313:U:OP2 | 19:CS:6:LYS:HB3 | 2.16 | 0.46 |
| 1:CA:1446:U:O2 | 1:CA:1456:G:O6 | 2.34 | 0.46 |
| 1:CA:16:A:C2' | 1:CA:17:U:H5' | 2.44 | 0.46 |
| 1:CA:262:A:C6 | 1:CA:263:A:C6 | 3.04 | 0.46 |
| 1:CA:445:G:C6 | 1:CA:490:G:C6 | 3.03 | 0.46 |
| 1:CA:458:C:N4 | 1:CA:474:G:H1 | 2.14 | 0.46 |
| 1:CA:542:G:C2 | 1:CA:543:C:C5 | 3.03 | 0.46 |
| 1:CA:560:U:H4' | 1:CA:561:U:O5' | 2.15 | 0.46 |
| 1:CA:577:G:N3 | 1:CA:578:C:C6 | 2.84 | 0.46 |
| 1:CA:675:A:H2' | 1:CA:676:A:H8 | 1.79 | 0.46 |
| 1:CA:805:C:O2' | 1:CA:806:C:H5' | 2.15 | 0.46 |
| 2:CB:97:TRP:HZ2 | 2:CB:102:LEU:HD13 | 1.80 | 0.46 |
| 2:CB:88:ALA:HB1 | 2:CB:222:ILE:HG21 | 1.98 | 0.46 |
| 3:CC:11:ARG:HB3 | 3:CC:15:THR:HB | 1.98 | 0.46 |
| 8:CH:11:THR:HG23 | 8:CH:14:ARG:NH1 | 2.30 | 0.46 |
| 8:CH:20:TYR:HA | 8:CH:65:TYR:CE2 | 2.51 | 0.46 |
| 1:CA:881:G:P | 12:CL:12:ARG:HH22 | 2.38 | 0.46 |
| 17:CQ:6:LEU:O | 17:CQ:58:GLU:HA | 2.15 | 0.46 |
| 20:CT:100:ILE:O | 20:CT:100:ILE:HG22 | 2.16 | 0.46 |
| 24:D2:45:SER:HA | 24:D2:47:ASN:HD21 | 1.80 | 0.46 |
| 27:D5:57:VAL:C | 27:D5:58:LEU:HG | 2.36 | 0.46 |
| 28:D6:30:THR:HB | 31:DA:2286:A:OP1 | 2.16 | 0.46 |
| 30:D8:31:HIS:O | 30:D8:33:ASN:N | 2.48 | 0.46 |
| 31:DA:1108:U:C4 | 31:DA:1109:C:O2 | 2.69 | 0.46 |
| 31:DA:1434:A:C2' | 31:DA:1435:G:H5' | 2.45 | 0.46 |
| 31:DA:1902:C:C2' | 31:DA:1903:G:O5' | 2.63 | 0.46 |
| 31:DA:2048:G:C6 | 31:DA:2049:G:C5 | 3.04 | 0.46 |
| 31:DA:2275:C:H5' | 31:DA:2275:C:H6 | 1.80 | 0.46 |
| 31:DA:2779:U:O4' | 31:DA:2779:U:O2 | 2.34 | 0.46 |
| 31:DA:708:C:N4 | 31:DA:723:G:H1 | 2.13 | 0.46 |
| 31:DA:90:U:O2' | 31:DA:92:A:H5'' | 2.16 | 0.46 |
| 32:DB:78:A:C2 | 32:DB:100:A:C4 | 3.04 | 0.46 |
| 33:DD:101:GLU:HG3 | 33:DD:102:LYS:N | 2.31 | 0.46 |
| 35:DF:160:ASN:C | 35:DF:160:ASN:ND2 | 2.68 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:DG:60:LEU:HD13 | 36:DG:60:LEU:C | 2.36 | 0.46 |
| 43:DR:50:HIS:NE2 | 43:DR:54:LEU:HD21 | 2.30 | 0.46 |
| 45:DT:56:GLY:C | 45:DT:59:THR:CG2 | 2.85 | 0.46 |
| 50:DY:8:LYS:H | 50:DY:28:LYS:NZ | 2.14 | 0.46 |
| 50:DY:75:ILE:CD1 | 50:DY:79:CYS:C | 2.77 | 0.46 |
| 1:AA:1012:U:H6 | 1:AA:1012:U:O5' | 1.99 | 0.46 |
| 1:AA:1031:G:H2' | 1:AA:1032:G:C8 | 2.50 | 0.46 |
| 1:AA:1271:G:OP1 | 1:AA:1314:C:H4' | 2.15 | 0.46 |
| 1:AA:374:A:C4 | 1:AA:375:U:C5 | 3.04 | 0.46 |
| 1:AA:928:G:C2 | 1:AA:1390:U:O2 | 2.68 | 0.46 |
| 2:AB:53:ARG:HA | 2:AB:56:ARG:HB2 | 1.97 | 0.46 |
| 3:AC:134:ILE:O | 3:AC:138:VAL:HG23 | 2.16 | 0.46 |
| 4:AD:33:MET:HE2 | 4:AD:37:PRO:HA | 1.95 | 0.46 |
| 8:AH:41:ARG:O | 8:AH:41:ARG:HG2 | 2.16 | 0.46 |
| 10:AJ:22:LYS:HZ2 | 10:AJ:88:LEU:HD23 | 1.80 | 0.46 |
| 27:B5:57:VAL:C | 27:B5:58:LEU:HG | 2.36 | 0.46 |
| 31:BA:1450(A):C:N4 | 31:BA:1451:C:H41 | 2.13 | 0.46 |
| 31:BA:1591:G:H8 | 31:BA:1591:G:C5' | 2.29 | 0.46 |
| 23:B1:44:PRO:HA | 31:BA:2231:C:OP1 | 2.16 | 0.46 |
| 31:BA:2629:A:N3 | 31:BA:2629:A:H2' | 2.30 | 0.46 |
| 31:BA:82:G:O2' | 31:BA:83:G:H5' | 2.15 | 0.46 |
| 37:BH:126:PRO:HB2 | 37:BH:130:ARG:NH1 | 2.30 | 0.46 |
| 39:BN:17:ASP:C | 39:BN:19:GLU:H | 2.18 | 0.46 |
| 39:BN:56:ASN:H | 39:BN:125:GLY:N | 2.14 | 0.46 |
| 42:BQ:22:LYS:CE | 42:BQ:22:LYS:HA | 2.29 | 0.46 |
| 48:BW:9:TYR:N | 48:BW:102:HIS:CD2 | 2.76 | 0.46 |
| 48:BW:70:TYR:OH | 48:BW:72:LYS:HD2 | 2.16 | 0.46 |
| 31:BA:139(A):G:C2 | 49:BX:44:GLU:OE1 | 2.69 | 0.46 |
| 50:BY:28:LYS:C | 50:BY:30:VAL:H | 2.19 | 0.46 |
| 50:BY:45:VAL:CG1 | 50:BY:62:GLU:OE2 | 2.64 | 0.46 |
| 50:BY:72:VAL:C | 50:BY:73:ARG:HG3 | 2.36 | 0.46 |
| 1:CA:1476:G:C6 | 1:CA:1477:C:N4 | 2.84 | 0.46 |
| 1:CA:338:A:C6 | 1:CA:339:C:C4 | 3.03 | 0.46 |
| 1:CA:754:C:H3' | 1:CA:754:C:O2 | 2.16 | 0.46 |
| 1:CA:779:C:H2' | 1:CA:780:A:O4' | 2.15 | 0.46 |
| 4:CD:14:ARG:HA | 4:CD:39:PRO:CB | 2.46 | 0.46 |
| 1:CA:923:A:C5' | 5:CE:21:ALA:HB2 | 2.46 | 0.46 |
| 8:CH:97:VAL:O | 8:CH:100:ILE:HG13 | 2.16 | 0.46 |
| 1:CA:1368:G:OP2 | 9:CI:112:LYS:HD3 | 2.16 | 0.46 |
| 18:CR:62:GLU:O | 18:CR:65:ILE:HD12 | 2.16 | 0.46 |
| 23:D1:33:LYS:NZ | 23:D1:35:THR:CG2 | 2.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:D2:30:ARG:N | 24:D2:30:ARG:CD | 2.76 | 0.46 |
| 30:D8:25:MET:HB2 | 41:DP:62:LEU:HD21 | 1.94 | 0.46 |
| 30:D8:26:LYS:HE2 | 30:D8:47:LYS:NZ | 2.30 | 0.46 |
| 30:D8:48:PHE:H | 30:D8:48:PHE:HD1 | 1.61 | 0.46 |
| 30:D8:50:LEU:HD12 | 30:D8:51:ALA:H | 1.81 | 0.46 |
| 31:DA:1042:G:C5' | 31:DA:1043:C:OP2 | 2.63 | 0.46 |
| 31:DA:1043:C:OP2 | 31:DA:1043:C:C6 | 2.69 | 0.46 |
| 31:DA:1142(A):A:C5 | 31:DA:1144:G:C5 | 3.04 | 0.46 |
| 31:DA:1241:A:H2' | 31:DA:1242:A:O5' | 2.16 | 0.46 |
| 31:DA:1886:C:O5' | 31:DA:1886:C:H6 | 1.99 | 0.46 |
| 31:DA:2092:U:C4 | 31:DA:2226:C:OP2 | 2.69 | 0.46 |
| 31:DA:2722:G:O2' | 43:DR:5:LYS:HB2 | 2.15 | 0.46 |
| 31:DA:327:G:C2 | 31:DA:336:C:C2 | 3.04 | 0.46 |
| 31:DA:373:U:H2' | 31:DA:374:A:C8 | 2.51 | 0.46 |
| 31:DA:873:G:H1 | 31:DA:904:C:H42 | 1.64 | 0.46 |
| 32:DB:13:A:O2' | 32:DB:15:A:O5' | 2.33 | 0.46 |
| 33:DD:35:LYS:H | 33:DD:64:ILE:HG23 | 1.81 | 0.46 |
| 34:DE:176:ILE:HD12 | 34:DE:176:ILE:N | 2.31 | 0.46 |
| 35:DF:36:VAL:O | 35:DF:40:GLN:HG3 | 2.15 | 0.46 |
| 37:DH:85:LYS:HE2 | 37:DH:145:ALA:N | 2.31 | 0.46 |
| 37:DH:153:LYS:HB2 | 37:DH:154:PRO:CD | 2.46 | 0.46 |
| 40:DO:17:ARG:HA | 40:DO:17:ARG:HD3 | 1.63 | 0.46 |
| 44:DS:106:ARG:HB3 | 44:DS:106:ARG:HE | 1.36 | 0.46 |
| 44:DS:58:LEU:O | 44:DS:59:LYS:O | 2.33 | 0.46 |
| 50:DY:28:LYS:CE | 50:DY:30:VAL:HG22 | 2.29 | 0.46 |
| 50:DY:41:GLY:O | 50:DY:42:VAL:C | 2.55 | 0.46 |
| 51:DZ:117:LEU:CB | 51:DZ:174:VAL:HG22 | 2.46 | 0.46 |
| 1:AA:1061:G:H5'' | 10:AJ:59:SER:OG | 2.16 | 0.45 |
| 1:AA:322:C:C5 | 1:AA:328:C:C5 | 2.99 | 0.45 |
| 1:AA:444:C:H2' | 1:AA:445:G:H8 | 1.81 | 0.45 |
| 3:AC:112:SER:O | 3:AC:116:VAL:HG23 | 2.16 | 0.45 |
| 10:AJ:75:ILE:HG13 | 10:AJ:76:ASN:N | 2.31 | 0.45 |
| 11:AK:48:ILE:HG22 | 11:AK:49:GLY:N | 2.32 | 0.45 |
| 13:AM:44:ARG:CB | 13:AM:46:LYS:HG2 | 2.45 | 0.45 |
| 15:AO:54:ARG:HG2 | 15:AO:58:MET:HE1 | 1.97 | 0.45 |
| 20:AT:89:ARG:C | 20:AT:91:LEU:H | 2.19 | 0.45 |
| 31:BA:2287:A:N3 | 31:BA:2289:G:C8 | 2.84 | 0.45 |
| 31:BA:2410:G:C2 | 31:BA:2411:A:H1' | 2.51 | 0.45 |
| 31:BA:2876:G:H4' | 45:BT:3:ARG:HD3 | 1.96 | 0.45 |
| 31:BA:481:G:HO2' | 31:BA:482:A:P | 2.39 | 0.45 |
| 31:BA:910:A:C8 | 42:BQ:13:GLN:HB2 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:910:A:H2' | 31:BA:2264:C:O2' | 2.16 | 0.45 |
| 31:BA:926:A:H8 | 31:BA:926:A:H5'' | 1.81 | 0.45 |
| 32:BB:86:G:C2' | 32:BB:87:G:C8 | 2.99 | 0.45 |
| 33:BD:173:VAL:CG2 | 33:BD:174:ILE:N | 2.78 | 0.45 |
| 34:BE:37:ARG:HD3 | 34:BE:44:TYR:CZ | 2.51 | 0.45 |
| 34:BE:28:ALA:O | 34:BE:93:VAL:HG23 | 2.16 | 0.45 |
| 43:BR:24:GLN:HE22 | 43:BR:36:THR:HG21 | 1.80 | 0.45 |
| 44:BS:56:LEU:O | 44:BS:56:LEU:HD23 | 2.16 | 0.45 |
| 45:BT:31:SER:OG | 45:BT:43:GLN:N | 2.49 | 0.45 |
| 45:BT:28:VAL:CG1 | 45:BT:46:GLU:HB2 | 2.45 | 0.45 |
| 46:BU:39:LEU:HA | 46:BU:39:LEU:HD23 | 1.56 | 0.45 |
| 47:BV:16:PRO:C | 47:BV:98:GLU:OE2 | 2.54 | 0.45 |
| 48:BW:46:PHE:O | 48:BW:50:VAL:HG12 | 2.15 | 0.45 |
| 1:CA:1014:A:H2 | 1:CA:1219:U:O2 | 1.98 | 0.45 |
| 1:CA:1498:U:H1' | 1:CA:1499:A:OP2 | 2.17 | 0.45 |
| 1:CA:261:U:C5 | 20:CT:79:ARG:CZ | 2.99 | 0.45 |
| 1:CA:286:G:C5 | 1:CA:287:U:C5 | 3.04 | 0.45 |
| 1:CA:674:G:H2' | 1:CA:675:A:C8 | 2.51 | 0.45 |
| 1:CA:930:C:C2' | 1:CA:931:C:H5' | 2.46 | 0.45 |
| 2:CB:16:HIS:CG | 2:CB:213:LEU:HD13 | 2.51 | 0.45 |
| 2:CB:7:VAL:HG12 | 2:CB:11:LEU:HD11 | 1.98 | 0.45 |
| 4:CD:172:PRO:O | 4:CD:187:ARG:NH1 | 2.44 | 0.45 |
| 6:CF:19:LEU:O | 6:CF:23:LYS:HG3 | 2.16 | 0.45 |
| 6:CF:67:MET:CE | 6:CF:75:LEU:HD12 | 2.46 | 0.45 |
| 8:CH:25:ASP:HB3 | 8:CH:58:TYR:CB | 2.46 | 0.45 |
| 9:CI:19:LEU:HB3 | 9:CI:59:PHE:HD2 | 1.81 | 0.45 |
| 11:CK:21:ILE:HB | 11:CK:84:VAL:HA | 1.98 | 0.45 |
| 16:CP:4:ILE:HD12 | 16:CP:4:ILE:N | 2.31 | 0.45 |
| 6:CF:99:ALA:HB3 | 18:CR:29:PHE:CE2 | 2.50 | 0.45 |
| 20:CT:10:LEU:O | 20:CT:12:ALA:N | 2.43 | 0.45 |
| 20:CT:71:THR:HG22 | 20:CT:72:LEU:H | 1.80 | 0.45 |
| 23:D1:21:ARG:HD3 | 23:D1:21:ARG:C | 2.36 | 0.45 |
| 30:D8:34:TRP:HD1 | 31:DA:2391:G:OP1 | 1.99 | 0.45 |
| 31:DA:1639:U:H4' | 31:DA:2699:C:H4' | 1.97 | 0.45 |
| 31:DA:1722:A:N6 | 31:DA:1741:A:H2 | 2.13 | 0.45 |
| 31:DA:195:A:H61 | 31:DA:198:C:H3' | 1.81 | 0.45 |
| 31:DA:2314:C:C2 | 31:DA:2315:G:C8 | 3.04 | 0.45 |
| 31:DA:272(G):C:H42 | 31:DA:363(C):G:H1 | 1.63 | 0.45 |
| 31:DA:675:A:C4 | 31:DA:804:A:C2 | 3.04 | 0.45 |
| 31:DA:719:C:O2' | 31:DA:720:C:H5' | 2.16 | 0.45 |
| 31:DA:878:A:N6 | 31:DA:900:A:C8 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:995:C:O2 | 46:DU:57:PHE:CD2 | 2.69 | 0.45 |
| 32:DB:94:C:H2' | 32:DB:95:C:C6 | 2.50 | 0.45 |
| 33:DD:96:HIS:CE1 | 33:DD:102:LYS:HD3 | 2.51 | 0.45 |
| 31:DA:2784:C:H1' | 34:DE:37:ARG:NH2 | 2.31 | 0.45 |
| 35:DF:162:LEU:HD12 | 35:DF:162:LEU:HA | 1.78 | 0.45 |
| 35:DF:20:LEU:HD13 | 35:DF:203:GLN:NE2 | 2.31 | 0.45 |
| 36:DG:13:GLU:HG3 | 36:DG:13:GLU:O | 2.16 | 0.45 |
| 38:DI:138:ILE:HG22 | 38:DI:139:GLN:H | 1.81 | 0.45 |
| 38:DI:5:LEU:HD21 | 38:DI:19:VAL:HG12 | 1.97 | 0.45 |
| 39:DN:78:TYR:CD1 | 39:DN:79:PRO:CB | 2.99 | 0.45 |
| 40:DO:34:THR:OG1 | 40:DO:35:VAL:N | 2.48 | 0.45 |
| 41:DP:75:ILE:N | 41:DP:75:ILE:CD1 | 2.70 | 0.45 |
| 43:DR:11:ASN:CG | 43:DR:12:ARG:N | 2.67 | 0.45 |
| 31:DA:1275:A:C8 | 43:DR:16:HIS:CD2 | 3.04 | 0.45 |
| 44:DS:57:LYS:HG2 | 44:DS:58:LEU:N | 2.30 | 0.45 |
| 46:DU:69:CYS:O | 46:DU:74:LEU:HD12 | 2.17 | 0.45 |
| 50:DY:31:LEU:HD13 | 50:DY:31:LEU:HA | 1.53 | 0.45 |
| 1:AA:382:A:C2 | 1:AA:383:A:C4 | 3.04 | 0.45 |
| 1:AA:389:A:H2' | 1:AA:390:C:C5' | 2.46 | 0.45 |
| 1:AA:457:C:H2' | 1:AA:458:C:C6 | 2.51 | 0.45 |
| 1:AA:527:G:O2' | 1:AA:528:C:H5' | 2.16 | 0.45 |
| 1:AA:577:G:H1' | 1:AA:816:A:C4 | 2.50 | 0.45 |
| 1:AA:600:C:O2' | 1:AA:601:C:H5' | 2.17 | 0.45 |
| 1:AA:730:G:O2' | 1:AA:766:A:H5' | 2.16 | 0.45 |
| 1:AA:826:C:H4' | 8:AH:12:ARG:HD3 | 1.98 | 0.45 |
| 4:AD:203:VAL:O | 4:AD:204:ILE:C | 2.55 | 0.45 |
| 11:AK:48:ILE:HG21 | 11:AK:63:LEU:HD13 | 1.98 | 0.45 |
| 1:AA:950:U:H6 | 13:AM:102:ARG:NH1 | 2.13 | 0.45 |
| 16:AP:22:THR:HG23 | 16:AP:32:TYR:HA | 1.98 | 0.45 |
| 20:AT:14:LYS:HA | 20:AT:17:ARG:HE | 1.81 | 0.45 |
| 20:AT:73:HIS:HB3 | 20:AT:74:LYS:H | 1.60 | 0.45 |
| 28:B6:20:ASN:CG | 28:B6:21:TYR:N | 2.70 | 0.45 |
| 30:B8:2:PRO:O | 30:B8:3:LYS:C | 2.53 | 0.45 |
| 31:BA:109:G:H2' | 31:BA:110:G:O4' | 2.16 | 0.45 |
| 31:BA:1364:G:H5'' | 31:BA:1365:A:OP2 | 2.17 | 0.45 |
| 31:BA:1416:G:O2' | 31:BA:1417:C:C6 | 2.70 | 0.45 |
| 31:BA:1902:C:C2' | 31:BA:1903:G:O5' | 2.64 | 0.45 |
| 31:BA:2186:G:H3' | 31:BA:2187:G:H5'' | 1.98 | 0.45 |
| 31:BA:2299:G:N1 | 31:BA:2318:G:C8 | 2.84 | 0.45 |
| 31:BA:2705:A:H2' | 31:BA:2706:G:O4' | 2.17 | 0.45 |
| 31:BA:271(H):G:O6 | 31:BA:271(Q):G:O6 | 2.33 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:2859:G:H4' | 31:BA:2860:A:OP1 | 2.16 | 0.45 |
| 31:BA:34:C:H3' | 31:BA:34:C:H6 | 1.81 | 0.45 |
| 31:BA:387:U:H4' | 31:BA:388:G:O5' | 2.16 | 0.45 |
| 31:BA:518:G:H2' | 31:BA:519:U:H6 | 1.80 | 0.45 |
| 33:BD:77:ALA:HB2 | 33:BD:97:TYR:CG | 2.50 | 0.45 |
| 34:BE:179:GLU:HB3 | 34:BE:181:LEU:HD22 | 1.97 | 0.45 |
| 35:BF:3:GLU:HB2 | 35:BF:20:LEU:H | 1.81 | 0.45 |
| 37:BH:43:VAL:CG1 | 37:BH:53:GLU:H | 2.28 | 0.45 |
| 37:BH:89:ILE:HD12 | 37:BH:89:ILE:C | 2.36 | 0.45 |
| 38:BI:5:LEU:HD21 | 38:BI:19:VAL:HG12 | 1.97 | 0.45 |
| 40:BO:16:ALA:HB2 | 40:BO:52:VAL:HG11 | 1.98 | 0.45 |
| 40:BO:73:ASP:OD2 | 45:BT:32:TYR:HE1 | 1.98 | 0.45 |
| 40:BO:9:GLU:O | 40:BO:83:ALA:HA | 2.17 | 0.45 |
| 30:B8:58:ILE:CG2 | 41:BP:49:ARG:CD | 2.94 | 0.45 |
| 42:BQ:30:GLY:CA | 42:BQ:107:ALA:HB2 | 2.44 | 0.45 |
| 44:BS:88:ASP:CG | 44:BS:89:ARG:N | 2.68 | 0.45 |
| 45:BT:56:GLY:C | 45:BT:59:THR:CG2 | 2.84 | 0.45 |
| 45:BT:66:VAL:HA | 45:BT:71:GLY:HA2 | 1.99 | 0.45 |
| 51:BZ:108:PRO:O | 51:BZ:109:ALA:C | 2.55 | 0.45 |
| 51:BZ:150:LEU:C | 51:BZ:151:HIS:HD2 | 2.19 | 0.45 |
| 1:CA:336:C:H2' | 1:CA:337:C:H6 | 1.80 | 0.45 |
| 1:CA:429:U:H4' | 1:CA:430:A:O5' | 2.15 | 0.45 |
| 1:CA:694:A:C2 | 1:CA:695:A:H1' | 2.50 | 0.45 |
| 1:CA:738:C:C4 | 1:CA:739:C:C5 | 3.05 | 0.45 |
| 1:CA:1346:A:C5' | 9:CI:120:ARG:HH12 | 2.29 | 0.45 |
| 15:CO:74:ASP:HA | 15:CO:75:PRO:HD2 | 1.78 | 0.45 |
| 16:CP:39:TYR:CE1 | 16:CP:41:PRO:HA | 2.51 | 0.45 |
| 28:D6:15:GLU:OE1 | 28:D6:18:ARG:CG | 2.65 | 0.45 |
| 31:DA:1131:G:OP1 | 39:DN:80:GLY:HA2 | 2.14 | 0.45 |
| 31:DA:2023:G:H4' | 31:DA:2617:C:O3' | 2.16 | 0.45 |
| 31:DA:2306:C:OP2 | 31:DA:2307:G:C8 | 2.69 | 0.45 |
| 31:DA:2402:C:C3' | 31:DA:2403:C:H5' | 2.45 | 0.45 |
| 31:DA:34:C:H3' | 31:DA:34:C:H6 | 1.81 | 0.45 |
| 31:DA:529:A:N6 | 31:DA:2041:U:C2 | 2.85 | 0.45 |
| 31:DA:614:U:H5' | 31:DA:614(C):A:N6 | 2.31 | 0.45 |
| 31:DA:716:A:H2' | 31:DA:717:G:O5' | 2.16 | 0.45 |
| 31:DA:795:C:H2' | 31:DA:796:C:C6 | 2.51 | 0.45 |
| 31:DA:838:C:C4 | 31:DA:839:U:C5 | 3.05 | 0.45 |
| 32:DB:65:C:N4 | 32:DB:109:C:C2 | 2.84 | 0.45 |
| 32:DB:14:U:H5' | 32:DB:71:C:O4' | 2.16 | 0.45 |
| 34:DE:28:ALA:O | 34:DE:93:VAL:HG23 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DF:65:TRP:HZ3 | 35:DF:73:ALA:O | 1.99 | 0.45 |
| 36:DG:139:LEU:HD23 | 36:DG:149:VAL:HG21 | 1.98 | 0.45 |
| 37:DH:90:LYS:CB | 37:DH:159:GLU:O | 2.61 | 0.45 |
| 31:DA:1190:G:O3' | 41:DP:35:HIS:HB3 | 2.16 | 0.45 |
| 41:DP:33:ARG:O | 41:DP:35:HIS:O | 2.34 | 0.45 |
| 41:DP:71:VAL:HG13 | 41:DP:72:PRO:N | 2.31 | 0.45 |
| 42:DQ:22:LYS:NZ | 42:DQ:25:ASP:OD1 | 2.49 | 0.45 |
| 43:DR:51:LEU:CD1 | 43:DR:70:LEU:HD21 | 2.46 | 0.45 |
| 45:DT:33:LYS:HB3 | 45:DT:41:ARG:HB3 | 1.97 | 0.45 |
| 31:DA:993:G:C5' | 47:DV:75:PHE:CE2 | 2.89 | 0.45 |
| 51:DZ:33:LEU:HD12 | 51:DZ:33:LEU:HA | 1.74 | 0.45 |
| 1:AA:994:A:H62 | 1:AA:1046:A:H2 | 1.64 | 0.45 |
| 1:AA:299:G:C5 | 1:AA:300:A:C6 | 3.05 | 0.45 |
| 1:AA:577:G:C1' | 1:AA:816:A:C4 | 3.00 | 0.45 |
| 1:AA:84:U:H5 | 1:AA:88:A:N7 | 2.14 | 0.45 |
| 1:AA:909:A:H2' | 1:AA:910:C:O4' | 2.16 | 0.45 |
| 3:AC:112:SER:HB3 | 3:AC:115:LEU:HD12 | 1.99 | 0.45 |
| 4:AD:82:ALA:O | 4:AD:83:SER:C | 2.55 | 0.45 |
| 6:AF:19:LEU:HD11 | 6:AF:59:TYR:CD2 | 2.51 | 0.45 |
| 13:AM:45:VAL:HA | 13:AM:48:LEU:HD13 | 1.97 | 0.45 |
| 24:B2:48:HIS:ND1 | 24:B2:48:HIS:O | 2.50 | 0.45 |
| 28:B6:11:LEU:HD11 | 28:B6:51:GLU:HB2 | 1.97 | 0.45 |
| 31:BA:1528:A:O2' | 31:BA:1528(A):A:C8 | 2.62 | 0.45 |
| 31:BA:1865:G:N2 | 31:BA:1877:A:C8 | 2.85 | 0.45 |
| 31:BA:197:A:H5' | 31:BA:197:A:H8 | 1.81 | 0.45 |
| 31:BA:2017:U:H5'' | 31:BA:2018:G:OP2 | 2.15 | 0.45 |
| 31:BA:2470:G:C6 | 31:BA:2471:C:C5 | 3.05 | 0.45 |
| 31:BA:2773:C:O2' | 31:BA:2774:C:H5' | 2.17 | 0.45 |
| 31:BA:601:C:O2 | 31:BA:605:C:H4' | 2.15 | 0.45 |
| 31:BA:745:G:H5'' | 31:BA:746:A:OP2 | 2.17 | 0.45 |
| 22:B0:77:ARG:NH2 | 31:BA:857:C:OP1 | 2.43 | 0.45 |
| 32:BB:71:C:O2 | 32:BB:71:C:C2' | 2.62 | 0.45 |
| 33:BD:70:TRP:CZ3 | 33:BD:146:GLU:OE2 | 2.69 | 0.45 |
| 32:BB:45:A:H1' | 36:BG:95:ARG:NH2 | 2.31 | 0.45 |
| 37:BH:68:THR:O | 37:BH:69:ARG:C | 2.54 | 0.45 |
| 38:BI:138:ILE:HG22 | 38:BI:139:GLN:N | 2.31 | 0.45 |
| 41:BP:140:ALA:O | 41:BP:141:ALA:CB | 2.64 | 0.45 |
| 45:BT:28:VAL:HG13 | 45:BT:46:GLU:CB | 2.44 | 0.45 |
| 31:BA:1225:G:OP1 | 47:BV:88:ARG:CB | 2.64 | 0.45 |
| 49:BX:55:ASN:HB2 | 49:BX:78:LYS:CD | 2.46 | 0.45 |
| 1:CA:1250:A:N6 | 1:CA:1251:A:C6 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1433:A:N1 | 1:CA:1434:A:C2 | 2.85 | 0.45 |
| 1:CA:41:G:H2' | 1:CA:42:G:H8 | 1.80 | 0.45 |
| 1:CA:586:C:H2' | 1:CA:587:G:H5' | 1.98 | 0.45 |
| 1:CA:602:A:C2 | 1:CA:637:G:C2 | 3.04 | 0.45 |
| 1:CA:657:G:N2 | 1:CA:750:G:C8 | 2.84 | 0.45 |
| 1:CA:96:U:O2' | 1:CA:97:G:H8 | 2.00 | 0.45 |
| 1:CA:981:U:O5' | 1:CA:981:U:H6 | 1.99 | 0.45 |
| 2:CB:25:ASN:HA | 2:CB:26:PRO:HD2 | 1.70 | 0.45 |
| 3:CC:125:GLU:HA | 3:CC:191:THR:CG2 | 2.45 | 0.45 |
| 4:CD:58:LEU:HD23 | 4:CD:206:PHE:CZ | 2.51 | 0.45 |
| 4:CD:96:LEU:N | 4:CD:96:LEU:HD22 | 2.30 | 0.45 |
| 5:CE:135:THR:O | 5:CE:138:ALA:HB3 | 2.16 | 0.45 |
| 1:CA:826:C:H4' | 8:CH:12:ARG:HD3 | 1.98 | 0.45 |
| 10:CJ:30:SER:HB2 | 10:CJ:80:LYS:HG3 | 1.98 | 0.45 |
| 10:CJ:49:VAL:HG11 | 14:CN:41:ARG:O | 2.16 | 0.45 |
| 11:CK:41:THR:CG2 | 11:CK:42:TRP:H | 2.29 | 0.45 |
| 11:CK:58:PRO:HA | 11:CK:90:GLY:HA2 | 1.99 | 0.45 |
| 19:CS:22:LEU:O | 19:CS:26:GLY:HA2 | 2.17 | 0.45 |
| 30:D8:58:ILE:CG2 | 41:DP:49:ARG:CD | 2.95 | 0.45 |
| 30:D8:59:LYS:HB3 | 30:D8:59:LYS:HE3 | 1.65 | 0.45 |
| 31:DA:1478:G:O2' | 31:DA:1558:A:C2 | 2.70 | 0.45 |
| 31:DA:1866:C:H2' | 31:DA:1876:A:O4' | 2.17 | 0.45 |
| 31:DA:2186:G:H3' | 31:DA:2187:G:H5'' | 1.98 | 0.45 |
| 31:DA:2584:U:H6 | 31:DA:2585:U:C5 | 2.34 | 0.45 |
| 31:DA:2803:C:OP2 | 31:DA:2803:C:H3' | 2.17 | 0.45 |
| 31:DA:480:A:OP2 | 50:DY:46:LYS:HD3 | 2.17 | 0.45 |
| 25:D3:46:ASN:ND2 | 31:DA:851:U:C4' | 2.79 | 0.45 |
| 31:DA:94:C:O2 | 31:DA:94:C:H2' | 2.15 | 0.45 |
| 31:DA:954:G:C4 | 31:DA:955:C:C6 | 3.03 | 0.45 |
| 32:DB:60:C:N3 | 32:DB:61:G:N7 | 2.63 | 0.45 |
| 35:DF:20:LEU:O | 35:DF:23:ASP:HB2 | 2.16 | 0.45 |
| 37:DH:157:TYR:O | 37:DH:158:HIS:HB2 | 2.17 | 0.45 |
| 41:DP:35:HIS:O | 41:DP:36:LYS:CB | 2.64 | 0.45 |
| 41:DP:38:GLN:HG3 | 41:DP:39:LYS:N | 2.24 | 0.45 |
| 43:DR:75:LEU:CD1 | 43:DR:75:LEU:C | 2.84 | 0.45 |
| 47:DV:40:LEU:HD12 | 47:DV:40:LEU:C | 2.37 | 0.45 |
| 47:DV:69:LYS:O | 47:DV:70:ILE:HG23 | 2.15 | 0.45 |
| 51:DZ:14:LYS:HB2 | 51:DZ:17:ALA:HB3 | 1.98 | 0.45 |
| 51:DZ:29:TYR:HA | 51:DZ:33:LEU:O | 2.16 | 0.45 |
| 1:AA:1085:U:C2 | 1:AA:1094:G:O6 | 2.70 | 0.45 |
| 1:AA:1128:C:O2' | 1:AA:1130:A:C8 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:AA:1206:G:O6 | 1:AA:1207:G:C6 | 2.69 | 0.45 |
| 1:AA:1250:A:N6 | 1:AA:1251:A:C6 | 2.84 | 0.45 |
| 1:AA:250:A:C1' | 1:AA:251:G:OP2 | 2.64 | 0.45 |
| 1:AA:867:G:N2 | 1:AA:868:C:C2 | 2.85 | 0.45 |
| 1:AA:940:C:H2' | 1:AA:941:G:H8 | 1.81 | 0.45 |
| 1:AA:951:G:C6 | 1:AA:1231:G:C6 | 3.04 | 0.45 |
| 9:AI:19:LEU:HB3 | 9:AI:59:PHE:HD2 | 1.82 | 0.45 |
| 10:AJ:32:ALA:HB3 | 10:AJ:76:ASN:HB3 | 1.97 | 0.45 |
| 13:AM:19:LEU:HD11 | 13:AM:56:LEU:HD11 | 1.98 | 0.45 |
| 27:B5:11:THR:CG2 | 31:BA:1264:G:H5' | 2.46 | 0.45 |
| 31:BA:1020:A:N1 | 31:BA:1141:U:O2' | 2.42 | 0.45 |
| 31:BA:1225:G:P | 47:BV:88:ARG:HB3 | 2.57 | 0.45 |
| 27:B5:11:THR:HG23 | 31:BA:1264:G:H5' | 1.99 | 0.45 |
| 31:BA:1300:U:O2' | 31:BA:1300:U:H5'' | 2.17 | 0.45 |
| 31:BA:1747(A):G:O2' | 31:BA:1748:G:H5' | 2.16 | 0.45 |
| 31:BA:1804:C:O2' | 31:BA:1805:U:H5' | 2.17 | 0.45 |
| 31:BA:2703:C:H2' | 31:BA:2704:C:C6 | 2.51 | 0.45 |
| 31:BA:272(J):C:H2' | 31:BA:274:G:OP1 | 2.15 | 0.45 |
| 31:BA:877:U:C2' | 31:BA:878:A:H5'' | 2.46 | 0.45 |
| 31:BA:2580:U:C4' | 34:BE:131:ALA:H | 2.28 | 0.45 |
| 36:BG:25:TYR:CZ | 36:BG:32:PRO:HD3 | 2.51 | 0.45 |
| 31:BA:2393:A:OP1 | 41:BP:62:LEU:HD12 | 2.17 | 0.45 |
| 44:BS:19:LYS:CG | 44:BS:19:LYS:O | 2.64 | 0.45 |
| 45:BT:27:THR:OG1 | 45:BT:28:VAL:N | 2.49 | 0.45 |
| 45:BT:38:ASN:ND2 | 45:BT:38:ASN:C | 2.69 | 0.45 |
| 47:BV:25:LEU:HD12 | 47:BV:94:LEU:HD22 | 1.99 | 0.45 |
| 50:BY:75:ILE:HD11 | 50:BY:80:GLY:N | 2.30 | 0.45 |
| 1:CA:1031:G:H2' | 1:CA:1032:G:C8 | 2.51 | 0.45 |
| 1:CA:1129:C:H4' | 1:CA:1130:A:H5' | 1.98 | 0.45 |
| 1:CA:112:G:N3 | 1:CA:112:G:H2' | 2.31 | 0.45 |
| 1:CA:1272:G:C6 | 1:CA:1273:G:N7 | 2.85 | 0.45 |
| 1:CA:1452:C:H5' | 1:CA:1456:G:C5 | 2.51 | 0.45 |
| 1:CA:299:G:C6 | 1:CA:300:A:C6 | 3.04 | 0.45 |
| 1:CA:688:G:H2' | 1:CA:689:C:H6 | 1.82 | 0.45 |
| 1:CA:688:G:H2' | 1:CA:689:C:C6 | 2.51 | 0.45 |
| 1:CA:577:G:H1' | 1:CA:816:A:N3 | 2.32 | 0.45 |
| 2:CB:144:ARG:HA | 2:CB:147:LYS:CB | 2.46 | 0.45 |
| 4:CD:112:VAL:HG13 | 4:CD:113:SER:N | 2.31 | 0.45 |
| 4:CD:146:ILE:HD12 | 4:CD:146:ILE:H | 1.80 | 0.45 |
| 4:CD:150:GLU:H | 4:CD:150:GLU:CD | 2.20 | 0.45 |
| 4:CD:18:LYS:C | 4:CD:19:LEU:HG | 2.37 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:CL:126:LYS:HE2 | 12:CL:128:ALA:H | 1.80 | 0.45 |
| 13:CM:94:ARG:O | 13:CM:96:LEU:HG | 2.16 | 0.45 |
| 14:CN:41:ARG:HG3 | 14:CN:42:ILE:HD13 | 1.97 | 0.45 |
| 19:CS:10:PHE:HE2 | 19:CS:37:ARG:O | 1.99 | 0.45 |
| 24:D2:25:VAL:HG13 | 24:D2:26:ARG:CD | 2.41 | 0.45 |
| 30:D8:58:ILE:O | 30:D8:61:LEU:HG | 2.16 | 0.45 |
| 31:DA:130:C:H2' | 31:DA:131:G:H5'' | 1.98 | 0.45 |
| 31:DA:1323:U:H2' | 31:DA:1324:G:H5' | 1.98 | 0.45 |
| 31:DA:1956:U:H2' | 31:DA:1957:C:H5' | 1.98 | 0.45 |
| 31:DA:197:A:H8 | 31:DA:197:A:H5' | 1.81 | 0.45 |
| 31:DA:2031:A:N3 | 31:DA:2455:G:O2' | 2.42 | 0.45 |
| 31:DA:2223:G:H2' | 31:DA:2224:G:C5' | 2.40 | 0.45 |
| 31:DA:2306:C:OP2 | 31:DA:2307:G:H8 | 2.00 | 0.45 |
| 31:DA:641:C:O2' | 31:DA:2350:C:OP1 | 2.29 | 0.45 |
| 31:DA:251:A:C5' | 41:DP:51:PHE:HZ | 2.29 | 0.45 |
| 31:DA:2704:C:H2' | 31:DA:2705:A:O4' | 2.16 | 0.45 |
| 30:D8:2:PRO:N | 31:DA:591:C:O2 | 2.49 | 0.45 |
| 31:DA:753:C:O5' | 31:DA:753:C:C6 | 2.70 | 0.45 |
| 31:DA:985:C:H2' | 31:DA:986:C:C6 | 2.48 | 0.45 |
| 32:DB:78:A:H2' | 32:DB:79:C:O4' | 2.16 | 0.45 |
| 33:DD:238:GLY:O | 33:DD:239:ARG:HB2 | 2.16 | 0.45 |
| 34:DE:51:PHE:CE1 | 34:DE:52:LEU:HG | 2.50 | 0.45 |
| 36:DG:86:MET:HB2 | 36:DG:87:PRO:HD2 | 1.98 | 0.45 |
| 37:DH:137:ASP:HB3 | 37:DH:140:LYS:H | 1.81 | 0.45 |
| 37:DH:138:LYS:C | 37:DH:140:LYS:N | 2.70 | 0.45 |
| 38:DI:9:LEU:N | 38:DI:13:GLY:HA2 | 2.27 | 0.45 |
| 38:DI:28:ASN:C | 38:DI:32:PRO:HG2 | 2.37 | 0.45 |
| 40:DO:87:ILE:CG2 | 40:DO:88:ASN:N | 2.79 | 0.45 |
| 42:DQ:20:ALA:CB | 42:DQ:98:LYS:HB3 | 2.47 | 0.45 |
| 43:DR:71:GLN:NE2 | 43:DR:71:GLN:HA | 2.26 | 0.45 |
| 44:DS:58:LEU:HA | 44:DS:58:LEU:HD12 | 1.81 | 0.45 |
| 44:DS:87:PHE:HE2 | 44:DS:97:ARG:NH2 | 2.05 | 0.45 |
| 45:DT:33:LYS:HD3 | 45:DT:33:LYS:HA | 1.44 | 0.45 |
| 48:DW:28:SER:O | 48:DW:29:LEU:C | 2.55 | 0.45 |
| 50:DY:45:VAL:HG22 | 50:DY:62:GLU:CB | 2.46 | 0.45 |
| 51:DZ:100:VAL:O | 51:DZ:101:PRO:O | 2.35 | 0.45 |
| 1:AA:1065:U:H4' | 1:AA:1066:C:O5' | 2.17 | 0.45 |
| 1:AA:1054:C:OP1 | 1:AA:1197:G:OP2 | 2.35 | 0.45 |
| 1:AA:830:G:C5 | 1:AA:831:U:C5 | 3.05 | 0.45 |
| 3:AC:36:ASP:HB3 | 3:AC:40:ARG:HH12 | 1.80 | 0.45 |
| 7:AG:101:LEU:O | 7:AG:105:VAL:HG23 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AK:105:VAL:HG23 | 11:AK:105:VAL:O | 2.15 | 0.45 |
| 16:AP:4:ILE:HG13 | 16:AP:21:VAL:CG1 | 2.30 | 0.45 |
| 19:AS:48:THR:HG22 | 19:AS:61:TYR:CD1 | 2.52 | 0.45 |
| 20:AT:61:SER:OG | 20:AT:65:LYS:HE3 | 2.17 | 0.45 |
| 22:B0:72:ARG:O | 22:B0:73:GLY:C | 2.52 | 0.45 |
| 24:B2:34:GLU:O | 24:B2:34:GLU:HG2 | 2.16 | 0.45 |
| 28:B6:40:CYS:SG | 28:B6:45:LYS:CD | 3.04 | 0.45 |
| 31:BA:1461:G:C2' | 31:BA:1462:C:H5' | 2.47 | 0.45 |
| 31:BA:1826:G:H2' | 31:BA:1827:C:H6 | 1.82 | 0.45 |
| 31:BA:2100:G:O6 | 31:BA:2189:U:O4 | 2.35 | 0.45 |
| 31:BA:251:A:C5' | 41:BP:51:PHE:HZ | 2.29 | 0.45 |
| 31:BA:2543:G:H8 | 31:BA:2543:G:H5' | 1.81 | 0.45 |
| 31:BA:1669:A:H5'' | 31:BA:2550:G:OP1 | 2.17 | 0.45 |
| 31:BA:2592:G:H2' | 31:BA:2593:U:O4' | 2.17 | 0.45 |
| 31:BA:362:U:C3' | 31:BA:362:U:C6 | 3.00 | 0.45 |
| 31:BA:448:U:H3' | 31:BA:449:A:H5' | 1.98 | 0.45 |
| 31:BA:699:A:H2' | 31:BA:700:G:O4' | 2.17 | 0.45 |
| 31:BA:873:G:H1 | 31:BA:904:C:H42 | 1.63 | 0.45 |
| 31:BA:990:A:OP2 | 31:BA:991:C:OP2 | 2.35 | 0.45 |
| 32:BB:15:A:H5' | 32:BB:16:G:H8 | 1.75 | 0.45 |
| 33:BD:33:LEU:O | 33:BD:35:LYS:N | 2.50 | 0.45 |
| 31:BA:2784:C:H1' | 34:BE:37:ARG:NH2 | 2.32 | 0.45 |
| 34:BE:57:LYS:O | 34:BE:59:VAL:N | 2.47 | 0.45 |
| 36:BG:91:ARG:O | 36:BG:91:ARG:HD2 | 2.16 | 0.45 |
| 37:BH:85:LYS:HE2 | 37:BH:145:ALA:N | 2.31 | 0.45 |
| 39:BN:75:TYR:CE2 | 39:BN:83:LYS:NZ | 2.85 | 0.45 |
| 39:BN:87:LEU:O | 39:BN:88:GLU:C | 2.54 | 0.45 |
| 41:BP:83:VAL:HG12 | 41:BP:112:LEU:HD21 | 1.98 | 0.45 |
| 49:BX:25:LYS:HG3 | 49:BX:26:TYR:CD1 | 2.51 | 0.45 |
| 50:BY:46:LYS:C | 50:BY:47:LYS:CD | 2.85 | 0.45 |
| 50:BY:80:GLY:O | 50:BY:81:LYS:HB2 | 2.17 | 0.45 |
| 51:BZ:48:PHE:HE2 | 51:BZ:71:VAL:HG11 | 1.82 | 0.45 |
| 1:CA:1098:C:N3 | 1:CA:1099:G:C8 | 2.84 | 0.45 |
| 1:CA:1350:A:H2' | 1:CA:1351:U:C6 | 2.51 | 0.45 |
| 1:CA:189(F):U:O4 | 17:CQ:63:ARG:N | 2.39 | 0.45 |
| 1:CA:49:U:C2 | 1:CA:361:G:N2 | 2.85 | 0.45 |
| 1:CA:509:A:H2' | 1:CA:510:A:N7 | 2.31 | 0.45 |
| 1:CA:542:G:H5' | 4:CD:41:GLY:CA | 2.46 | 0.45 |
| 1:CA:655:A:C2 | 1:CA:754:C:N4 | 2.85 | 0.45 |
| 1:CA:69:G:C2 | 1:CA:70:G:C8 | 3.05 | 0.45 |
| 1:CA:827:U:H6 | 1:CA:827:U:O5' | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:160:ASP:O | 2:CB:183:PRO:HD2 | 2.16 | 0.45 |
| 2:CB:19:HIS:CG | 2:CB:20:GLU:N | 2.84 | 0.45 |
| 4:CD:61:LYS:HA | 4:CD:203:VAL:HG22 | 1.98 | 0.45 |
| 9:CI:124:GLN:HB3 | 9:CI:125:TYR:H | 1.45 | 0.45 |
| 10:CJ:84:GLN:O | 10:CJ:88:LEU:CB | 2.64 | 0.45 |
| 13:CM:19:LEU:HD11 | 13:CM:56:LEU:HD11 | 1.98 | 0.45 |
| 1:CA:1216:G:H5'' | 14:CN:5:ALA:HB2 | 1.99 | 0.45 |
| 24:D2:14:ARG:HE | 24:D2:14:ARG:HB3 | 1.64 | 0.45 |
| 25:D3:9:VAL:HG11 | 25:D3:55:ARG:HG3 | 1.96 | 0.45 |
| 31:DA:1025:G:H8 | 31:DA:1025:G:OP1 | 1.99 | 0.45 |
| 29:D7:13:ALA:HB1 | 31:DA:125:G:H1' | 1.98 | 0.45 |
| 31:DA:1327:C:O2' | 31:DA:1328:G:H5' | 2.17 | 0.45 |
| 31:DA:1341:U:C2' | 31:DA:1397:U:O2 | 2.64 | 0.45 |
| 31:DA:1341:U:H2' | 31:DA:1397:U:O2 | 2.17 | 0.45 |
| 31:DA:1465:G:C2 | 31:DA:1466:G:C4 | 3.05 | 0.45 |
| 31:DA:174:C:H2' | 31:DA:175:G:H5'' | 1.98 | 0.45 |
| 31:DA:2228:G:C5 | 31:DA:2229:C:C4 | 3.04 | 0.45 |
| 31:DA:226:G:H21 | 31:DA:228:A:H62 | 1.65 | 0.45 |
| 31:DA:21:A:O2' | 31:DA:22:C:H5' | 2.16 | 0.45 |
| 31:DA:2327:A:C6 | 31:DA:2328:A:C6 | 3.04 | 0.45 |
| 31:DA:2333:A:C2' | 31:DA:2334:G:OP2 | 2.65 | 0.45 |
| 31:DA:2776:A:N1 | 31:DA:2778:A:C2 | 2.85 | 0.45 |
| 31:DA:2836:U:C4 | 31:DA:2883:A:N6 | 2.85 | 0.45 |
| 31:DA:493:G:H2' | 31:DA:494:G:H5'' | 1.99 | 0.45 |
| 31:DA:13:A:N1 | 31:DA:525:U:H2' | 2.32 | 0.45 |
| 31:DA:916:G:O2' | 31:DA:917:A:H5'' | 2.16 | 0.45 |
| 31:DA:848:G:C4 | 31:DA:933:A:C8 | 3.04 | 0.45 |
| 35:DF:108:LYS:O | 35:DF:111:ALA:HB3 | 2.16 | 0.45 |
| 36:DG:37:VAL:O | 36:DG:94:LEU:HG | 2.16 | 0.45 |
| 37:DH:99:VAL:O | 37:DH:102:ALA:HB3 | 2.16 | 0.45 |
| 41:DP:124:LYS:HG2 | 41:DP:143:GLY:HA3 | 1.98 | 0.45 |
| 45:DT:57:PHE:O | 45:DT:58:ASN:ND2 | 2.49 | 0.45 |
| 46:DU:17:ILE:HG23 | 46:DU:39:LEU:HD12 | 1.98 | 0.45 |
| 46:DU:61:TRP:O | 46:DU:62:ILE:C | 2.53 | 0.45 |
| 49:DX:34:ALA:C | 49:DX:36:LYS:N | 2.69 | 0.45 |
| 50:DY:45:VAL:HG11 | 50:DY:60:PHE:C | 2.36 | 0.45 |
| 1:AA:1130:A:H1' | 1:AA:1146:A:C2 | 2.52 | 0.45 |
| 1:AA:945:G:N1 | 1:AA:1337:G:C2 | 2.84 | 0.45 |
| 1:AA:942:G:C2 | 1:AA:1342:C:C2 | 3.05 | 0.45 |
| 1:AA:336:C:H2' | 1:AA:337:C:H6 | 1.82 | 0.45 |
| 1:AA:561:U:HO2' | 1:AA:562:C:P | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:675:A:H2' | 1:AA:676:A:H8 | 1.82 | 0.45 |
| 8:AH:25:ASP:HB3 | 8:AH:58:TYR:CB | 2.47 | 0.45 |
| 13:AM:29:ARG:HA | 13:AM:32:GLU:HB3 | 1.99 | 0.45 |
| 16:AP:4:ILE:N | 16:AP:4:ILE:HD12 | 2.32 | 0.45 |
| 27:B5:31:VAL:HB | 27:B5:32:PRO:HD2 | 1.98 | 0.45 |
| 31:BA:2023:G:H4' | 31:BA:2617:C:O3' | 2.16 | 0.45 |
| 31:BA:2102:U:C4 | 31:BA:2103:C:N4 | 2.85 | 0.45 |
| 31:BA:2392:A:O4' | 31:BA:2392:A:N3 | 2.48 | 0.45 |
| 31:BA:2469:A:O2' | 42:BQ:56:ARG:CG | 2.60 | 0.45 |
| 31:BA:282:A:C4 | 31:BA:359:A:C2 | 3.05 | 0.45 |
| 31:BA:686:G:N2 | 31:BA:788:A:H61 | 2.15 | 0.45 |
| 31:BA:916:G:O2' | 31:BA:917:A:H5'' | 2.16 | 0.45 |
| 35:BF:81:PRO:HB3 | 35:BF:87:GLY:O | 2.17 | 0.45 |
| 36:BG:63:ILE:HD13 | 36:BG:141:PHE:CE2 | 2.51 | 0.45 |
| 32:BB:42:C:O2 | 36:BG:93:THR:N | 2.49 | 0.45 |
| 37:BH:45:VAL:CG1 | 37:BH:46:GLU:N | 2.76 | 0.45 |
| 39:BN:112:LEU:HD12 | 39:BN:112:LEU:C | 2.35 | 0.45 |
| 40:BO:12:ASP:C | 40:BO:99:PHE:HE2 | 2.19 | 0.45 |
| 46:BU:92:ARG:NH1 | 47:BV:11:GLN:O | 2.50 | 0.45 |
| 47:BV:62:LEU:CB | 47:BV:98:GLU:HA | 2.43 | 0.45 |
| 50:BY:68:HIS:H | 50:BY:71:LYS:NZ | 2.11 | 0.45 |
| 1:CA:99:U:O2' | 1:CA:100:C:H5' | 2.17 | 0.45 |
| 1:CA:1190:G:OP1 | 3:CC:5:ILE:N | 2.42 | 0.45 |
| 1:CA:11:G:C6 | 1:CA:12:U:C4 | 3.05 | 0.45 |
| 1:CA:33:A:H2' | 1:CA:34:C:C6 | 2.52 | 0.45 |
| 1:CA:683:G:C6 | 1:CA:684:A:C6 | 3.05 | 0.45 |
| 2:CB:142:LEU:C | 2:CB:142:LEU:HD23 | 2.37 | 0.45 |
| 5:CE:39:GLY:O | 5:CE:69:VAL:N | 2.40 | 0.45 |
| 1:CA:1061:G:H5'' | 10:CJ:59:SER:OG | 2.17 | 0.45 |
| 12:CL:93:LEU:O | 12:CL:94:PRO:C | 2.54 | 0.45 |
| 25:D3:36:VAL:HG23 | 25:D3:36:VAL:O | 2.16 | 0.45 |
| 31:DA:1225:G:P | 47:DV:88:ARG:HB3 | 2.57 | 0.45 |
| 31:DA:1531:C:H5' | 31:DA:1532:C:OP2 | 2.16 | 0.45 |
| 31:DA:2100:G:O6 | 31:DA:2189:U:O4 | 2.34 | 0.45 |
| 31:DA:858:U:O2 | 31:DA:2268:A:H2' | 2.17 | 0.45 |
| 31:DA:2592:G:H2' | 31:DA:2593:U:O4' | 2.16 | 0.45 |
| 31:DA:2801:A:O2' | 31:DA:2895:U:C4' | 2.61 | 0.45 |
| 31:DA:2808:U:O2' | 31:DA:2809:A:H5' | 2.16 | 0.45 |
| 31:DA:309:G:N3 | 31:DA:329:G:O2' | 2.45 | 0.45 |
| 31:DA:547:A:O2' | 31:DA:548:A:OP2 | 2.30 | 0.45 |
| 31:DA:616:G:H2' | 31:DA:618:C:O4' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DB:31:C:O2 | 32:DB:52:A:H2 | 2.00 | 0.45 |
| 32:DB:2:C:H2' | 32:DB:3:C:H6 | 1.81 | 0.45 |
| 31:DA:1797:C:O2' | 33:DD:259:THR:HB | 2.16 | 0.45 |
| 34:DE:111:ARG:HD2 | 34:DE:160:TYR:CD1 | 2.52 | 0.45 |
| 35:DF:89:VAL:CG1 | 35:DF:90:PHE:N | 2.70 | 0.45 |
| 36:DG:67:LYS:HD2 | 36:DG:67:LYS:H | 1.80 | 0.45 |
| 37:DH:117:PRO:HA | 37:DH:123:PHE:HE1 | 1.82 | 0.45 |
| 39:DN:99:LEU:HD22 | 39:DN:99:LEU:HA | 1.61 | 0.45 |
| 43:DR:100:LEU:HD11 | 43:DR:113:LEU:HD13 | 1.98 | 0.45 |
| 44:DS:95:HIS:O | 44:DS:98:VAL:CG2 | 2.65 | 0.45 |
| 45:DT:87:ASP:OD1 | 45:DT:87:ASP:N | 2.49 | 0.45 |
| 49:DX:29:TRP:CE3 | 49:DX:76:ARG:HB3 | 2.51 | 0.45 |
| 49:DX:77:LYS:HD3 | 49:DX:78:LYS:HD2 | 1.97 | 0.45 |
| 50:DY:90:LEU:HD12 | 50:DY:91:GLU:HG2 | 1.97 | 0.45 |
| 51:DZ:104:PHE:HA | 51:DZ:139:VAL:HB | 1.99 | 0.45 |
| 1:AA:1250:A:C6 | 1:AA:1251:A:C6 | 3.05 | 0.45 |
| 1:AA:374:A:C6 | 1:AA:375:U:C4 | 3.05 | 0.45 |
| 1:AA:509:A:H2' | 1:AA:510:A:N7 | 2.32 | 0.45 |
| 1:AA:673:G:H2' | 1:AA:674:G:H8 | 1.79 | 0.45 |
| 1:AA:764:C:C2 | 1:AA:765:G:C8 | 3.05 | 0.45 |
| 1:AA:948:C:C5 | 13:AM:106:ASN:ND2 | 2.84 | 0.45 |
| 2:AB:144:ARG:HA | 2:AB:147:LYS:CB | 2.46 | 0.45 |
| 2:AB:67:THR:HG21 | 2:AB:155:LEU:HD21 | 1.99 | 0.45 |
| 2:AB:24:TRP:CZ3 | 2:AB:26:PRO:HA | 2.52 | 0.45 |
| 2:AB:84:GLU:HB3 | 2:AB:219:VAL:CG2 | 2.34 | 0.45 |
| 5:AE:80:ILE:HD11 | 5:AE:138:ALA:HB1 | 1.98 | 0.45 |
| 5:AE:6:PHE:HD2 | 5:AE:36:ASP:HB3 | 1.81 | 0.45 |
| 9:AI:50:LEU:HD22 | 9:AI:55:ALA:O | 2.16 | 0.45 |
| 24:B2:14:ARG:CD | 24:B2:57:ILE:HB | 2.47 | 0.45 |
| 28:B6:10:LEU:CD2 | 28:B6:10:LEU:N | 2.80 | 0.45 |
| 30:B8:32:LEU:HB2 | 30:B8:34:TRP:H | 1.82 | 0.45 |
| 31:BA:1353:A:H5'' | 33:BD:38:LYS:NZ | 2.32 | 0.45 |
| 31:BA:2461:C:H2' | 31:BA:2462:U:H6 | 1.81 | 0.45 |
| 31:BA:2655:G:O2' | 31:BA:2656:U:H5 | 1.99 | 0.45 |
| 31:BA:2807:G:H22 | 31:BA:2892:A:N6 | 2.15 | 0.45 |
| 31:BA:2885:C:H2' | 31:BA:2886:G:O5' | 2.17 | 0.45 |
| 32:BB:28:C:H2' | 32:BB:29:A:O4' | 2.17 | 0.45 |
| 33:BD:12:SER:O | 33:BD:16:MET:HB2 | 2.17 | 0.45 |
| 33:BD:13:ARG:HA | 33:BD:16:MET:HE3 | 1.97 | 0.45 |
| 33:BD:25:THR:CG2 | 33:BD:25:THR:O | 2.62 | 0.45 |
| 31:BA:2820:A:C8 | 34:BE:109:LYS:HE3 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BE:111:ARG:HD2 | 34:BE:160:TYR:CE1 | 2.52 | 0.45 |
| 34:BE:114:ALA:HB3 | 34:BE:160:TYR:HB3 | 1.98 | 0.45 |
| 34:BE:70:ALA:O | 34:BE:72:VAL:C | 2.55 | 0.45 |
| 34:BE:51:PHE:HB3 | 34:BE:76:ARG:HB3 | 1.98 | 0.45 |
| 35:BF:136:THR:HG22 | 35:BF:140:LEU:CD2 | 2.47 | 0.45 |
| 37:BH:118:PRO:HG2 | 37:BH:121:ILE:HD12 | 1.98 | 0.45 |
| 39:BN:55:VAL:HG12 | 39:BN:125:GLY:HA3 | 1.98 | 0.45 |
| 43:BR:5:LYS:N | 43:BR:5:LYS:CD | 2.79 | 0.45 |
| 46:BU:92:ARG:HH22 | 47:BV:10:LYS:HG2 | 1.81 | 0.45 |
| 48:BW:8:ARG:HA | 48:BW:102:HIS:CD2 | 2.52 | 0.45 |
| 49:BX:31:HIS:C | 49:BX:31:HIS:CD2 | 2.90 | 0.45 |
| 51:BZ:127:LYS:HB3 | 51:BZ:162:GLU:HG3 | 1.99 | 0.45 |
| 1:CA:1128:C:N3 | 1:CA:1139:G:C6 | 2.85 | 0.45 |
| 1:CA:1254:C:OP1 | 10:CJ:45:ARG:HG2 | 2.16 | 0.45 |
| 1:CA:1507:A:C8 | 1:CA:1530:G:N2 | 2.84 | 0.45 |
| 1:CA:28:G:C6 | 1:CA:29:G:C5 | 3.05 | 0.45 |
| 1:CA:939:G:C6 | 1:CA:940:C:N4 | 2.85 | 0.45 |
| 2:CB:67:THR:HG21 | 2:CB:155:LEU:HD21 | 1.99 | 0.45 |
| 2:CB:15:VAL:HG21 | 2:CB:209:ARG:HH21 | 1.82 | 0.45 |
| 3:CC:155:GLY:O | 3:CC:196:LEU:HD13 | 2.16 | 0.45 |
| 5:CE:147:ASP:N | 5:CE:147:ASP:OD2 | 2.50 | 0.45 |
| 6:CF:76:ALA:O | 6:CF:80:ARG:HG3 | 2.17 | 0.45 |
| 8:CH:44:PHE:HA | 8:CH:79:VAL:CG1 | 2.46 | 0.45 |
| 25:D3:46:ASN:O | 25:D3:50:VAL:HG22 | 2.17 | 0.45 |
| 30:D8:30:ARG:HB2 | 31:DA:2393:A:OP1 | 2.17 | 0.45 |
| 31:DA:1316:U:H2' | 31:DA:1317:A:C8 | 2.52 | 0.45 |
| 31:DA:1517:G:H2' | 31:DA:1518:U:O4' | 2.16 | 0.45 |
| 31:DA:1518:U:H2' | 31:DA:1519:G:O4' | 2.17 | 0.45 |
| 31:DA:231:C:O2' | 31:DA:232:G:H5' | 2.17 | 0.45 |
| 31:DA:375:C:H2' | 31:DA:376:C:C6 | 2.52 | 0.45 |
| 31:DA:878:A:H2' | 31:DA:879:G:H5' | 1.97 | 0.45 |
| 31:DA:930:U:O4' | 31:DA:930:U:O2 | 2.32 | 0.45 |
| 32:DB:75:G:N3 | 51:DZ:85:HIS:CE1 | 2.85 | 0.45 |
| 32:DB:7:G:O5' | 44:DS:29:PHE:CE1 | 2.70 | 0.45 |
| 33:DD:3:VAL:H | 33:DD:20:ASP:HB2 | 1.82 | 0.45 |
| 31:DA:1141:U:P | 39:DN:25:ARG:HH12 | 2.40 | 0.45 |
| 40:DO:50:GLY:C | 40:DO:52:VAL:N | 2.70 | 0.45 |
| 44:DS:16:ASN:HB3 | 44:DS:20:ARG:NH2 | 2.32 | 0.45 |
| 44:DS:95:HIS:O | 44:DS:97:ARG:O | 2.33 | 0.45 |
| 46:DU:112:ARG:HG2 | 46:DU:112:ARG:HH11 | 1.82 | 0.45 |
| 47:DV:22:VAL:O | 47:DV:23:GLU:CB | 2.53 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:DV:66:ARG:HD3 | 47:DV:67:GLY:N | 2.32 | 0.45 |
| 49:DX:31:HIS:CD2 | 49:DX:31:HIS:C | 2.90 | 0.45 |
| 50:DY:28:LYS:C | 50:DY:30:VAL:H | 2.20 | 0.45 |
| 50:DY:75:ILE:HA | 50:DY:75:ILE:HD13 | 1.50 | 0.45 |
| 1:AA:115:G:H4' | 1:AA:116:A:O5' | 2.16 | 0.45 |
| 1:AA:1237:C:H42 | 1:AA:1337:G:H1 | 1.65 | 0.45 |
| 1:AA:1433:A:C6 | 1:AA:1468:A:C4 | 3.05 | 0.45 |
| 1:AA:185:A:C6 | 1:AA:186:C:N4 | 2.85 | 0.45 |
| 1:AA:303:A:C5 | 1:AA:304:U:C5 | 3.05 | 0.45 |
| 1:AA:410:G:OP2 | 4:AD:25:ARG:HG3 | 2.17 | 0.45 |
| 1:AA:447:G:C6 | 1:AA:485:G:H1' | 2.51 | 0.45 |
| 1:AA:612:C:O2 | 1:AA:629:G:N2 | 2.50 | 0.45 |
| 1:AA:665:A:H1' | 1:AA:733:A:O4' | 2.17 | 0.45 |
| 3:AC:11:ARG:HB3 | 3:AC:15:THR:HB | 1.98 | 0.45 |
| 13:AM:81:LEU:HD11 | 13:AM:88:ARG:HH12 | 1.82 | 0.45 |
| 15:AO:55:GLY:O | 15:AO:56:LEU:C | 2.55 | 0.45 |
| 16:AP:50:LYS:HD3 | 16:AP:51:VAL:N | 2.31 | 0.45 |
| 1:AA:192:U:H4' | 20:AT:57:ARG:HD2 | 1.98 | 0.45 |
| 23:B1:13:ILE:HG21 | 23:B1:63:ALA:HB3 | 1.99 | 0.45 |
| 28:B6:43:CYS:O | 28:B6:44:ARG:CB | 2.65 | 0.45 |
| 28:B6:48:VAL:O | 28:B6:49:HIS:O | 2.35 | 0.45 |
| 31:BA:1272:A:OP2 | 31:BA:1647:G:OP1 | 2.35 | 0.45 |
| 31:BA:1545:A:C2' | 31:BA:1546:C:O5' | 2.64 | 0.45 |
| 31:BA:1593:G:H2' | 31:BA:1594:G:C8 | 2.52 | 0.45 |
| 31:BA:1803:A:H2 | 31:BA:1822:G:N3 | 2.14 | 0.45 |
| 31:BA:2314:C:C2 | 31:BA:2315:G:C8 | 3.05 | 0.45 |
| 31:BA:2630:G:C8 | 31:BA:2894:G:C2 | 3.04 | 0.45 |
| 31:BA:2850:A:C2 | 31:BA:2851:A:C4 | 3.05 | 0.45 |
| 31:BA:854:G:H2' | 31:BA:855:G:H8 | 1.81 | 0.45 |
| 31:BA:997:G:C2' | 31:BA:998:C:H5' | 2.47 | 0.45 |
| 33:BD:213:ARG:HD2 | 33:BD:213:ARG:HA | 1.72 | 0.45 |
| 33:BD:246:PRO:HG2 | 33:BD:255:LYS:HG2 | 1.99 | 0.45 |
| 34:BE:120:TRP:CD2 | 34:BE:155:LYS:HD3 | 2.52 | 0.45 |
| 34:BE:65:GLY:C | 34:BE:67:PHE:N | 2.70 | 0.45 |
| 31:BA:1952:A:C6 | 40:BO:22:ILE:HD12 | 2.52 | 0.45 |
| 43:BR:9:LYS:O | 43:BR:10:LEU:CG | 2.64 | 0.45 |
| 44:BS:95:HIS:O | 44:BS:96:GLY:C | 2.54 | 0.45 |
| 45:BT:35:LYS:C | 45:BT:37:GLY:N | 2.71 | 0.45 |
| 48:BW:29:LEU:HG | 48:BW:33:ARG:HD2 | 1.99 | 0.45 |
| 50:BY:45:VAL:HG21 | 50:BY:62:GLU:N | 2.31 | 0.45 |
| 42:BQ:141:GLN:HB3 | 51:BZ:70:LEU:HD13 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1054:C:C2' | 1:CA:1055:A:H5'' | 2.46 | 0.45 |
| 1:CA:1137:C:H6 | 1:CA:1137:C:H3' | 1.82 | 0.45 |
| 1:CA:1142:G:H3' | 1:CA:1143:G:C8 | 2.51 | 0.45 |
| 1:CA:1210:C:H4' | 1:CA:1214:C:C4 | 2.52 | 0.45 |
| 1:CA:1226:C:N4 | 13:CM:104:ARG:HD2 | 2.32 | 0.45 |
| 1:CA:946:A:C2 | 1:CA:1236:A:C2 | 3.05 | 0.45 |
| 1:CA:1496:C:H2' | 1:CA:1497:G:O4' | 2.17 | 0.45 |
| 1:CA:1499:A:H1' | 1:CA:1520:G:H5' | 1.99 | 0.45 |
| 1:CA:201:C:H42 | 1:CA:203:U:H1' | 1.82 | 0.45 |
| 1:CA:498:U:H2' | 1:CA:498:U:O2 | 2.15 | 0.45 |
| 1:CA:577:G:C4 | 1:CA:578:C:C5 | 3.05 | 0.45 |
| 1:CA:683:G:C2 | 1:CA:708:C:N3 | 2.84 | 0.45 |
| 2:CB:35:GLU:HA | 2:CB:39:ILE:O | 2.17 | 0.45 |
| 4:CD:10:ARG:HA | 4:CD:13:ARG:HG3 | 1.98 | 0.45 |
| 5:CE:6:PHE:HD2 | 5:CE:36:ASP:HB3 | 1.81 | 0.45 |
| 7:CG:111:ARG:CZ | 7:CG:122:HIS:HB3 | 2.47 | 0.45 |
| 7:CG:36:LYS:HB2 | 7:CG:36:LYS:NZ | 2.32 | 0.45 |
| 8:CH:103:VAL:HG21 | 8:CH:109:ILE:C | 2.36 | 0.45 |
| 11:CK:33:THR:HG22 | 11:CK:39:PRO:HA | 1.99 | 0.45 |
| 15:CO:37:ASN:N | 15:CO:37:ASN:ND2 | 2.62 | 0.45 |
| 15:CO:66:LEU:O | 15:CO:69:TYR:HB3 | 2.17 | 0.45 |
| 20:CT:92:LEU:C | 20:CT:94:ALA:H | 2.19 | 0.45 |
| 25:D3:6:VAL:HG12 | 25:D3:54:VAL:CG1 | 2.47 | 0.45 |
| 27:D5:49:CYS:O | 27:D5:50:GLY:C | 2.55 | 0.45 |
| 29:D7:31:LEU:O | 29:D7:32:LYS:C | 2.54 | 0.45 |
| 31:DA:109:G:H2' | 31:DA:110:G:O4' | 2.17 | 0.45 |
| 31:DA:973:A:O4' | 31:DA:1188:U:C6 | 2.70 | 0.45 |
| 31:DA:1221:C:H2' | 31:DA:1221(A):C:H6 | 1.82 | 0.45 |
| 31:DA:142:A:C5' | 31:DA:142(A):C:H5 | 2.30 | 0.45 |
| 31:DA:1475:G:H5' | 31:DA:1476:C:OP2 | 2.17 | 0.45 |
| 31:DA:1722:A:C2 | 31:DA:1740:G:H2' | 2.52 | 0.45 |
| 22:D0:16:SER:CB | 31:DA:2262:U:OP2 | 2.65 | 0.45 |
| 31:DA:2540:C:C2' | 31:DA:2541:A:H5' | 2.47 | 0.45 |
| 31:DA:271(P):C:O3' | 38:DI:42:SER:OG | 2.34 | 0.45 |
| 31:DA:2849:U:H5' | 31:DA:2867:G:H21 | 1.82 | 0.45 |
| 31:DA:608:A:C6 | 31:DA:609:A:C6 | 3.04 | 0.45 |
| 24:D2:41:ILE:HG13 | 31:DA:94(A):G:H22 | 1.82 | 0.45 |
| 36:DG:18:GLU:HG2 | 36:DG:175:LEU:HD21 | 1.98 | 0.45 |
| 36:DG:63:ILE:HD13 | 36:DG:141:PHE:CE2 | 2.51 | 0.45 |
| 37:DH:126:PRO:HB2 | 37:DH:130:ARG:HH12 | 1.81 | 0.45 |
| 39:DN:78:TYR:N | 39:DN:79:PRO:HD3 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:DO:3:GLN:HG3 | 40:DO:4:PRO:HD2 | 1.99 | 0.45 |
| 44:DS:90:GLY:C | 44:DS:92:TYR:H | 2.19 | 0.45 |
| 45:DT:68:TYR:CD2 | 45:DT:68:TYR:N | 2.84 | 0.45 |
| 46:DU:104:GLN:HB2 | 47:DV:43:GLU:CD | 2.37 | 0.45 |
| 1:AA:195:A:H1' | 1:AA:222:U:O2' | 2.16 | 0.45 |
| 1:AA:28:G:C6 | 1:AA:29:G:C5 | 3.05 | 0.45 |
| 1:AA:601:C:H2' | 1:AA:602:A:C8 | 2.52 | 0.45 |
| 1:AA:675:A:N6 | 1:AA:715:A:H61 | 2.15 | 0.45 |
| 1:AA:981:U:H6 | 1:AA:981:U:O5' | 2.00 | 0.45 |
| 3:AC:16:ARG:CZ | 3:AC:16:ARG:HB2 | 2.46 | 0.45 |
| 5:AE:78:HIS:HE1 | 5:AE:142:LEU:HD23 | 1.81 | 0.45 |
| 6:AF:50:TYR:CE1 | 18:AR:77:GLY:HA2 | 2.52 | 0.45 |
| 6:AF:54:LYS:O | 6:AF:56:PRO:HD3 | 2.17 | 0.45 |
| 8:AH:80:ILE:HG22 | 8:AH:80:ILE:O | 2.17 | 0.45 |
| 10:AJ:4:ILE:HG23 | 10:AJ:98:ILE:HG23 | 1.99 | 0.45 |
| 12:AL:92:ASP:C | 12:AL:93:LEU:HD23 | 2.38 | 0.45 |
| 17:AQ:7:THR:HA | 17:AQ:57:VAL:O | 2.17 | 0.45 |
| 20:AT:26:ASN:HB3 | 20:AT:71:THR:OG1 | 2.17 | 0.45 |
| 24:B2:12:GLU:C | 24:B2:14:ARG:N | 2.69 | 0.45 |
| 30:B8:39:LYS:HG2 | 30:B8:39:LYS:O | 2.17 | 0.45 |
| 31:BA:1491:G:O2' | 33:BD:101:GLU:HB2 | 2.17 | 0.45 |
| 31:BA:1517:G:O2' | 31:BA:1518:U:H5' | 2.17 | 0.45 |
| 31:BA:1826:G:H4' | 33:BD:242:ARG:CZ | 2.47 | 0.45 |
| 22:B0:16:SER:CB | 31:BA:2262:U:OP2 | 2.64 | 0.45 |
| 28:B6:30:THR:HB | 31:BA:2286:A:OP1 | 2.17 | 0.45 |
| 31:BA:2753:A:HO2' | 31:BA:2754:U:H6 | 1.59 | 0.45 |
| 31:BA:2870:C:H2' | 31:BA:2871:C:C5' | 2.47 | 0.45 |
| 31:BA:287:C:H2' | 31:BA:288:C:H6 | 1.82 | 0.45 |
| 31:BA:363(C):G:H2' | 31:BA:363(D):G:H8 | 1.81 | 0.45 |
| 31:BA:384:U:H2' | 31:BA:385:C:H6 | 1.82 | 0.45 |
| 31:BA:878:A:C6 | 31:BA:900:A:C8 | 3.05 | 0.45 |
| 31:BA:993:G:H1' | 47:BV:91:TYR:CE1 | 2.52 | 0.45 |
| 33:BD:267:SER:HA | 33:BD:270:ILE:CD1 | 2.47 | 0.45 |
| 33:BD:33:LEU:HB3 | 33:BD:34:VAL:H | 1.34 | 0.45 |
| 37:BH:153:LYS:HB2 | 37:BH:154:PRO:CD | 2.47 | 0.45 |
| 39:BN:46:VAL:HG13 | 39:BN:48:MET:HG3 | 1.99 | 0.45 |
| 42:BQ:20:ALA:C | 42:BQ:22:LYS:N | 2.70 | 0.45 |
| 42:BQ:57:HIS:CE1 | 42:BQ:116:GLU:HB3 | 2.52 | 0.45 |
| 31:BA:2870:C:C5' | 43:BR:65:LEU:HD21 | 2.47 | 0.45 |
| 45:BT:50:ILE:HD11 | 45:BT:102:ILE:CD1 | 2.40 | 0.45 |
| 49:BX:73:ARG:H | 49:BX:74:PRO:HD3 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1092:A:C2 | 1:CA:1183:A:C2 | 3.05 | 0.45 |
| 1:CA:195:A:H1' | 1:CA:222:U:O2' | 2.17 | 0.45 |
| 1:CA:741:G:H2' | 1:CA:742:G:O4' | 2.17 | 0.45 |
| 2:CB:19:HIS:CG | 2:CB:20:GLU:H | 2.35 | 0.45 |
| 3:CC:153:VAL:HG12 | 3:CC:154:SER:N | 2.32 | 0.45 |
| 4:CD:62:GLN:NE2 | 4:CD:62:GLN:HA | 2.32 | 0.45 |
| 7:CG:101:LEU:O | 7:CG:105:VAL:HG23 | 2.16 | 0.45 |
| 8:CH:64:LYS:HG2 | 8:CH:79:VAL:HG21 | 1.98 | 0.45 |
| 7:CG:150:ALA:HB2 | 11:CK:50:TYR:CE1 | 2.51 | 0.45 |
| 12:CL:20:LYS:H | 12:CL:20:LYS:HD3 | 1.81 | 0.45 |
| 15:CO:18:PHE:O | 15:CO:19:PRO:C | 2.55 | 0.45 |
| 17:CQ:74:LEU:HA | 17:CQ:74:LEU:HD22 | 1.74 | 0.45 |
| 20:CT:55:ILE:O | 20:CT:58:LYS:N | 2.50 | 0.45 |
| 23:D1:11:ARG:HG3 | 23:D1:61:ARG:O | 2.17 | 0.45 |
| 24:D2:30:ARG:CZ | 24:D2:30:ARG:HB3 | 2.47 | 0.45 |
| 30:D8:29:LYS:O | 30:D8:30:ARG:C | 2.55 | 0.45 |
| 31:DA:1174:A:OP1 | 31:DA:1175:U:OP1 | 2.35 | 0.45 |
| 31:DA:123:G:H2' | 31:DA:124:G:O4' | 2.17 | 0.45 |
| 31:DA:1368:G:C2 | 31:DA:1369:G:C8 | 3.05 | 0.45 |
| 31:DA:132:G:H1 | 31:DA:147:U:H3 | 1.65 | 0.45 |
| 31:DA:154:G:N1 | 31:DA:154(A):C:N4 | 2.62 | 0.45 |
| 31:DA:157:U:H6 | 31:DA:157:U:OP2 | 2.00 | 0.45 |
| 31:DA:1822:G:C5' | 31:DA:1822:G:H8 | 2.16 | 0.45 |
| 31:DA:2273:A:H2' | 31:DA:2274:A:C8 | 2.52 | 0.45 |
| 31:DA:2517:C:O2' | 31:DA:2542:A:N1 | 2.40 | 0.45 |
| 31:DA:287:C:H2' | 31:DA:288:C:H6 | 1.82 | 0.45 |
| 31:DA:2630:G:C8 | 31:DA:2894:G:C2 | 3.05 | 0.45 |
| 31:DA:384:U:H2' | 31:DA:385:C:H6 | 1.80 | 0.45 |
| 31:DA:455:C:HO2' | 31:DA:472:A:H2 | 1.64 | 0.45 |
| 31:DA:530:G:C5 | 31:DA:2022:U:H5'' | 2.52 | 0.45 |
| 31:DA:855:G:C5 | 31:DA:856:C:C5 | 3.05 | 0.45 |
| 32:DB:27:C:N4 | 32:DB:28:C:C4 | 2.85 | 0.45 |
| 34:DE:152:LYS:HG2 | 39:DN:78:TYR:CE2 | 2.49 | 0.45 |
| 39:DN:68:GLU:HA | 39:DN:86:PRO:HB2 | 1.98 | 0.45 |
| 43:DR:3:HIS:O | 43:DR:4:LEU:CB | 2.65 | 0.45 |
| 49:DX:80:ILE:O | 49:DX:81:VAL:CB | 2.65 | 0.45 |
| 49:DX:93:GLU:HG3 | 49:DX:93:GLU:O | 2.16 | 0.45 |
| 51:DZ:108:PRO:O | 51:DZ:109:ALA:C | 2.56 | 0.45 |
| 51:DZ:150:LEU:C | 51:DZ:151:HIS:HD2 | 2.20 | 0.45 |
| 1:AA:1503:A:O2' | 1:AA:1504:G:C5' | 2.64 | 0.45 |
| 1:AA:292:G:N2 | 1:AA:309:G:C4 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:432:A:N7 | 1:AA:433:C:C4 | 2.85 | 0.45 |
| 1:AA:521:G:O2' | 1:AA:522:C:H5' | 2.17 | 0.45 |
| 1:AA:989:C:H1' | 1:AA:1016:A:H2 | 1.82 | 0.45 |
| 4:AD:173:TRP:CD1 | 4:AD:174:LEU:HG | 2.51 | 0.45 |
| 11:AK:33:THR:HG22 | 11:AK:39:PRO:HA | 1.99 | 0.45 |
| 1:AA:1217:C:OP1 | 14:AN:9:LYS:HD2 | 2.17 | 0.45 |
| 15:AO:17:ARG:CG | 15:AO:26:GLU:HG3 | 2.47 | 0.45 |
| 15:AO:62:GLN:O | 15:AO:65:ARG:HB2 | 2.17 | 0.45 |
| 22:B0:84:LEU:N | 22:B0:84:LEU:HD12 | 2.31 | 0.45 |
| 23:B1:11:ARG:HB3 | 23:B1:12:PRO:CD | 2.47 | 0.45 |
| 24:B2:32:LEU:C | 24:B2:32:LEU:HD12 | 2.37 | 0.45 |
| 31:BA:1042:G:H3' | 31:BA:1043:C:O4' | 2.17 | 0.45 |
| 31:BA:108:U:O2 | 31:BA:109:G:C8 | 2.70 | 0.45 |
| 31:BA:1174:A:OP1 | 31:BA:1175:U:OP1 | 2.35 | 0.45 |
| 31:BA:1448:G:H1' | 31:BA:1528:A:H61 | 1.79 | 0.45 |
| 31:BA:1450(A):C:C4 | 31:BA:1451:C:N4 | 2.84 | 0.45 |
| 31:BA:1642:G:H2' | 31:BA:1643:G:O4' | 2.17 | 0.45 |
| 31:BA:1742:G:C3' | 31:BA:1742:G:C8 | 2.99 | 0.45 |
| 31:BA:1815:A:H8 | 31:BA:1815:A:OP1 | 2.00 | 0.45 |
| 31:BA:1891:G:C6 | 31:BA:1892:C:N3 | 2.85 | 0.45 |
| 31:BA:2494:G:C4 | 31:BA:2495:G:C8 | 3.04 | 0.45 |
| 31:BA:2621:A:O2' | 34:BE:159:HIS:HB2 | 2.17 | 0.45 |
| 31:BA:2895:U:C5 | 31:BA:2896:C:C5 | 3.04 | 0.45 |
| 31:BA:491:G:H2' | 31:BA:492:A:C8 | 2.51 | 0.45 |
| 31:BA:580:C:H2' | 31:BA:581:C:C6 | 2.52 | 0.45 |
| 31:BA:607:U:N3 | 31:BA:621:A:H2 | 1.95 | 0.45 |
| 31:BA:814:C:C4 | 41:BP:27:HIS:NE2 | 2.85 | 0.45 |
| 31:BA:934:G:H2' | 31:BA:935:C:C6 | 2.52 | 0.45 |
| 33:BD:25:THR:HB | 33:BD:82:ILE:H | 1.82 | 0.45 |
| 33:BD:43:ARG:HH11 | 33:BD:44:ASN:ND2 | 2.15 | 0.45 |
| 33:BD:70:TRP:CZ2 | 33:BD:150:LYS:HD3 | 2.52 | 0.45 |
| 36:BG:13:GLU:O | 36:BG:13:GLU:HG3 | 2.16 | 0.45 |
| 39:BN:78:TYR:N | 39:BN:79:PRO:CD | 2.80 | 0.45 |
| 45:BT:121:ILE:O | 45:BT:124:ASP:HB2 | 2.17 | 0.45 |
| 48:BW:37:ARG:HG2 | 48:BW:38:TYR:CE2 | 2.51 | 0.45 |
| 49:BX:80:ILE:O | 49:BX:81:VAL:CB | 2.61 | 0.45 |
| 51:BZ:39:VAL:CG2 | 51:BZ:44:PHE:HB2 | 2.46 | 0.45 |
| 1:CA:1088:G:C6 | 1:CA:1089:G:C6 | 3.04 | 0.45 |
| 1:CA:1187:G:C6 | 1:CA:1188:A:C6 | 3.05 | 0.45 |
| 1:CA:1392:G:H22 | 1:CA:1502:A:H8 | 1.63 | 0.45 |
| 1:CA:292:G:N2 | 1:CA:309:G:C4 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:342:C:H2' | 1:CA:343:U:O4' | 2.17 | 0.45 |
| 1:CA:355:C:H5' | 1:CA:389:A:OP2 | 2.17 | 0.45 |
| 1:CA:39:G:C2 | 1:CA:40:C:C6 | 3.05 | 0.45 |
| 1:CA:664:G:N2 | 1:CA:741:G:H1 | 2.14 | 0.45 |
| 1:CA:877:C:H5'' | 8:CH:88:LYS:CD | 2.45 | 0.45 |
| 3:CC:66:VAL:O | 3:CC:66:VAL:HG12 | 2.17 | 0.45 |
| 4:CD:41:GLY:O | 4:CD:43:HIS:N | 2.51 | 0.45 |
| 6:CF:19:LEU:HD11 | 6:CF:59:TYR:CD2 | 2.52 | 0.45 |
| 6:CF:19:LEU:HD11 | 6:CF:59:TYR:CG | 2.51 | 0.45 |
| 8:CH:33:GLU:HG2 | 8:CH:59:LEU:HD11 | 1.99 | 0.45 |
| 11:CK:21:ILE:CD1 | 11:CK:82:VAL:HG13 | 2.46 | 0.45 |
| 12:CL:46:LYS:O | 12:CL:47:LYS:C | 2.55 | 0.45 |
| 13:CM:19:LEU:HB3 | 13:CM:25:ILE:HG21 | 1.99 | 0.45 |
| 16:CP:51:VAL:HG12 | 16:CP:51:VAL:O | 2.15 | 0.45 |
| 17:CQ:63:ARG:HG2 | 17:CQ:64:PRO:HD2 | 1.99 | 0.45 |
| 19:CS:29:ARG:O | 19:CS:31:ILE:HG22 | 2.17 | 0.45 |
| 24:D2:18:PRO:O | 24:D2:19:VAL:C | 2.56 | 0.45 |
| 28:D6:48:VAL:CG2 | 28:D6:48:VAL:O | 2.65 | 0.45 |
| 31:DA:1110:G:H4' | 31:DA:1110:G:OP1 | 2.17 | 0.45 |
| 31:DA:1005:C:C2 | 31:DA:1143:A:C6 | 3.05 | 0.45 |
| 31:DA:1313:U:H2' | 31:DA:1610:A:C2 | 2.52 | 0.45 |
| 31:DA:1417:C:H2' | 31:DA:1418:G:H5' | 1.98 | 0.45 |
| 31:DA:142:A:N6 | 31:DA:1596:A:H5' | 2.33 | 0.45 |
| 31:DA:143:G:H2' | 31:DA:143(A):C:C6 | 2.52 | 0.45 |
| 31:DA:1605:C:O4' | 31:DA:1610:A:C6 | 2.70 | 0.45 |
| 31:DA:1608:A:H1' | 31:DA:1610:A:OP2 | 2.17 | 0.45 |
| 31:DA:1695:G:N2 | 31:DA:1696:G:C8 | 2.84 | 0.45 |
| 31:DA:176:G:O2' | 31:DA:177:G:H5' | 2.16 | 0.45 |
| 31:DA:2228:G:C5 | 31:DA:2229:C:C5 | 3.04 | 0.45 |
| 31:DA:2258:C:H4' | 31:DA:2259:G:OP2 | 2.17 | 0.45 |
| 30:D8:4:MET:HE1 | 31:DA:593:G:O4' | 2.17 | 0.45 |
| 31:DA:671:C:H2' | 31:DA:672:C:H6 | 1.80 | 0.45 |
| 33:DD:34:VAL:O | 33:DD:34:VAL:HG13 | 2.17 | 0.45 |
| 34:DE:119:ARG:HD2 | 34:DE:120:TRP:CE2 | 2.51 | 0.45 |
| 35:DF:78:ILE:H | 35:DF:78:ILE:CD1 | 2.21 | 0.45 |
| 31:DA:2746:U:H4' | 37:DH:138:LYS:HB3 | 1.98 | 0.45 |
| 38:DI:79:ILE:HA | 38:DI:80:PRO:HD3 | 1.67 | 0.45 |
| 40:DO:12:ASP:C | 40:DO:99:PHE:HE2 | 2.21 | 0.45 |
| 42:DQ:23:GLY:O | 42:DQ:99:PRO:O | 2.35 | 0.45 |
| 44:DS:42:ASP:C | 44:DS:44:LYS:N | 2.70 | 0.45 |
| 44:DS:89:ARG:HE | 44:DS:90:GLY:N | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:DT:45:PHE:CE2 | 45:DT:63:VAL:HG22 | 2.52 | 0.45 |
| 47:DV:27:ALA:O | 47:DV:28:GLU:C | 2.56 | 0.45 |
| 47:DV:72:VAL:CG1 | 47:DV:73:SER:N | 2.74 | 0.45 |
| 48:DW:46:PHE:O | 48:DW:50:VAL:HG12 | 2.17 | 0.45 |
| 50:DY:45:VAL:HG22 | 50:DY:62:GLU:CA | 2.46 | 0.45 |
| 50:DY:76:CYS:O | 50:DY:96:ILE:HD12 | 2.17 | 0.45 |
| 51:DZ:135:GLU:O | 51:DZ:136:PHE:HB3 | 2.16 | 0.45 |
| 51:DZ:73:GLN:HG2 | 51:DZ:87:ASP:CG | 2.37 | 0.45 |
| 1:AA:102:G:H2' | 1:AA:103:C:C6 | 2.42 | 0.44 |
| 1:AA:1158:C:C2' | 1:AA:1158:C:O2 | 2.65 | 0.44 |
| 1:AA:1238:A:N6 | 1:AA:1299:A:N6 | 2.61 | 0.44 |
| 1:AA:176:C:H2' | 1:AA:177:C:H6 | 1.77 | 0.44 |
| 1:AA:234:C:C2 | 1:AA:235:C:C5 | 3.06 | 0.44 |
| 1:AA:303:A:H2' | 1:AA:304:U:O4' | 2.17 | 0.44 |
| 1:AA:764:C:H2' | 1:AA:765:G:O5' | 2.17 | 0.44 |
| 1:AA:929:G:H1 | 1:AA:1388:C:N4 | 2.07 | 0.44 |
| 1:AA:407:G:HO2' | 4:AD:116:GLN:HG3 | 1.83 | 0.44 |
| 1:AA:620:C:C2 | 4:AD:135:LEU:HG | 2.51 | 0.44 |
| 4:AD:196:LEU:N | 4:AD:196:LEU:HD12 | 2.32 | 0.44 |
| 7:AG:111:ARG:CZ | 7:AG:122:HIS:HB3 | 2.47 | 0.44 |
| 8:AH:10:LEU:CD2 | 8:AH:10:LEU:N | 2.80 | 0.44 |
| 11:AK:21:ILE:CD1 | 11:AK:82:VAL:HG13 | 2.48 | 0.44 |
| 16:AP:9:PHE:CE2 | 16:AP:18:ARG:HB2 | 2.52 | 0.44 |
| 17:AQ:18:THR:OG1 | 17:AQ:69:LYS:NZ | 2.46 | 0.44 |
| 23:B1:67:ILE:HD12 | 23:B1:68:PRO:HD2 | 1.99 | 0.44 |
| 24:B2:56:GLN:N | 24:B2:56:GLN:CD | 2.70 | 0.44 |
| 25:B3:52:HIS:CD2 | 32:BB:83:G:H4' | 2.51 | 0.44 |
| 30:B8:39:LYS:CG | 30:B8:39:LYS:O | 2.65 | 0.44 |
| 31:BA:107:C:N3 | 31:BA:108:U:C5 | 2.85 | 0.44 |
| 31:BA:1107:G:C6 | 31:BA:1108:U:N3 | 2.85 | 0.44 |
| 31:BA:1049:C:H1' | 31:BA:1113:U:O2' | 2.17 | 0.44 |
| 31:BA:1478:G:O2' | 31:BA:1558:A:H2 | 2.00 | 0.44 |
| 31:BA:1673:U:C4 | 34:BE:129:HIS:HD2 | 2.34 | 0.44 |
| 31:BA:1741:A:N7 | 31:BA:1742:G:N1 | 2.65 | 0.44 |
| 31:BA:174:C:C2' | 31:BA:175:G:H5'' | 2.47 | 0.44 |
| 31:BA:1865:G:H8 | 31:BA:1865:G:H5'' | 1.83 | 0.44 |
| 31:BA:2023:G:C2 | 31:BA:2024:G:C8 | 3.05 | 0.44 |
| 31:BA:251:A:C5 | 31:BA:252:G:H1' | 2.52 | 0.44 |
| 31:BA:2552:U:C2 | 31:BA:2554:U:C5' | 3.00 | 0.44 |
| 31:BA:2889:C:H2' | 31:BA:2891:G:O4' | 2.17 | 0.44 |
| 31:BA:478:A:C6 | 31:BA:480:A:C6 | 3.05 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:839:U:H2' | 31:BA:840:C:C6 | 2.52 | 0.44 |
| 32:BB:1:U:C6 | 32:BB:2:C:C5 | 3.05 | 0.44 |
| 32:BB:33:G:C2 | 32:BB:50:G:C2 | 3.05 | 0.44 |
| 33:BD:108:PRO:HD2 | 33:BD:111:LEU:HG | 2.00 | 0.44 |
| 33:BD:121:PRO:HB3 | 33:BD:135:PHE:CE1 | 2.52 | 0.44 |
| 33:BD:132:PRO:HG3 | 33:BD:190:TYR:CE1 | 2.53 | 0.44 |
| 38:BI:138:ILE:HG22 | 38:BI:139:GLN:H | 1.82 | 0.44 |
| 38:BI:28:ASN:C | 38:BI:32:PRO:HG2 | 2.37 | 0.44 |
| 42:BQ:8:LYS:CD | 42:BQ:9:TYR:H | 2.29 | 0.44 |
| 43:BR:2:ARG:CB | 43:BR:5:LYS:HE3 | 2.46 | 0.44 |
| 32:BB:8:U:O2' | 44:BS:40:ILE:HD13 | 2.17 | 0.44 |
| 49:BX:44:GLU:HB2 | 49:BX:49:VAL:O | 2.17 | 0.44 |
| 50:BY:16:ALA:HA | 50:BY:21:LYS:HD2 | 1.99 | 0.44 |
| 51:BZ:124:ILE:CG1 | 51:BZ:125:LEU:N | 2.80 | 0.44 |
| 1:CA:1260:C:H4' | 1:CA:1284:C:H5' | 1.99 | 0.44 |
| 1:CA:376:G:N3 | 1:CA:389:A:C2 | 2.84 | 0.44 |
| 1:CA:473:G:C2 | 1:CA:474:G:C8 | 3.04 | 0.44 |
| 1:CA:451:A:C5 | 1:CA:481:G:C6 | 3.06 | 0.44 |
| 1:CA:509:A:C2 | 1:CA:510:A:C2 | 3.05 | 0.44 |
| 1:CA:552:U:H2' | 1:CA:553:A:H5' | 1.97 | 0.44 |
| 1:CA:718:G:H1' | 11:CK:116:HIS:HA | 1.99 | 0.44 |
| 1:CA:735:C:H6 | 1:CA:735:C:O5' | 2.00 | 0.44 |
| 10:CJ:22:LYS:C | 10:CJ:24:VAL:H | 2.20 | 0.44 |
| 14:CN:13:THR:N | 14:CN:14:PRO:CD | 2.80 | 0.44 |
| 18:CR:25:THR:O | 18:CR:26:LEU:HD23 | 2.17 | 0.44 |
| 1:CA:323:U:OP1 | 20:CT:26:ASN:ND2 | 2.49 | 0.44 |
| 23:D1:76:ARG:CB | 23:D1:78:LYS:HE3 | 2.46 | 0.44 |
| 24:D2:47:ASN:C | 24:D2:49:LYS:N | 2.69 | 0.44 |
| 29:D7:19:ARG:HG2 | 29:D7:19:ARG:NH1 | 2.33 | 0.44 |
| 31:DA:1178:C:H2' | 31:DA:1179:C:H6 | 1.81 | 0.44 |
| 31:DA:1336:A:H2' | 31:DA:1337:G:C8 | 2.52 | 0.44 |
| 31:DA:1696:G:C3' | 31:DA:1697:G:H5'' | 2.47 | 0.44 |
| 31:DA:1742:G:N7 | 31:DA:1743:C:C2 | 2.84 | 0.44 |
| 31:DA:1839:G:C8 | 31:DA:1839:G:C5' | 2.99 | 0.44 |
| 31:DA:2019:A:C2' | 31:DA:2020:A:O5' | 2.64 | 0.44 |
| 31:DA:2287:A:N1 | 31:DA:2346:A:H2 | 2.15 | 0.44 |
| 31:DA:2839:G:H5' | 43:DR:46:GLY:HA2 | 1.98 | 0.44 |
| 31:DA:732:C:O2' | 31:DA:733:G:H5' | 2.17 | 0.44 |
| 31:DA:768:G:C6 | 31:DA:769:G:C5 | 3.05 | 0.44 |
| 31:DA:825:C:C3' | 31:DA:825:C:C6 | 3.00 | 0.44 |
| 31:DA:892:G:C5 | 31:DA:893:C:C5 | 3.05 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:2621:A:O2' | 34:DE:159:HIS:HB2 | 2.18 | 0.44 |
| 34:DE:4:ILE:HG23 | 34:DE:4:ILE:O | 2.17 | 0.44 |
| 35:DF:24:LEU:O | 35:DF:25:PRO:C | 2.56 | 0.44 |
| 36:DG:118:ARG:HB2 | 36:DG:181:ARG:CZ | 2.48 | 0.44 |
| 31:DA:1952:A:C5 | 40:DO:22:ILE:HD11 | 2.51 | 0.44 |
| 31:DA:810:U:O2 | 41:DP:33:ARG:HD3 | 2.16 | 0.44 |
| 43:DR:41:ALA:HB1 | 43:DR:114:VAL:CG2 | 2.46 | 0.44 |
| 44:DS:20:ARG:HA | 44:DS:20:ARG:HD3 | 1.64 | 0.44 |
| 44:DS:97:ARG:HD2 | 44:DS:98:VAL:N | 2.32 | 0.44 |
| 47:DV:79:VAL:HG23 | 47:DV:82:ARG:HD3 | 1.99 | 0.44 |
| 1:AA:1210:C:H4' | 1:AA:1214:C:C4 | 2.53 | 0.44 |
| 1:AA:1423:G:H2' | 1:AA:1424:C:C6 | 2.52 | 0.44 |
| 1:AA:435:C:N4 | 1:AA:436:C:H41 | 2.14 | 0.44 |
| 1:AA:450:G:OP1 | 16:AP:43:LYS:NZ | 2.50 | 0.44 |
| 1:AA:458:C:H2' | 1:AA:460:G:C8 | 2.52 | 0.44 |
| 1:AA:602:A:C2 | 1:AA:637:G:C2 | 3.05 | 0.44 |
| 1:AA:683:G:C6 | 1:AA:684:A:C6 | 3.05 | 0.44 |
| 1:AA:798:G:OP1 | 11:AK:122:LYS:NZ | 2.50 | 0.44 |
| 1:AA:562:C:N4 | 1:AA:884:U:C6 | 2.85 | 0.44 |
| 2:AB:74:LYS:C | 2:AB:78:GLN:HG3 | 2.38 | 0.44 |
| 6:AF:6:VAL:C | 6:AF:7:ASN:HD22 | 2.20 | 0.44 |
| 7:AG:37:ASN:HD21 | 9:AI:40:LEU:HD22 | 1.82 | 0.44 |
| 12:AL:25:PRO:O | 12:AL:27:LEU:HD22 | 2.17 | 0.44 |
| 13:AM:52:GLU:O | 13:AM:56:LEU:HB2 | 2.17 | 0.44 |
| 1:AA:1316:G:H1 | 19:AS:5:LEU:CD2 | 2.30 | 0.44 |
| 22:B0:14:ARG:HE | 22:B0:14:ARG:HB2 | 1.44 | 0.44 |
| 30:B8:2:PRO:N | 31:BA:591:C:O2 | 2.50 | 0.44 |
| 31:BA:1115:G:H2' | 31:BA:1116:C:O4' | 2.17 | 0.44 |
| 31:BA:1275:A:N3 | 31:BA:1276:A:H1' | 2.32 | 0.44 |
| 31:BA:154:G:O5' | 31:BA:154:G:H8 | 2.01 | 0.44 |
| 31:BA:1857:G:H2' | 31:BA:1858:G:O4' | 2.17 | 0.44 |
| 31:BA:1899:G:C2' | 31:BA:1900:A:OP2 | 2.65 | 0.44 |
| 31:BA:189:G:H2' | 31:BA:205:G:N2 | 2.33 | 0.44 |
| 31:BA:528:A:C2 | 31:BA:2042:A:H2' | 2.52 | 0.44 |
| 31:BA:2334:G:H4' | 31:BA:2335:A:OP2 | 2.16 | 0.44 |
| 31:BA:826:U:OP1 | 31:BA:2428:G:H3' | 2.16 | 0.44 |
| 31:BA:2543:G:H2' | 31:BA:2544:G:C8 | 2.52 | 0.44 |
| 31:BA:2746:U:H4' | 37:BH:138:LYS:HB3 | 1.99 | 0.44 |
| 31:BA:49:A:C4' | 31:BA:50:U:H5' | 2.45 | 0.44 |
| 31:BA:705:A:H2' | 31:BA:706:A:O4' | 2.18 | 0.44 |
| 31:BA:769:G:O2' | 31:BA:770:G:H5' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 31:BA:814:C:N4 | 41:BP:27:HIS:NE2 | 2.64 | 0.44 |
| 31:BA:996:A:O4' | 46:BU:92:ARG:NH2 | 2.50 | 0.44 |
| 32:BB:93:G:H2' | 32:BB:94:C:C6 | 2.52 | 0.44 |
| 31:BA:1816:G:H8 | 33:BD:62:TYR:CZ | 2.34 | 0.44 |
| 35:BF:41:LEU:N | 35:BF:41:LEU:HD23 | 2.33 | 0.44 |
| 36:BG:96:ARG:HB2 | 36:BG:97:ASP:H | 1.64 | 0.44 |
| 40:BO:87:ILE:HD13 | 40:BO:87:ILE:HA | 1.58 | 0.44 |
| 41:BP:35:HIS:O | 41:BP:36:LYS:CB | 2.65 | 0.44 |
| 42:BQ:72:LYS:HB3 | 42:BQ:94:VAL:HG23 | 1.99 | 0.44 |
| 43:BR:34:ILE:HD12 | 43:BR:34:ILE:HA | 1.60 | 0.44 |
| 43:BR:36:THR:HB | 43:BR:37:THR:H | 1.54 | 0.44 |
| 43:BR:8:ARG:HB3 | 43:BR:9:LYS:H | 1.59 | 0.44 |
| 43:BR:9:LYS:O | 43:BR:10:LEU:HD23 | 2.17 | 0.44 |
| 44:BS:101:LEU:O | 44:BS:102:ALA:O | 2.35 | 0.44 |
| 47:BV:79:VAL:HG23 | 47:BV:82:ARG:HD2 | 1.99 | 0.44 |
| 51:BZ:4:ARG:HD3 | 51:BZ:60:GLU:OE1 | 2.18 | 0.44 |
| 1:CA:1113:C:H2' | 1:CA:1114:C:H6 | 1.82 | 0.44 |
| 1:CA:267:C:OP1 | 17:CQ:67:LYS:HD2 | 2.16 | 0.44 |
| 1:CA:299:G:C6 | 1:CA:300:A:N1 | 2.86 | 0.44 |
| 1:CA:359:U:H2' | 1:CA:360:A:H8 | 1.81 | 0.44 |
| 1:CA:411:A:OP1 | 4:CD:30:LYS:NZ | 2.49 | 0.44 |
| 1:CA:562:C:H4' | 1:CA:563:A:O5' | 2.16 | 0.44 |
| 1:CA:564:C:H2' | 1:CA:565:U:H5' | 1.99 | 0.44 |
| 1:CA:615:C:H2' | 1:CA:616:G:O4' | 2.18 | 0.44 |
| 1:CA:989:C:H1' | 1:CA:1016:A:H2 | 1.82 | 0.44 |
| 2:CB:163:PHE:HD2 | 2:CB:185:ILE:CG1 | 2.30 | 0.44 |
| 4:CD:61:LYS:NZ | 4:CD:62:GLN:NE2 | 2.66 | 0.44 |
| 8:CH:100:ILE:HA | 8:CH:101:PRO:HD3 | 1.83 | 0.44 |
| 12:CL:102:ARG:NH1 | 12:CL:102:ARG:CG | 2.77 | 0.44 |
| 12:CL:22:SER:O | 12:CL:24:VAL:N | 2.49 | 0.44 |
| 1:CA:1217:C:OP1 | 14:CN:9:LYS:HD2 | 2.17 | 0.44 |
| 8:CH:91:ARG:NH1 | 17:CQ:33:GLY:HA3 | 2.33 | 0.44 |
| 23:D1:10:LYS:CG | 23:D1:11:ARG:N | 2.80 | 0.44 |
| 23:D1:13:ILE:HG21 | 23:D1:63:ALA:HB3 | 1.99 | 0.44 |
| 24:D2:30:ARG:HA | 24:D2:33:MET:SD | 2.58 | 0.44 |
| 25:D3:52:HIS:CD2 | 32:DB:83:G:H5'' | 2.52 | 0.44 |
| 31:DA:1042:G:H3' | 31:DA:1043:C:O4' | 2.17 | 0.44 |
| 31:DA:1049:C:O2 | 31:DA:1049:C:H2' | 2.16 | 0.44 |
| 31:DA:1528(A):A:H2' | 31:DA:1529:G:O4' | 2.17 | 0.44 |
| 31:DA:1578:U:C2' | 31:DA:1579:A:H5' | 2.47 | 0.44 |
| 31:DA:174:C:C2' | 31:DA:175:G:H5'' | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:1819:A:OP1 | 33:DD:158:ALA:HB2 | 2.17 | 0.44 |
| 31:DA:1857:G:H2' | 31:DA:1858:G:O4' | 2.17 | 0.44 |
| 31:DA:2287:A:H2 | 31:DA:2346:A:N1 | 2.13 | 0.44 |
| 31:DA:2452:C:N4 | 31:DA:2453:A:N6 | 2.65 | 0.44 |
| 31:DA:2552:U:C2 | 31:DA:2554:U:C5' | 3.00 | 0.44 |
| 31:DA:2577:A:H5'' | 31:DA:2578:G:C5' | 2.43 | 0.44 |
| 31:DA:697:C:C2 | 31:DA:698:C:C5 | 3.05 | 0.44 |
| 31:DA:792:G:C3' | 31:DA:793:A:H5' | 2.47 | 0.44 |
| 31:DA:816:C:H2' | 31:DA:817:C:H6 | 1.82 | 0.44 |
| 31:DA:90:U:O2' | 31:DA:92:A:C5' | 2.66 | 0.44 |
| 33:DD:69:ARG:NH2 | 33:DD:128:GLY:O | 2.44 | 0.44 |
| 33:DD:25:THR:O | 33:DD:27:THR:CB | 2.65 | 0.44 |
| 33:DD:267:SER:O | 33:DD:268:ARG:CB | 2.65 | 0.44 |
| 33:DD:35:LYS:HD3 | 33:DD:64:ILE:N | 2.32 | 0.44 |
| 33:DD:35:LYS:CA | 33:DD:64:ILE:HG22 | 2.46 | 0.44 |
| 34:DE:65:GLY:HA2 | 34:DE:70:ALA:HB2 | 1.97 | 0.44 |
| 36:DG:55:LYS:NZ | 36:DG:148:MET:O | 2.50 | 0.44 |
| 37:DH:163:TYR:H | 37:DH:163:TYR:HD1 | 1.64 | 0.44 |
| 37:DH:43:VAL:CG2 | 37:DH:43:VAL:O | 2.62 | 0.44 |
| 38:DI:27:ARG:CG | 38:DI:27:ARG:HH11 | 2.30 | 0.44 |
| 41:DP:48:PRO:CG | 41:DP:49:ARG:H | 2.22 | 0.44 |
| 42:DQ:70:PRO:CA | 42:DQ:95:ALA:HB2 | 2.47 | 0.44 |
| 44:DS:16:ASN:HB3 | 44:DS:20:ARG:HH21 | 1.82 | 0.44 |
| 44:DS:28:VAL:O | 44:DS:89:ARG:CG | 2.66 | 0.44 |
| 45:DT:16:ARG:H | 45:DT:79:HIS:HD2 | 1.65 | 0.44 |
| 46:DU:95:LEU:HD22 | 47:DV:4:ILE:HD13 | 1.97 | 0.44 |
| 47:DV:66:ARG:HH11 | 47:DV:66:ARG:HG3 | 1.81 | 0.44 |
| 24:D2:29:LYS:HZ2 | 49:DX:9:LEU:HA | 1.81 | 0.44 |
| 51:DZ:121:HIS:ND1 | 51:DZ:169:GLU:OE2 | 2.50 | 0.44 |
| 42:DQ:140:ALA:CB | 51:DZ:53:ILE:HG13 | 2.31 | 0.44 |
| 1:AA:1137:C:H3' | 1:AA:1137:C:H6 | 1.82 | 0.44 |
| 1:AA:1289:A:H2' | 1:AA:1290:G:O4' | 2.18 | 0.44 |
| 1:AA:1496:C:H4' | 31:BA:1920:C:O2' | 2.17 | 0.44 |
| 1:AA:66:G:H5' | 1:AA:173:U:O4 | 2.17 | 0.44 |
| 1:AA:189(K):U:H2' | 1:AA:189(L):G:H8 | 1.82 | 0.44 |
| 1:AA:255:G:H2' | 1:AA:256:U:C6 | 2.53 | 0.44 |
| 1:AA:271:C:O2' | 1:AA:272:C:H5' | 2.17 | 0.44 |
| 1:AA:382:A:C2 | 1:AA:383:A:C5 | 3.06 | 0.44 |
| 2:AB:118:LEU:HD11 | 2:AB:141:GLU:HG2 | 1.99 | 0.44 |
| 2:AB:97:TRP:CH2 | 2:AB:176:GLU:OE2 | 2.71 | 0.44 |
| 2:AB:97:TRP:HH2 | 2:AB:176:GLU:CD | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:AD:13:ARG:HD2 | 4:AD:38:TYR:O | 2.17 | 0.44 |
| 5:AE:11:ILE:HG22 | 5:AE:12:LEU:N | 2.32 | 0.44 |
| 8:AH:25:ASP:HA | 8:AH:59:LEU:O | 2.17 | 0.44 |
| 10:AJ:50:ILE:N | 10:AJ:50:ILE:HD13 | 2.33 | 0.44 |
| 1:AA:718:G:H1' | 11:AK:116:HIS:HA | 1.98 | 0.44 |
| 11:AK:57:THR:HG23 | 11:AK:58:PRO:HD2 | 2.00 | 0.44 |
| 20:AT:71:THR:HG22 | 20:AT:72:LEU:H | 1.82 | 0.44 |
| 27:B5:56:LYS:O | 27:B5:57:VAL:O | 2.35 | 0.44 |
| 28:B6:33:LYS:HA | 28:B6:33:LYS:HD3 | 1.71 | 0.44 |
| 31:BA:1108:U:C4 | 31:BA:1109:C:O2 | 2.71 | 0.44 |
| 31:BA:1241:A:H2' | 31:BA:1242:A:O5' | 2.17 | 0.44 |
| 31:BA:1484:G:N2 | 31:BA:1505:C:N4 | 2.62 | 0.44 |
| 31:BA:1510:G:H2' | 31:BA:1511:C:C6 | 2.53 | 0.44 |
| 31:BA:2099:U:O2 | 31:BA:2099:U:H2' | 2.17 | 0.44 |
| 31:BA:2439:A:C5' | 31:BA:2439:A:C8 | 3.00 | 0.44 |
| 31:BA:327:G:C2 | 31:BA:336:C:C2 | 3.05 | 0.44 |
| 31:BA:357:A:N3 | 31:BA:358:U:O2 | 2.50 | 0.44 |
| 31:BA:515:A:H1' | 31:BA:581:C:H1' | 1.99 | 0.44 |
| 32:BB:78:A:H2' | 32:BB:79:C:O4' | 2.18 | 0.44 |
| 33:BD:25:THR:O | 33:BD:27:THR:CB | 2.64 | 0.44 |
| 33:BD:27:THR:O | 33:BD:28:GLU:HB2 | 2.17 | 0.44 |
| 33:BD:36:PRO:HA | 33:BD:62:TYR:O | 2.18 | 0.44 |
| 34:BE:44:TYR:O | 34:BE:45:THR:HB | 2.17 | 0.44 |
| 36:BG:13:GLU:O | 36:BG:14:GLU:CB | 2.65 | 0.44 |
| 36:BG:60:LEU:HA | 36:BG:63:ILE:HG12 | 2.00 | 0.44 |
| 37:BH:44:VAL:O | 37:BH:46:GLU:CD | 2.55 | 0.44 |
| 37:BH:47:GLU:C | 37:BH:49:VAL:H | 2.21 | 0.44 |
| 38:BI:72:LEU:HD12 | 38:BI:138:ILE:CG2 | 2.36 | 0.44 |
| 39:BN:46:VAL:CG1 | 39:BN:48:MET:HG3 | 2.47 | 0.44 |
| 42:BQ:141:GLN:CD | 51:BZ:72:ARG:HG2 | 2.38 | 0.44 |
| 42:BQ:7:MET:O | 42:BQ:10:ARG:NE | 2.50 | 0.44 |
| 43:BR:41:ALA:O | 43:BR:44:LEU:N | 2.49 | 0.44 |
| 31:BA:1754:C:OP1 | 45:BT:96:ARG:NH1 | 2.50 | 0.44 |
| 46:BU:90:VAL:O | 46:BU:91:ASP:C | 2.55 | 0.44 |
| 49:BX:60:ARG:CG | 49:BX:72:LYS:H | 2.30 | 0.44 |
| 50:BY:8:LYS:HB2 | 50:BY:28:LYS:HZ3 | 1.83 | 0.44 |
| 1:CA:1077:G:C6 | 1:CA:1081:G:O6 | 2.70 | 0.44 |
| 1:CA:1116:C:N4 | 1:CA:1117:G:N7 | 2.66 | 0.44 |
| 1:CA:1169:A:C2' | 1:CA:1170:A:H8 | 2.29 | 0.44 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:H6 | 1.82 | 0.44 |
| 1:CA:155:C:C2 | 1:CA:156:G:N7 | 2.86 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:176:C:H2' | 1:CA:177:C:H6 | 1.80 | 0.44 |
| 1:CA:935:A:H2' | 1:CA:936:C:C6 | 2.52 | 0.44 |
| 2:CB:187:LEU:HA | 2:CB:201:ILE:O | 2.18 | 0.44 |
| 4:CD:173:TRP:CD1 | 4:CD:174:LEU:HG | 2.52 | 0.44 |
| 4:CD:190:ASP:O | 4:CD:191:ARG:C | 2.55 | 0.44 |
| 5:CE:18:ARG:HE | 5:CE:25:ARG:HB3 | 1.82 | 0.44 |
| 6:CF:19:LEU:HD21 | 6:CF:59:TYR:CE2 | 2.53 | 0.44 |
| 8:CH:10:LEU:HD23 | 8:CH:10:LEU:H | 1.81 | 0.44 |
| 9:CI:118:LYS:HB3 | 9:CI:118:LYS:HZ3 | 1.82 | 0.44 |
| 1:CA:552:U:C4' | 12:CL:86:ARG:HG2 | 2.44 | 0.44 |
| 15:CO:20:GLY:O | 15:CO:21:ASP:HB3 | 2.16 | 0.44 |
| 16:CP:1:MET:HG2 | 16:CP:2:VAL:O | 2.17 | 0.44 |
| 17:CQ:52:LYS:H | 17:CQ:52:LYS:HD2 | 1.83 | 0.44 |
| 17:CQ:45:HIS:O | 17:CQ:73:VAL:HG23 | 2.17 | 0.44 |
| 20:CT:73:HIS:O | 20:CT:74:LYS:C | 2.55 | 0.44 |
| 22:D0:11:ARG:O | 22:D0:14:ARG:NH2 | 2.51 | 0.44 |
| 22:D0:51:VAL:N | 22:D0:62:LEU:HD12 | 2.32 | 0.44 |
| 23:D1:12:PRO:HD2 | 23:D1:62:VAL:CG2 | 2.42 | 0.44 |
| 23:D1:26:ARG:HB2 | 23:D1:34:THR:HB | 2.00 | 0.44 |
| 24:D2:53:LEU:HA | 24:D2:56:GLN:NE2 | 2.33 | 0.44 |
| 27:D5:36:CYS:O | 27:D5:38:ALA:N | 2.44 | 0.44 |
| 30:D8:39:LYS:HE2 | 30:D8:39:LYS:O | 2.18 | 0.44 |
| 31:DA:1122:G:C2 | 31:DA:1123:C:C6 | 3.06 | 0.44 |
| 31:DA:1416:G:HO2' | 31:DA:1417:C:H6 | 1.60 | 0.44 |
| 31:DA:1549:C:O2' | 31:DA:1550:C:H5' | 2.18 | 0.44 |
| 31:DA:1784:A:H4' | 31:DA:1785:A:C5' | 2.48 | 0.44 |
| 31:DA:17:G:C6 | 31:DA:18:C:N4 | 2.86 | 0.44 |
| 31:DA:1865:G:H5' | 31:DA:1866:C:OP2 | 2.17 | 0.44 |
| 31:DA:1884:A:C2 | 31:DA:1885:A:C4 | 3.05 | 0.44 |
| 23:D1:18:ILE:HD13 | 31:DA:188:G:OP1 | 2.18 | 0.44 |
| 31:DA:1956:U:C2' | 31:DA:1957:C:H5' | 2.47 | 0.44 |
| 31:DA:196:A:C5 | 31:DA:805:G:C6 | 3.05 | 0.44 |
| 31:DA:221:A:N6 | 31:DA:265:A:C8 | 2.85 | 0.44 |
| 31:DA:2296:U:H4' | 31:DA:2297:C:OP1 | 2.16 | 0.44 |
| 31:DA:2468:G:C6 | 31:DA:2481:G:C4 | 3.05 | 0.44 |
| 31:DA:2555:U:C5 | 31:DA:2556:C:C2 | 3.05 | 0.44 |
| 31:DA:262:A:H2' | 31:DA:263:C:O4' | 2.17 | 0.44 |
| 31:DA:271(H):G:O6 | 31:DA:271(Q):G:O6 | 2.36 | 0.44 |
| 31:DA:357:A:N3 | 31:DA:358:U:O2 | 2.50 | 0.44 |
| 31:DA:778:G:C5 | 31:DA:779:U:C4 | 3.06 | 0.44 |
| 31:DA:1902:C:H4' | 33:DD:244:ARG:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DD:35:LYS:CG | 33:DD:64:ILE:H | 2.30 | 0.44 |
| 31:DA:745:G:P | 34:DE:133:LYS:HE3 | 2.58 | 0.44 |
| 31:DA:320:A:OP2 | 35:DF:137:LYS:HE2 | 2.17 | 0.44 |
| 36:DG:6:ALA:HB3 | 36:DG:104:GLU:OE1 | 2.16 | 0.44 |
| 37:DH:85:LYS:HZ3 | 37:DH:145:ALA:HA | 1.82 | 0.44 |
| 37:DH:41:MET:HG3 | 37:DH:53:GLU:O | 2.18 | 0.44 |
| 39:DN:78:TYR:N | 39:DN:79:PRO:CD | 2.81 | 0.44 |
| 31:DA:196:A:C4' | 41:DP:46:LYS:HE2 | 2.47 | 0.44 |
| 41:DP:85:LEU:HB3 | 41:DP:114:ILE:HD12 | 1.98 | 0.44 |
| 41:DP:97:PRO:O | 41:DP:98:GLU:CB | 2.46 | 0.44 |
| 44:DS:92:TYR:HB2 | 44:DS:97:ARG:HH22 | 1.82 | 0.44 |
| 45:DT:28:VAL:O | 45:DT:29:ARG:CD | 2.65 | 0.44 |
| 45:DT:38:ASN:C | 45:DT:38:ASN:ND2 | 2.71 | 0.44 |
| 45:DT:24:PRO:HA | 45:DT:49:VAL:O | 2.17 | 0.44 |
| 46:DU:50:ARG:NH2 | 47:DV:75:PHE:CD2 | 2.85 | 0.44 |
| 46:DU:83:LEU:C | 46:DU:88:ILE:HD11 | 2.37 | 0.44 |
| 46:DU:61:TRP:CE2 | 46:DU:94:ASN:HA | 2.52 | 0.44 |
| 47:DV:1:MET:H1 | 47:DV:44:LYS:HD2 | 1.81 | 0.44 |
| 27:D5:25:LEU:HD11 | 48:DW:19:LEU:HB3 | 2.00 | 0.44 |
| 49:DX:38:GLU:CD | 49:DX:38:GLU:N | 2.69 | 0.44 |
| 51:DZ:54:HIS:ND1 | 51:DZ:101:PRO:HD3 | 2.32 | 0.44 |
| 51:DZ:44:PHE:C | 51:DZ:44:PHE:CD1 | 2.90 | 0.44 |
| 1:AA:1113:C:H2' | 1:AA:1114:C:H6 | 1.82 | 0.44 |
| 1:AA:1226:C:N4 | 13:AM:104:ARG:HD2 | 2.33 | 0.44 |
| 1:AA:61:G:OP1 | 20:AT:10:LEU:HD11 | 2.18 | 0.44 |
| 1:AA:69:G:C2 | 1:AA:70:G:C8 | 3.06 | 0.44 |
| 1:AA:731:G:C6 | 1:AA:732:C:N4 | 2.86 | 0.44 |
| 1:AA:865:A:H2 | 1:AA:918:A:H4' | 1.82 | 0.44 |
| 1:AA:930:C:C4 | 1:AA:931:C:C5 | 3.06 | 0.44 |
| 2:AB:15:VAL:C | 2:AB:16:HIS:CG | 2.91 | 0.44 |
| 2:AB:163:PHE:HD2 | 2:AB:185:ILE:CG1 | 2.31 | 0.44 |
| 3:AC:165:THR:O | 3:AC:165:THR:HG23 | 2.18 | 0.44 |
| 4:AD:159:ARG:O | 4:AD:163:GLU:N | 2.51 | 0.44 |
| 4:AD:61:LYS:CA | 4:AD:203:VAL:HG22 | 2.48 | 0.44 |
| 4:AD:43:HIS:CE1 | 4:AD:46:LYS:HZ2 | 2.35 | 0.44 |
| 6:AF:81:ILE:O | 6:AF:82:ARG:C | 2.55 | 0.44 |
| 9:AI:21:PRO:HA | 9:AI:58:ARG:O | 2.16 | 0.44 |
| 11:AK:57:THR:CG2 | 11:AK:58:PRO:HD2 | 2.47 | 0.44 |
| 12:AL:46:LYS:CG | 12:AL:47:LYS:N | 2.80 | 0.44 |
| 1:AA:750:G:H21 | 15:AO:24:SER:H | 1.65 | 0.44 |
| 16:AP:68:ASP:C | 16:AP:70:ALA:H | 2.20 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:B1:28:GLY:C | 23:B1:30:VAL:H | 2.19 | 0.44 |
| 23:B1:41:ARG:NH2 | 31:BA:205:G:O6 | 2.50 | 0.44 |
| 24:B2:53:LEU:HA | 24:B2:56:GLN:NE2 | 2.32 | 0.44 |
| 25:B3:39:ASP:OD1 | 25:B3:44:ARG:HG3 | 2.16 | 0.44 |
| 29:B7:15:THR:CG2 | 29:B7:16:HIS:CE1 | 3.01 | 0.44 |
| 29:B7:31:LEU:O | 29:B7:32:LYS:C | 2.54 | 0.44 |
| 31:BA:130:C:H2' | 31:BA:131:G:H5'' | 1.99 | 0.44 |
| 31:BA:1497:U:C2' | 31:BA:1497:U:O2 | 2.64 | 0.44 |
| 31:BA:1721:G:N1 | 31:BA:1739:U:OP2 | 2.51 | 0.44 |
| 31:BA:1948:G:H2' | 31:BA:1949:G:C5' | 2.47 | 0.44 |
| 31:BA:2006:C:H6 | 31:BA:2006:C:O5' | 2.00 | 0.44 |
| 31:BA:2226:C:O5' | 31:BA:2226:C:H6 | 2.01 | 0.44 |
| 31:BA:2306:C:OP2 | 31:BA:2307:G:C8 | 2.70 | 0.44 |
| 31:BA:271(F):C:C4 | 31:BA:271(G):C:C5 | 3.06 | 0.44 |
| 31:BA:529:A:N6 | 31:BA:2041:U:C2 | 2.86 | 0.44 |
| 31:BA:782:A:H5' | 31:BA:783:A:C2 | 2.53 | 0.44 |
| 31:BA:786:C:O2' | 31:BA:787:U:H5' | 2.17 | 0.44 |
| 31:BA:78:A:C6 | 31:BA:109:G:C6 | 3.05 | 0.44 |
| 31:BA:966:G:H2' | 31:BA:967:C:C6 | 2.53 | 0.44 |
| 36:BG:135:LEU:HD23 | 36:BG:140:ILE:HD11 | 1.99 | 0.44 |
| 39:BN:121:LYS:HD2 | 39:BN:123:TYR:CE1 | 2.51 | 0.44 |
| 41:BP:131:SER:O | 41:BP:132:LYS:C | 2.55 | 0.44 |
| 45:BT:41:ARG:NH1 | 45:BT:43:GLN:HB2 | 2.32 | 0.44 |
| 47:BV:79:VAL:CG2 | 47:BV:82:ARG:HD2 | 2.48 | 0.44 |
| 31:BA:993:G:N3 | 47:BV:91:TYR:HE1 | 2.16 | 0.44 |
| 49:BX:65:ARG:HE | 49:BX:65:ARG:HA | 1.82 | 0.44 |
| 49:BX:82:GLN:OE1 | 49:BX:83:VAL:HG22 | 2.18 | 0.44 |
| 49:BX:49:VAL:CG1 | 49:BX:87:GLN:HG2 | 2.47 | 0.44 |
| 1:CA:103:C:OP2 | 20:CT:14:LYS:HD3 | 2.18 | 0.44 |
| 1:CA:253:U:H2' | 1:CA:254:G:H8 | 1.82 | 0.44 |
| 1:CA:450:G:H1 | 1:CA:483:C:N4 | 2.14 | 0.44 |
| 1:CA:734:G:H2' | 1:CA:735:C:C6 | 2.52 | 0.44 |
| 2:CB:68:ILE:HG13 | 2:CB:161:ALA:HB3 | 1.98 | 0.44 |
| 4:CD:22:LYS:HB2 | 4:CD:26:CYS:SG | 2.56 | 0.44 |
| 6:CF:12:PRO:HB3 | 6:CF:58:GLY:N | 2.32 | 0.44 |
| 1:CA:134:A:N6 | 16:CP:25:ARG:NH1 | 2.65 | 0.44 |
| 16:CP:36:ILE:O | 16:CP:36:ILE:HG13 | 2.18 | 0.44 |
| 6:CF:100:ASN:ND2 | 18:CR:23:LYS:HE3 | 2.32 | 0.44 |
| 28:D6:16:CYS:O | 28:D6:17:LYS:CB | 2.57 | 0.44 |
| 31:DA:1368:G:N2 | 31:DA:1369:G:C4 | 2.85 | 0.44 |
| 31:DA:1548:C:O2' | 31:DA:1549:C:H5' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:D6:46:HIS:ND1 | 31:DA:2371:G:O2' | 2.49 | 0.44 |
| 31:DA:2409:G:H2' | 31:DA:2410:G:O4' | 2.17 | 0.44 |
| 31:DA:2741:A:H2' | 31:DA:2742:C:O4' | 2.16 | 0.44 |
| 31:DA:806:C:OP2 | 41:DP:39:LYS:CG | 2.65 | 0.44 |
| 31:DA:995:C:O2 | 39:DN:4:TYR:OH | 2.34 | 0.44 |
| 32:DB:45:A:C2' | 32:DB:46:A:H5' | 2.48 | 0.44 |
| 33:DD:166:GLN:HE21 | 33:DD:166:GLN:CA | 2.30 | 0.44 |
| 33:DD:267:SER:HA | 33:DD:270:ILE:CD1 | 2.48 | 0.44 |
| 34:DE:101:ARG:HA | 34:DE:101:ARG:HD3 | 1.82 | 0.44 |
| 34:DE:147:PRO:HB2 | 34:DE:149:ARG:HG2 | 1.98 | 0.44 |
| 35:DF:106:ARG:HG2 | 35:DF:106:ARG:H | 1.53 | 0.44 |
| 36:DG:125:PHE:HE2 | 36:DG:173:LEU:HD12 | 1.80 | 0.44 |
| 37:DH:94:TYR:N | 37:DH:94:TYR:CD1 | 2.84 | 0.44 |
| 39:DN:40:PRO:CA | 46:DU:64:ARG:NH2 | 2.78 | 0.44 |
| 39:DN:65:LYS:NZ | 39:DN:66:LYS:H | 2.14 | 0.44 |
| 44:DS:24:LEU:HB3 | 44:DS:85:VAL:CG1 | 2.47 | 0.44 |
| 1:AA:1128:C:N3 | 1:AA:1139:G:C6 | 2.86 | 0.44 |
| 1:AA:1194:U:H4' | 5:AE:22:GLY:HA2 | 1.99 | 0.44 |
| 1:AA:1320:C:H5' | 19:AS:70:LYS:CG | 2.48 | 0.44 |
| 1:AA:939:G:H1' | 1:AA:1375:A:C2 | 2.53 | 0.44 |
| 1:AA:664:G:N2 | 1:AA:741:G:H1 | 2.15 | 0.44 |
| 2:AB:19:HIS:CG | 2:AB:20:GLU:N | 2.85 | 0.44 |
| 4:AD:19:LEU:HB2 | 4:AD:21:LEU:HD23 | 1.98 | 0.44 |
| 5:AE:127:ASN:O | 5:AE:131:ILE:HG12 | 2.18 | 0.44 |
| 5:AE:57:LYS:O | 5:AE:61:TYR:CD2 | 2.70 | 0.44 |
| 10:AJ:24:VAL:O | 10:AJ:28:ARG:HG3 | 2.18 | 0.44 |
| 10:AJ:6:ILE:HD11 | 10:AJ:72:VAL:HB | 1.99 | 0.44 |
| 11:AK:57:THR:HG22 | 11:AK:59:TYR:N | 2.32 | 0.44 |
| 11:AK:91:ARG:O | 11:AK:95:ILE:HG12 | 2.17 | 0.44 |
| 12:AL:60:LEU:HA | 12:AL:60:LEU:HD13 | 1.80 | 0.44 |
| 14:AN:3:ARG:HB3 | 14:AN:3:ARG:NH1 | 2.32 | 0.44 |
| 18:AR:71:LYS:O | 18:AR:72:ARG:C | 2.55 | 0.44 |
| 23:B1:33:LYS:C | 23:B1:34:THR:HG22 | 2.38 | 0.44 |
| 27:B5:40:LYS:HE3 | 27:B5:49:CYS:SG | 2.57 | 0.44 |
| 30:B8:30:ARG:NH2 | 41:BP:62:LEU:HB2 | 2.33 | 0.44 |
| 31:BA:176:G:O2' | 31:BA:177:G:H5' | 2.17 | 0.44 |
| 1:AA:1409:C:H4' | 31:BA:1915:U:O4 | 2.18 | 0.44 |
| 31:BA:1667:G:H22 | 31:BA:1992:G:H5'' | 1.82 | 0.44 |
| 31:BA:2101:G:C6 | 31:BA:2102:U:C4 | 3.06 | 0.44 |
| 31:BA:2262:U:H4' | 31:BA:2328:A:C2 | 2.53 | 0.44 |
| 31:BA:2347:C:H2' | 31:BA:2348:U:C6 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:BA:2473:U:C4 | 31:BA:2474:C:C5 | 3.06 | 0.44 |
| 27:B5:34:PRO:HG3 | 31:BA:2885:C:O2' | 2.18 | 0.44 |
| 31:BA:614:U:O4' | 31:BA:614:U:O2 | 2.35 | 0.44 |
| 31:BA:951:C:C2' | 31:BA:952:G:H5' | 2.48 | 0.44 |
| 31:BA:1816:G:C8 | 33:BD:62:TYR:CZ | 3.06 | 0.44 |
| 33:BD:83:GLU:HB2 | 33:BD:92:ILE:HD12 | 1.98 | 0.44 |
| 34:BE:28:ALA:HB3 | 34:BE:93:VAL:CG2 | 2.48 | 0.44 |
| 35:BF:157:VAL:HB | 35:BF:194:MET:HB3 | 1.99 | 0.44 |
| 36:BG:19:LEU:HG | 36:BG:175:LEU:CD1 | 2.47 | 0.44 |
| 36:BG:96:ARG:O | 36:BG:99:MET:HB3 | 2.17 | 0.44 |
| 37:BH:99:VAL:O | 37:BH:102:ALA:HB3 | 2.18 | 0.44 |
| 39:BN:78:TYR:CD1 | 39:BN:79:PRO:CB | 3.00 | 0.44 |
| 40:BO:61:VAL:O | 40:BO:84:ALA:HA | 2.17 | 0.44 |
| 45:BT:33:LYS:HA | 45:BT:33:LYS:HD3 | 1.47 | 0.44 |
| 46:BU:92:ARG:NH2 | 47:BV:11:GLN:H | 2.14 | 0.44 |
| 49:BX:62:LYS:HG3 | 49:BX:62:LYS:O | 2.17 | 0.44 |
| 50:BY:75:ILE:CD1 | 50:BY:79:CYS:C | 2.80 | 0.44 |
| 1:CA:1157:A:N3 | 1:CA:1181:G:N3 | 2.65 | 0.44 |
| 1:CA:1245:A:C6 | 1:CA:1246:C:C4 | 3.06 | 0.44 |
| 1:CA:1289:A:H2' | 1:CA:1290:G:O4' | 2.17 | 0.44 |
| 1:CA:284:G:H2' | 1:CA:285:G:H8 | 1.82 | 0.44 |
| 1:CA:356:A:C2 | 1:CA:368:U:O2 | 2.70 | 0.44 |
| 1:CA:414:A:H2' | 1:CA:415:A:O4' | 2.17 | 0.44 |
| 1:CA:577:G:C1' | 1:CA:816:A:C4 | 3.01 | 0.44 |
| 1:CA:601:C:H2' | 1:CA:602:A:C8 | 2.52 | 0.44 |
| 1:CA:79:G:H1' | 1:CA:80:G:O5' | 2.18 | 0.44 |
| 1:CA:881:G:P | 12:CL:12:ARG:NH2 | 2.90 | 0.44 |
| 3:CC:134:ILE:O | 3:CC:138:VAL:HG23 | 2.18 | 0.44 |
| 5:CE:127:ASN:O | 5:CE:131:ILE:HG12 | 2.17 | 0.44 |
| 10:CJ:44:VAL:HG12 | 10:CJ:45:ARG:N | 2.32 | 0.44 |
| 7:CG:150:ALA:HA | 11:CK:59:TYR:HB3 | 1.98 | 0.44 |
| 1:CA:948:C:C5 | 13:CM:106:ASN:ND2 | 2.85 | 0.44 |
| 23:D1:21:ARG:HH12 | 31:DA:380:U:P | 2.40 | 0.44 |
| 24:D2:48:HIS:ND1 | 24:D2:48:HIS:O | 2.51 | 0.44 |
| 27:D5:30:LEU:O | 27:D5:31:VAL:HG13 | 2.17 | 0.44 |
| 27:D5:31:VAL:HB | 27:D5:32:PRO:HD2 | 1.99 | 0.44 |
| 30:D8:62:LEU:N | 30:D8:63:PRO:CD | 2.80 | 0.44 |
| 31:DA:1438:U:O2' | 31:DA:1439:A:H5' | 2.18 | 0.44 |
| 31:DA:1638:C:H5'' | 31:DA:2710:C:O2' | 2.18 | 0.44 |
| 31:DA:1721:G:N1 | 31:DA:1739:U:OP2 | 2.50 | 0.44 |
| 31:DA:2016:U:H2' | 31:DA:2017:U:H6 | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:2615:U:H2' | 31:DA:2616:C:H6 | 1.82 | 0.44 |
| 31:DA:2664:G:H2' | 31:DA:2665:A:O5' | 2.16 | 0.44 |
| 31:DA:2690:C:OP2 | 43:DR:14:SER:HB3 | 2.18 | 0.44 |
| 31:DA:2729:G:H2' | 31:DA:2730:C:C6 | 2.52 | 0.44 |
| 31:DA:2752:C:H2' | 31:DA:2753:A:H5' | 1.99 | 0.44 |
| 31:DA:39:C:H2' | 31:DA:40:C:C6 | 2.52 | 0.44 |
| 31:DA:658:C:H2' | 31:DA:659:C:C6 | 2.53 | 0.44 |
| 31:DA:750:A:C2 | 31:DA:753:C:C6 | 3.06 | 0.44 |
| 32:DB:74:U:C3' | 32:DB:75:G:H5'' | 2.47 | 0.44 |
| 33:DD:223:GLY:HA2 | 33:DD:231:HIS:CD2 | 2.53 | 0.44 |
| 38:DI:138:ILE:HG22 | 38:DI:139:GLN:N | 2.32 | 0.44 |
| 39:DN:75:TYR:CD2 | 39:DN:83:LYS:NZ | 2.82 | 0.44 |
| 43:DR:38:VAL:HG12 | 43:DR:42:LYS:HD2 | 1.99 | 0.44 |
| 49:DX:31:HIS:CD2 | 49:DX:33:LYS:H | 2.35 | 0.44 |
| 49:DX:41:ASN:O | 49:DX:45:THR:CG2 | 2.66 | 0.44 |
| 1:AA:102:G:C6 | 1:AA:103:C:C4 | 3.05 | 0.44 |
| 1:AA:1038:C:H2' | 1:AA:1039:C:C6 | 2.53 | 0.44 |
| 1:AA:1058:G:C5 | 1:AA:1059:C:C4 | 3.05 | 0.44 |
| 1:AA:1142:G:H3' | 1:AA:1143:G:C8 | 2.52 | 0.44 |
| 1:AA:11:G:C6 | 1:AA:12:U:C4 | 3.05 | 0.44 |
| 1:AA:945:G:O6 | 1:AA:1337:G:C6 | 2.71 | 0.44 |
| 1:AA:782:A:H4' | 1:AA:1514:C:O2' | 2.18 | 0.44 |
| 1:AA:977:A:C2' | 1:AA:978:A:H5' | 2.47 | 0.44 |
| 1:AA:977:A:HO2' | 1:AA:981:U:H3 | 1.65 | 0.44 |
| 7:AG:124:LEU:O | 7:AG:128:ALA:HB2 | 2.17 | 0.44 |
| 5:AE:143:ARG:NH1 | 8:AH:77:GLU:OE2 | 2.51 | 0.44 |
| 8:AH:44:PHE:HA | 8:AH:79:VAL:CG1 | 2.46 | 0.44 |
| 1:AA:1348:U:H4' | 9:AI:120:ARG:HH11 | 1.82 | 0.44 |
| 11:AK:67:ASP:O | 11:AK:71:LYS:HG3 | 2.18 | 0.44 |
| 1:AA:552:U:C4' | 12:AL:86:ARG:HG2 | 2.45 | 0.44 |
| 1:AA:624:C:C4' | 16:AP:10:GLY:HA2 | 2.36 | 0.44 |
| 20:AT:30:LYS:O | 20:AT:30:LYS:HD2 | 2.18 | 0.44 |
| 28:B6:26:ASN:ND2 | 28:B6:32:ASN:OD1 | 2.51 | 0.44 |
| 31:BA:1342:A:H5' | 31:BA:1398:C:OP1 | 2.17 | 0.44 |
| 31:BA:1639:U:O2' | 31:BA:1640:C:H5'' | 2.16 | 0.44 |
| 31:BA:174:C:H2' | 31:BA:175:G:H5'' | 1.98 | 0.44 |
| 31:BA:1796:U:H2' | 31:BA:1797:C:H6 | 1.81 | 0.44 |
| 31:BA:2299:G:C6 | 31:BA:2318:G:C8 | 3.05 | 0.44 |
| 31:BA:2323:G:H2' | 31:BA:2324:C:O4' | 2.16 | 0.44 |
| 31:BA:2584:U:H2' | 31:BA:2585:U:C6 | 2.53 | 0.44 |
| 31:BA:2605:U:H2' | 31:BA:2606:C:C6 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:2610:C:C4' | 31:BA:2611:U:OP2 | 2.64 | 0.44 |
| 31:BA:2893:G:H4' | 31:BA:2894:G:H8 | 1.83 | 0.44 |
| 31:BA:325:G:O2' | 31:BA:326:G:H5' | 2.17 | 0.44 |
| 31:BA:311:A:N3 | 31:BA:331:A:H3' | 2.33 | 0.44 |
| 31:BA:855:G:C6 | 31:BA:856:C:N4 | 2.86 | 0.44 |
| 31:BA:854:G:H2' | 31:BA:855:G:C8 | 2.52 | 0.44 |
| 31:BA:912:C:N3 | 31:BA:913:U:C5 | 2.86 | 0.44 |
| 31:BA:848:G:C4 | 31:BA:933:A:H8 | 2.34 | 0.44 |
| 33:BD:241:PRO:O | 33:BD:243:GLY:N | 2.50 | 0.44 |
| 33:BD:253:GLN:HB3 | 33:BD:255:LYS:HE2 | 2.00 | 0.44 |
| 35:BF:65:TRP:O | 35:BF:67:GLN:N | 2.50 | 0.44 |
| 36:BG:67:LYS:N | 36:BG:67:LYS:HD2 | 2.33 | 0.44 |
| 38:BI:114:LEU:O | 38:BI:115:ALA:HB3 | 2.18 | 0.44 |
| 38:BI:124:GLY:N | 38:BI:142:VAL:HG23 | 2.32 | 0.44 |
| 39:BN:65:LYS:O | 39:BN:69:GLN:CB | 2.66 | 0.44 |
| 41:BP:127:ALA:HB3 | 41:BP:130:PHE:CE2 | 2.53 | 0.44 |
| 41:BP:57:THR:HB | 41:BP:59:LEU:N | 2.32 | 0.44 |
| 31:BA:2415:G:O3' | 41:BP:66:GLY:HA3 | 2.17 | 0.44 |
| 43:BR:53:HIS:HA | 43:BR:56:LYS:HB2 | 1.98 | 0.44 |
| 32:BB:117:G:H4' | 44:BS:55:ALA:HB1 | 1.98 | 0.44 |
| 45:BT:24:PRO:HA | 45:BT:49:VAL:O | 2.18 | 0.44 |
| 46:BU:47:TYR:HA | 46:BU:50:ARG:NH2 | 2.32 | 0.44 |
| 50:BY:46:LYS:HB3 | 50:BY:47:LYS:H | 1.64 | 0.44 |
| 1:CA:1058:G:C5 | 1:CA:1059:C:C4 | 3.06 | 0.44 |
| 1:CA:1316:G:H1 | 19:CS:5:LEU:CD2 | 2.31 | 0.44 |
| 1:CA:564:C:C2' | 1:CA:565:U:H5' | 2.48 | 0.44 |
| 1:CA:691:G:H1' | 1:CA:696:A:N6 | 2.31 | 0.44 |
| 1:CA:925:G:O4' | 1:CA:1502:A:C5 | 2.71 | 0.44 |
| 1:CA:977:A:C2' | 1:CA:978:A:H5' | 2.47 | 0.44 |
| 5:CE:11:ILE:HG22 | 5:CE:12:LEU:N | 2.32 | 0.44 |
| 11:CK:73:MET:SD | 11:CK:103:LEU:HD22 | 2.57 | 0.44 |
| 11:CK:67:ASP:O | 11:CK:71:LYS:HG3 | 2.17 | 0.44 |
| 12:CL:60:LEU:HD13 | 12:CL:60:LEU:HA | 1.81 | 0.44 |
| 12:CL:87:GLY:H | 12:CL:99:HIS:H | 1.66 | 0.44 |
| 23:D1:85:LEU:HB3 | 23:D1:87:PRO:HD2 | 1.99 | 0.44 |
| 24:D2:15:LYS:CA | 24:D2:18:PRO:HD2 | 2.46 | 0.44 |
| 29:D7:48:LYS:HD2 | 31:DA:125:G:N2 | 2.33 | 0.44 |
| 31:DA:1024:G:OP2 | 31:DA:1025:G:H3' | 2.17 | 0.44 |
| 31:DA:108:U:O2 | 31:DA:109:G:C8 | 2.70 | 0.44 |
| 31:DA:1247:A:OP1 | 35:DF:95:ARG:NH2 | 2.41 | 0.44 |
| 31:DA:1405:U:C2' | 31:DA:1406:U:O5' | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:2347:C:H2' | 31:DA:2348:U:C6 | 2.52 | 0.44 |
| 31:DA:271(M):G:H2' | 31:DA:271(N):U:H5' | 1.99 | 0.44 |
| 31:DA:287:C:N3 | 31:DA:288:C:C5 | 2.86 | 0.44 |
| 31:DA:287:C:C2' | 31:DA:288:C:O5' | 2.66 | 0.44 |
| 31:DA:355:G:C2 | 31:DA:356:G:C8 | 3.06 | 0.44 |
| 31:DA:470:A:C2 | 31:DA:471:A:C4 | 3.05 | 0.44 |
| 32:DB:15:A:H2' | 32:DB:16:G:OP1 | 2.17 | 0.44 |
| 32:DB:86:G:C2' | 32:DB:87:G:C8 | 3.01 | 0.44 |
| 33:DD:182:LEU:O | 33:DD:271:ILE:HD12 | 2.17 | 0.44 |
| 33:DD:253:GLN:HB3 | 33:DD:255:LYS:NZ | 2.33 | 0.44 |
| 33:DD:66:ASP:OD1 | 33:DD:68:LYS:O | 2.35 | 0.44 |
| 34:DE:116:VAL:HG13 | 34:DE:122:PHE:CD2 | 2.53 | 0.44 |
| 34:DE:134:ILE:H | 34:DE:134:ILE:CD1 | 2.30 | 0.44 |
| 35:DF:66:PRO:O | 35:DF:67:GLN:CB | 2.46 | 0.44 |
| 37:DH:158:HIS:CE1 | 37:DH:170:ARG:N | 2.85 | 0.44 |
| 37:DH:85:LYS:HE2 | 37:DH:145:ALA:H | 1.82 | 0.44 |
| 38:DI:52:ARG:HE | 38:DI:52:ARG:HB3 | 1.41 | 0.44 |
| 40:DO:106:LEU:HD23 | 40:DO:106:LEU:HA | 1.72 | 0.44 |
| 42:DQ:22:LYS:CA | 42:DQ:22:LYS:HE2 | 2.34 | 0.44 |
| 44:DS:26:LEU:HD22 | 44:DS:87:PHE:HE1 | 1.77 | 0.44 |
| 44:DS:88:ASP:CG | 44:DS:89:ARG:N | 2.70 | 0.44 |
| 47:DV:36:PRO:CD | 47:DV:60:GLU:O | 2.65 | 0.44 |
| 47:DV:94:LEU:C | 47:DV:94:LEU:HD23 | 2.38 | 0.44 |
| 50:DY:83:THR:HG23 | 50:DY:94:LYS:HB2 | 2.00 | 0.44 |
| 51:DZ:157:LEU:HA | 51:DZ:158:PRO:HD2 | 1.87 | 0.44 |
| 1:AA:1067:A:N3 | 1:AA:1068:G:N9 | 2.66 | 0.44 |
| 1:AA:1187:G:C6 | 1:AA:1188:A:C6 | 3.05 | 0.44 |
| 1:AA:1490:C:O2' | 1:AA:1491:G:H5' | 2.18 | 0.44 |
| 1:AA:392:G:O2' | 1:AA:393:A:H5' | 2.18 | 0.44 |
| 1:AA:791:G:C5 | 1:AA:792:A:N7 | 2.85 | 0.44 |
| 1:AA:824:C:H4' | 8:AH:1:MET:H1 | 1.83 | 0.44 |
| 7:AG:12:LEU:HD13 | 7:AG:24:THR:OG1 | 2.17 | 0.44 |
| 11:AK:99:GLN:C | 11:AK:101:SER:H | 2.20 | 0.44 |
| 11:AK:58:PRO:HA | 11:AK:90:GLY:HA2 | 1.99 | 0.44 |
| 12:AL:62:SER:C | 12:AL:64:TYR:N | 2.71 | 0.44 |
| 17:AQ:6:LEU:O | 17:AQ:58:GLU:HA | 2.18 | 0.44 |
| 20:AT:55:ILE:O | 20:AT:56:MET:C | 2.55 | 0.44 |
| 22:B0:26:TYR:O | 22:B0:27:GLU:C | 2.55 | 0.44 |
| 22:B0:41:ARG:CB | 31:BA:2330:G:H1' | 2.47 | 0.44 |
| 23:B1:11:ARG:CB | 23:B1:12:PRO:CD | 2.96 | 0.44 |
| 23:B1:26:ARG:CB | 23:B1:34:THR:HB | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:B1:41:ARG:CG | 23:B1:41:ARG:NH1 | 2.56 | 0.44 |
| 23:B1:87:PRO:CD | 23:B1:88:LYS:N | 2.77 | 0.44 |
| 24:B2:15:LYS:CA | 24:B2:18:PRO:HD2 | 2.46 | 0.44 |
| 24:B2:38:GLN:HB3 | 24:B2:38:GLN:HE21 | 1.59 | 0.44 |
| 31:BA:1696:G:C3' | 31:BA:1697:G:H5'' | 2.48 | 0.44 |
| 31:BA:1822:G:C5' | 31:BA:1822:G:C8 | 2.95 | 0.44 |
| 31:BA:2324:C:H5'' | 31:BA:2325:G:H5' | 2.00 | 0.44 |
| 31:BA:464:U:C2' | 31:BA:465:G:H5' | 2.47 | 0.44 |
| 31:BA:685:A:C8 | 31:BA:774:A:C6 | 3.06 | 0.44 |
| 31:BA:860:U:C5 | 31:BA:917:A:N7 | 2.85 | 0.44 |
| 31:BA:90:U:O2 | 31:BA:90:U:C2' | 2.50 | 0.44 |
| 32:BB:88:C:C4 | 32:BB:89:G:C6 | 3.06 | 0.44 |
| 33:BD:61:LEU:O | 33:BD:63:ARG:NH1 | 2.51 | 0.44 |
| 33:BD:64:ILE:CG1 | 33:BD:64:ILE:O | 2.65 | 0.44 |
| 31:BA:727:A:C2 | 33:BD:9:TYR:CD2 | 3.05 | 0.44 |
| 35:BF:29:ASN:OD1 | 35:BF:29:ASN:C | 2.56 | 0.44 |
| 36:BG:45:GLU:HB2 | 36:BG:47:LYS:CG | 2.48 | 0.44 |
| 37:BH:85:LYS:HZ2 | 37:BH:133:VAL:CB | 2.29 | 0.44 |
| 41:BP:78:PRO:HB2 | 41:BP:111:ARG:HE | 1.83 | 0.44 |
| 47:BV:47:VAL:CG2 | 47:BV:49:THR:HB | 2.47 | 0.44 |
| 49:BX:89:ILE:O | 49:BX:89:ILE:HG23 | 2.18 | 0.44 |
| 1:CA:1250:A:C6 | 1:CA:1251:A:C6 | 3.06 | 0.44 |
| 1:CA:1285:A:H4' | 1:CA:1286:A:O5' | 2.18 | 0.44 |
| 1:CA:939:G:H1' | 1:CA:1375:A:C2 | 2.53 | 0.44 |
| 1:CA:189(K):U:H2' | 1:CA:189(L):G:H8 | 1.82 | 0.44 |
| 1:CA:483:C:H3' | 1:CA:484:G:H5'' | 1.99 | 0.44 |
| 1:CA:64:G:H4' | 1:CA:65:U:H5'' | 1.99 | 0.44 |
| 1:CA:989:C:H1' | 1:CA:1016:A:C2 | 2.53 | 0.44 |
| 2:CB:15:VAL:C | 2:CB:16:HIS:CG | 2.91 | 0.44 |
| 3:CC:108:ASN:HD22 | 3:CC:111:LEU:HD12 | 1.83 | 0.44 |
| 4:CD:108:LEU:HG | 4:CD:110:PHE:HE1 | 1.83 | 0.44 |
| 5:CE:72:GLN:O | 5:CE:73:ASN:HB2 | 2.17 | 0.44 |
| 7:CG:18:TYR:CE2 | 7:CG:59:LEU:HB2 | 2.53 | 0.44 |
| 8:CH:1:MET:HE2 | 8:CH:1:MET:N | 2.32 | 0.44 |
| 8:CH:80:ILE:HG22 | 8:CH:80:ILE:O | 2.17 | 0.44 |
| 10:CJ:4:ILE:HG23 | 10:CJ:98:ILE:HG23 | 1.99 | 0.44 |
| 10:CJ:32:ALA:HB3 | 10:CJ:76:ASN:HB3 | 1.99 | 0.44 |
| 1:CA:798:G:OP1 | 11:CK:122:LYS:NZ | 2.50 | 0.44 |
| 11:CK:57:THR:HG23 | 11:CK:58:PRO:HD2 | 2.00 | 0.44 |
| 7:CG:149:ARG:HD3 | 11:CK:59:TYR:CE1 | 2.52 | 0.44 |
| 11:CK:23:ALA:HB3 | 11:CK:86:GLY:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:CR:44:LEU:O | 18:CR:45:SER:C | 2.56 | 0.44 |
| 1:CA:986:A:H1' | 19:CS:54:GLY:O | 2.17 | 0.44 |
| 20:CT:58:LYS:HE3 | 20:CT:62:LEU:HD12 | 1.98 | 0.44 |
| 20:CT:84:LEU:HD13 | 20:CT:84:LEU:C | 2.38 | 0.44 |
| 30:D8:22:VAL:HB | 30:D8:53:PRO:CB | 2.47 | 0.44 |
| 30:D8:32:LEU:CB | 30:D8:35:GLN:N | 2.64 | 0.44 |
| 31:DA:1015:G:H2' | 31:DA:1016:G:H5' | 2.00 | 0.44 |
| 31:DA:1356:G:C5 | 31:DA:1357:U:C5 | 3.06 | 0.44 |
| 31:DA:1754:C:OP1 | 45:DT:96:ARG:NH1 | 2.50 | 0.44 |
| 31:DA:526:A:N3 | 31:DA:2044:C:H1' | 2.33 | 0.44 |
| 31:DA:2092:U:C5 | 31:DA:2226:C:OP2 | 2.71 | 0.44 |
| 31:DA:2200:C:H2' | 31:DA:2200:C:O2 | 2.18 | 0.44 |
| 31:DA:2359:C:N4 | 31:DA:2360:A:C6 | 2.86 | 0.44 |
| 31:DA:237:C:C2' | 31:DA:238:C:H5' | 2.48 | 0.44 |
| 31:DA:271(M):G:N7 | 31:DA:271(O):C:N4 | 2.66 | 0.44 |
| 31:DA:2747:G:O6 | 31:DA:2755:C:H5'' | 2.18 | 0.44 |
| 31:DA:536:A:H2' | 31:DA:537:C:H6 | 1.82 | 0.44 |
| 31:DA:873:G:N2 | 31:DA:905:U:O2 | 2.51 | 0.44 |
| 33:DD:70:TRP:CZ2 | 33:DD:150:LYS:HD3 | 2.53 | 0.44 |
| 37:DH:43:VAL:CG1 | 37:DH:53:GLU:H | 2.29 | 0.44 |
| 46:DU:8:VAL:HG11 | 46:DU:12:ARG:CZ | 2.48 | 0.44 |
| 48:DW:54:ALA:CB | 48:DW:107:LEU:HD22 | 2.48 | 0.44 |
| 48:DW:37:ARG:HG2 | 48:DW:38:TYR:CE2 | 2.52 | 0.44 |
| 1:AA:1034:G:N2 | 1:AA:1035:A:N6 | 2.65 | 0.44 |
| 1:AA:1157:A:N3 | 1:AA:1181:G:N3 | 2.65 | 0.44 |
| 1:AA:117:G:O2' | 1:AA:118:U:H5' | 2.18 | 0.44 |
| 1:AA:127:G:C2 | 1:AA:128:G:C8 | 3.06 | 0.44 |
| 1:AA:134:A:N6 | 16:AP:25:ARG:NH1 | 2.63 | 0.44 |
| 1:AA:165:C:H2' | 1:AA:166:G:H8 | 1.82 | 0.44 |
| 1:AA:316:G:OP2 | 1:AA:351:G:O2' | 2.35 | 0.44 |
| 1:AA:343:U:N3 | 1:AA:347:G:N1 | 2.65 | 0.44 |
| 1:AA:350:G:O2' | 1:AA:351:G:H5' | 2.18 | 0.44 |
| 1:AA:425:G:N2 | 1:AA:426:G:C1' | 2.81 | 0.44 |
| 1:AA:499:A:H4' | 1:AA:500:G:H5' | 2.00 | 0.44 |
| 1:AA:635:G:O2' | 1:AA:636:U:H5' | 2.18 | 0.44 |
| 2:AB:28:PHE:HD2 | 2:AB:194:PRO:HD3 | 1.83 | 0.44 |
| 2:AB:44:LEU:O | 2:AB:47:THR:N | 2.51 | 0.44 |
| 3:AC:19:GLU:O | 3:AC:40:ARG:NH2 | 2.49 | 0.44 |
| 5:AE:11:ILE:HB | 5:AE:31:LEU:O | 2.18 | 0.44 |
| 5:AE:128:PRO:O | 5:AE:129:ILE:C | 2.55 | 0.44 |
| 7:AG:49:ILE:HG22 | 7:AG:49:ILE:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:84:GLN:O | 10:AJ:88:LEU:CB | 2.66 | 0.44 |
| 11:AK:23:ALA:HB3 | 11:AK:86:GLY:O | 2.17 | 0.44 |
| 10:AJ:62:HIS:CE1 | 14:AN:61:TRP:CH2 | 3.06 | 0.44 |
| 19:AS:9:VAL:O | 19:AS:11:VAL:N | 2.50 | 0.44 |
| 23:B1:78:LYS:HZ3 | 23:B1:93:GLU:HB2 | 1.82 | 0.44 |
| 24:B2:55:ARG:CG | 24:B2:55:ARG:O | 2.65 | 0.44 |
| 30:B8:4:MET:SD | 30:B8:61:LEU:CD1 | 3.02 | 0.44 |
| 31:BA:1509(A):A:C4 | 31:BA:1509(B):A:C8 | 3.06 | 0.44 |
| 31:BA:1517:G:H2' | 31:BA:1518:U:O4' | 2.18 | 0.44 |
| 31:BA:1518:U:H2' | 31:BA:1519:G:O4' | 2.18 | 0.44 |
| 31:BA:1685:C:O2' | 31:BA:1686:C:H5' | 2.18 | 0.44 |
| 31:BA:21:A:O2' | 31:BA:22:C:H5' | 2.18 | 0.44 |
| 31:BA:225:A:C2' | 31:BA:226:G:H5' | 2.48 | 0.44 |
| 31:BA:2286:A:O2' | 31:BA:2286:A:H8 | 1.97 | 0.44 |
| 31:BA:2422:A:C4' | 31:BA:2423:U:OP1 | 2.63 | 0.44 |
| 31:BA:606:U:H4' | 31:BA:658:C:H4' | 2.00 | 0.44 |
| 31:BA:693:C:H2' | 31:BA:694:U:H6 | 1.82 | 0.44 |
| 32:BB:20:C:C2' | 32:BB:21:G:H5' | 2.35 | 0.44 |
| 33:BD:28:GLU:CB | 33:BD:29:PRO:CD | 2.95 | 0.44 |
| 31:BA:727:A:H2 | 33:BD:9:TYR:CD2 | 2.36 | 0.44 |
| 37:BH:41:MET:HG3 | 37:BH:53:GLU:O | 2.17 | 0.44 |
| 38:BI:99:GLU:O | 38:BI:102:SER:HB3 | 2.18 | 0.44 |
| 39:BN:129:PRO:O | 39:BN:130:HIS:CB | 2.66 | 0.44 |
| 48:BW:54:ALA:CB | 48:BW:107:LEU:HD22 | 2.48 | 0.44 |
| 50:BY:13:VAL:HG12 | 50:BY:73:ARG:O | 2.18 | 0.44 |
| 50:BY:7:VAL:HB | 50:BY:8:LYS:CD | 2.48 | 0.44 |
| 1:CA:1055:A:N3 | 3:CC:156:ARG:NH1 | 2.63 | 0.44 |
| 1:CA:174:C:H6 | 1:CA:174:C:O5' | 2.01 | 0.44 |
| 1:CA:193:C:H2' | 1:CA:194:C:C6 | 2.53 | 0.44 |
| 1:CA:222:U:H2' | 1:CA:223:U:C6 | 2.53 | 0.44 |
| 1:CA:243:A:C2 | 1:CA:246:A:C8 | 3.06 | 0.44 |
| 1:CA:330:C:C2' | 1:CA:331:G:H5' | 2.47 | 0.44 |
| 1:CA:343:U:N3 | 1:CA:347:G:N1 | 2.65 | 0.44 |
| 1:CA:457:C:H2' | 1:CA:458:C:C6 | 2.51 | 0.44 |
| 1:CA:458:C:H2' | 1:CA:460:G:C8 | 2.52 | 0.44 |
| 1:CA:556:C:O2' | 1:CA:557:G:H5' | 2.18 | 0.44 |
| 1:CA:563:A:C8 | 1:CA:567:G:O4' | 2.71 | 0.44 |
| 1:CA:801:U:H2' | 1:CA:802:A:H8 | 1.83 | 0.44 |
| 3:CC:112:SER:O | 3:CC:116:VAL:HG23 | 2.18 | 0.44 |
| 5:CE:11:ILE:HD12 | 5:CE:105:VAL:HA | 2.00 | 0.44 |
| 1:CA:933:G:O6 | 7:CG:3:ARG:NH2 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:D1:25:LYS:O | 23:D1:26:ARG:CG | 2.66 | 0.44 |
| 24:D2:12:GLU:C | 24:D2:14:ARG:H | 2.20 | 0.44 |
| 30:D8:61:LEU:HA | 30:D8:61:LEU:HD23 | 1.79 | 0.44 |
| 31:DA:1374:G:H2' | 31:DA:1375:C:C6 | 2.52 | 0.44 |
| 31:DA:1416:G:OP2 | 31:DA:1416:G:H4' | 2.17 | 0.44 |
| 31:DA:1575:C:O2' | 31:DA:1576:U:H5' | 2.18 | 0.44 |
| 31:DA:1593:G:H2' | 31:DA:1594:G:C8 | 2.53 | 0.44 |
| 31:DA:1686:C:H2' | 31:DA:1687:G:H5' | 1.99 | 0.44 |
| 31:DA:1694:C:O2' | 31:DA:1695:G:C5 | 2.71 | 0.44 |
| 31:DA:2057:A:H2' | 31:DA:2058:A:C8 | 2.52 | 0.44 |
| 31:DA:2712:U:O2' | 31:DA:2712(A):A:P | 2.76 | 0.44 |
| 31:DA:466:A:H2 | 31:DA:795:C:O2 | 2.01 | 0.44 |
| 31:DA:528:A:C2 | 31:DA:2043:C:C4' | 2.99 | 0.44 |
| 31:DA:993:G:OP1 | 47:DV:75:PHE:CE2 | 2.70 | 0.44 |
| 32:DB:8:U:O2' | 44:DS:40:ILE:HD13 | 2.18 | 0.44 |
| 33:DD:30:GLU:CG | 33:DD:63:ARG:NH2 | 2.81 | 0.44 |
| 35:DF:84:VAL:C | 35:DF:86:GLY:N | 2.70 | 0.44 |
| 36:DG:91:ARG:HD2 | 36:DG:91:ARG:O | 2.17 | 0.44 |
| 37:DH:84:SER:O | 37:DH:85:LYS:HB3 | 2.17 | 0.44 |
| 37:DH:85:LYS:HZ3 | 37:DH:145:ALA:HB2 | 1.83 | 0.44 |
| 38:DI:83:ALA:HB3 | 38:DI:123:LEU:HD21 | 2.00 | 0.44 |
| 40:DO:112:MET:CE | 40:DO:112:MET:HA | 2.48 | 0.44 |
| 41:DP:100:LEU:HD12 | 41:DP:100:LEU:HA | 1.71 | 0.44 |
| 43:DR:29:LEU:HA | 43:DR:29:LEU:HD12 | 1.64 | 0.44 |
| 45:DT:34:VAL:O | 45:DT:35:LYS:CB | 2.65 | 0.44 |
| 47:DV:15:GLU:O | 47:DV:98:GLU:CD | 2.56 | 0.44 |
| 50:DY:45:VAL:HG21 | 50:DY:62:GLU:H | 1.81 | 0.44 |
| 1:AA:1446:U:O2 | 1:AA:1456:G:O6 | 2.36 | 0.44 |
| 1:AA:1412:C:H42 | 1:AA:1488:G:H1 | 1.66 | 0.44 |
| 1:AA:24:U:O2' | 1:AA:25:C:H5' | 2.17 | 0.44 |
| 1:AA:386:C:C2' | 1:AA:387:U:C5' | 2.85 | 0.44 |
| 1:AA:602:A:C2 | 1:AA:603:U:C2 | 3.06 | 0.44 |
| 1:AA:64:G:H4' | 1:AA:65:U:H5'' | 1.99 | 0.44 |
| 2:AB:16:HIS:CG | 2:AB:213:LEU:HD13 | 2.53 | 0.44 |
| 3:AC:125:GLU:HA | 3:AC:191:THR:CG2 | 2.46 | 0.44 |
| 5:AE:32:VAL:CG2 | 5:AE:58:ALA:HB1 | 2.48 | 0.44 |
| 7:AG:108:ALA:O | 7:AG:111:ARG:HB2 | 2.18 | 0.44 |
| 15:AO:20:GLY:O | 15:AO:21:ASP:HB3 | 2.18 | 0.44 |
| 18:AR:65:ILE:H | 18:AR:65:ILE:HG13 | 1.59 | 0.44 |
| 11:AK:111:ASP:HA | 18:AR:84:LYS:HE2 | 2.00 | 0.44 |
| 20:AT:36:LEU:HD13 | 20:AT:36:LEU:HA | 1.84 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 31:BA:1309:G:H2' | 31:BA:1310:G:H5' | 2.00 | 0.44 |
| 31:BA:1416:G:O2' | 31:BA:1417:C:H6 | 2.01 | 0.44 |
| 31:BA:1445(A):C:H2' | 31:BA:1446:C:H6 | 1.83 | 0.44 |
| 31:BA:1464:C:O2' | 31:BA:1528:A:H1' | 2.17 | 0.44 |
| 31:BA:1891:G:C5 | 31:BA:1892:C:C4 | 3.06 | 0.44 |
| 31:BA:196:A:C4' | 41:BP:46:LYS:HE2 | 2.48 | 0.44 |
| 31:BA:2019:A:C2' | 31:BA:2020:A:O5' | 2.66 | 0.44 |
| 31:BA:2065:C:H2' | 31:BA:2066:C:H6 | 1.81 | 0.44 |
| 30:B8:27:THR:OG1 | 31:BA:2361:A:O5' | 2.36 | 0.44 |
| 31:BA:2544:G:O2' | 31:BA:2545:G:H5' | 2.18 | 0.44 |
| 31:BA:1783:A:C2 | 31:BA:2587:A:C4 | 3.05 | 0.44 |
| 31:BA:271(F):C:H2' | 31:BA:271(G):C:C6 | 2.42 | 0.44 |
| 23:B1:69:LYS:NZ | 31:BA:372:G:OP2 | 2.36 | 0.44 |
| 31:BA:372:G:HO2' | 31:BA:373:U:P | 2.41 | 0.44 |
| 31:BA:461:C:C2' | 31:BA:462:C:H5' | 2.48 | 0.44 |
| 31:BA:609:A:H2' | 31:BA:610:G:O5' | 2.18 | 0.44 |
| 31:BA:723:G:H2' | 31:BA:724:U:O4' | 2.17 | 0.44 |
| 31:BA:864:G:N2 | 31:BA:913:U:C2 | 2.85 | 0.44 |
| 31:BA:876:C:C4 | 31:BA:877:U:C4 | 3.06 | 0.44 |
| 33:BD:132:PRO:O | 33:BD:136:ILE:CD1 | 2.66 | 0.44 |
| 33:BD:35:LYS:CE | 33:BD:65:ILE:HG22 | 2.48 | 0.44 |
| 35:BF:53:THR:C | 35:BF:55:GLY:N | 2.71 | 0.44 |
| 38:BI:5:LEU:HD21 | 38:BI:19:VAL:CG1 | 2.48 | 0.44 |
| 39:BN:19:GLU:CG | 39:BN:20:GLY:N | 2.78 | 0.44 |
| 39:BN:69:GLN:HE21 | 39:BN:69:GLN:HB3 | 1.54 | 0.44 |
| 41:BP:71:VAL:HG13 | 41:BP:72:PRO:CD | 2.48 | 0.44 |
| 42:BQ:6:ARG:HA | 42:BQ:6:ARG:HD3 | 1.81 | 0.44 |
| 43:BR:23:ASN:N | 43:BR:23:ASN:HD22 | 2.16 | 0.44 |
| 45:BT:28:VAL:HG22 | 45:BT:46:GLU:CA | 2.48 | 0.44 |
| 47:BV:79:VAL:HB | 47:BV:80:GLN:H | 1.67 | 0.44 |
| 51:BZ:67:LEU:N | 51:BZ:67:LEU:CD1 | 2.81 | 0.44 |
| 1:CA:1386:G:N3 | 1:CA:1387:G:C8 | 2.86 | 0.44 |
| 1:CA:143:A:N1 | 1:CA:220:G:O6 | 2.50 | 0.44 |
| 1:CA:17:U:O2' | 1:CA:1079:G:H1' | 2.18 | 0.44 |
| 1:CA:801:U:H2' | 1:CA:802:A:C8 | 2.52 | 0.44 |
| 1:CA:93:G:N1 | 1:CA:96:U:C4 | 2.86 | 0.44 |
| 4:CD:105:VAL:CG1 | 4:CD:105:VAL:O | 2.66 | 0.44 |
| 8:CH:86:ILE:CB | 8:CH:133:LEU:HD22 | 2.46 | 0.44 |
| 9:CI:50:LEU:HD22 | 9:CI:55:ALA:O | 2.18 | 0.44 |
| 20:CT:53:LEU:HG | 20:CT:53:LEU:H | 1.60 | 0.44 |
| 23:D1:78:LYS:HZ3 | 23:D1:93:GLU:HB2 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:D2:32:LEU:HA | 24:D2:32:LEU:HD13 | 1.59 | 0.44 |
| 31:DA:1445(A):C:C2 | 31:DA:1446:C:C5 | 3.06 | 0.44 |
| 31:DA:1741:A:C8 | 31:DA:1742:G:C2 | 3.06 | 0.44 |
| 31:DA:2094:G:O2' | 31:DA:2095:C:H5' | 2.16 | 0.44 |
| 31:DA:2711:A:OP1 | 31:DA:2712(A):A:P | 2.76 | 0.44 |
| 31:DA:271(P):C:C2' | 31:DA:271(Q):G:C5' | 2.95 | 0.44 |
| 31:DA:302:C:O2' | 31:DA:303:U:H5' | 2.18 | 0.44 |
| 31:DA:449:A:OP1 | 35:DF:84:VAL:O | 2.36 | 0.44 |
| 31:DA:901:A:H2' | 31:DA:901:A:N3 | 2.33 | 0.44 |
| 31:DA:951:C:HO2' | 31:DA:952:G:H5' | 1.82 | 0.44 |
| 34:DE:101:ARG:HD2 | 34:DE:169:ASN:HD22 | 1.83 | 0.44 |
| 34:DE:37:ARG:HD3 | 34:DE:44:TYR:CZ | 2.52 | 0.44 |
| 34:DE:44:TYR:O | 34:DE:45:THR:HB | 2.18 | 0.44 |
| 36:DG:128:ARG:O | 36:DG:129:GLY:C | 2.56 | 0.44 |
| 36:DG:13:GLU:O | 36:DG:14:GLU:CB | 2.66 | 0.44 |
| 38:DI:99:GLU:O | 38:DI:102:SER:HB3 | 2.17 | 0.44 |
| 40:DO:61:VAL:O | 40:DO:84:ALA:HA | 2.17 | 0.44 |
| 41:DP:65:ARG:C | 41:DP:66:GLY:O | 2.56 | 0.44 |
| 42:DQ:16:ARG:HG3 | 42:DQ:17:LEU:H | 1.81 | 0.44 |
| 42:DQ:63:LYS:HG2 | 42:DQ:65:PHE:CZ | 2.53 | 0.44 |
| 43:DR:56:LYS:HE3 | 43:DR:94:TYR:CZ | 2.53 | 0.44 |
| 44:DS:61:ASN:O | 44:DS:65:VAL:HG23 | 2.17 | 0.44 |
| 45:DT:30:VAL:CG2 | 45:DT:31:SER:N | 2.76 | 0.44 |
| 47:DV:47:VAL:CG2 | 47:DV:49:THR:HB | 2.48 | 0.44 |
| 24:D2:26:ARG:CB | 49:DX:5:TYR:HB3 | 2.48 | 0.44 |
| 51:DZ:101:PRO:HA | 51:DZ:123:ASP:HB3 | 2.00 | 0.44 |
| 51:DZ:150:LEU:C | 51:DZ:151:HIS:CD2 | 2.90 | 0.44 |
| 51:DZ:19:ARG:HH11 | 51:DZ:19:ARG:HG2 | 1.81 | 0.44 |
| 1:AA:102:G:C4 | 1:AA:103:C:C6 | 3.06 | 0.43 |
| 1:AA:112:G:H2' | 1:AA:112:G:N3 | 2.32 | 0.43 |
| 1:AA:1242:C:H5'' | 21:AU:10:ARG:HH12 | 1.83 | 0.43 |
| 1:AA:1367:C:N3 | 1:AA:1368:G:C8 | 2.86 | 0.43 |
| 1:AA:185:A:N6 | 1:AA:186:C:N4 | 2.66 | 0.43 |
| 1:AA:524:G:H8 | 1:AA:524:G:O5' | 2.01 | 0.43 |
| 1:AA:73:G:N2 | 1:AA:76:C:C2 | 2.86 | 0.43 |
| 1:AA:840:C:H4' | 1:AA:848:C:O2 | 2.17 | 0.43 |
| 1:AA:935:A:H2' | 1:AA:936:C:C6 | 2.52 | 0.43 |
| 1:AA:92:C:H2' | 1:AA:93:G:H8 | 1.83 | 0.43 |
| 2:AB:154:LEU:HD23 | 2:AB:154:LEU:H | 1.82 | 0.43 |
| 5:AE:147:ASP:OD2 | 5:AE:147:ASP:N | 2.51 | 0.43 |
| 6:AF:15:ASP:CG | 6:AF:18:GLN:HE21 | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:AH:113:SER:C | 8:AH:114:THR:HG22 | 2.37 | 0.43 |
| 10:AJ:51:ARG:HG3 | 10:AJ:60:ARG:C | 2.38 | 0.43 |
| 15:AO:82:ILE:HG12 | 15:AO:87:ILE:CB | 2.44 | 0.43 |
| 30:B8:14:VAL:CG1 | 30:B8:22:VAL:HG13 | 2.46 | 0.43 |
| 31:BA:1043:C:C6 | 31:BA:1043:C:OP2 | 2.71 | 0.43 |
| 31:BA:1139:G:O2' | 31:BA:1143:A:N1 | 2.46 | 0.43 |
| 31:BA:1472:A:H2' | 31:BA:1473:G:C5' | 2.48 | 0.43 |
| 31:BA:414:C:H4' | 31:BA:1879:C:O2 | 2.17 | 0.43 |
| 31:BA:2689:U:H4' | 31:BA:2690:C:H5' | 2.00 | 0.43 |
| 31:BA:284:U:H2' | 31:BA:285:C:H6 | 1.82 | 0.43 |
| 31:BA:658:C:H2' | 31:BA:659:C:C6 | 2.53 | 0.43 |
| 31:BA:708:C:O2 | 31:BA:708:C:C2' | 2.66 | 0.43 |
| 31:BA:950:G:C6 | 31:BA:951:C:C4 | 3.06 | 0.43 |
| 32:BB:15:A:H1' | 32:BB:110:G:C4 | 2.54 | 0.43 |
| 32:BB:15:A:H2' | 32:BB:16:G:OP1 | 2.17 | 0.43 |
| 32:BB:45:A:H2' | 32:BB:46:A:H5' | 1.99 | 0.43 |
| 33:BD:186:HIS:C | 33:BD:186:HIS:CD2 | 2.91 | 0.43 |
| 31:BA:1797:C:O2' | 33:BD:259:THR:HB | 2.18 | 0.43 |
| 31:BA:574:C:N3 | 34:BE:145:LYS:HE2 | 2.32 | 0.43 |
| 35:BF:101:LEU:HD12 | 35:BF:102:PRO:N | 2.32 | 0.43 |
| 35:BF:24:LEU:O | 35:BF:25:PRO:C | 2.56 | 0.43 |
| 36:BG:128:ARG:O | 36:BG:129:GLY:C | 2.56 | 0.43 |
| 37:BH:85:LYS:HZ2 | 37:BH:133:VAL:CG2 | 2.30 | 0.43 |
| 39:BN:125:GLY:CA | 39:BN:126:PRO:O | 2.65 | 0.43 |
| 31:BA:631:A:OP1 | 41:BP:64:LYS:HE2 | 2.18 | 0.43 |
| 42:BQ:48:GLU:O | 42:BQ:52:VAL:HG13 | 2.18 | 0.43 |
| 42:BQ:70:PRO:HA | 42:BQ:95:ALA:HB2 | 2.00 | 0.43 |
| 44:BS:53:SER:C | 44:BS:55:ALA:N | 2.71 | 0.43 |
| 44:BS:80:LEU:HD12 | 44:BS:80:LEU:H | 1.83 | 0.43 |
| 40:BO:104:ARG:NH1 | 45:BT:35:LYS:HD3 | 2.33 | 0.43 |
| 45:BT:90:GLN:HG2 | 45:BT:120:ARG:CZ | 2.48 | 0.43 |
| 47:BV:19:LYS:HE2 | 47:BV:20:LEU:N | 2.32 | 0.43 |
| 49:BX:65:ARG:NE | 49:BX:66:LEU:N | 2.66 | 0.43 |
| 49:BX:59:VAL:HG22 | 49:BX:74:PRO:O | 2.17 | 0.43 |
| 42:BQ:141:GLN:C | 51:BZ:70:LEU:HD13 | 2.39 | 0.43 |
| 1:CA:1173:G:C5 | 1:CA:1174:G:N7 | 2.86 | 0.43 |
| 1:CA:292:G:H1 | 1:CA:308:C:H42 | 1.66 | 0.43 |
| 1:CA:356:A:C2' | 1:CA:357:G:O5' | 2.66 | 0.43 |
| 1:CA:583:A:H2' | 1:CA:584:G:O4' | 2.18 | 0.43 |
| 2:CB:166:ASP:CB | 2:CB:169:LYS:HB2 | 2.46 | 0.43 |
| 2:CB:44:LEU:H | 2:CB:44:LEU:CD1 | 2.23 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:61:LYS:CA | 4:CD:203:VAL:HG22 | 2.48 | 0.43 |
| 4:CD:68:TYR:HD1 | 4:CD:68:TYR:H | 1.60 | 0.43 |
| 7:CG:37:ASN:HD21 | 9:CI:40:LEU:HD22 | 1.83 | 0.43 |
| 7:CG:79:ARG:NE | 7:CG:84:ASN:HD21 | 2.16 | 0.43 |
| 11:CK:85:ARG:HA | 11:CK:112:THR:OG1 | 2.18 | 0.43 |
| 12:CL:70:ILE:HG13 | 12:CL:100:ILE:HD12 | 2.00 | 0.43 |
| 13:CM:29:ARG:HA | 13:CM:32:GLU:HB3 | 1.99 | 0.43 |
| 19:CS:4:SER:O | 19:CS:5:LEU:HB2 | 2.18 | 0.43 |
| 20:CT:29:LYS:O | 20:CT:33:ILE:HG12 | 2.18 | 0.43 |
| 23:D1:85:LEU:CB | 23:D1:87:PRO:HD3 | 2.48 | 0.43 |
| 25:D3:6:VAL:CG1 | 25:D3:54:VAL:CG1 | 2.91 | 0.43 |
| 31:DA:1034:G:H2' | 31:DA:1035:U:O4' | 2.17 | 0.43 |
| 31:DA:1115:G:H2' | 31:DA:1116:C:O4' | 2.17 | 0.43 |
| 31:DA:1364:G:H5'' | 31:DA:1365:A:OP2 | 2.17 | 0.43 |
| 31:DA:1450(A):C:C4 | 31:DA:1451:C:N4 | 2.86 | 0.43 |
| 31:DA:1509(A):A:C4 | 31:DA:1509(B):A:C8 | 3.05 | 0.43 |
| 31:DA:1510:G:H2' | 31:DA:1511:C:C6 | 2.52 | 0.43 |
| 31:DA:2232:U:O2' | 31:DA:2233:U:H5' | 2.18 | 0.43 |
| 31:DA:2270:G:C2' | 31:DA:2271:G:H5' | 2.48 | 0.43 |
| 22:D0:41:ARG:CB | 31:DA:2330:G:H1' | 2.48 | 0.43 |
| 22:D0:20:ARG:HG3 | 31:DA:2356:C:H4' | 2.00 | 0.43 |
| 31:DA:945:A:C6 | 31:DA:2448:A:C4 | 3.06 | 0.43 |
| 31:DA:2448:A:H4' | 31:DA:2449:U:OP2 | 2.17 | 0.43 |
| 31:DA:2469:A:O2' | 42:DQ:56:ARG:CG | 2.60 | 0.43 |
| 31:DA:2579:C:H2' | 31:DA:2580:U:O4' | 2.18 | 0.43 |
| 31:DA:2885:C:H2' | 31:DA:2886:G:O5' | 2.18 | 0.43 |
| 31:DA:511:U:C5 | 31:DA:512:G:C5 | 3.06 | 0.43 |
| 31:DA:775:G:C4 | 31:DA:794:G:C8 | 3.05 | 0.43 |
| 31:DA:84:A:H5'' | 50:DY:9:LYS:CD | 2.47 | 0.43 |
| 31:DA:8:A:H2' | 31:DA:9:U:H5 | 1.77 | 0.43 |
| 32:DB:82:G:C2' | 32:DB:83:G:C5' | 2.90 | 0.43 |
| 32:DB:87:G:H3' | 32:DB:88:C:C5' | 2.44 | 0.43 |
| 33:DD:125:ILE:HG13 | 33:DD:137:PRO:CG | 2.48 | 0.43 |
| 33:DD:186:HIS:CD2 | 33:DD:188:GLU:N | 2.59 | 0.43 |
| 33:DD:231:HIS:ND1 | 33:DD:232:PRO:HD2 | 2.33 | 0.43 |
| 33:DD:249:PRO:HD2 | 33:DD:250:TRP:CZ3 | 2.52 | 0.43 |
| 33:DD:31:LYS:O | 33:DD:31:LYS:HG3 | 2.17 | 0.43 |
| 33:DD:35:LYS:HG2 | 33:DD:64:ILE:H | 1.79 | 0.43 |
| 34:DE:13:ARG:HA | 34:DE:21:VAL:O | 2.18 | 0.43 |
| 34:DE:77:ILE:CG2 | 34:DE:78:LEU:N | 2.80 | 0.43 |
| 37:DH:85:LYS:NZ | 37:DH:145:ALA:CA | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:DI:99:GLU:HG3 | 38:DI:103:ARG:NH1 | 2.32 | 0.43 |
| 38:DI:9:LEU:HB2 | 38:DI:12:LEU:O | 2.18 | 0.43 |
| 39:DN:30:ILE:O | 39:DN:34:LEU:HD22 | 2.18 | 0.43 |
| 41:DP:107:LYS:C | 41:DP:109:GLY:N | 2.68 | 0.43 |
| 45:DT:121:ILE:O | 45:DT:124:ASP:HB2 | 2.18 | 0.43 |
| 45:DT:41:ARG:NH1 | 45:DT:43:GLN:HB2 | 2.33 | 0.43 |
| 45:DT:78:LEU:O | 45:DT:79:HIS:ND1 | 2.51 | 0.43 |
| 49:DX:60:ARG:CG | 49:DX:72:LYS:H | 2.31 | 0.43 |
| 50:DY:81:LYS:HD3 | 50:DY:97:ARG:CG | 2.48 | 0.43 |
| 1:AA:1173:G:C5 | 1:AA:1174:G:N7 | 2.85 | 0.43 |
| 1:AA:1423:G:H5' | 40:BO:49:ARG:NH2 | 2.20 | 0.43 |
| 1:AA:22:G:H4' | 1:AA:885:G:C8 | 2.53 | 0.43 |
| 1:AA:418:C:N3 | 1:AA:426:G:C2 | 2.86 | 0.43 |
| 1:AA:540:G:H2' | 1:AA:541:G:O4' | 2.17 | 0.43 |
| 1:AA:293:G:H4' | 1:AA:609:A:N1 | 2.32 | 0.43 |
| 1:AA:669:U:C2 | 1:AA:670:G:C8 | 3.06 | 0.43 |
| 1:AA:921:U:H2' | 1:AA:922:G:O4' | 2.18 | 0.43 |
| 5:AE:11:ILE:HD12 | 5:AE:105:VAL:HA | 2.00 | 0.43 |
| 8:AH:91:ARG:NH1 | 17:AQ:33:GLY:HA3 | 2.33 | 0.43 |
| 9:AI:118:LYS:O | 9:AI:119:ALA:HB3 | 2.18 | 0.43 |
| 9:AI:81:ILE:O | 9:AI:85:LEU:HG | 2.18 | 0.43 |
| 16:AP:39:TYR:CD1 | 16:AP:40:ASP:N | 2.86 | 0.43 |
| 24:B2:45:SER:HA | 24:B2:47:ASN:ND2 | 2.33 | 0.43 |
| 31:BA:1504:C:O2' | 31:BA:1505:C:C5' | 2.66 | 0.43 |
| 31:BA:1810:A:H2' | 31:BA:1811:G:O4' | 2.17 | 0.43 |
| 1:AA:1407:C:O2 | 31:BA:1912:A:C2 | 2.72 | 0.43 |
| 31:BA:2094:G:O2' | 31:BA:2095:C:H5' | 2.16 | 0.43 |
| 31:BA:284:U:H2' | 31:BA:285:C:C6 | 2.53 | 0.43 |
| 31:BA:596:G:C5 | 31:BA:597:U:C5 | 3.06 | 0.43 |
| 31:BA:671:C:C6 | 31:BA:671:C:C5' | 2.97 | 0.43 |
| 31:BA:768:G:C6 | 31:BA:769:G:C5 | 3.06 | 0.43 |
| 31:BA:90:U:O2' | 31:BA:92:A:H5'' | 2.18 | 0.43 |
| 31:BA:917:A:C8 | 31:BA:917:A:H5' | 2.53 | 0.43 |
| 34:BE:13:ARG:HA | 34:BE:21:VAL:O | 2.18 | 0.43 |
| 34:BE:203:LYS:C | 34:BE:203:LYS:HD2 | 2.38 | 0.43 |
| 35:BF:106:ARG:HG2 | 35:BF:106:ARG:H | 1.57 | 0.43 |
| 36:BG:127:GLY:O | 36:BG:128:ARG:C | 2.56 | 0.43 |
| 37:BH:117:PRO:HB3 | 37:BH:123:PHE:HD1 | 1.82 | 0.43 |
| 37:BH:148:ILE:O | 37:BH:162:ILE:HD11 | 2.19 | 0.43 |
| 38:BI:38:LEU:O | 38:BI:40:THR:HG23 | 2.19 | 0.43 |
| 38:BI:60:GLU:HA | 38:BI:63:ALA:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BO:26:LYS:HE3 | 40:BO:37:ASP:OD1 | 2.18 | 0.43 |
| 41:BP:106:LEU:HD12 | 41:BP:106:LEU:HA | 1.84 | 0.43 |
| 43:BR:74:LYS:O | 43:BR:77:ARG:HB2 | 2.19 | 0.43 |
| 50:BY:81:LYS:HD3 | 50:BY:97:ARG:CG | 2.47 | 0.43 |
| 51:BZ:121:HIS:HB2 | 51:BZ:171:ILE:HA | 2.00 | 0.43 |
| 51:BZ:121:HIS:ND1 | 51:BZ:169:GLU:OE2 | 2.51 | 0.43 |
| 1:CA:1012:U:H6 | 1:CA:1012:U:O5' | 2.00 | 0.43 |
| 1:CA:1169:A:C2' | 1:CA:1170:A:C8 | 2.96 | 0.43 |
| 1:CA:119:A:N7 | 1:CA:288:A:C2 | 2.86 | 0.43 |
| 1:CA:1237:C:H42 | 1:CA:1337:G:H1 | 1.64 | 0.43 |
| 1:CA:1458:G:H2' | 1:CA:1459:C:H6 | 1.84 | 0.43 |
| 1:CA:273:A:N6 | 1:CA:274:A:N6 | 2.66 | 0.43 |
| 1:CA:292:G:N7 | 1:CA:293:G:H1' | 2.33 | 0.43 |
| 1:CA:51:A:H4' | 1:CA:52:G:C5' | 2.48 | 0.43 |
| 1:CA:579:G:C5 | 1:CA:580:U:C4 | 3.06 | 0.43 |
| 1:CA:595:G:H1' | 1:CA:596:C:H5 | 1.83 | 0.43 |
| 1:CA:60:A:H4' | 1:CA:61:G:O5' | 2.19 | 0.43 |
| 1:CA:719:C:O2' | 18:CR:49:LYS:HB3 | 2.18 | 0.43 |
| 2:CB:102:LEU:HD12 | 2:CB:102:LEU:N | 2.33 | 0.43 |
| 2:CB:118:LEU:HD11 | 2:CB:141:GLU:HG2 | 1.99 | 0.43 |
| 2:CB:154:LEU:HD23 | 2:CB:154:LEU:H | 1.83 | 0.43 |
| 7:CG:145:ALA:O | 7:CG:146:GLU:HB2 | 2.18 | 0.43 |
| 8:CH:27:PRO:HA | 8:CH:58:TYR:HA | 1.99 | 0.43 |
| 15:CO:57:LEU:HD23 | 15:CO:57:LEU:HA | 1.80 | 0.43 |
| 15:CO:62:GLN:O | 15:CO:65:ARG:HB2 | 2.18 | 0.43 |
| 22:D0:14:ARG:HD2 | 31:DA:2280:G:O6 | 2.18 | 0.43 |
| 22:D0:65:GLY:HA2 | 22:D0:84:LEU:CD2 | 2.48 | 0.43 |
| 23:D1:11:ARG:CB | 23:D1:12:PRO:CD | 2.95 | 0.43 |
| 23:D1:63:ALA:O | 23:D1:64:ALA:C | 2.56 | 0.43 |
| 23:D1:64:ALA:O | 23:D1:65:SER:HB3 | 2.17 | 0.43 |
| 24:D2:14:ARG:CD | 24:D2:57:ILE:HB | 2.48 | 0.43 |
| 30:D8:35:GLN:HB3 | 30:D8:35:GLN:HE21 | 1.55 | 0.43 |
| 31:DA:1039:G:O2' | 31:DA:1040:C:H5' | 2.18 | 0.43 |
| 31:DA:1154:G:O5' | 31:DA:1154:G:H8 | 2.01 | 0.43 |
| 31:DA:1175:U:H4' | 31:DA:1176:G:H2' | 2.00 | 0.43 |
| 31:DA:1411:C:O2' | 31:DA:1412:A:H5' | 2.17 | 0.43 |
| 31:DA:749:C:C5 | 31:DA:1618:A:C6 | 3.06 | 0.43 |
| 31:DA:1805:U:O2 | 33:DD:50:THR:HB | 2.18 | 0.43 |
| 31:DA:1810:A:H2' | 31:DA:1811:G:O4' | 2.18 | 0.43 |
| 31:DA:1897:G:H2' | 31:DA:1898:U:O4' | 2.18 | 0.43 |
| 31:DA:1992:G:C2 | 31:DA:1997:G:C5 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:2387:U:H5'' | 31:DA:2388:A:OP2 | 2.17 | 0.43 |
| 31:DA:2391:G:O6 | 31:DA:2425:A:H8 | 2.00 | 0.43 |
| 31:DA:338:G:H2' | 31:DA:339:U:C6 | 2.53 | 0.43 |
| 31:DA:465:G:C6 | 31:DA:466:A:N6 | 2.86 | 0.43 |
| 31:DA:540:C:H2' | 31:DA:541:C:H6 | 1.83 | 0.43 |
| 31:DA:740:U:H2' | 31:DA:741:G:H8 | 1.83 | 0.43 |
| 31:DA:855:G:C6 | 31:DA:856:C:C4 | 3.06 | 0.43 |
| 31:DA:921:G:H2' | 31:DA:922:U:C6 | 2.54 | 0.43 |
| 33:DD:79:VAL:CG2 | 33:DD:111:LEU:HD11 | 2.48 | 0.43 |
| 37:DH:157:TYR:CD1 | 37:DH:171:LEU:N | 2.85 | 0.43 |
| 37:DH:89:ILE:HB | 37:DH:90:LYS:H | 1.61 | 0.43 |
| 38:DI:124:GLY:N | 38:DI:142:VAL:HG23 | 2.33 | 0.43 |
| 40:DO:6:THR:HG22 | 40:DO:7:TYR:N | 2.33 | 0.43 |
| 41:DP:17:LYS:O | 41:DP:19:VAL:HG23 | 2.18 | 0.43 |
| 42:DQ:27:VAL:HG23 | 51:DZ:81:ARG:HH22 | 1.84 | 0.43 |
| 43:DR:67:LEU:O | 43:DR:70:LEU:O | 2.36 | 0.43 |
| 47:DV:40:LEU:CD1 | 47:DV:40:LEU:C | 2.86 | 0.43 |
| 48:DW:7:ALA:N | 48:DW:103:ILE:O | 2.45 | 0.43 |
| 1:AA:1142:G:H2' | 1:AA:1143:G:O4' | 2.19 | 0.43 |
| 1:AA:262:A:N1 | 1:AA:263:A:C6 | 2.85 | 0.43 |
| 1:AA:321:A:N6 | 1:AA:329:A:OP2 | 2.52 | 0.43 |
| 1:AA:375:U:C4 | 1:AA:376:G:N7 | 2.87 | 0.43 |
| 1:AA:66:G:H4' | 1:AA:173:U:C4 | 2.53 | 0.43 |
| 1:AA:790:A:C6 | 1:AA:791:G:C6 | 3.06 | 0.43 |
| 5:AE:71:LEU:HD11 | 5:AE:114:GLY:HA3 | 2.00 | 0.43 |
| 7:AG:145:ALA:O | 7:AG:146:GLU:HB2 | 2.18 | 0.43 |
| 7:AG:149:ARG:O | 7:AG:149:ARG:HG2 | 2.19 | 0.43 |
| 8:AH:36:LEU:HD23 | 8:AH:36:LEU:HA | 1.80 | 0.43 |
| 11:AK:83:ILE:HA | 11:AK:109:VAL:O | 2.18 | 0.43 |
| 13:AM:76:ALA:HA | 13:AM:79:LYS:HD2 | 2.00 | 0.43 |
| 14:AN:13:THR:N | 14:AN:14:PRO:CD | 2.81 | 0.43 |
| 1:AA:976:G:P | 14:AN:32:SER:H | 2.40 | 0.43 |
| 17:AQ:8:GLY:HA3 | 17:AQ:22:LEU:O | 2.18 | 0.43 |
| 30:B8:31:HIS:O | 30:B8:33:ASN:N | 2.51 | 0.43 |
| 31:BA:107:C:C4 | 31:BA:108:U:C5 | 3.05 | 0.43 |
| 31:BA:1721:G:N2 | 31:BA:1739:U:OP2 | 2.51 | 0.43 |
| 31:BA:1930:G:O2' | 31:BA:1931:U:P | 2.76 | 0.43 |
| 31:BA:481:G:C4 | 31:BA:507:A:C2 | 3.07 | 0.43 |
| 31:BA:774:A:N1 | 31:BA:787:U:O2' | 2.46 | 0.43 |
| 31:BA:783:A:C3' | 31:BA:783:A:C8 | 3.01 | 0.43 |
| 33:BD:159:ALA:C | 33:BD:161:THR:H | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BD:17:THR:CG2 | 33:BD:205:VAL:N | 2.61 | 0.43 |
| 33:BD:65:ILE:HD11 | 33:BD:67:PHE:CZ | 2.46 | 0.43 |
| 38:BI:52:ARG:HE | 38:BI:52:ARG:HB3 | 1.51 | 0.43 |
| 39:BN:75:TYR:HD1 | 39:BN:75:TYR:N | 2.14 | 0.43 |
| 39:BN:82:LEU:CD1 | 39:BN:82:LEU:H | 2.23 | 0.43 |
| 41:BP:96:THR:HG22 | 41:BP:126:VAL:HG23 | 2.00 | 0.43 |
| 46:BU:45:TYR:O | 46:BU:49:HIS:CG | 2.71 | 0.43 |
| 46:BU:74:LEU:N | 46:BU:74:LEU:CD1 | 2.77 | 0.43 |
| 49:BX:34:ALA:N | 49:BX:35:THR:HG22 | 2.34 | 0.43 |
| 50:BY:7:VAL:HB | 50:BY:8:LYS:CE | 2.48 | 0.43 |
| 1:CA:1038:C:H2' | 1:CA:1039:C:C6 | 2.54 | 0.43 |
| 1:CA:117:G:O2' | 1:CA:118:U:H5' | 2.18 | 0.43 |
| 1:CA:173:U:C6 | 1:CA:197:A:C2 | 3.07 | 0.43 |
| 1:CA:432:A:N7 | 1:CA:433:C:C4 | 2.85 | 0.43 |
| 1:CA:445:G:N3 | 1:CA:446:G:C8 | 2.86 | 0.43 |
| 1:CA:521:G:O2' | 1:CA:522:C:H5' | 2.18 | 0.43 |
| 1:CA:567:G:C2 | 1:CA:568:G:H1' | 2.53 | 0.43 |
| 1:CA:721:G:N1 | 1:CA:733:A:C2 | 2.86 | 0.43 |
| 1:CA:782:A:O3' | 1:CA:1515:C:H4' | 2.18 | 0.43 |
| 1:CA:883:C:C2' | 1:CA:884:U:H5' | 2.48 | 0.43 |
| 1:CA:928:G:C2 | 1:CA:1390:U:O2 | 2.71 | 0.43 |
| 3:CC:127:ARG:HD2 | 3:CC:127:ARG:N | 2.33 | 0.43 |
| 9:CI:5:TYR:CD2 | 9:CI:18:PHE:CE2 | 3.07 | 0.43 |
| 22:D0:47:PRO:HB3 | 22:D0:51:VAL:HG12 | 1.99 | 0.43 |
| 31:DA:1407:C:C2' | 31:DA:1407:C:O2 | 2.65 | 0.43 |
| 31:DA:1476:C:C2' | 31:DA:1477:A:O5' | 2.66 | 0.43 |
| 31:DA:1495:A:H2' | 31:DA:1496:A:C2 | 2.53 | 0.43 |
| 31:DA:1914:C:H2' | 31:DA:1915:U:O4' | 2.18 | 0.43 |
| 31:DA:2085:C:O2' | 31:DA:2086:U:H5' | 2.18 | 0.43 |
| 31:DA:2288:A:H8 | 31:DA:2288:A:O5' | 2.01 | 0.43 |
| 31:DA:2338:G:O2' | 31:DA:2339:G:H5' | 2.18 | 0.43 |
| 31:DA:2291:U:O2' | 31:DA:2374:C:O2 | 2.33 | 0.43 |
| 31:DA:2464:C:HO2' | 31:DA:2465:C:P | 2.39 | 0.43 |
| 31:DA:2659:G:H5'' | 31:DA:2659:G:H8 | 1.83 | 0.43 |
| 31:DA:2687:U:C4 | 31:DA:2688:U:C5 | 3.07 | 0.43 |
| 31:DA:2827:C:H2' | 31:DA:2828:C:C6 | 2.53 | 0.43 |
| 31:DA:705:A:C2 | 31:DA:706:A:C4 | 3.06 | 0.43 |
| 31:DA:783:A:H3' | 31:DA:783:A:C8 | 2.54 | 0.43 |
| 31:DA:807:U:C2' | 31:DA:808:G:O5' | 2.66 | 0.43 |
| 32:DB:87:G:C2' | 32:DB:88:C:H5'' | 2.48 | 0.43 |
| 32:DB:88:C:C4 | 32:DB:89:G:C6 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DD:209:ALA:O | 33:DD:210:GLY:O | 2.35 | 0.43 |
| 37:DH:83:TYR:N | 37:DH:83:TYR:CD1 | 2.86 | 0.43 |
| 40:DO:87:ILE:HG23 | 40:DO:91:LEU:HA | 2.01 | 0.43 |
| 31:DA:637:A:OP1 | 41:DP:133:SER:HB3 | 2.18 | 0.43 |
| 45:DT:35:LYS:C | 45:DT:37:GLY:N | 2.71 | 0.43 |
| 47:DV:23:GLU:O | 47:DV:24:LYS:C | 2.55 | 0.43 |
| 50:DY:80:GLY:O | 50:DY:81:LYS:CB | 2.66 | 0.43 |
| 51:DZ:121:HIS:HB2 | 51:DZ:171:ILE:HA | 2.00 | 0.43 |
| 1:AA:1014:A:H2 | 1:AA:1219:U:O2 | 2.00 | 0.43 |
| 1:AA:1055:A:N3 | 3:AC:156:ARG:NH1 | 2.64 | 0.43 |
| 1:AA:108:G:H5'' | 1:AA:109:A:C5' | 2.46 | 0.43 |
| 1:AA:1125:U:C2' | 1:AA:1126:U:OP2 | 2.66 | 0.43 |
| 1:AA:327:A:C5 | 1:AA:329:A:C5 | 3.05 | 0.43 |
| 1:AA:724:G:C2 | 1:AA:725:G:C8 | 3.05 | 0.43 |
| 1:AA:666:G:C6 | 1:AA:741:G:C5 | 3.06 | 0.43 |
| 1:AA:575:G:HO2' | 1:AA:821:G:H5' | 1.83 | 0.43 |
| 1:AA:833:U:C2 | 1:AA:834:C:C5 | 3.07 | 0.43 |
| 1:AA:853:G:H2' | 1:AA:854:G:C8 | 2.45 | 0.43 |
| 1:AA:93:G:N1 | 1:AA:96:U:C4 | 2.87 | 0.43 |
| 1:AA:989:C:H1' | 1:AA:1016:A:C2 | 2.53 | 0.43 |
| 1:AA:995:C:H1' | 14:AN:8:GLU:OE2 | 2.17 | 0.43 |
| 3:AC:6:HIS:HD2 | 3:AC:8:ILE:H | 1.65 | 0.43 |
| 4:AD:90:GLY:O | 4:AD:94:LEU:CD1 | 2.65 | 0.43 |
| 5:AE:114:GLY:O | 5:AE:115:VAL:O | 2.37 | 0.43 |
| 5:AE:137:GLU:O | 5:AE:141:GLN:HG3 | 2.18 | 0.43 |
| 5:AE:7:GLU:O | 5:AE:8:GLU:HB3 | 2.19 | 0.43 |
| 8:AH:104:ARG:CZ | 8:AH:138:TRP:CH2 | 3.00 | 0.43 |
| 1:AA:881:G:P | 12:AL:12:ARG:NH2 | 2.91 | 0.43 |
| 12:AL:46:LYS:CG | 12:AL:47:LYS:H | 2.22 | 0.43 |
| 1:AA:523:A:N6 | 12:AL:53:ARG:HH12 | 2.16 | 0.43 |
| 12:AL:70:ILE:HD12 | 12:AL:70:ILE:N | 2.32 | 0.43 |
| 17:AQ:74:LEU:HA | 17:AQ:74:LEU:HD22 | 1.75 | 0.43 |
| 18:AR:71:LYS:O | 18:AR:74:ARG:HB2 | 2.18 | 0.43 |
| 24:B2:30:ARG:HB3 | 24:B2:30:ARG:CZ | 2.47 | 0.43 |
| 24:B2:32:LEU:HD21 | 31:BA:61:G:O2' | 2.18 | 0.43 |
| 30:B8:8:LYS:HB3 | 30:B8:12:LYS:HE3 | 1.99 | 0.43 |
| 31:BA:1771:C:H1' | 31:BA:1786:A:C8 | 2.53 | 0.43 |
| 31:BA:1882:C:C5' | 31:BA:1883:G:OP2 | 2.55 | 0.43 |
| 31:BA:2078:C:O2' | 31:BA:2079:U:H5' | 2.18 | 0.43 |
| 31:BA:225:A:H2' | 31:BA:226:G:H5' | 1.99 | 0.43 |
| 31:BA:2359:C:N4 | 31:BA:2360:A:C6 | 2.87 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:2399:G:C6 | 31:BA:2400:G:C5 | 3.06 | 0.43 |
| 31:BA:2740:A:C6 | 31:BA:2764:A:C8 | 3.07 | 0.43 |
| 31:BA:721:C:C2 | 31:BA:722:A:C8 | 3.06 | 0.43 |
| 31:BA:902:C:O2' | 31:BA:903:C:H5' | 2.18 | 0.43 |
| 31:BA:906:G:H2' | 31:BA:907:U:O5' | 2.18 | 0.43 |
| 31:BA:870:A:C2 | 31:BA:908:C:C2 | 3.06 | 0.43 |
| 31:BA:848:G:C4 | 31:BA:933:A:C8 | 3.06 | 0.43 |
| 35:BF:7:TYR:HB3 | 35:BF:16:GLY:CA | 2.49 | 0.43 |
| 36:BG:63:ILE:HD13 | 36:BG:141:PHE:CZ | 2.53 | 0.43 |
| 37:BH:126:PRO:HB2 | 37:BH:130:ARG:HH12 | 1.83 | 0.43 |
| 44:BS:66:ALA:HA | 44:BS:69:VAL:HG12 | 2.01 | 0.43 |
| 45:BT:33:LYS:N | 45:BT:33:LYS:HZ2 | 2.15 | 0.43 |
| 45:BT:34:VAL:O | 45:BT:35:LYS:CB | 2.65 | 0.43 |
| 47:BV:16:PRO:O | 47:BV:98:GLU:OE2 | 2.37 | 0.43 |
| 50:BY:34:LYS:HE2 | 50:BY:34:LYS:HB3 | 1.74 | 0.43 |
| 50:BY:88:LYS:O | 50:BY:89:PHE:CB | 2.66 | 0.43 |
| 32:BB:92:C:H5'' | 51:BZ:79:ARG:HH22 | 1.84 | 0.43 |
| 1:CA:1503:A:O2' | 1:CA:1504:G:C5' | 2.65 | 0.43 |
| 1:CA:198:G:C2 | 1:CA:199:G:C8 | 3.06 | 0.43 |
| 1:CA:288:A:H2' | 1:CA:289:G:H4' | 2.00 | 0.43 |
| 1:CA:418:C:N3 | 1:CA:426:G:C2 | 2.87 | 0.43 |
| 1:CA:443:C:N3 | 1:CA:444:C:C5 | 2.86 | 0.43 |
| 1:CA:573:A:H2' | 1:CA:574:A:C8 | 2.54 | 0.43 |
| 1:CA:60:A:P | 1:CA:60:A:C8 | 3.07 | 0.43 |
| 1:CA:612:C:C2' | 1:CA:613:C:H5' | 2.48 | 0.43 |
| 1:CA:642:A:C5 | 8:CH:115:SER:HA | 2.53 | 0.43 |
| 1:CA:659:U:C2' | 1:CA:660:G:C5' | 2.95 | 0.43 |
| 1:CA:748:C:C4' | 1:CA:749:C:O5' | 2.58 | 0.43 |
| 1:CA:949:A:C6 | 1:CA:1233:G:C2 | 3.06 | 0.43 |
| 2:CB:105:PHE:C | 2:CB:107:THR:H | 2.21 | 0.43 |
| 3:CC:77:ILE:C | 3:CC:83:ARG:HB3 | 2.39 | 0.43 |
| 4:CD:19:LEU:HB2 | 4:CD:21:LEU:HD23 | 2.00 | 0.43 |
| 4:CD:59:ARG:HA | 4:CD:59:ARG:NE | 2.34 | 0.43 |
| 7:CG:108:ALA:O | 7:CG:111:ARG:HB2 | 2.19 | 0.43 |
| 8:CH:25:ASP:HA | 8:CH:59:LEU:O | 2.17 | 0.43 |
| 9:CI:6:GLY:HA3 | 9:CI:84:ALA:HB2 | 2.00 | 0.43 |
| 20:CT:74:LYS:C | 20:CT:76:ALA:H | 2.22 | 0.43 |
| 23:D1:33:LYS:C | 23:D1:34:THR:HG22 | 2.38 | 0.43 |
| 24:D2:14:ARG:CZ | 24:D2:57:ILE:HG22 | 2.48 | 0.43 |
| 27:D5:20:ARG:HG2 | 27:D5:23:HIS:CD2 | 2.53 | 0.43 |
| 31:DA:1043:C:O2' | 31:DA:1044:G:C8 | 2.58 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:1899:G:C2' | 31:DA:1900:A:OP2 | 2.66 | 0.43 |
| 31:DA:2078:C:O2' | 31:DA:2079:U:H5' | 2.19 | 0.43 |
| 31:DA:2400:G:C5 | 31:DA:2401:U:C5 | 3.06 | 0.43 |
| 31:DA:2635:C:C2' | 31:DA:2636:U:O5' | 2.66 | 0.43 |
| 31:DA:271(F):C:C4 | 31:DA:271(G):C:C5 | 3.07 | 0.43 |
| 31:DA:2787:C:O2 | 34:DE:61:ARG:NH1 | 2.50 | 0.43 |
| 31:DA:2821:A:H2' | 31:DA:2822:G:H8 | 1.82 | 0.43 |
| 31:DA:463:G:N1 | 31:DA:467:G:C6 | 2.87 | 0.43 |
| 31:DA:27:G:C4 | 31:DA:512:G:C2 | 3.07 | 0.43 |
| 31:DA:860:U:C5 | 31:DA:917:A:N7 | 2.86 | 0.43 |
| 32:DB:75:G:H5' | 32:DB:75:G:C8 | 2.42 | 0.43 |
| 31:DA:444:C:C4' | 35:DF:49:ALA:HB2 | 2.49 | 0.43 |
| 36:DG:41:GLN:HG2 | 36:DG:155:MET:CB | 2.38 | 0.43 |
| 36:DG:60:LEU:HA | 36:DG:63:ILE:HG12 | 2.00 | 0.43 |
| 39:DN:30:ILE:CD1 | 39:DN:99:LEU:HD11 | 2.48 | 0.43 |
| 42:DQ:35:VAL:HG23 | 42:DQ:100:GLY:C | 2.38 | 0.43 |
| 43:DR:56:LYS:HE2 | 43:DR:87:TYR:CB | 2.49 | 0.43 |
| 48:DW:92:ARG:O | 48:DW:93:ALA:HB3 | 2.17 | 0.43 |
| 50:DY:66:PRO:O | 50:DY:67:LEU:CB | 2.66 | 0.43 |
| 51:DZ:118:GLN:O | 51:DZ:120:ILE:HG12 | 2.18 | 0.43 |
| 1:AA:1168:A:C6 | 1:AA:1169:A:C6 | 3.07 | 0.43 |
| 1:AA:1209:C:O2' | 1:AA:1210:C:H5' | 2.18 | 0.43 |
| 1:AA:1285:A:H4' | 1:AA:1286:A:O5' | 2.18 | 0.43 |
| 1:AA:136:C:N4 | 1:AA:227:G:H1 | 2.17 | 0.43 |
| 1:AA:397:A:N3 | 1:AA:397:A:H5'' | 2.34 | 0.43 |
| 1:AA:473:G:C2 | 1:AA:474:G:C8 | 3.07 | 0.43 |
| 1:AA:560:U:H4' | 1:AA:561:U:O5' | 2.16 | 0.43 |
| 1:AA:587:G:O2' | 1:AA:588:G:OP2 | 2.32 | 0.43 |
| 1:AA:615:C:H2' | 1:AA:616:G:O4' | 2.18 | 0.43 |
| 1:AA:739:C:O2 | 1:AA:739:C:H2' | 2.19 | 0.43 |
| 9:AI:5:TYR:CD2 | 9:AI:18:PHE:CE2 | 3.06 | 0.43 |
| 13:AM:68:GLY:O | 13:AM:70:LEU:N | 2.51 | 0.43 |
| 10:AJ:62:HIS:CE1 | 14:AN:61:TRP:HH2 | 2.36 | 0.43 |
| 15:AO:17:ARG:HG2 | 15:AO:26:GLU:HG3 | 1.99 | 0.43 |
| 17:AQ:50:LYS:HE3 | 17:AQ:51:TYR:HE1 | 1.82 | 0.43 |
| 1:AA:130:A:C8 | 17:AQ:63:ARG:HG3 | 2.52 | 0.43 |
| 1:AA:986:A:H1' | 19:AS:54:GLY:O | 2.18 | 0.43 |
| 20:AT:38:LYS:HA | 20:AT:41:ILE:HD11 | 2.01 | 0.43 |
| 24:B2:14:ARG:NH1 | 24:B2:57:ILE:CG2 | 2.78 | 0.43 |
| 31:BA:1589:C:H2' | 31:BA:1590:U:C6 | 2.53 | 0.43 |
| 31:BA:2402:C:C3' | 31:BA:2403:C:H5' | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:2437:U:H2' | 31:BA:2438:U:C6 | 2.54 | 0.43 |
| 31:BA:2557:G:H2' | 31:BA:2558:C:H6 | 1.83 | 0.43 |
| 31:BA:2624:G:H2' | 31:BA:2625:G:H5' | 2.01 | 0.43 |
| 31:BA:2663:G:C6 | 31:BA:2664:G:C5 | 3.06 | 0.43 |
| 31:BA:1638:C:H5'' | 31:BA:2710:C:O2' | 2.18 | 0.43 |
| 31:BA:271(S):G:C5 | 31:BA:271(T):C:C5 | 3.06 | 0.43 |
| 31:BA:2808:U:C4 | 31:BA:2809:A:N7 | 2.87 | 0.43 |
| 31:BA:2808:U:O2' | 31:BA:2809:A:H5' | 2.17 | 0.43 |
| 31:BA:2788:C:O2' | 31:BA:2809:A:N3 | 2.45 | 0.43 |
| 32:BB:46:A:C2' | 32:BB:47:C:O5' | 2.67 | 0.43 |
| 33:BD:62:TYR:CE1 | 33:BD:64:ILE:HA | 2.53 | 0.43 |
| 36:BG:37:VAL:O | 36:BG:94:LEU:HG | 2.18 | 0.43 |
| 38:BI:128:LEU:HB3 | 38:BI:129:THR:H | 1.57 | 0.43 |
| 43:BR:74:LYS:CD | 43:BR:77:ARG:HH21 | 2.30 | 0.43 |
| 43:BR:83:ILE:O | 43:BR:84:ALA:C | 2.57 | 0.43 |
| 46:BU:88:ILE:HA | 46:BU:90:VAL:HG23 | 2.01 | 0.43 |
| 47:BV:69:LYS:HB2 | 47:BV:93:GLU:OE2 | 2.18 | 0.43 |
| 31:BA:64:A:O3' | 49:BX:68:ARG:O | 2.36 | 0.43 |
| 50:BY:41:GLY:O | 50:BY:42:VAL:C | 2.56 | 0.43 |
| 50:BY:45:VAL:HG22 | 50:BY:62:GLU:CB | 2.48 | 0.43 |
| 51:BZ:128:VAL:HG23 | 51:BZ:160:GLY:O | 2.19 | 0.43 |
| 1:CA:1065:U:H4' | 1:CA:1066:C:O5' | 2.19 | 0.43 |
| 1:CA:1067:A:N3 | 1:CA:1068:G:N9 | 2.67 | 0.43 |
| 1:CA:1079:G:H2' | 1:CA:1080:A:C8 | 2.52 | 0.43 |
| 1:CA:1118:C:H1' | 1:CA:1179:A:C4 | 2.53 | 0.43 |
| 1:CA:1293:G:O2' | 1:CA:1294:G:P | 2.76 | 0.43 |
| 1:CA:374:A:C4 | 1:CA:375:U:C5 | 3.07 | 0.43 |
| 1:CA:600:C:O2' | 1:CA:601:C:H5' | 2.18 | 0.43 |
| 1:CA:665:A:H1' | 1:CA:733:A:O4' | 2.17 | 0.43 |
| 1:CA:930:C:C4 | 1:CA:931:C:C5 | 3.06 | 0.43 |
| 8:CH:31:PHE:O | 8:CH:35:ILE:HG13 | 2.18 | 0.43 |
| 8:CH:38:ILE:O | 8:CH:42:GLU:HB2 | 2.19 | 0.43 |
| 10:CJ:51:ARG:HG3 | 10:CJ:60:ARG:C | 2.37 | 0.43 |
| 12:CL:44:THR:HA | 12:CL:45:PRO:HD3 | 1.86 | 0.43 |
| 12:CL:50:SER:O | 12:CL:51:ALA:HB2 | 2.17 | 0.43 |
| 12:CL:62:SER:C | 12:CL:64:TYR:N | 2.71 | 0.43 |
| 13:CM:45:VAL:HA | 13:CM:48:LEU:HD13 | 1.99 | 0.43 |
| 18:CR:40:LEU:O | 18:CR:43:PHE:HB2 | 2.17 | 0.43 |
| 20:CT:100:ILE:HD12 | 20:CT:100:ILE:N | 2.33 | 0.43 |
| 24:D2:49:LYS:HD3 | 31:DA:76:C:H5'' | 2.00 | 0.43 |
| 27:D5:31:VAL:O | 27:D5:39:MET:HA | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:D8:38:GLY:C | 30:D8:40:GLU:H | 2.22 | 0.43 |
| 31:DA:1338:G:O2' | 31:DA:1339:G:H5' | 2.18 | 0.43 |
| 31:DA:1740:G:H4' | 31:DA:1741:A:OP1 | 2.18 | 0.43 |
| 31:DA:1742:G:C8 | 31:DA:1742:G:C3' | 3.01 | 0.43 |
| 31:DA:1826:G:H2' | 31:DA:1827:C:C6 | 2.54 | 0.43 |
| 31:DA:1882:C:C5' | 31:DA:1883:G:OP2 | 2.58 | 0.43 |
| 31:DA:2259:G:C2 | 31:DA:2282:G:C6 | 3.07 | 0.43 |
| 31:DA:225:A:H2' | 31:DA:226:G:H5' | 2.00 | 0.43 |
| 31:DA:2564:A:C6 | 31:DA:2565:A:C6 | 3.06 | 0.43 |
| 31:DA:2772:C:H2' | 31:DA:2773:C:H6 | 1.83 | 0.43 |
| 33:DD:35:LYS:H | 33:DD:64:ILE:CG2 | 2.30 | 0.43 |
| 35:DF:8:GLN:HG3 | 35:DF:8:GLN:O | 2.17 | 0.43 |
| 38:DI:10:GLU:C | 38:DI:12:LEU:H | 2.21 | 0.43 |
| 39:DN:25:ARG:CG | 39:DN:25:ARG:HH11 | 2.28 | 0.43 |
| 40:DO:2:ILE:N | 40:DO:2:ILE:HD13 | 2.33 | 0.43 |
| 41:DP:48:PRO:CG | 41:DP:49:ARG:N | 2.81 | 0.43 |
| 42:DQ:36:ALA:O | 42:DQ:100:GLY:N | 2.50 | 0.43 |
| 43:DR:9:LYS:O | 43:DR:10:LEU:CG | 2.66 | 0.43 |
| 46:DU:61:TRP:CD2 | 46:DU:94:ASN:HA | 2.54 | 0.43 |
| 46:DU:80:ILE:HD13 | 46:DU:80:ILE:HA | 1.83 | 0.43 |
| 46:DU:92:ARG:NH2 | 47:DV:11:GLN:H | 2.16 | 0.43 |
| 47:DV:62:LEU:HD12 | 47:DV:96:ILE:HD13 | 1.99 | 0.43 |
| 49:DX:65:ARG:O | 49:DX:66:LEU:CB | 2.66 | 0.43 |
| 49:DX:60:ARG:HG2 | 49:DX:72:LYS:H | 1.83 | 0.43 |
| 49:DX:89:ILE:O | 49:DX:89:ILE:CG2 | 2.65 | 0.43 |
| 50:DY:41:GLY:O | 50:DY:43:ASN:OD1 | 2.37 | 0.43 |
| 51:DZ:42:VAL:HG13 | 51:DZ:43:GLU:H | 1.84 | 0.43 |
| 1:AA:12:U:H4' | 1:AA:526:C:O2' | 2.18 | 0.43 |
| 1:AA:273:A:N6 | 1:AA:274:A:N6 | 2.67 | 0.43 |
| 1:AA:503:C:O2 | 1:AA:510:A:H2 | 2.02 | 0.43 |
| 2:AB:174:VAL:O | 2:AB:178:ARG:HB2 | 2.18 | 0.43 |
| 3:AC:153:VAL:HG12 | 3:AC:154:SER:N | 2.34 | 0.43 |
| 4:AD:62:GLN:HA | 4:AD:62:GLN:NE2 | 2.33 | 0.43 |
| 10:AJ:22:LYS:C | 10:AJ:24:VAL:H | 2.21 | 0.43 |
| 14:AN:46:GLU:O | 14:AN:50:LYS:HG3 | 2.18 | 0.43 |
| 17:AQ:60:ILE:HG12 | 17:AQ:61:GLU:N | 2.33 | 0.43 |
| 17:AQ:59:ILE:HG21 | 17:AQ:71:PHE:HB3 | 1.97 | 0.43 |
| 31:BA:1044:G:N1 | 31:BA:1112:G:O6 | 2.51 | 0.43 |
| 31:BA:1106:A:H2' | 31:BA:1107:G:C8 | 2.54 | 0.43 |
| 31:BA:1436:G:H2' | 31:BA:1437:C:O4' | 2.19 | 0.43 |
| 31:BA:1667:G:H4' | 31:BA:1668:A:OP1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:1689:A:H62 | 31:BA:1698:A:H2 | 1.66 | 0.43 |
| 31:BA:1946:U:H2' | 31:BA:1947:C:H6 | 1.83 | 0.43 |
| 31:BA:2103:C:C2 | 31:BA:2187:G:N1 | 2.87 | 0.43 |
| 31:BA:2662:A:H5' | 31:BA:2663:G:H1' | 2.01 | 0.43 |
| 31:BA:2681:C:H2' | 31:BA:2681:C:O2 | 2.19 | 0.43 |
| 31:BA:388:G:O2' | 31:BA:389:G:N7 | 2.46 | 0.43 |
| 31:BA:672:C:O2' | 31:BA:673:C:H5' | 2.19 | 0.43 |
| 31:BA:683:C:H6 | 31:BA:683:C:O5' | 2.01 | 0.43 |
| 31:BA:921:G:H2' | 31:BA:922:U:C6 | 2.54 | 0.43 |
| 34:BE:119:ARG:HB3 | 34:BE:120:TRP:CD1 | 2.53 | 0.43 |
| 34:BE:147:PRO:HB2 | 34:BE:149:ARG:HG2 | 2.01 | 0.43 |
| 34:BE:24:THR:HG23 | 34:BE:184:VAL:HG23 | 2.00 | 0.43 |
| 34:BE:34:VAL:HG23 | 34:BE:34:VAL:O | 2.18 | 0.43 |
| 35:BF:7:TYR:HB3 | 35:BF:16:GLY:N | 2.33 | 0.43 |
| 26:B4:14:ILE:CB | 36:BG:5:VAL:HG13 | 2.49 | 0.43 |
| 37:BH:46:GLU:O | 37:BH:47:GLU:HB2 | 2.19 | 0.43 |
| 40:BO:1:MET:HB2 | 40:BO:32:TYR:HB3 | 2.00 | 0.43 |
| 1:CA:1034:G:N2 | 1:CA:1035:A:N6 | 2.67 | 0.43 |
| 1:CA:1138:G:N1 | 1:CA:1140:C:C2 | 2.87 | 0.43 |
| 1:CA:1311:G:N2 | 1:CA:1327:C:C2 | 2.87 | 0.43 |
| 1:CA:1366:C:H2' | 1:CA:1367:C:C6 | 2.53 | 0.43 |
| 1:CA:148:G:C2 | 1:CA:149:A:N7 | 2.87 | 0.43 |
| 1:CA:234:C:C2 | 1:CA:235:C:C5 | 3.06 | 0.43 |
| 1:CA:537:G:OP1 | 12:CL:113:ARG:NH2 | 2.51 | 0.43 |
| 1:CA:69:G:N2 | 1:CA:70:G:C4 | 2.87 | 0.43 |
| 1:CA:764:C:C2' | 1:CA:765:G:O5' | 2.67 | 0.43 |
| 1:CA:824:C:H4' | 8:CH:1:MET:H1 | 1.83 | 0.43 |
| 1:CA:855:G:C2 | 1:CA:856:C:C2 | 3.07 | 0.43 |
| 1:CA:9:G:N3 | 1:CA:9:G:H2' | 2.33 | 0.43 |
| 13:CM:68:GLY:O | 13:CM:70:LEU:N | 2.52 | 0.43 |
| 14:CN:12:ARG:C | 14:CN:14:PRO:CD | 2.87 | 0.43 |
| 1:CA:995:C:H1' | 14:CN:8:GLU:OE2 | 2.18 | 0.43 |
| 19:CS:69:HIS:HB2 | 19:CS:74:PHE:CE2 | 2.51 | 0.43 |
| 20:CT:26:ASN:HB3 | 20:CT:71:THR:OG1 | 2.19 | 0.43 |
| 24:D2:14:ARG:NH1 | 24:D2:57:ILE:CG2 | 2.79 | 0.43 |
| 26:D4:2:LYS:CB | 32:DB:40:U:O4 | 2.66 | 0.43 |
| 30:D8:37:SER:HB2 | 30:D8:38:GLY:H | 1.46 | 0.43 |
| 30:D8:51:ALA:CA | 30:D8:53:PRO:HD2 | 2.48 | 0.43 |
| 31:DA:1028:A:N3 | 31:DA:2486:G:O2' | 2.38 | 0.43 |
| 31:DA:105:C:H2' | 31:DA:106:C:H6 | 1.83 | 0.43 |
| 31:DA:1495:A:OP2 | 31:DA:1495:A:O4' | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:1545:A:H2' | 31:DA:1546:C:O5' | 2.18 | 0.43 |
| 31:DA:154:G:O5' | 31:DA:154:G:H8 | 2.01 | 0.43 |
| 31:DA:2408:U:H2' | 31:DA:2409:G:C8 | 2.53 | 0.43 |
| 31:DA:2645:G:C3' | 31:DA:2646:C:H5' | 2.48 | 0.43 |
| 31:DA:2674:G:H2' | 31:DA:2675:A:O4' | 2.18 | 0.43 |
| 31:DA:2880:C:H1' | 43:DR:92:GLY:O | 2.18 | 0.43 |
| 31:DA:292:C:H2' | 31:DA:293:U:H6 | 1.83 | 0.43 |
| 34:DE:116:VAL:HG13 | 34:DE:122:PHE:CB | 2.48 | 0.43 |
| 35:DF:64:ILE:HD12 | 35:DF:65:TRP:CE2 | 2.54 | 0.43 |
| 36:DG:111:LEU:N | 36:DG:112:PRO:CD | 2.82 | 0.43 |
| 38:DI:78:THR:OG1 | 38:DI:141:LYS:HD2 | 2.19 | 0.43 |
| 39:DN:45:ASN:N | 39:DN:45:ASN:ND2 | 2.63 | 0.43 |
| 41:DP:127:ALA:HB3 | 41:DP:130:PHE:CE2 | 2.54 | 0.43 |
| 42:DQ:141:GLN:CD | 51:DZ:70:LEU:HB3 | 2.39 | 0.43 |
| 42:DQ:19:GLY:O | 42:DQ:21:THR:N | 2.48 | 0.43 |
| 43:DR:23:ASN:N | 43:DR:23:ASN:HD22 | 2.15 | 0.43 |
| 44:DS:54:LEU:HD22 | 44:DS:58:LEU:O | 2.19 | 0.43 |
| 45:DT:109:GLU:HA | 45:DT:112:ARG:HG2 | 1.99 | 0.43 |
| 46:DU:90:VAL:HG11 | 47:DV:40:LEU:HB3 | 2.01 | 0.43 |
| 47:DV:61:VAL:HG12 | 47:DV:99:ILE:HB | 2.00 | 0.43 |
| 31:DA:1614:A:H62 | 48:DW:87:PRO:HA | 1.83 | 0.43 |
| 49:DX:76:ARG:HD2 | 49:DX:77:LYS:HB2 | 1.99 | 0.43 |
| 1:AA:1138:G:N1 | 1:AA:1140:C:C2 | 2.86 | 0.43 |
| 1:AA:1203:C:H2' | 1:AA:1204:A:C8 | 2.53 | 0.43 |
| 1:AA:1260:C:H4' | 1:AA:1284:C:H5' | 2.00 | 0.43 |
| 1:AA:1347:G:O2' | 1:AA:1348:U:P | 2.77 | 0.43 |
| 1:AA:1386:G:C2 | 1:AA:1387:G:N7 | 2.86 | 0.43 |
| 1:AA:148:G:C2 | 1:AA:149:A:N7 | 2.86 | 0.43 |
| 1:AA:318:G:N3 | 1:AA:319:G:C8 | 2.87 | 0.43 |
| 1:AA:356:A:C2' | 1:AA:357:G:O5' | 2.66 | 0.43 |
| 1:AA:414:A:H2' | 1:AA:415:A:O4' | 2.17 | 0.43 |
| 1:AA:539:A:H2' | 1:AA:540:G:H8 | 1.79 | 0.43 |
| 1:AA:574:A:H5'' | 1:AA:575:G:OP2 | 2.19 | 0.43 |
| 1:AA:625:G:H2' | 1:AA:626:U:H6 | 1.83 | 0.43 |
| 1:AA:673:G:C2 | 1:AA:674:G:C6 | 3.06 | 0.43 |
| 1:AA:801:U:H2' | 1:AA:802:A:C8 | 2.54 | 0.43 |
| 1:AA:577:G:H1' | 1:AA:816:A:N3 | 2.33 | 0.43 |
| 1:AA:949:A:C6 | 1:AA:1233:G:C2 | 3.07 | 0.43 |
| 2:AB:17:PHE:H | 2:AB:17:PHE:HD2 | 1.66 | 0.43 |
| 2:AB:163:PHE:CD2 | 2:AB:185:ILE:HG13 | 2.52 | 0.43 |
| 2:AB:88:ALA:HB1 | 2:AB:222:ILE:HG21 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:77:ILE:O | 3:AC:83:ARG:HB3 | 2.18 | 0.43 |
| 4:AD:96:LEU:N | 4:AD:96:LEU:HD22 | 2.34 | 0.43 |
| 5:AE:110:LEU:HD12 | 5:AE:118:ILE:HG21 | 2.01 | 0.43 |
| 5:AE:132:ALA:O | 5:AE:133:TYR:C | 2.56 | 0.43 |
| 6:AF:100:ASN:ND2 | 18:AR:23:LYS:HE3 | 2.33 | 0.43 |
| 6:AF:8:ILE:HG22 | 6:AF:9:VAL:H | 1.82 | 0.43 |
| 9:AI:17:VAL:HG22 | 9:AI:63:ILE:CG1 | 2.49 | 0.43 |
| 12:AL:50:SER:O | 12:AL:51:ALA:HB2 | 2.19 | 0.43 |
| 12:AL:53:ARG:HG2 | 12:AL:53:ARG:HH11 | 1.84 | 0.43 |
| 1:AA:1329:A:P | 13:AM:28:ALA:HB3 | 2.58 | 0.43 |
| 20:AT:100:ILE:O | 20:AT:100:ILE:HG22 | 2.19 | 0.43 |
| 24:B2:47:ASN:ND2 | 24:B2:48:HIS:H | 2.16 | 0.43 |
| 27:B5:41:PRO:O | 27:B5:44:THR:OG1 | 2.35 | 0.43 |
| 30:B8:29:LYS:HB2 | 30:B8:44:LYS:HG2 | 1.99 | 0.43 |
| 30:B8:48:PHE:N | 30:B8:48:PHE:CD1 | 2.85 | 0.43 |
| 31:BA:1478:G:O2' | 31:BA:1558:A:C2 | 2.72 | 0.43 |
| 31:BA:1884:A:C2 | 31:BA:1885:A:C4 | 3.06 | 0.43 |
| 31:BA:1900:A:N1 | 31:BA:1970:A:C6 | 2.87 | 0.43 |
| 31:BA:2094:G:OP1 | 38:BI:22:LYS:HD3 | 2.19 | 0.43 |
| 31:BA:2096:U:H3 | 31:BA:2193:G:H1 | 1.66 | 0.43 |
| 31:BA:2280:G:C2' | 31:BA:2281:C:H5' | 2.49 | 0.43 |
| 31:BA:286:C:N4 | 31:BA:356:G:C6 | 2.87 | 0.43 |
| 32:BB:93:G:H2' | 32:BB:94:C:H6 | 1.84 | 0.43 |
| 31:BA:1673:U:C5 | 34:BE:129:HIS:CD2 | 3.07 | 0.43 |
| 36:BG:101:ILE:HG23 | 36:BG:102:PHE:N | 2.33 | 0.43 |
| 36:BG:96:ARG:O | 36:BG:97:ASP:C | 2.56 | 0.43 |
| 31:BA:1131:G:OP1 | 39:BN:80:GLY:HA2 | 2.19 | 0.43 |
| 40:BO:106:LEU:HA | 40:BO:106:LEU:HD23 | 1.81 | 0.43 |
| 45:BT:15:VAL:O | 45:BT:15:VAL:HG22 | 2.19 | 0.43 |
| 47:BV:1:MET:H1 | 47:BV:44:LYS:HD2 | 1.84 | 0.43 |
| 47:BV:5:VAL:HG22 | 47:BV:6:LYS:N | 2.34 | 0.43 |
| 48:BW:111:HIS:CG | 48:BW:112:GLY:N | 2.84 | 0.43 |
| 49:BX:57:LEU:O | 49:BX:76:ARG:N | 2.44 | 0.43 |
| 49:BX:65:ARG:O | 49:BX:66:LEU:HB3 | 2.18 | 0.43 |
| 49:BX:77:LYS:CD | 49:BX:78:LYS:HG3 | 2.48 | 0.43 |
| 50:BY:39:VAL:CG1 | 50:BY:40:GLU:H | 2.25 | 0.43 |
| 51:BZ:125:LEU:HD23 | 51:BZ:126:VAL:H | 1.82 | 0.43 |
| 1:CA:1054:C:OP1 | 1:CA:1197:G:OP2 | 2.36 | 0.43 |
| 1:CA:1209:C:O2' | 1:CA:1210:C:H5' | 2.18 | 0.43 |
| 1:CA:272:C:H2' | 1:CA:273:A:C8 | 2.54 | 0.43 |
| 1:CA:439:A:C4 | 1:CA:496:A:C2 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:579:G:C6 | 1:CA:580:U:C4 | 3.07 | 0.43 |
| 1:CA:929:G:H1 | 1:CA:1388:C:N4 | 2.06 | 0.43 |
| 4:CD:11:LEU:C | 4:CD:13:ARG:N | 2.69 | 0.43 |
| 6:CF:79:LEU:HD12 | 6:CF:88:VAL:HG11 | 2.00 | 0.43 |
| 7:CG:124:LEU:O | 7:CG:128:ALA:HB2 | 2.18 | 0.43 |
| 9:CI:79:LEU:HD13 | 9:CI:79:LEU:C | 2.39 | 0.43 |
| 1:CA:523:A:N1 | 12:CL:92:ASP:HB2 | 2.34 | 0.43 |
| 15:CO:55:GLY:O | 15:CO:56:LEU:C | 2.57 | 0.43 |
| 16:CP:74:LEU:HB3 | 16:CP:79:VAL:HG11 | 2.01 | 0.43 |
| 20:CT:18:GLN:O | 20:CT:19:SER:C | 2.56 | 0.43 |
| 20:CT:89:ARG:C | 20:CT:91:LEU:H | 2.22 | 0.43 |
| 22:D0:47:PRO:HB2 | 22:D0:51:VAL:O | 2.19 | 0.43 |
| 27:D5:42:PRO:HB2 | 27:D5:43:HIS:HD2 | 1.83 | 0.43 |
| 27:D5:56:LYS:O | 27:D5:57:VAL:O | 2.36 | 0.43 |
| 30:D8:4:MET:CE | 31:DA:593:G:O4' | 2.67 | 0.43 |
| 31:DA:1006:C:C2 | 31:DA:1138:G:N2 | 2.86 | 0.43 |
| 31:DA:1458:C:H4' | 31:DA:1459:G:C4 | 2.54 | 0.43 |
| 31:DA:1891:G:C6 | 31:DA:1892:C:N3 | 2.86 | 0.43 |
| 31:DA:1902:C:O2' | 33:DD:244:ARG:CB | 2.65 | 0.43 |
| 31:DA:2087:G:O5' | 31:DA:2087:G:H8 | 2.02 | 0.43 |
| 31:DA:2251:G:C8 | 31:DA:2450:A:H4' | 2.54 | 0.43 |
| 31:DA:250:G:C6 | 31:DA:251:A:C6 | 3.07 | 0.43 |
| 31:DA:2583:G:H2' | 31:DA:2584:U:O2 | 2.18 | 0.43 |
| 31:DA:2610:C:C4' | 31:DA:2611:U:OP2 | 2.65 | 0.43 |
| 31:DA:2813:A:H2' | 31:DA:2814:C:O4' | 2.18 | 0.43 |
| 31:DA:2849:U:H5' | 31:DA:2867:G:N2 | 2.33 | 0.43 |
| 31:DA:354:G:H3' | 31:DA:354:G:C8 | 2.53 | 0.43 |
| 31:DA:528:A:C2' | 31:DA:529:A:C5' | 2.95 | 0.43 |
| 31:DA:838:C:H2' | 31:DA:839:U:H6 | 1.84 | 0.43 |
| 31:DA:867:C:C6 | 31:DA:868:U:C5 | 3.06 | 0.43 |
| 32:DB:21:G:C6 | 32:DB:63:G:C6 | 3.07 | 0.43 |
| 34:DE:51:PHE:HD1 | 34:DE:52:LEU:HD12 | 1.83 | 0.43 |
| 36:DG:127:GLY:O | 36:DG:128:ARG:C | 2.57 | 0.43 |
| 37:DH:32:GLU:C | 37:DH:33:LEU:HD23 | 2.38 | 0.43 |
| 38:DI:60:GLU:HA | 38:DI:63:ALA:HB3 | 2.00 | 0.43 |
| 41:DP:39:LYS:HE3 | 41:DP:42:SER:CB | 2.49 | 0.43 |
| 42:DQ:52:VAL:HA | 42:DQ:55:VAL:CG1 | 2.46 | 0.43 |
| 32:DB:38:C:C1' | 44:DS:95:HIS:HE2 | 2.32 | 0.43 |
| 46:DU:27:LEU:HA | 46:DU:30:LYS:HB2 | 2.01 | 0.43 |
| 46:DU:83:LEU:HD13 | 46:DU:113:ALA:HB2 | 2.01 | 0.43 |
| 49:DX:27:THR:OG1 | 49:DX:77:LYS:HA | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:DZ:148:ASP:HB2 | 51:DZ:149:SER:H | 1.56 | 0.43 |
| 1:AA:1304:G:C6 | 1:AA:1305:G:N1 | 2.87 | 0.43 |
| 1:AA:1368:G:OP2 | 9:AI:112:LYS:CD | 2.67 | 0.43 |
| 1:AA:155:C:C2 | 1:AA:156:G:N7 | 2.87 | 0.43 |
| 1:AA:451:A:C5 | 1:AA:481:G:C6 | 3.07 | 0.43 |
| 4:AD:8:VAL:O | 4:AD:10:ARG:N | 2.51 | 0.43 |
| 5:AE:15:ARG:CZ | 5:AE:26:PHE:CE2 | 3.02 | 0.43 |
| 5:AE:32:VAL:CB | 5:AE:58:ALA:HB1 | 2.48 | 0.43 |
| 7:AG:79:ARG:NE | 7:AG:84:ASN:HD21 | 2.16 | 0.43 |
| 8:AH:97:VAL:HA | 8:AH:100:ILE:HD11 | 2.01 | 0.43 |
| 9:AI:83:ARG:HH21 | 9:AI:102:LEU:CD2 | 2.32 | 0.43 |
| 12:AL:68:ALA:HA | 12:AL:96:VAL:HG13 | 2.01 | 0.43 |
| 15:AO:39:LEU:O | 15:AO:42:HIS:HB3 | 2.19 | 0.43 |
| 16:AP:39:TYR:CE1 | 16:AP:41:PRO:CA | 3.02 | 0.43 |
| 17:AQ:5:VAL:CG1 | 17:AQ:6:LEU:N | 2.82 | 0.43 |
| 19:AS:29:ARG:HD2 | 19:AS:30:LEU:N | 2.33 | 0.43 |
| 19:AS:69:HIS:HB2 | 19:AS:74:PHE:CE2 | 2.51 | 0.43 |
| 20:AT:73:HIS:O | 20:AT:74:LYS:C | 2.57 | 0.43 |
| 24:B2:53:LEU:O | 24:B2:54:LYS:HB2 | 2.19 | 0.43 |
| 31:BA:1239:G:H2' | 31:BA:1240:U:O4' | 2.18 | 0.43 |
| 31:BA:1313:U:H5'' | 31:BA:1314:C:OP2 | 2.19 | 0.43 |
| 31:BA:1891:G:C6 | 31:BA:1892:C:C4 | 3.07 | 0.43 |
| 31:BA:1987:G:H2' | 31:BA:1988:C:H6 | 1.83 | 0.43 |
| 31:BA:2031:A:H8 | 31:BA:2031:A:OP1 | 2.02 | 0.43 |
| 31:BA:2503:A:H4' | 31:BA:2504:U:OP1 | 2.19 | 0.43 |
| 31:BA:2704:C:H2' | 31:BA:2705:A:O4' | 2.19 | 0.43 |
| 31:BA:2716:U:O2' | 31:BA:2717:G:H5' | 2.18 | 0.43 |
| 31:BA:492:A:H2' | 31:BA:493:G:O4' | 2.19 | 0.43 |
| 31:BA:656:G:H2' | 31:BA:657:U:O5' | 2.19 | 0.43 |
| 31:BA:705:A:C2' | 31:BA:706:A:H5' | 2.49 | 0.43 |
| 31:BA:921:G:O2' | 31:BA:922:U:H5' | 2.19 | 0.43 |
| 31:BA:995:C:C2 | 39:BN:4:TYR:CZ | 3.06 | 0.43 |
| 32:BB:15:A:H1' | 32:BB:110:G:C8 | 2.53 | 0.43 |
| 33:BD:45:ASN:CG | 33:BD:46:GLN:N | 2.71 | 0.43 |
| 34:BE:51:PHE:HD1 | 34:BE:52:LEU:HD12 | 1.83 | 0.43 |
| 35:BF:27:GLU:O | 35:BF:112:MET:HE2 | 2.19 | 0.43 |
| 35:BF:9:ILE:HG12 | 35:BF:14:PRO:HA | 2.01 | 0.43 |
| 35:BF:96:ASP:OD1 | 35:BF:96:ASP:C | 2.57 | 0.43 |
| 37:BH:94:TYR:N | 37:BH:94:TYR:HD1 | 2.17 | 0.43 |
| 43:BR:56:LYS:HE3 | 43:BR:94:TYR:CZ | 2.54 | 0.43 |
| 45:BT:42:ILE:HD13 | 45:BT:83:ILE:CD1 | 2.47 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:BV:19:LYS:CG | 47:BV:20:LEU:N | 2.39 | 0.43 |
| 48:BW:95:ILE:O | 48:BW:95:ILE:HG13 | 2.17 | 0.43 |
| 49:BX:29:TRP:CE3 | 49:BX:76:ARG:HB3 | 2.53 | 0.43 |
| 31:BA:1341:U:N3 | 49:BX:77:LYS:HE2 | 2.32 | 0.43 |
| 1:CA:1125:U:C2' | 1:CA:1126:U:OP2 | 2.66 | 0.43 |
| 1:CA:1168:A:C6 | 1:CA:1169:A:C6 | 3.07 | 0.43 |
| 1:CA:262:A:C6 | 1:CA:263:A:N6 | 2.87 | 0.43 |
| 1:CA:437:U:H5'' | 4:CD:155:LEU:CD1 | 2.47 | 0.43 |
| 1:CA:623:C:C4 | 1:CA:624:C:C5 | 3.07 | 0.43 |
| 1:CA:625:G:H2' | 1:CA:626:U:C6 | 2.54 | 0.43 |
| 2:CB:163:PHE:HD2 | 2:CB:185:ILE:HB | 1.84 | 0.43 |
| 2:CB:93:VAL:HG11 | 2:CB:97:TRP:HD1 | 1.84 | 0.43 |
| 4:CD:135:LEU:O | 4:CD:136:PRO:C | 2.56 | 0.43 |
| 6:CF:89:MET:HG2 | 6:CF:89:MET:O | 2.18 | 0.43 |
| 9:CI:81:ILE:O | 9:CI:85:LEU:HG | 2.18 | 0.43 |
| 10:CJ:6:ILE:HD11 | 10:CJ:72:VAL:HB | 2.00 | 0.43 |
| 16:CP:74:LEU:HA | 16:CP:74:LEU:HD23 | 1.77 | 0.43 |
| 16:CP:82:GLN:HE21 | 16:CP:82:GLN:N | 2.17 | 0.43 |
| 22:D0:72:ARG:NH2 | 22:D0:75:LEU:HD12 | 2.34 | 0.43 |
| 30:D8:22:VAL:HB | 30:D8:53:PRO:HB2 | 2.01 | 0.43 |
| 30:D8:32:LEU:CA | 30:D8:34:TRP:H | 2.31 | 0.43 |
| 31:DA:1107:G:C6 | 31:DA:1108:U:N3 | 2.87 | 0.43 |
| 31:DA:1106:A:H2' | 31:DA:1107:G:C8 | 2.54 | 0.43 |
| 31:DA:1158:C:HO2' | 31:DA:1159:U:C5' | 2.27 | 0.43 |
| 31:DA:1379:A:HO2' | 31:DA:1380:G:P | 2.30 | 0.43 |
| 31:DA:1528:A:O2' | 31:DA:1528(A):A:C8 | 2.63 | 0.43 |
| 31:DA:1686:C:C2' | 31:DA:1687:G:H5' | 2.48 | 0.43 |
| 31:DA:1884:A:C2 | 31:DA:1885:A:C8 | 3.07 | 0.43 |
| 31:DA:2101:G:C6 | 31:DA:2102:U:C4 | 3.06 | 0.43 |
| 31:DA:2274:A:C5 | 31:DA:2276:G:C8 | 3.06 | 0.43 |
| 31:DA:2304:G:H22 | 31:DA:2312:U:H3 | 1.65 | 0.43 |
| 31:DA:2689:U:C4' | 31:DA:2690:C:H5' | 2.49 | 0.43 |
| 31:DA:623:G:H2' | 31:DA:624:C:C6 | 2.54 | 0.43 |
| 31:DA:691:C:O2' | 31:DA:692:C:H5' | 2.18 | 0.43 |
| 31:DA:699:A:H2' | 31:DA:700:G:O4' | 2.18 | 0.43 |
| 31:DA:912:C:N3 | 31:DA:913:U:C5 | 2.86 | 0.43 |
| 33:DD:25:THR:CG2 | 33:DD:82:ILE:N | 2.82 | 0.43 |
| 34:DE:21:VAL:O | 34:DE:23:VAL:HG22 | 2.19 | 0.43 |
| 35:DF:7:TYR:HB3 | 35:DF:16:GLY:N | 2.34 | 0.43 |
| 35:DF:65:TRP:CZ3 | 35:DF:73:ALA:O | 2.72 | 0.43 |
| 37:DH:89:ILE:HG13 | 37:DH:129:THR:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:DH:71:LEU:HD12 | 37:DH:71:LEU:HA | 1.80 | 0.43 |
| 39:DN:5:VAL:HA | 39:DN:6:PRO:HD3 | 1.45 | 0.43 |
| 42:DQ:88:GLY:O | 42:DQ:89:ASN:CB | 2.66 | 0.43 |
| 31:DA:2334:G:H5' | 44:DS:13:ARG:HB3 | 1.99 | 0.43 |
| 44:DS:30:ARG:O | 44:DS:30:ARG:HG3 | 2.18 | 0.43 |
| 47:DV:80:GLN:HA | 47:DV:81:TYR:HA | 1.73 | 0.43 |
| 50:DY:71:LYS:HZ3 | 50:DY:71:LYS:CB | 2.29 | 0.43 |
| 1:AA:1433:A:N1 | 1:AA:1434:A:C2 | 2.86 | 0.43 |
| 1:AA:1496:C:H2' | 1:AA:1497:G:O4' | 2.19 | 0.43 |
| 1:AA:234:C:H2' | 1:AA:235:C:C6 | 2.50 | 0.43 |
| 1:AA:342:C:H2' | 1:AA:343:U:O4' | 2.18 | 0.43 |
| 1:AA:543:C:N3 | 1:AA:544:G:N7 | 2.67 | 0.43 |
| 1:AA:556:C:O2' | 1:AA:557:G:H5' | 2.18 | 0.43 |
| 1:AA:563:A:C5 | 1:AA:567:G:C4 | 3.07 | 0.43 |
| 1:AA:644:G:C6 | 1:AA:645:C:C5 | 3.07 | 0.43 |
| 3:AC:155:GLY:O | 3:AC:196:LEU:HD13 | 2.19 | 0.43 |
| 7:AG:25:ALA:O | 7:AG:29:LYS:HG2 | 2.18 | 0.43 |
| 8:AH:102:ARG:N | 8:AH:102:ARG:NE | 2.61 | 0.43 |
| 10:AJ:48:THR:HG23 | 10:AJ:62:HIS:HB3 | 2.00 | 0.43 |
| 12:AL:93:LEU:O | 12:AL:94:PRO:C | 2.57 | 0.43 |
| 13:AM:60:VAL:HG12 | 13:AM:66:LEU:HD21 | 2.00 | 0.43 |
| 14:AN:15:LYS:HA | 14:AN:15:LYS:HD3 | 1.85 | 0.43 |
| 19:AS:29:ARG:O | 19:AS:31:ILE:HG22 | 2.18 | 0.43 |
| 20:AT:58:LYS:HE3 | 20:AT:62:LEU:HD12 | 2.00 | 0.43 |
| 23:B1:21:ARG:HH12 | 31:BA:380:U:P | 2.42 | 0.43 |
| 25:B3:11:SER:HG | 25:B3:13:ILE:HG12 | 1.84 | 0.43 |
| 26:B4:23:GLU:O | 26:B4:24:THR:CB | 2.66 | 0.43 |
| 31:BA:1039:G:O2' | 31:BA:1040:C:H5' | 2.18 | 0.43 |
| 31:BA:1141:U:OP2 | 39:BN:63:THR:OG1 | 2.28 | 0.43 |
| 31:BA:1550:C:O2' | 31:BA:1551:C:H5' | 2.19 | 0.43 |
| 31:BA:1558:A:H1' | 31:BA:1559:G:OP2 | 2.19 | 0.43 |
| 31:BA:1635:G:H2' | 31:BA:1636:C:H6 | 1.84 | 0.43 |
| 31:BA:1803:A:C2 | 31:BA:1822:G:N3 | 2.87 | 0.43 |
| 31:BA:1819:A:OP1 | 33:BD:158:ALA:HB2 | 2.18 | 0.43 |
| 31:BA:1839:G:C5' | 31:BA:1839:G:C8 | 3.02 | 0.43 |
| 31:BA:2287:A:C4 | 31:BA:2289:G:N7 | 2.86 | 0.43 |
| 31:BA:444:C:H4' | 35:BF:49:ALA:HB2 | 2.01 | 0.43 |
| 31:BA:610:G:H2' | 31:BA:611:C:H6 | 1.83 | 0.43 |
| 31:BA:64:A:O2' | 31:BA:65:C:H5' | 2.19 | 0.43 |
| 31:BA:755:C:H2' | 31:BA:756:C:H6 | 1.83 | 0.43 |
| 32:BB:74:U:C3' | 32:BB:75:G:H5'' | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BD:266:SER:O | 33:BD:267:SER:HB2 | 2.17 | 0.43 |
| 33:BD:28:GLU:CB | 33:BD:29:PRO:HD3 | 2.48 | 0.43 |
| 34:BE:21:VAL:HA | 34:BE:22:PRO:HD2 | 1.89 | 0.43 |
| 34:BE:56:PRO:C | 34:BE:58:ARG:H | 2.22 | 0.43 |
| 36:BG:139:LEU:HD23 | 36:BG:149:VAL:HG21 | 2.01 | 0.43 |
| 37:BH:158:HIS:CE1 | 37:BH:170:ARG:N | 2.86 | 0.43 |
| 37:BH:83:TYR:CD1 | 37:BH:83:TYR:N | 2.87 | 0.43 |
| 38:BI:9:LEU:HB2 | 38:BI:12:LEU:O | 2.19 | 0.43 |
| 41:BP:101:VAL:O | 41:BP:103:ALA:N | 2.50 | 0.43 |
| 30:B8:59:LYS:CD | 41:BP:50:ARG:HB3 | 2.44 | 0.43 |
| 43:BR:116:LEU:HD23 | 43:BR:116:LEU:HA | 1.74 | 0.43 |
| 44:BS:59:LYS:CE | 44:BS:68:GLN:HE22 | 2.29 | 0.43 |
| 46:BU:84:LYS:C | 46:BU:86:ALA:H | 2.21 | 0.43 |
| 46:BU:65:ILE:CG1 | 46:BU:96:ALA:HB3 | 2.47 | 0.43 |
| 47:BV:62:LEU:HD12 | 47:BV:96:ILE:HD13 | 2.01 | 0.43 |
| 48:BW:80:PRO:O | 48:BW:100:THR:HG22 | 2.18 | 0.43 |
| 50:BY:7:VAL:HG11 | 50:BY:8:LYS:HZ3 | 1.84 | 0.43 |
| 51:BZ:98:MET:HE3 | 51:BZ:99:TYR:O | 2.19 | 0.43 |
| 1:CA:1099:G:H2' | 1:CA:1099:G:N3 | 2.34 | 0.43 |
| 1:CA:1130:A:H1' | 1:CA:1146:A:C2 | 2.53 | 0.43 |
| 1:CA:1271:G:OP1 | 1:CA:1314:C:H4' | 2.19 | 0.43 |
| 1:CA:1378:C:N4 | 1:CA:1379:G:C2 | 2.87 | 0.43 |
| 1:CA:769:G:H4' | 1:CA:1513:A:H4' | 2.01 | 0.43 |
| 1:CA:102:G:O2' | 1:CA:151:A:N3 | 2.44 | 0.43 |
| 1:CA:327:A:C6 | 1:CA:329:A:C5 | 3.07 | 0.43 |
| 1:CA:563:A:C5 | 1:CA:567:G:C4 | 3.07 | 0.43 |
| 1:CA:644:G:C6 | 1:CA:645:C:C5 | 3.06 | 0.43 |
| 1:CA:812:C:OP1 | 1:CA:903:G:H1' | 2.19 | 0.43 |
| 3:CC:16:ARG:CZ | 3:CC:16:ARG:HB2 | 2.49 | 0.43 |
| 4:CD:12:CYS:SG | 4:CD:19:LEU:O | 2.76 | 0.43 |
| 8:CH:102:ARG:N | 8:CH:102:ARG:NE | 2.59 | 0.43 |
| 10:CJ:35:SER:OG | 10:CJ:73:ASP:HB2 | 2.19 | 0.43 |
| 15:CO:2:PRO:HB2 | 15:CO:3:ILE:H | 1.66 | 0.43 |
| 17:CQ:52:LYS:HB3 | 17:CQ:52:LYS:HE3 | 1.80 | 0.43 |
| 19:CS:9:VAL:O | 19:CS:11:VAL:N | 2.52 | 0.43 |
| 22:D0:70:GLN:O | 22:D0:77:ARG:HA | 2.19 | 0.43 |
| 23:D1:26:ARG:CB | 23:D1:34:THR:HB | 2.49 | 0.43 |
| 30:D8:43:GLN:O | 30:D8:44:LYS:CD | 2.66 | 0.43 |
| 31:DA:1259:G:H2' | 31:DA:1260:G:C8 | 2.54 | 0.43 |
| 31:DA:1404:C:O2 | 31:DA:1404:C:H2' | 2.17 | 0.43 |
| 31:DA:1462:C:H2' | 31:DA:1463:C:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:1628:G:H2' | 31:DA:1629:U:H6 | 1.84 | 0.43 |
| 31:DA:1856:G:C2' | 31:DA:1857:G:H5' | 2.49 | 0.43 |
| 31:DA:1892:C:C2' | 31:DA:1893:C:H5' | 2.48 | 0.43 |
| 31:DA:2405:G:H4' | 31:DA:2406:U:OP2 | 2.19 | 0.43 |
| 31:DA:243:U:C2' | 31:DA:244:A:H5' | 2.49 | 0.43 |
| 31:DA:2619:C:H2' | 31:DA:2620:C:C6 | 2.53 | 0.43 |
| 31:DA:2648:C:H2' | 31:DA:2649:U:H6 | 1.83 | 0.43 |
| 31:DA:271(N):U:C6 | 31:DA:271(N):U:OP1 | 2.72 | 0.43 |
| 31:DA:362:U:H3' | 31:DA:362:U:C6 | 2.54 | 0.43 |
| 31:DA:223:A:O2' | 31:DA:420:C:O2 | 2.31 | 0.43 |
| 31:DA:449:A:H2' | 31:DA:450:G:C5' | 2.49 | 0.43 |
| 31:DA:656:G:C2' | 31:DA:657:U:O5' | 2.67 | 0.43 |
| 31:DA:733:G:H8 | 31:DA:733:G:O5' | 2.01 | 0.43 |
| 31:DA:905:U:C2' | 31:DA:906:G:H5' | 2.49 | 0.43 |
| 31:DA:934:G:H2' | 31:DA:935:C:H6 | 1.84 | 0.43 |
| 32:DB:33:G:C2' | 32:DB:34:U:H5' | 2.49 | 0.43 |
| 32:DB:46:A:C2' | 32:DB:47:C:O5' | 2.67 | 0.43 |
| 32:DB:75:G:C5' | 32:DB:75:G:C8 | 2.98 | 0.43 |
| 33:DD:224:ALA:O | 33:DD:225:ALA:CB | 2.67 | 0.43 |
| 33:DD:83:GLU:HB2 | 33:DD:92:ILE:HD12 | 1.98 | 0.43 |
| 34:DE:114:ALA:HB3 | 34:DE:160:TYR:HB3 | 2.00 | 0.43 |
| 34:DE:101:ARG:HG3 | 34:DE:169:ASN:ND2 | 2.33 | 0.43 |
| 34:DE:203:LYS:HD2 | 34:DE:203:LYS:C | 2.38 | 0.43 |
| 35:DF:132:VAL:CG2 | 35:DF:133:ASN:H | 2.31 | 0.43 |
| 38:DI:27:ARG:HG2 | 38:DI:27:ARG:HH11 | 1.84 | 0.43 |
| 38:DI:35:LEU:O | 38:DI:36:ALA:HB2 | 2.19 | 0.43 |
| 39:DN:121:LYS:HA | 39:DN:121:LYS:HD3 | 1.80 | 0.43 |
| 41:DP:101:VAL:CG2 | 41:DP:107:LYS:HA | 2.49 | 0.43 |
| 43:DR:9:LYS:O | 43:DR:10:LEU:HD23 | 2.18 | 0.43 |
| 43:DR:52:ILE:H | 43:DR:52:ILE:HG12 | 1.71 | 0.43 |
| 43:DR:92:GLY:HA2 | 43:DR:94:TYR:CZ | 2.54 | 0.43 |
| 44:DS:90:GLY:C | 44:DS:92:TYR:N | 2.72 | 0.43 |
| 49:DX:28:PHE:CD1 | 49:DX:28:PHE:N | 2.87 | 0.43 |
| 31:DA:329:G:OP2 | 50:DY:71:LYS:CE | 2.67 | 0.43 |
| 1:AA:1014:A:C2 | 19:AS:34:TRP:CE2 | 3.07 | 0.43 |
| 1:AA:949:A:C2 | 1:AA:1233:G:N3 | 2.86 | 0.43 |
| 1:AA:1245:A:C6 | 1:AA:1246:C:C4 | 3.07 | 0.43 |
| 1:AA:1423:G:H2' | 1:AA:1424:C:H6 | 1.82 | 0.43 |
| 1:AA:333:G:O2' | 1:AA:334:C:H5' | 2.19 | 0.43 |
| 1:AA:356:A:C2 | 1:AA:368:U:O2 | 2.71 | 0.43 |
| 1:AA:738:C:C4 | 1:AA:739:C:C5 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:754:C:H3' | 1:AA:754:C:O2 | 2.19 | 0.43 |
| 2:AB:238:LEU:O | 2:AB:240:GLN:N | 2.46 | 0.43 |
| 2:AB:25:ASN:HA | 2:AB:26:PRO:HD2 | 1.68 | 0.43 |
| 3:AC:77:ILE:C | 3:AC:83:ARG:HB3 | 2.39 | 0.43 |
| 4:AD:63:LYS:HE3 | 4:AD:63:LYS:HB2 | 1.76 | 0.43 |
| 8:AH:109:ILE:HD11 | 8:AH:120:THR:CG2 | 2.49 | 0.43 |
| 9:AI:46:ALA:HA | 9:AI:78:LYS:HZ1 | 1.84 | 0.43 |
| 9:AI:48:GLU:N | 9:AI:49:PRO:CD | 2.82 | 0.43 |
| 9:AI:6:GLY:HA3 | 9:AI:84:ALA:HB2 | 2.01 | 0.43 |
| 11:AK:73:MET:SD | 11:AK:103:LEU:HD22 | 2.59 | 0.43 |
| 12:AL:64:TYR:O | 12:AL:65:GLU:HB2 | 2.19 | 0.43 |
| 15:AO:74:ASP:HA | 15:AO:75:PRO:HD2 | 1.80 | 0.43 |
| 24:B2:37:PHE:CE2 | 24:B2:39:ALA:O | 2.72 | 0.43 |
| 31:BA:2506:U:H4' | 31:BA:2507:C:OP1 | 2.17 | 0.43 |
| 31:BA:2510:C:H2' | 31:BA:2511:U:O4' | 2.19 | 0.43 |
| 31:BA:2635:C:C2' | 31:BA:2636:U:O5' | 2.66 | 0.43 |
| 31:BA:2785:C:H2' | 31:BA:2786:U:O4' | 2.19 | 0.43 |
| 31:BA:511:U:C5 | 31:BA:512:G:C5 | 3.07 | 0.43 |
| 31:BA:893:C:H2' | 31:BA:894:C:O5' | 2.19 | 0.43 |
| 31:BA:971:C:H2' | 31:BA:972:G:C5' | 2.49 | 0.43 |
| 31:BA:981:A:C2 | 31:BA:2027:G:N3 | 2.87 | 0.43 |
| 33:BD:182:LEU:HD23 | 33:BD:182:LEU:HA | 1.76 | 0.43 |
| 33:BD:205:VAL:HG12 | 33:BD:205:VAL:O | 2.19 | 0.43 |
| 31:BA:1902:C:H4' | 33:BD:244:ARG:HA | 2.00 | 0.43 |
| 34:BE:116:VAL:HG13 | 34:BE:122:PHE:CB | 2.49 | 0.43 |
| 37:BH:138:LYS:O | 37:BH:140:LYS:N | 2.52 | 0.43 |
| 38:BI:132:PRO:C | 38:BI:133:HIS:CD2 | 2.92 | 0.43 |
| 38:BI:44:LEU:HA | 38:BI:44:LEU:HD23 | 1.60 | 0.43 |
| 41:BP:121:LYS:HG3 | 41:BP:122:PRO:HD2 | 2.01 | 0.43 |
| 32:BB:38:C:C1' | 44:BS:95:HIS:HE2 | 2.31 | 0.43 |
| 45:BT:29:ARG:HD2 | 45:BT:29:ARG:HA | 1.49 | 0.43 |
| 46:BU:88:ILE:O | 46:BU:89:GLU:C | 2.57 | 0.43 |
| 49:BX:36:LYS:O | 49:BX:38:GLU:N | 2.52 | 0.43 |
| 50:BY:8:LYS:CD | 50:BY:8:LYS:N | 2.80 | 0.43 |
| 51:BZ:11:GLU:HB2 | 51:BZ:13:GLU:OE2 | 2.19 | 0.43 |
| 1:CA:1142:G:H2' | 1:CA:1143:G:O4' | 2.18 | 0.43 |
| 1:CA:1348:U:H4' | 9:CI:120:ARG:HH11 | 1.84 | 0.43 |
| 1:CA:1431:C:H2' | 1:CA:1432:G:O4' | 2.19 | 0.43 |
| 1:CA:159:G:C4 | 1:CA:161:A:OP2 | 2.71 | 0.43 |
| 1:CA:438:G:OP1 | 4:CD:125:HIS:HE1 | 2.02 | 0.43 |
| 1:CA:499:A:H4' | 1:CA:500:G:H5' | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:577:G:C2 | 1:CA:578:C:C6 | 3.07 | 0.43 |
| 1:CA:617:G:N1 | 1:CA:618:C:C4 | 2.87 | 0.43 |
| 1:CA:790:A:N6 | 1:CA:791:G:C6 | 2.87 | 0.43 |
| 1:CA:914:A:C2' | 1:CA:915:A:H5' | 2.48 | 0.43 |
| 1:CA:865:A:H2 | 1:CA:918:A:H4' | 1.84 | 0.43 |
| 1:CA:966:G:H5'' | 1:CA:969:A:N7 | 2.33 | 0.43 |
| 2:CB:163:PHE:CD2 | 2:CB:185:ILE:HG13 | 2.51 | 0.43 |
| 4:CD:65:ARG:HG3 | 4:CD:75:PHE:CD1 | 2.54 | 0.43 |
| 5:CE:110:LEU:HD12 | 5:CE:118:ILE:HG21 | 2.01 | 0.43 |
| 6:CF:100:ASN:N | 18:CR:23:LYS:HZ2 | 2.16 | 0.43 |
| 6:CF:15:ASP:CG | 6:CF:18:GLN:HE21 | 2.22 | 0.43 |
| 7:CG:25:ALA:O | 7:CG:29:LYS:HG2 | 2.18 | 0.43 |
| 9:CI:48:GLU:H | 9:CI:49:PRO:HD2 | 1.83 | 0.43 |
| 11:CK:11:LYS:HB3 | 11:CK:12:ARG:H | 1.64 | 0.43 |
| 15:CO:39:LEU:O | 15:CO:42:HIS:HB3 | 2.18 | 0.43 |
| 15:CO:54:ARG:HG2 | 15:CO:58:MET:CE | 2.49 | 0.43 |
| 18:CR:63:GLN:OE1 | 18:CR:66:LEU:HD23 | 2.19 | 0.43 |
| 20:CT:46:GLU:CG | 20:CT:48:LYS:HE2 | 2.49 | 0.43 |
| 20:CT:75:ASN:HD22 | 20:CT:75:ASN:H | 1.66 | 0.43 |
| 30:D8:32:LEU:N | 30:D8:32:LEU:CD1 | 2.77 | 0.43 |
| 31:DA:11:G:O2' | 31:DA:12:U:H5' | 2.19 | 0.43 |
| 31:DA:1221:C:H2' | 31:DA:1221(A):C:C6 | 2.54 | 0.43 |
| 31:DA:1436:G:H2' | 31:DA:1437:C:O4' | 2.19 | 0.43 |
| 31:DA:1602:U:H3' | 31:DA:1603:A:H5' | 2.01 | 0.43 |
| 31:DA:1930:G:O2' | 31:DA:1931:U:P | 2.77 | 0.43 |
| 31:DA:2078:C:C4 | 31:DA:2079:U:C4 | 3.07 | 0.43 |
| 31:DA:2078:C:C2' | 31:DA:2079:U:H5' | 2.48 | 0.43 |
| 31:DA:2334:G:H4' | 31:DA:2335:A:OP2 | 2.19 | 0.43 |
| 31:DA:2808:U:H2' | 31:DA:2809:A:O5' | 2.18 | 0.43 |
| 31:DA:30:G:H2' | 31:DA:31:C:C6 | 2.54 | 0.43 |
| 31:DA:325:G:O2' | 31:DA:326:G:H5' | 2.18 | 0.43 |
| 31:DA:363(C):G:H2' | 31:DA:363(D):G:C8 | 2.54 | 0.43 |
| 31:DA:506:G:H4' | 31:DA:509:C:O2 | 2.19 | 0.43 |
| 31:DA:901:A:H3' | 31:DA:902:C:H6 | 1.82 | 0.43 |
| 31:DA:910:A:C6 | 31:DA:911:A:C6 | 3.07 | 0.43 |
| 33:DD:223:GLY:CA | 33:DD:231:HIS:CD2 | 3.02 | 0.43 |
| 33:DD:28:GLU:CB | 33:DD:29:PRO:CD | 2.97 | 0.43 |
| 33:DD:78:LYS:HE3 | 33:DD:78:LYS:HB2 | 1.84 | 0.43 |
| 34:DE:11:MET:HB2 | 34:DE:23:VAL:O | 2.19 | 0.43 |
| 35:DF:140:LEU:O | 35:DF:141:ALA:C | 2.57 | 0.43 |
| 37:DH:153:LYS:CG | 37:DH:154:PRO:N | 2.79 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DI:62:LYS:HE2 | 38:DI:134:PRO:HG2 | 2.00 | 0.43 |
| 38:DI:4:ILE:HD11 | 38:DI:44:LEU:HD23 | 2.01 | 0.43 |
| 39:DN:121:LYS:HD3 | 39:DN:122:VAL:N | 2.34 | 0.43 |
| 39:DN:39:ARG:HG2 | 39:DN:41:ASP:HB2 | 2.00 | 0.43 |
| 31:DA:2415:G:O3' | 41:DP:66:GLY:HA3 | 2.18 | 0.43 |
| 42:DQ:31:ASP:O | 42:DQ:133:ARG:O | 2.36 | 0.43 |
| 45:DT:29:ARG:HG3 | 45:DT:30:VAL:H | 1.84 | 0.43 |
| 49:DX:31:HIS:HD2 | 49:DX:33:LYS:N | 2.16 | 0.43 |
| 50:DY:100:ALA:O | 50:DY:101:LYS:HB2 | 2.18 | 0.43 |
| 50:DY:7:VAL:HB | 50:DY:8:LYS:CD | 2.49 | 0.43 |
| 1:AA:1293:G:O2' | 1:AA:1294:G:P | 2.77 | 0.42 |
| 1:AA:1311:G:N2 | 1:AA:1327:C:C2 | 2.86 | 0.42 |
| 1:AA:460:G:N2 | 1:AA:471:G:C8 | 2.87 | 0.42 |
| 1:AA:564:C:H2' | 1:AA:565:U:H5' | 2.01 | 0.42 |
| 1:AA:684:A:H2' | 1:AA:685:G:H8 | 1.81 | 0.42 |
| 1:AA:827:U:H6 | 1:AA:827:U:O5' | 2.01 | 0.42 |
| 1:AA:99:U:O2' | 1:AA:100:C:H5' | 2.19 | 0.42 |
| 3:AC:11:ARG:O | 3:AC:13:GLY:N | 2.52 | 0.42 |
| 6:AF:30:LEU:HG | 6:AF:30:LEU:H | 1.65 | 0.42 |
| 11:AK:84:VAL:HG11 | 11:AK:95:ILE:HD11 | 2.00 | 0.42 |
| 12:AL:119:LYS:HB2 | 12:AL:120:TYR:HD1 | 1.83 | 0.42 |
| 12:AL:21:LYS:HD2 | 12:AL:21:LYS:N | 2.34 | 0.42 |
| 24:B2:44:LEU:HD13 | 24:B2:44:LEU:HA | 1.54 | 0.42 |
| 28:B6:11:LEU:O | 28:B6:23:THR:HA | 2.19 | 0.42 |
| 31:BA:1003:G:N2 | 31:BA:1153:C:C2 | 2.87 | 0.42 |
| 31:BA:1161:C:H1' | 47:BV:8:GLY:O | 2.19 | 0.42 |
| 31:BA:1464:C:C2' | 31:BA:1528:A:H8 | 2.30 | 0.42 |
| 31:BA:1686:C:C2' | 31:BA:1687:G:H5' | 2.48 | 0.42 |
| 31:BA:1686:C:H2' | 31:BA:1687:G:H5' | 1.99 | 0.42 |
| 30:B8:31:HIS:ND1 | 31:BA:2419:U:O4 | 2.51 | 0.42 |
| 31:BA:197:A:N6 | 31:BA:2430:A:H2' | 2.34 | 0.42 |
| 31:BA:271(N):U:C6 | 31:BA:271(N):U:OP1 | 2.72 | 0.42 |
| 31:BA:2747:G:O6 | 31:BA:2755:C:H5'' | 2.19 | 0.42 |
| 31:BA:324:A:N6 | 31:BA:338:G:O2' | 2.50 | 0.42 |
| 31:BA:620:G:H5' | 31:BA:620:G:N3 | 2.33 | 0.42 |
| 31:BA:774:A:H2 | 31:BA:787:U:HO2' | 1.58 | 0.42 |
| 31:BA:901:A:H2' | 31:BA:901:A:N3 | 2.34 | 0.42 |
| 33:BD:233:HIS:CD2 | 33:BD:233:HIS:N | 2.85 | 0.42 |
| 34:BE:3:GLY:HA3 | 34:BE:81:ILE:CG1 | 2.49 | 0.42 |
| 35:BF:176:LEU:HD21 | 35:BF:180:GLY:O | 2.19 | 0.42 |
| 36:BG:111:LEU:N | 36:BG:112:PRO:CD | 2.81 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BH:71:LEU:HD12 | 37:BH:71:LEU:HA | 1.80 | 0.42 |
| 37:BH:83:TYR:HA | 37:BH:135:GLY:O | 2.19 | 0.42 |
| 38:BI:99:GLU:HG3 | 38:BI:103:ARG:NH1 | 2.34 | 0.42 |
| 31:BA:2873:A:C2 | 43:BR:6:SER:HB2 | 2.53 | 0.42 |
| 44:BS:54:LEU:HD22 | 44:BS:58:LEU:O | 2.19 | 0.42 |
| 44:BS:92:TYR:HB2 | 44:BS:97:ARG:HH22 | 1.84 | 0.42 |
| 46:BU:12:ARG:HA | 46:BU:15:LYS:HG2 | 2.00 | 0.42 |
| 48:BW:82:LEU:HD12 | 48:BW:82:LEU:HA | 1.76 | 0.42 |
| 49:BX:73:ARG:H | 49:BX:74:PRO:CD | 2.31 | 0.42 |
| 49:BX:89:ILE:O | 49:BX:89:ILE:CG2 | 2.65 | 0.42 |
| 50:BY:45:VAL:CG1 | 50:BY:46:LYS:H | 2.32 | 0.42 |
| 1:CA:1015:A:N6 | 1:CA:1016:A:C6 | 2.86 | 0.42 |
| 1:CA:1347:G:O2' | 1:CA:1348:U:P | 2.77 | 0.42 |
| 1:CA:1516:G:H2' | 1:CA:1518:A:OP2 | 2.19 | 0.42 |
| 1:CA:228:A:H2' | 1:CA:229:U:O4' | 2.19 | 0.42 |
| 1:CA:303:A:H2' | 1:CA:304:U:O4' | 2.19 | 0.42 |
| 1:CA:668:G:O2' | 15:CO:46:HIS:HD2 | 2.02 | 0.42 |
| 1:CA:81:U:H2' | 1:CA:82:U:C5 | 2.54 | 0.42 |
| 1:CA:963:G:H1 | 1:CA:972:C:N4 | 2.17 | 0.42 |
| 5:CE:32:VAL:CG2 | 5:CE:58:ALA:HB1 | 2.48 | 0.42 |
| 9:CI:18:PHE:O | 9:CI:61:ALA:HA | 2.20 | 0.42 |
| 11:CK:69:ALA:HB1 | 11:CK:103:LEU:HD23 | 2.01 | 0.42 |
| 1:CA:1329:A:P | 13:CM:28:ALA:HB3 | 2.59 | 0.42 |
| 14:CN:3:ARG:NH1 | 14:CN:3:ARG:HB3 | 2.34 | 0.42 |
| 18:CR:53:ARG:HH21 | 18:CR:60:ALA:H | 1.64 | 0.42 |
| 20:CT:53:LEU:HD21 | 20:CT:92:LEU:CD1 | 2.49 | 0.42 |
| 20:CT:84:LEU:HD13 | 20:CT:85:MET:N | 2.34 | 0.42 |
| 28:D6:11:LEU:HD23 | 28:D6:26:ASN:H | 1.83 | 0.42 |
| 31:DA:1144:G:C6 | 31:DA:1145:C:N4 | 2.86 | 0.42 |
| 31:DA:1206:G:C6 | 31:DA:1207:C:C4 | 3.07 | 0.42 |
| 31:DA:1553:A:C6 | 31:DA:1555:G:C4 | 3.06 | 0.42 |
| 31:DA:1613:G:C2 | 31:DA:1619:G:C5 | 3.07 | 0.42 |
| 31:DA:528:A:N1 | 31:DA:2043:C:O5' | 2.52 | 0.42 |
| 31:DA:2096:U:H3 | 31:DA:2193:G:H1 | 1.66 | 0.42 |
| 31:DA:323:G:O2' | 31:DA:1205:U:N3 | 2.42 | 0.42 |
| 31:DA:478:A:N1 | 31:DA:500:G:H4' | 2.34 | 0.42 |
| 31:DA:492:A:H2' | 31:DA:493:G:O4' | 2.19 | 0.42 |
| 31:DA:855:G:H2' | 31:DA:856:C:C6 | 2.53 | 0.42 |
| 31:DA:882:G:H8 | 31:DA:882:G:O5' | 2.00 | 0.42 |
| 31:DA:953:A:N3 | 31:DA:954:G:C8 | 2.87 | 0.42 |
| 32:DB:15:A:H1' | 32:DB:110:G:C4 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DE:61:ARG:C | 34:DE:63:LEU:H | 2.23 | 0.42 |
| 35:DF:22:ALA:HA | 35:DF:26:ALA:HA | 2.00 | 0.42 |
| 37:DH:150:ALA:O | 37:DH:151:ILE:C | 2.58 | 0.42 |
| 38:DI:56:LYS:HA | 38:DI:59:ALA:CB | 2.45 | 0.42 |
| 39:DN:55:VAL:HG12 | 39:DN:125:GLY:HA3 | 2.01 | 0.42 |
| 31:DA:2265:U:H4' | 42:DQ:13:GLN:HE22 | 1.84 | 0.42 |
| 42:DQ:74:TYR:O | 42:DQ:89:ASN:N | 2.48 | 0.42 |
| 46:DU:92:ARG:O | 46:DU:93:LYS:C | 2.57 | 0.42 |
| 47:DV:66:ARG:NH2 | 47:DV:94:LEU:HD12 | 2.34 | 0.42 |
| 48:DW:2:GLU:OE1 | 48:DW:72:LYS:NZ | 2.49 | 0.42 |
| 49:DX:36:LYS:HZ2 | 49:DX:39:ILE:N | 2.16 | 0.42 |
| 50:DY:27:VAL:CB | 50:DY:29:GLU:OE1 | 2.67 | 0.42 |
| 50:DY:45:VAL:HG13 | 50:DY:62:GLU:CG | 2.49 | 0.42 |
| 51:DZ:38:TYR:O | 51:DZ:38:TYR:CD1 | 2.72 | 0.42 |
| 51:DZ:4:ARG:HD3 | 51:DZ:60:GLU:OE1 | 2.19 | 0.42 |
| 42:DQ:141:GLN:CD | 51:DZ:72:ARG:HG2 | 2.40 | 0.42 |
| 1:AA:159:G:C4 | 1:AA:161:A:OP2 | 2.72 | 0.42 |
| 1:AA:267:C:OP1 | 17:AQ:67:LYS:HD2 | 2.19 | 0.42 |
| 1:AA:436:C:O2' | 1:AA:437:U:P | 2.77 | 0.42 |
| 1:AA:577:G:H2' | 1:AA:578:C:H6 | 1.84 | 0.42 |
| 1:AA:60:A:H4' | 1:AA:61:G:O5' | 2.19 | 0.42 |
| 1:AA:60:A:C8 | 1:AA:60:A:OP2 | 2.72 | 0.42 |
| 1:AA:644:G:H2' | 1:AA:645:C:H5' | 2.02 | 0.42 |
| 1:AA:801:U:H2' | 1:AA:802:A:H8 | 1.84 | 0.42 |
| 1:AA:9:G:N3 | 1:AA:9:G:H2' | 2.34 | 0.42 |
| 2:AB:190:THR:C | 2:AB:192:SER:H | 2.22 | 0.42 |
| 4:AD:36:ARG:C | 4:AD:38:TYR:H | 2.22 | 0.42 |
| 8:AH:27:PRO:HA | 8:AH:58:TYR:HA | 2.02 | 0.42 |
| 1:AA:1346:A:C5' | 9:AI:120:ARG:HH12 | 2.31 | 0.42 |
| 10:AJ:30:SER:HB2 | 10:AJ:80:LYS:HG3 | 2.01 | 0.42 |
| 10:AJ:54:PHE:HZ | 10:AJ:55:LYS:HZ2 | 1.62 | 0.42 |
| 11:AK:69:ALA:HB1 | 11:AK:103:LEU:HD23 | 2.01 | 0.42 |
| 13:AM:54:VAL:O | 13:AM:58:GLU:HB2 | 2.20 | 0.42 |
| 18:AR:25:THR:HG22 | 18:AR:42:ARG:NH1 | 2.29 | 0.42 |
| 18:AR:44:LEU:O | 18:AR:45:SER:C | 2.57 | 0.42 |
| 22:B0:47:PRO:HB2 | 22:B0:51:VAL:O | 2.19 | 0.42 |
| 30:B8:11:LYS:O | 41:BP:65:ARG:HD2 | 2.19 | 0.42 |
| 31:BA:1465:G:N1 | 31:BA:1466:G:C5 | 2.88 | 0.42 |
| 31:BA:1495:A:H2' | 31:BA:1496:A:C2 | 2.54 | 0.42 |
| 31:BA:1497:U:H5'' | 31:BA:1498:C:C5 | 2.55 | 0.42 |
| 31:BA:1545:A:H2' | 31:BA:1546:C:O5' | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1799:G:N7 | 33:BD:179:SER:OG | 2.45 | 0.42 |
| 31:BA:2031:A:O4' | 31:BA:2031:A:OP1 | 2.37 | 0.42 |
| 31:BA:2328:A:H2' | 31:BA:2329:G:H8 | 1.81 | 0.42 |
| 31:BA:445:C:O2' | 31:BA:446:G:H5' | 2.19 | 0.42 |
| 31:BA:774:A:H2 | 31:BA:787:U:O2' | 2.00 | 0.42 |
| 31:BA:981:A:H2 | 31:BA:2027:G:N3 | 2.17 | 0.42 |
| 32:BB:2:C:H2' | 32:BB:3:C:C6 | 2.54 | 0.42 |
| 26:B4:2:LYS:CB | 32:BB:40:U:O4 | 2.67 | 0.42 |
| 33:BD:206:LEU:HD23 | 33:BD:206:LEU:HA | 1.53 | 0.42 |
| 35:BF:65:TRP:HZ3 | 35:BF:73:ALA:O | 2.02 | 0.42 |
| 41:BP:71:VAL:HG13 | 41:BP:72:PRO:N | 2.34 | 0.42 |
| 46:BU:45:TYR:O | 46:BU:49:HIS:HB2 | 2.19 | 0.42 |
| 47:BV:90:PRO:CD | 47:BV:91:TYR:N | 2.82 | 0.42 |
| 47:BV:69:LYS:CB | 47:BV:93:GLU:CD | 2.87 | 0.42 |
| 48:BW:4:LYS:CB | 48:BW:106:ILE:HG22 | 2.35 | 0.42 |
| 50:BY:46:LYS:O | 50:BY:47:LYS:CE | 2.67 | 0.42 |
| 1:CA:1057:G:C4 | 1:CA:1204:A:C2 | 3.07 | 0.42 |
| 1:CA:1305:G:H5' | 21:CU:4:GLY:HA3 | 2.01 | 0.42 |
| 1:CA:192:U:H4' | 20:CT:57:ARG:HD2 | 2.00 | 0.42 |
| 1:CA:274:A:H4' | 1:CA:275:G:OP1 | 2.18 | 0.42 |
| 1:CA:328:C:H4' | 1:CA:329:A:H5' | 2.01 | 0.42 |
| 1:CA:373:A:O2' | 1:CA:374:A:H5' | 2.19 | 0.42 |
| 1:CA:541:G:H2' | 1:CA:542:G:C8 | 2.54 | 0.42 |
| 1:CA:604:G:N7 | 1:CA:605:U:C5 | 2.87 | 0.42 |
| 1:CA:673:G:C2 | 1:CA:674:G:C6 | 3.06 | 0.42 |
| 3:CC:165:THR:O | 3:CC:165:THR:HG23 | 2.18 | 0.42 |
| 8:CH:9:MET:O | 8:CH:12:ARG:HB2 | 2.19 | 0.42 |
| 9:CI:83:ARG:HH21 | 9:CI:102:LEU:CD2 | 2.32 | 0.42 |
| 1:CA:1371:G:OP1 | 9:CI:11:LYS:HG2 | 2.19 | 0.42 |
| 10:CJ:50:ILE:N | 10:CJ:50:ILE:HD13 | 2.34 | 0.42 |
| 11:CK:62:GLN:O | 11:CK:63:LEU:C | 2.57 | 0.42 |
| 18:CR:22:VAL:HG11 | 18:CR:42:ARG:O | 2.20 | 0.42 |
| 20:CT:38:LYS:HA | 20:CT:41:ILE:HD11 | 2.01 | 0.42 |
| 24:D2:41:ILE:CG2 | 24:D2:42:GLY:N | 2.78 | 0.42 |
| 26:D4:19:GLY:O | 26:D4:21:VAL:N | 2.52 | 0.42 |
| 31:DA:1450(A):C:N4 | 31:DA:1451:C:H41 | 2.17 | 0.42 |
| 31:DA:140:G:N2 | 31:DA:1596:A:H4' | 2.35 | 0.42 |
| 31:DA:1628:G:O2' | 31:DA:1629:U:H5' | 2.19 | 0.42 |
| 31:DA:2103:C:C2 | 31:DA:2187:G:N1 | 2.87 | 0.42 |
| 31:DA:2392:A:N3 | 31:DA:2392:A:O4' | 2.52 | 0.42 |
| 31:DA:2416:C:N4 | 31:DA:2417:C:N4 | 2.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:2422:A:C4' | 31:DA:2423:U:OP1 | 2.66 | 0.42 |
| 31:DA:2452:C:N4 | 31:DA:2453:A:C6 | 2.87 | 0.42 |
| 31:DA:2592:G:N7 | 31:DA:2593:U:C5 | 2.87 | 0.42 |
| 31:DA:363(D):G:C6 | 31:DA:363(E):U:O4 | 2.72 | 0.42 |
| 33:DD:121:PRO:HB3 | 33:DD:135:PHE:CE1 | 2.54 | 0.42 |
| 33:DD:166:GLN:HE21 | 33:DD:166:GLN:HA | 1.83 | 0.42 |
| 33:DD:210:GLY:HA2 | 33:DD:213:ARG:HB2 | 2.01 | 0.42 |
| 31:DA:2631:G:H22 | 34:DE:61:ARG:HH12 | 1.63 | 0.42 |
| 37:DH:85:LYS:HE2 | 37:DH:141:VAL:O | 2.20 | 0.42 |
| 37:DH:47:GLU:C | 37:DH:49:VAL:H | 2.23 | 0.42 |
| 38:DI:88:ILE:HD11 | 38:DI:142:VAL:HB | 2.00 | 0.42 |
| 41:DP:39:LYS:HD3 | 41:DP:40:SER:H | 1.84 | 0.42 |
| 41:DP:45:LEU:HD22 | 41:DP:46:LYS:N | 2.32 | 0.42 |
| 42:DQ:88:GLY:O | 42:DQ:89:ASN:HB2 | 2.19 | 0.42 |
| 43:DR:51:LEU:HD23 | 43:DR:51:LEU:HA | 1.74 | 0.42 |
| 45:DT:92:GLY:HA2 | 45:DT:114:LEU:HB3 | 2.01 | 0.42 |
| 47:DV:90:PRO:CD | 47:DV:91:TYR:N | 2.82 | 0.42 |
| 50:DY:13:VAL:HG11 | 50:DY:72:VAL:HB | 2.01 | 0.42 |
| 1:AA:272:C:H2' | 1:AA:273:A:C8 | 2.54 | 0.42 |
| 1:AA:355:C:N3 | 1:AA:356:A:C8 | 2.87 | 0.42 |
| 1:AA:445:G:N3 | 1:AA:446:G:C8 | 2.87 | 0.42 |
| 1:AA:709:G:H2' | 1:AA:710:G:C8 | 2.52 | 0.42 |
| 1:AA:832:C:N3 | 1:AA:855:G:C2 | 2.87 | 0.42 |
| 1:AA:84:U:H6 | 1:AA:84:U:H3' | 1.85 | 0.42 |
| 1:AA:973:G:C3' | 1:AA:974:A:H5'' | 2.44 | 0.42 |
| 2:AB:88:ALA:CB | 2:AB:219:VAL:HG13 | 2.44 | 0.42 |
| 2:AB:29:ALA:C | 2:AB:31:TYR:N | 2.73 | 0.42 |
| 3:AC:100:ALA:O | 3:AC:101:LEU:HB2 | 2.18 | 0.42 |
| 3:AC:127:ARG:HD2 | 3:AC:127:ARG:N | 2.34 | 0.42 |
| 3:AC:22:TRP:HE3 | 3:AC:23:TYR:O | 2.02 | 0.42 |
| 3:AC:47:LEU:HD23 | 3:AC:52:LEU:HD13 | 2.00 | 0.42 |
| 3:AC:48:TYR:O | 3:AC:51:GLY:N | 2.51 | 0.42 |
| 4:AD:192:GLU:CD | 4:AD:192:GLU:H | 2.23 | 0.42 |
| 5:AE:18:ARG:HE | 5:AE:25:ARG:HB3 | 1.84 | 0.42 |
| 8:AH:38:ILE:O | 8:AH:42:GLU:HB2 | 2.18 | 0.42 |
| 9:AI:49:PRO:HA | 9:AI:101:PHE:CE1 | 2.54 | 0.42 |
| 10:AJ:99:LYS:HA | 10:AJ:99:LYS:HD3 | 1.91 | 0.42 |
| 11:AK:23:ALA:HB1 | 11:AK:88:GLY:HA3 | 2.00 | 0.42 |
| 13:AM:9:ILE:HD12 | 13:AM:9:ILE:N | 2.34 | 0.42 |
| 15:AO:54:ARG:HG2 | 15:AO:58:MET:CE | 2.49 | 0.42 |
| 18:AR:44:LEU:O | 18:AR:45:SER:O | 2.37 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:B0:49:LYS:N | 22:B0:80:HIS:ND1 | 2.65 | 0.42 |
| 24:B2:14:ARG:HB3 | 24:B2:14:ARG:HE | 1.68 | 0.42 |
| 24:B2:26:ARG:CB | 49:BX:5:TYR:HB3 | 2.49 | 0.42 |
| 26:B4:20:ASN:O | 26:B4:24:THR:HA | 2.19 | 0.42 |
| 27:B5:40:LYS:HZ1 | 27:B5:49:CYS:CB | 2.31 | 0.42 |
| 30:B8:22:VAL:HB | 30:B8:53:PRO:CB | 2.49 | 0.42 |
| 30:B8:51:ALA:CA | 30:B8:53:PRO:HD2 | 2.49 | 0.42 |
| 31:BA:1405:U:C2' | 31:BA:1406:U:O5' | 2.67 | 0.42 |
| 31:BA:1436:G:C3' | 31:BA:1437:C:H5'' | 2.49 | 0.42 |
| 31:BA:1531:C:H5'' | 31:BA:1532:C:C6 | 2.50 | 0.42 |
| 31:BA:1678:G:H8 | 31:BA:1678:G:C5' | 2.33 | 0.42 |
| 31:BA:2287:A:H2 | 31:BA:2346:A:N1 | 2.13 | 0.42 |
| 31:BA:2802:G:OP2 | 31:BA:2803:C:OP2 | 2.36 | 0.42 |
| 31:BA:2859:G:O5' | 31:BA:2859:G:H8 | 2.01 | 0.42 |
| 31:BA:358:U:C3' | 31:BA:358:U:C6 | 3.02 | 0.42 |
| 31:BA:894:C:H2' | 31:BA:895:U:H5' | 2.00 | 0.42 |
| 31:BA:975:C:OP2 | 31:BA:975:C:H4' | 2.20 | 0.42 |
| 32:BB:7:G:C2 | 32:BB:115:G:C2 | 3.07 | 0.42 |
| 33:BD:3:VAL:H | 33:BD:20:ASP:HB2 | 1.83 | 0.42 |
| 33:BD:94:LEU:HD22 | 33:BD:94:LEU:C | 2.39 | 0.42 |
| 34:BE:116:VAL:HG13 | 34:BE:122:PHE:CD2 | 2.55 | 0.42 |
| 35:BF:20:LEU:HD13 | 35:BF:203:GLN:NE2 | 2.34 | 0.42 |
| 36:BG:16:ARG:HB2 | 36:BG:17:PRO:CD | 2.49 | 0.42 |
| 38:BI:75:LEU:HD11 | 38:BI:105:HIS:HE1 | 1.84 | 0.42 |
| 40:BO:22:ILE:HD13 | 40:BO:22:ILE:HA | 1.57 | 0.42 |
| 42:BQ:31:ASP:O | 42:BQ:133:ARG:O | 2.36 | 0.42 |
| 31:BA:995:C:N3 | 46:BU:57:PHE:CZ | 2.87 | 0.42 |
| 46:BU:69:CYS:HB3 | 46:BU:106:PHE:CE2 | 2.54 | 0.42 |
| 46:BU:90:VAL:HG11 | 47:BV:40:LEU:HB3 | 2.01 | 0.42 |
| 47:BV:66:ARG:HD3 | 47:BV:67:GLY:C | 2.39 | 0.42 |
| 49:BX:34:ALA:O | 49:BX:36:LYS:N | 2.52 | 0.42 |
| 24:B2:29:LYS:HZ2 | 49:BX:9:LEU:HA | 1.83 | 0.42 |
| 1:CA:1085:U:C2 | 1:CA:1094:G:O6 | 2.73 | 0.42 |
| 1:CA:1446:U:HO2' | 1:CA:1447:A:H8 | 1.54 | 0.42 |
| 1:CA:189:G:N1 | 1:CA:189(L):G:C6 | 2.86 | 0.42 |
| 1:CA:407:G:HO2' | 4:CD:116:GLN:HG3 | 1.84 | 0.42 |
| 1:CA:508:C:OP1 | 4:CD:209:ARG:NH2 | 2.52 | 0.42 |
| 1:CA:518:C:H2' | 1:CA:530:G:N3 | 2.34 | 0.42 |
| 1:CA:644:G:H2' | 1:CA:645:C:H5' | 2.02 | 0.42 |
| 1:CA:663:A:O3' | 18:CR:64:ARG:NH2 | 2.52 | 0.42 |
| 1:CA:562:C:N4 | 1:CA:884:U:C6 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:CB:69:LEU:HB2 | 2:CB:159:PRO:HG2 | 2.01 | 0.42 |
| 5:CE:102:ALA:HB2 | 5:CE:120:THR:OG1 | 2.20 | 0.42 |
| 7:CG:26:PHE:CG | 7:CG:62:PHE:HE1 | 2.38 | 0.42 |
| 8:CH:38:ILE:HD11 | 8:CH:118:VAL:O | 2.19 | 0.42 |
| 8:CH:109:ILE:HD11 | 8:CH:120:THR:CG2 | 2.49 | 0.42 |
| 8:CH:91:ARG:CG | 8:CH:91:ARG:HH11 | 2.32 | 0.42 |
| 18:CR:59:SER:H | 18:CR:62:GLU:CD | 2.22 | 0.42 |
| 20:CT:100:ILE:O | 20:CT:102:GLY:N | 2.52 | 0.42 |
| 24:D2:46:GLN:HE21 | 24:D2:47:ASN:HA | 1.83 | 0.42 |
| 41:BP:121:LYS:HE3 | 25:D3:2:PRO:HG3 | 2.02 | 0.42 |
| 29:D7:48:LYS:CD | 29:D7:48:LYS:N | 2.82 | 0.42 |
| 31:DA:1141:U:H4' | 31:DA:1142(A):A:O4' | 2.19 | 0.42 |
| 31:DA:1142(A):A:C4 | 31:DA:1144:G:N7 | 2.87 | 0.42 |
| 31:DA:1472:A:H2' | 31:DA:1473:G:C5' | 2.49 | 0.42 |
| 31:DA:1501:C:H2' | 31:DA:1502:C:H6 | 1.84 | 0.42 |
| 31:DA:174:C:O2 | 31:DA:174:C:H2' | 2.19 | 0.42 |
| 31:DA:1904:G:H2' | 31:DA:1905:C:O4' | 2.20 | 0.42 |
| 31:DA:2102:U:C4 | 31:DA:2103:C:N4 | 2.87 | 0.42 |
| 31:DA:265:A:H1' | 31:DA:266:G:O4' | 2.19 | 0.42 |
| 31:DA:271(F):C:C2 | 31:DA:271(G):C:C5 | 3.07 | 0.42 |
| 31:DA:322:A:C5 | 31:DA:340:A:C2 | 3.07 | 0.42 |
| 31:DA:36:G:C5 | 31:DA:37:C:C5 | 3.08 | 0.42 |
| 31:DA:575:A:OP2 | 31:DA:2055:C:N4 | 2.38 | 0.42 |
| 31:DA:643:A:C2 | 31:DA:644:A:C4 | 3.07 | 0.42 |
| 31:DA:712:G:N2 | 31:DA:720:C:C2 | 2.88 | 0.42 |
| 31:DA:801:G:N7 | 35:DF:53:THR:CG2 | 2.83 | 0.42 |
| 25:D3:49:LYS:HD2 | 31:DA:851:U:C5' | 2.49 | 0.42 |
| 32:DB:28:C:N3 | 32:DB:29:A:N7 | 2.68 | 0.42 |
| 33:DD:115:GLN:HG2 | 33:DD:116:GLN:O | 2.19 | 0.42 |
| 34:DE:21:VAL:CG2 | 34:DE:21:VAL:O | 2.67 | 0.42 |
| 34:DE:57:LYS:O | 34:DE:59:VAL:N | 2.50 | 0.42 |
| 35:DF:132:VAL:HG22 | 35:DF:133:ASN:H | 1.84 | 0.42 |
| 41:DP:126:VAL:HA | 41:DP:145:PRO:HB2 | 2.02 | 0.42 |
| 45:DT:33:LYS:O | 45:DT:40:THR:O | 2.37 | 0.42 |
| 45:DT:61:PHE:CZ | 45:DT:76:PHE:HB2 | 2.53 | 0.42 |
| 48:DW:40:ASN:O | 48:DW:41:LYS:HG2 | 2.19 | 0.42 |
| 49:DX:89:ILE:HG23 | 49:DX:89:ILE:O | 2.20 | 0.42 |
| 50:DY:10:GLY:C | 50:DY:27:VAL:HG22 | 2.40 | 0.42 |
| 1:AA:1279:A:O2' | 1:AA:1282:C:N4 | 2.52 | 0.42 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:C6 | 2.54 | 0.42 |
| 1:AA:1442(A):G:H8 | 45:BT:118:ARG:NH1 | 2.14 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:AA:228:A:H2' | 1:AA:229:U:O4' | 2.18 | 0.42 |
| 1:AA:437:U:H5'' | 4:AD:155:LEU:CD1 | 2.46 | 0.42 |
| 1:AA:673:G:N1 | 1:AA:674:G:C6 | 2.87 | 0.42 |
| 1:AA:79:G:H1' | 1:AA:80:G:O5' | 2.20 | 0.42 |
| 4:AD:100:ARG:NH1 | 4:AD:137:SER:HA | 2.34 | 0.42 |
| 4:AD:108:LEU:HD12 | 4:AD:108:LEU:HA | 1.87 | 0.42 |
| 4:AD:64:LEU:O | 4:AD:65:ARG:C | 2.57 | 0.42 |
| 6:AF:12:PRO:HG3 | 6:AF:55:ASP:HB3 | 2.01 | 0.42 |
| 9:AI:48:GLU:H | 9:AI:49:PRO:HD2 | 1.83 | 0.42 |
| 14:AN:12:ARG:C | 14:AN:14:PRO:CD | 2.88 | 0.42 |
| 18:AR:22:VAL:HG11 | 18:AR:42:ARG:O | 2.19 | 0.42 |
| 23:B1:47:GLN:O | 23:B1:48:LYS:O | 2.37 | 0.42 |
| 31:BA:108:U:C2 | 31:BA:109:G:C8 | 3.07 | 0.42 |
| 31:BA:1126:A:H4' | 31:BA:1127:A:O5' | 2.19 | 0.42 |
| 31:BA:1142(A):A:C5 | 31:BA:1144:G:C5 | 3.07 | 0.42 |
| 31:BA:1173:G:H5' | 31:BA:1174:A:P | 2.59 | 0.42 |
| 31:BA:1313:U:C2' | 31:BA:1313:U:O2 | 2.67 | 0.42 |
| 31:BA:1379:A:HO2' | 31:BA:1380:G:P | 2.26 | 0.42 |
| 31:BA:1528(A):A:H2' | 31:BA:1529:G:O4' | 2.19 | 0.42 |
| 31:BA:1649:G:C6 | 31:BA:2009:G:O6 | 2.73 | 0.42 |
| 31:BA:1951:U:O2 | 31:BA:1953:A:H8 | 2.01 | 0.42 |
| 31:BA:1979:C:H2' | 31:BA:1980:G:H5' | 2.02 | 0.42 |
| 31:BA:2291:U:H2' | 31:BA:2292:C:C6 | 2.55 | 0.42 |
| 31:BA:2702:U:OP1 | 31:BA:2702:U:O4' | 2.37 | 0.42 |
| 31:BA:90:U:O2' | 31:BA:92:A:C5' | 2.67 | 0.42 |
| 31:BA:917:A:C5' | 31:BA:917:A:H8 | 2.32 | 0.42 |
| 32:BB:60:C:N3 | 32:BB:61:G:N7 | 2.68 | 0.42 |
| 33:BD:218:ARG:HB3 | 33:BD:219:PRO:HD2 | 2.00 | 0.42 |
| 39:BN:18:ALA:O | 39:BN:21:LYS:HB2 | 2.19 | 0.42 |
| 43:BR:101:ALA:O | 43:BR:102:GLU:CB | 2.68 | 0.42 |
| 49:BX:65:ARG:O | 49:BX:66:LEU:CB | 2.67 | 0.42 |
| 50:BY:75:ILE:HD13 | 50:BY:75:ILE:HA | 1.47 | 0.42 |
| 42:BQ:141:GLN:NE2 | 51:BZ:72:ARG:HG2 | 2.34 | 0.42 |
| 1:CA:1014:A:C2 | 1:CA:1219:U:O2 | 2.72 | 0.42 |
| 1:CA:1141:C:H3' | 1:CA:1141:C:H6 | 1.85 | 0.42 |
| 1:CA:1478:C:C2 | 1:CA:1479:C:C5 | 3.07 | 0.42 |
| 1:CA:337:C:H2' | 1:CA:338:A:C8 | 2.54 | 0.42 |
| 1:CA:675:A:H2' | 1:CA:676:A:C8 | 2.54 | 0.42 |
| 1:CA:996:A:H2' | 1:CA:997:U:C6 | 2.55 | 0.42 |
| 2:CB:161:ALA:HB1 | 2:CB:185:ILE:HD11 | 2.01 | 0.42 |
| 3:CC:106:VAL:HG12 | 3:CC:108:ASN:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:438:G:H4' | 4:CD:123:HIS:HD1 | 1.84 | 0.42 |
| 4:CD:173:TRP:HA | 4:CD:187:ARG:NH1 | 2.34 | 0.42 |
| 4:CD:78:LEU:O | 4:CD:81:GLU:HB3 | 2.19 | 0.42 |
| 8:CH:104:ARG:CZ | 8:CH:138:TRP:CH2 | 3.02 | 0.42 |
| 8:CH:113:SER:C | 8:CH:114:THR:HG22 | 2.39 | 0.42 |
| 10:CJ:7:LYS:HD3 | 10:CJ:71:LEU:HD11 | 2.02 | 0.42 |
| 11:CK:84:VAL:HG11 | 11:CK:95:ILE:HD11 | 2.00 | 0.42 |
| 12:CL:31:PRO:HB2 | 12:CL:32:PHE:CD2 | 2.55 | 0.42 |
| 13:CM:60:VAL:HG12 | 13:CM:66:LEU:HD21 | 2.01 | 0.42 |
| 20:CT:96:GLY:O | 20:CT:97:ALA:HB3 | 2.20 | 0.42 |
| 25:D3:12:PRO:HA | 25:D3:15:TYR:CD1 | 2.54 | 0.42 |
| 28:D6:26:ASN:ND2 | 28:D6:32:ASN:OD1 | 2.52 | 0.42 |
| 31:DA:1275:A:N3 | 31:DA:1276:A:H1' | 2.34 | 0.42 |
| 31:DA:1462:C:H2' | 31:DA:1463:C:H6 | 1.85 | 0.42 |
| 31:DA:1654:A:H2' | 31:DA:1655:A:H8 | 1.83 | 0.42 |
| 31:DA:1827:C:O2' | 31:DA:1970:A:N3 | 2.42 | 0.42 |
| 31:DA:2192:G:C2 | 31:DA:2193:G:C8 | 3.08 | 0.42 |
| 31:DA:2290:G:O2' | 31:DA:2381:C:H1' | 2.19 | 0.42 |
| 31:DA:2280:G:O2' | 31:DA:2388:A:N1 | 2.39 | 0.42 |
| 31:DA:26:G:C6 | 31:DA:27:G:C6 | 3.08 | 0.42 |
| 31:DA:38:A:H2' | 31:DA:39:C:C6 | 2.54 | 0.42 |
| 31:DA:580:C:H2' | 31:DA:581:C:H6 | 1.82 | 0.42 |
| 31:DA:631:A:OP1 | 41:DP:64:LYS:HE2 | 2.19 | 0.42 |
| 31:DA:705:A:H2' | 31:DA:706:A:O4' | 2.19 | 0.42 |
| 27:D5:2:ALA:N | 31:DA:747:U:C2 | 2.88 | 0.42 |
| 31:DA:685:A:C8 | 31:DA:774:A:C6 | 3.07 | 0.42 |
| 33:DD:27:THR:O | 33:DD:28:GLU:HB2 | 2.19 | 0.42 |
| 33:DD:35:LYS:N | 33:DD:64:ILE:CG2 | 2.83 | 0.42 |
| 33:DD:25:THR:CG2 | 33:DD:82:ILE:H | 2.32 | 0.42 |
| 36:DG:174:GLU:HG3 | 36:DG:180:PHE:CE1 | 2.55 | 0.42 |
| 38:DI:44:LEU:HA | 38:DI:44:LEU:HD23 | 1.58 | 0.42 |
| 39:DN:16:ILE:O | 39:DN:54:VAL:HA | 2.19 | 0.42 |
| 39:DN:46:VAL:O | 39:DN:47:ALA:HB3 | 2.19 | 0.42 |
| 40:DO:80:ASP:OD2 | 45:DT:64:ARG:NH2 | 2.53 | 0.42 |
| 41:DP:86:LYS:HB3 | 41:DP:118:GLY:HA3 | 2.00 | 0.42 |
| 42:DQ:141:GLN:NE2 | 51:DZ:72:ARG:HG2 | 2.34 | 0.42 |
| 31:DA:2469:A:HO2' | 42:DQ:56:ARG:HG2 | 1.82 | 0.42 |
| 49:DX:73:ARG:H | 49:DX:74:PRO:HD3 | 1.84 | 0.42 |
| 50:DY:34:LYS:HB3 | 50:DY:34:LYS:HE2 | 1.75 | 0.42 |
| 50:DY:45:VAL:HG13 | 50:DY:46:LYS:H | 1.84 | 0.42 |
| 50:DY:52:SER:HA | 50:DY:53:PRO:HD3 | 1.93 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1090:U:C2 | 1:AA:1091:U:C6 | 3.07 | 0.42 |
| 1:AA:1116:C:N4 | 1:AA:1117:G:N7 | 2.66 | 0.42 |
| 1:AA:1272:G:C6 | 1:AA:1273:G:N7 | 2.87 | 0.42 |
| 1:AA:1320:C:H2' | 1:AA:1321:C:O4' | 2.20 | 0.42 |
| 1:AA:1409:C:OP1 | 31:BA:1916:A:H2 | 2.03 | 0.42 |
| 1:AA:1442(A):G:N2 | 45:BT:119:LYS:HA | 2.35 | 0.42 |
| 1:AA:926:G:C6 | 1:AA:1505:G:C6 | 3.07 | 0.42 |
| 1:AA:1499:A:H1' | 1:AA:1520:G:H5' | 2.00 | 0.42 |
| 1:AA:66:G:C4' | 1:AA:173:U:C5 | 2.97 | 0.42 |
| 1:AA:270:A:C5 | 1:AA:271:C:C4 | 3.08 | 0.42 |
| 1:AA:292:G:H1 | 1:AA:308:C:H42 | 1.68 | 0.42 |
| 1:AA:359:U:O2' | 1:AA:360:A:H5' | 2.19 | 0.42 |
| 1:AA:383:A:OP1 | 1:AA:454:C:O2' | 2.32 | 0.42 |
| 1:AA:450:G:N7 | 1:AA:481:G:C6 | 2.88 | 0.42 |
| 1:AA:55:A:C4 | 1:AA:56:U:C5 | 3.07 | 0.42 |
| 1:AA:741:G:H2' | 1:AA:742:G:O4' | 2.19 | 0.42 |
| 1:AA:763:G:C5 | 1:AA:764:C:C5 | 3.08 | 0.42 |
| 1:AA:81:U:H2' | 1:AA:82:U:C5 | 2.55 | 0.42 |
| 1:AA:874:G:C2' | 1:AA:875:C:H5' | 2.49 | 0.42 |
| 2:AB:70:PHE:O | 2:AB:92:TYR:HA | 2.20 | 0.42 |
| 4:AD:18:LYS:C | 4:AD:19:LEU:HG | 2.39 | 0.42 |
| 6:AF:63:TYR:HB3 | 6:AF:65:VAL:HG12 | 2.02 | 0.42 |
| 7:AG:26:PHE:CG | 7:AG:62:PHE:HE1 | 2.36 | 0.42 |
| 8:AH:9:MET:O | 8:AH:12:ARG:HB2 | 2.19 | 0.42 |
| 8:AH:77:GLU:CG | 8:AH:78:GLN:H | 2.33 | 0.42 |
| 9:AI:18:PHE:O | 9:AI:61:ALA:HA | 2.19 | 0.42 |
| 10:AJ:7:LYS:HD3 | 10:AJ:71:LEU:HD11 | 2.01 | 0.42 |
| 12:AL:46:LYS:O | 12:AL:47:LYS:C | 2.58 | 0.42 |
| 14:AN:32:SER:O | 14:AN:40:CYS:HA | 2.20 | 0.42 |
| 16:AP:49:LEU:O | 16:AP:50:LYS:HB2 | 2.19 | 0.42 |
| 17:AQ:62:SER:OG | 17:AQ:72:ARG:HB2 | 2.19 | 0.42 |
| 18:AR:70:ILE:HG23 | 18:AR:79:LEU:HD13 | 2.01 | 0.42 |
| 23:B1:21:ARG:HD3 | 23:B1:21:ARG:C | 2.40 | 0.42 |
| 27:B5:5:PRO:O | 27:B5:6:VAL:HG23 | 2.19 | 0.42 |
| 30:B8:59:LYS:HE3 | 30:B8:59:LYS:HB3 | 1.64 | 0.42 |
| 31:BA:1038:C:O2 | 31:BA:1038:C:H2' | 2.19 | 0.42 |
| 31:BA:1175:U:H4' | 31:BA:1176:G:H2' | 2.00 | 0.42 |
| 31:BA:1549:C:H2' | 31:BA:1550:C:H6 | 1.83 | 0.42 |
| 31:BA:1380:G:N2 | 31:BA:1570:A:C2 | 2.88 | 0.42 |
| 31:BA:1694:C:O2' | 31:BA:1695:G:C5 | 2.72 | 0.42 |
| 31:BA:1722:A:C2 | 31:BA:1740:G:H2' | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1722:A:C6 | 31:BA:1741:A:C2 | 3.06 | 0.42 |
| 31:BA:1884:A:C2 | 31:BA:1885:A:C8 | 3.06 | 0.42 |
| 31:BA:2664:G:H2' | 31:BA:2665:A:O5' | 2.19 | 0.42 |
| 31:BA:2801:A:O2' | 31:BA:2895:U:C4' | 2.62 | 0.42 |
| 31:BA:353:G:H2' | 31:BA:354:G:O5' | 2.19 | 0.42 |
| 31:BA:384:U:O2' | 31:BA:385:C:H5' | 2.20 | 0.42 |
| 31:BA:547:A:H2' | 31:BA:547:A:N3 | 2.34 | 0.42 |
| 31:BA:868:U:C4 | 31:BA:869:G:N7 | 2.87 | 0.42 |
| 32:BB:75:G:N3 | 51:BZ:85:HIS:CE1 | 2.87 | 0.42 |
| 33:BD:166:GLN:CA | 33:BD:166:GLN:HE21 | 2.32 | 0.42 |
| 35:BF:126:VAL:HG21 | 35:BF:129:PHE:CZ | 2.55 | 0.42 |
| 35:BF:153:SER:HA | 35:BF:172:TRP:O | 2.19 | 0.42 |
| 35:BF:199:TRP:CZ3 | 35:BF:203:GLN:HG3 | 2.55 | 0.42 |
| 35:BF:53:THR:H | 35:BF:56:GLU:HB2 | 1.83 | 0.42 |
| 38:BI:77:LEU:O | 38:BI:104:GLN:OE1 | 2.38 | 0.42 |
| 41:BP:16:ARG:NH1 | 41:BP:18:ARG:HG2 | 2.35 | 0.42 |
| 45:BT:35:LYS:O | 45:BT:38:ASN:N | 2.53 | 0.42 |
| 46:BU:12:ARG:O | 46:BU:15:LYS:HG3 | 2.19 | 0.42 |
| 46:BU:92:ARG:HH22 | 47:BV:10:LYS:CA | 2.31 | 0.42 |
| 47:BV:96:ILE:HG23 | 47:BV:97:LYS:H | 1.85 | 0.42 |
| 47:BV:96:ILE:HG22 | 47:BV:97:LYS:N | 2.35 | 0.42 |
| 1:CA:949:A:C2 | 1:CA:1233:G:N3 | 2.88 | 0.42 |
| 1:CA:236:G:C5 | 1:CA:237:C:C5 | 3.07 | 0.42 |
| 1:CA:527:G:O2' | 1:CA:528:C:H5' | 2.19 | 0.42 |
| 1:CA:628:G:C2 | 1:CA:629:G:C4 | 3.07 | 0.42 |
| 1:CA:666:G:C6 | 1:CA:741:G:C5 | 3.07 | 0.42 |
| 1:CA:782:A:H4' | 1:CA:1514:C:O2' | 2.19 | 0.42 |
| 2:CB:204:ASN:HB3 | 2:CB:210:SER:HB3 | 2.01 | 0.42 |
| 2:CB:93:VAL:HG11 | 2:CB:97:TRP:CD1 | 2.54 | 0.42 |
| 6:CF:14:LEU:HA | 6:CF:14:LEU:HD23 | 1.93 | 0.42 |
| 7:CG:49:ILE:O | 7:CG:49:ILE:HG22 | 2.19 | 0.42 |
| 9:CI:48:GLU:N | 9:CI:49:PRO:CD | 2.82 | 0.42 |
| 10:CJ:48:THR:HA | 10:CJ:62:HIS:CB | 2.49 | 0.42 |
| 11:CK:83:ILE:HA | 11:CK:109:VAL:O | 2.19 | 0.42 |
| 10:CJ:62:HIS:CE1 | 14:CN:61:TRP:HH2 | 2.36 | 0.42 |
| 19:CS:29:ARG:HD2 | 19:CS:30:LEU:N | 2.34 | 0.42 |
| 1:CA:61:G:OP1 | 20:CT:10:LEU:HD11 | 2.19 | 0.42 |
| 22:D0:72:ARG:HH21 | 22:D0:75:LEU:HD13 | 1.83 | 0.42 |
| 28:D6:11:LEU:HB2 | 28:D6:24:GLU:C | 2.40 | 0.42 |
| 31:DA:1794:U:O2' | 31:DA:1795:C:H5' | 2.19 | 0.42 |
| 31:DA:225:A:C2' | 31:DA:226:G:H5' | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:2563:U:O2 | 31:DA:2565:A:C8 | 2.72 | 0.42 |
| 31:DA:2648:C:H2' | 31:DA:2649:U:C6 | 2.55 | 0.42 |
| 31:DA:2748:A:N6 | 31:DA:2749:A:C6 | 2.87 | 0.42 |
| 31:DA:2892:A:C8 | 31:DA:2892:A:H3' | 2.54 | 0.42 |
| 31:DA:672:C:H2' | 31:DA:673:C:C6 | 2.55 | 0.42 |
| 31:DA:917:A:H2' | 31:DA:918:A:O4' | 2.19 | 0.42 |
| 31:DA:993:G:H1' | 47:DV:91:TYR:HD1 | 1.82 | 0.42 |
| 31:DA:997:G:C2' | 31:DA:998:C:H5' | 2.49 | 0.42 |
| 32:DB:49:C:H2' | 32:DB:50:G:H8 | 1.84 | 0.42 |
| 32:DB:66:A:C6 | 32:DB:109:C:C5 | 3.08 | 0.42 |
| 33:DD:16:MET:HG2 | 33:DD:211:ARG:HH21 | 1.84 | 0.42 |
| 33:DD:83:GLU:OE1 | 33:DD:104:TYR:CE2 | 2.73 | 0.42 |
| 34:DE:4:ILE:HG12 | 34:DE:28:ALA:HB1 | 2.01 | 0.42 |
| 35:DF:39:TRP:HA | 35:DF:99:TYR:OH | 2.20 | 0.42 |
| 36:DG:107:LEU:HD23 | 36:DG:111:LEU:HD12 | 2.02 | 0.42 |
| 36:DG:43:LEU:HD22 | 36:DG:43:LEU:N | 2.34 | 0.42 |
| 36:DG:45:GLU:HB2 | 36:DG:47:LYS:CG | 2.48 | 0.42 |
| 39:DN:69:GLN:HB3 | 39:DN:69:GLN:HE21 | 1.56 | 0.42 |
| 40:DO:108:GLU:HG2 | 40:DO:108:GLU:H | 1.39 | 0.42 |
| 41:DP:18:ARG:HB3 | 41:DP:18:ARG:HE | 1.70 | 0.42 |
| 41:DP:88:LEU:HD12 | 41:DP:88:LEU:HA | 1.79 | 0.42 |
| 42:DQ:79:LEU:O | 42:DQ:80:GLU:OE2 | 2.38 | 0.42 |
| 43:DR:12:ARG:HH11 | 43:DR:12:ARG:HG3 | 1.84 | 0.42 |
| 45:DT:100:TYR:O | 45:DT:103:ARG:HG3 | 2.18 | 0.42 |
| 47:DV:43:GLU:HA | 47:DV:48:GLY:CA | 2.49 | 0.42 |
| 47:DV:47:VAL:CG1 | 47:DV:48:GLY:H | 2.10 | 0.42 |
| 48:DW:75:TYR:CE2 | 48:DW:104:THR:HB | 2.54 | 0.42 |
| 49:DX:11:PRO:HB2 | 49:DX:13:LEU:CD2 | 2.49 | 0.42 |
| 49:DX:8:ILE:H | 49:DX:8:ILE:HD12 | 1.85 | 0.42 |
| 50:DY:37:VAL:HG23 | 50:DY:67:LEU:HB3 | 2.01 | 0.42 |
| 1:AA:1064:G:H1' | 1:AA:1065:U:OP2 | 2.19 | 0.42 |
| 1:AA:373:A:O2' | 1:AA:374:A:H5' | 2.20 | 0.42 |
| 1:AA:450:G:H1 | 1:AA:483:C:N4 | 2.17 | 0.42 |
| 1:AA:473:G:H2' | 1:AA:474:G:C8 | 2.52 | 0.42 |
| 1:AA:567:G:C2 | 1:AA:568:G:H1' | 2.54 | 0.42 |
| 1:AA:694:A:C2 | 1:AA:695:A:H1' | 2.54 | 0.42 |
| 1:AA:933:G:O6 | 7:AG:3:ARG:NH2 | 2.52 | 0.42 |
| 2:AB:98:LEU:HB2 | 2:AB:101:MET:HE2 | 2.01 | 0.42 |
| 2:AB:158:LEU:N | 2:AB:158:LEU:HD12 | 2.33 | 0.42 |
| 2:AB:23:ARG:O | 2:AB:23:ARG:HG2 | 2.20 | 0.42 |
| 4:AD:43:HIS:HB3 | 4:AD:46:LYS:HD2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:91:LEU:HD12 | 5:AE:120:THR:HG22 | 2.02 | 0.42 |
| 5:AE:7:GLU:HB2 | 5:AE:35:GLY:O | 2.19 | 0.42 |
| 6:AF:55:ASP:HA | 6:AF:56:PRO:HD2 | 1.95 | 0.42 |
| 6:AF:19:LEU:HD21 | 6:AF:59:TYR:CE2 | 2.54 | 0.42 |
| 12:AL:82:VAL:CG1 | 12:AL:83:VAL:N | 2.77 | 0.42 |
| 1:AA:564:C:N3 | 17:AQ:31:LEU:HD11 | 2.35 | 0.42 |
| 20:AT:18:GLN:O | 20:AT:19:SER:C | 2.58 | 0.42 |
| 1:AA:261:U:C5 | 20:AT:79:ARG:CZ | 3.02 | 0.42 |
| 20:AT:53:LEU:HD21 | 20:AT:92:LEU:CD1 | 2.50 | 0.42 |
| 23:B1:26:ARG:HD3 | 23:B1:34:THR:HB | 2.02 | 0.42 |
| 25:B3:11:SER:HA | 25:B3:12:PRO:HD3 | 1.75 | 0.42 |
| 31:BA:123:G:H2' | 31:BA:124:G:O4' | 2.18 | 0.42 |
| 31:BA:1602:U:H3' | 31:BA:1603:A:H5' | 2.00 | 0.42 |
| 31:BA:1670:C:O2 | 34:BE:129:HIS:CE1 | 2.72 | 0.42 |
| 31:BA:1696:G:C6 | 31:BA:1697:G:C5 | 3.08 | 0.42 |
| 31:BA:2025:C:H2' | 31:BA:2026:C:C6 | 2.54 | 0.42 |
| 31:BA:2192:G:C2 | 31:BA:2193:G:C8 | 3.07 | 0.42 |
| 31:BA:2290:G:O2' | 31:BA:2381:C:H1' | 2.20 | 0.42 |
| 31:BA:2555:U:C5 | 31:BA:2556:C:C2 | 3.07 | 0.42 |
| 31:BA:2558:C:C4 | 31:BA:2559:C:C5 | 3.07 | 0.42 |
| 31:BA:2694:G:C6 | 31:BA:2695:C:C4 | 3.08 | 0.42 |
| 31:BA:271(F):C:C2 | 31:BA:271(G):C:C5 | 3.07 | 0.42 |
| 31:BA:271(P):C:C2' | 31:BA:271(Q):G:C5' | 2.97 | 0.42 |
| 31:BA:2789:C:C2' | 31:BA:2790:A:OP2 | 2.67 | 0.42 |
| 31:BA:355:G:C2 | 31:BA:356:G:C8 | 3.07 | 0.42 |
| 31:BA:671:C:H2' | 31:BA:672:C:H6 | 1.85 | 0.42 |
| 31:BA:878:A:N6 | 31:BA:900:A:C8 | 2.87 | 0.42 |
| 32:BB:15:A:O2' | 32:BB:110:G:C8 | 2.67 | 0.42 |
| 32:BB:44:G:C5' | 32:BB:45:A:OP1 | 2.62 | 0.42 |
| 33:BD:125:ILE:HG13 | 33:BD:137:PRO:CG | 2.49 | 0.42 |
| 34:BE:48:GLN:HE22 | 34:BE:64:LYS:HE2 | 1.84 | 0.42 |
| 34:BE:61:ARG:C | 34:BE:63:LEU:H | 2.22 | 0.42 |
| 35:BF:140:LEU:HA | 35:BF:140:LEU:HD13 | 1.84 | 0.42 |
| 36:BG:68:PRO:HB2 | 36:BG:90:LEU:HG | 2.00 | 0.42 |
| 38:BI:88:ILE:CD1 | 38:BI:123:LEU:HD23 | 2.50 | 0.42 |
| 39:BN:78:TYR:CD1 | 39:BN:79:PRO:CG | 3.02 | 0.42 |
| 42:BQ:88:GLY:O | 42:BQ:89:ASN:CB | 2.66 | 0.42 |
| 46:BU:10:ARG:O | 46:BU:11:ARG:C | 2.56 | 0.42 |
| 46:BU:91:ASP:O | 46:BU:92:ARG:CB | 2.68 | 0.42 |
| 47:BV:45:THR:HG22 | 47:BV:45:THR:O | 2.20 | 0.42 |
| 47:BV:72:VAL:O | 47:BV:89:GLN:O | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:BY:39:VAL:O | 50:BY:40:GLU:CG | 2.67 | 0.42 |
| 1:CA:1064:G:H1' | 1:CA:1065:U:OP2 | 2.19 | 0.42 |
| 1:CA:1066:C:H3' | 1:CA:1067:A:C8 | 2.55 | 0.42 |
| 1:CA:1327:C:OP1 | 21:CU:20:LYS:HB3 | 2.19 | 0.42 |
| 1:CA:386:C:C2' | 1:CA:387:U:C5' | 2.86 | 0.42 |
| 1:CA:406:G:C2 | 1:CA:407:G:C8 | 3.08 | 0.42 |
| 1:CA:617:G:C6 | 1:CA:618:C:C5 | 3.07 | 0.42 |
| 1:CA:617:G:N2 | 1:CA:618:C:C2 | 2.87 | 0.42 |
| 1:CA:673:G:C2 | 1:CA:674:G:C5 | 3.07 | 0.42 |
| 1:CA:840:C:H4' | 1:CA:848:C:O2 | 2.19 | 0.42 |
| 2:CB:102:LEU:O | 2:CB:105:PHE:HB2 | 2.20 | 0.42 |
| 3:CC:77:ILE:O | 3:CC:83:ARG:HB3 | 2.19 | 0.42 |
| 1:CA:620:C:C2 | 4:CD:135:LEU:HG | 2.55 | 0.42 |
| 4:CD:79:PHE:CD2 | 4:CD:79:PHE:C | 2.93 | 0.42 |
| 5:CE:131:ILE:O | 5:CE:134:ALA:HB3 | 2.20 | 0.42 |
| 5:CE:7:GLU:HB2 | 5:CE:35:GLY:O | 2.19 | 0.42 |
| 6:CF:30:LEU:CB | 6:CF:35:ALA:HB3 | 2.46 | 0.42 |
| 9:CI:77:ILE:O | 9:CI:81:ILE:HG12 | 2.19 | 0.42 |
| 13:CM:76:ALA:HA | 13:CM:79:LYS:HD2 | 2.01 | 0.42 |
| 17:CQ:22:LEU:HD12 | 17:CQ:40:LYS:O | 2.20 | 0.42 |
| 1:CA:719:C:H1' | 18:CR:49:LYS:HB3 | 2.00 | 0.42 |
| 18:CR:73:ALA:CB | 18:CR:79:LEU:HD12 | 2.42 | 0.42 |
| 20:CT:55:ILE:O | 20:CT:56:MET:C | 2.57 | 0.42 |
| 30:D8:2:PRO:O | 30:D8:3:LYS:C | 2.57 | 0.42 |
| 31:DA:1484:G:N2 | 31:DA:1505:C:N4 | 2.60 | 0.42 |
| 31:DA:1629:U:H2' | 31:DA:1630:G:C8 | 2.55 | 0.42 |
| 31:DA:1722:A:C6 | 31:DA:1741:A:C2 | 3.08 | 0.42 |
| 31:DA:2345:G:N3 | 31:DA:2381:C:H2' | 2.35 | 0.42 |
| 31:DA:2473:U:O2 | 31:DA:2473:U:H2' | 2.19 | 0.42 |
| 31:DA:286:C:N4 | 31:DA:356:G:C6 | 2.88 | 0.42 |
| 31:DA:413:C:O5' | 31:DA:413:C:H6 | 2.03 | 0.42 |
| 31:DA:676:A:N1 | 31:DA:802:A:N1 | 2.68 | 0.42 |
| 31:DA:874:G:N2 | 31:DA:904:C:C2 | 2.87 | 0.42 |
| 31:DA:900:A:C4 | 31:DA:901:A:C8 | 3.07 | 0.42 |
| 33:DD:28:GLU:CB | 33:DD:29:PRO:HD3 | 2.49 | 0.42 |
| 36:DG:88:ILE:HG22 | 36:DG:89:GLY:N | 2.35 | 0.42 |
| 36:DG:92:VAL:HG22 | 36:DG:93:THR:N | 2.34 | 0.42 |
| 36:DG:96:ARG:O | 36:DG:99:MET:HB3 | 2.19 | 0.42 |
| 38:DI:88:ILE:CD1 | 38:DI:123:LEU:HD23 | 2.48 | 0.42 |
| 38:DI:136:VAL:HG22 | 38:DI:136:VAL:O | 2.19 | 0.42 |
| 38:DI:13:GLY:O | 38:DI:15:VAL:N | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:DO:7:TYR:CE1 | 40:DO:20:MET:HB2 | 2.55 | 0.42 |
| 42:DQ:26:TYR:HD1 | 42:DQ:27:VAL:O | 2.02 | 0.42 |
| 43:DR:18:LEU:HD23 | 43:DR:18:LEU:HA | 1.80 | 0.42 |
| 31:DA:995:C:N3 | 46:DU:57:PHE:CZ | 2.87 | 0.42 |
| 31:DA:1225:G:OP1 | 47:DV:88:ARG:CB | 2.67 | 0.42 |
| 51:DZ:5:LEU:HA | 51:DZ:5:LEU:HD23 | 1.63 | 0.42 |
| 1:AA:1387:G:N3 | 1:AA:1387:G:H2' | 2.35 | 0.42 |
| 1:AA:836:G:C6 | 1:AA:851:G:C5 | 3.07 | 0.42 |
| 2:AB:102:LEU:N | 2:AB:102:LEU:HD12 | 2.34 | 0.42 |
| 2:AB:187:LEU:HA | 2:AB:201:ILE:O | 2.19 | 0.42 |
| 4:AD:144:ASP:O | 4:AD:146:ILE:HD12 | 2.19 | 0.42 |
| 7:AG:87:VAL:HA | 7:AG:88:PRO:HD3 | 1.94 | 0.42 |
| 9:AI:111:ARG:HG2 | 9:AI:112:LYS:N | 2.35 | 0.42 |
| 9:AI:114:TYR:N | 9:AI:114:TYR:HD2 | 2.13 | 0.42 |
| 11:AK:27:ASN:OD1 | 11:AK:28:THR:N | 2.53 | 0.42 |
| 18:AR:53:ARG:HH21 | 18:AR:60:ALA:H | 1.66 | 0.42 |
| 28:B6:44:ARG:O | 28:B6:45:LYS:CG | 2.60 | 0.42 |
| 30:B8:50:LEU:HD12 | 30:B8:51:ALA:H | 1.83 | 0.42 |
| 31:BA:1404:C:O2 | 31:BA:1404:C:H2' | 2.19 | 0.42 |
| 31:BA:1480:G:C6 | 31:BA:1481:U:N3 | 2.87 | 0.42 |
| 31:BA:1512:U:O2' | 31:BA:1513:C:H5' | 2.19 | 0.42 |
| 31:BA:1549:C:O2' | 31:BA:1550:C:H5' | 2.20 | 0.42 |
| 31:BA:1677:A:H2' | 31:BA:1678:G:C8 | 2.53 | 0.42 |
| 31:BA:1892:C:C2' | 31:BA:1893:C:H5' | 2.50 | 0.42 |
| 31:BA:1973:G:C5 | 31:BA:1974:C:C5 | 3.07 | 0.42 |
| 31:BA:2078:C:C2' | 31:BA:2079:U:H5' | 2.49 | 0.42 |
| 31:BA:2411:A:H2' | 31:BA:2411:A:N3 | 2.33 | 0.42 |
| 31:BA:2526:G:C6 | 31:BA:2527:C:C4 | 3.08 | 0.42 |
| 31:BA:2702:U:OP1 | 31:BA:2702:U:C2 | 2.73 | 0.42 |
| 31:BA:353:G:C2' | 31:BA:354:G:O5' | 2.67 | 0.42 |
| 31:BA:358:U:H3' | 31:BA:358:U:C6 | 2.50 | 0.42 |
| 31:BA:375:C:H2' | 31:BA:376:C:C6 | 2.55 | 0.42 |
| 31:BA:491:G:O2' | 31:BA:492:A:H5' | 2.19 | 0.42 |
| 31:BA:510:C:O2' | 31:BA:511:U:H5' | 2.19 | 0.42 |
| 32:BB:21:G:O6 | 32:BB:63:G:C4 | 2.73 | 0.42 |
| 32:BB:73:A:C4 | 32:BB:105:A:C2 | 3.07 | 0.42 |
| 34:BE:144:ARG:HB3 | 34:BE:145:LYS:H | 1.43 | 0.42 |
| 35:BF:3:GLU:C | 35:BF:24:LEU:HG | 2.39 | 0.42 |
| 37:BH:41:MET:HE1 | 37:BH:55:PRO:HD3 | 2.02 | 0.42 |
| 37:BH:85:LYS:HZ3 | 37:BH:145:ALA:CB | 2.33 | 0.42 |
| 39:BN:15:LEU:HD21 | 39:BN:55:VAL:CG2 | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BQ:42:ILE:HG22 | 42:BQ:47:ILE:HG13 | 2.01 | 0.42 |
| 43:BR:44:LEU:O | 43:BR:45:ARG:C | 2.56 | 0.42 |
| 44:BS:33:LYS:C | 44:BS:34:HIS:HD2 | 2.23 | 0.42 |
| 44:BS:61:ASN:O | 44:BS:65:VAL:HG23 | 2.19 | 0.42 |
| 45:BT:68:TYR:C | 45:BT:70:VAL:H | 2.22 | 0.42 |
| 45:BT:89:VAL:HB | 45:BT:91:ARG:HG2 | 2.02 | 0.42 |
| 47:BV:62:LEU:HD22 | 47:BV:98:GLU:CB | 2.35 | 0.42 |
| 51:BZ:118:GLN:O | 51:BZ:120:ILE:HG12 | 2.19 | 0.42 |
| 51:BZ:76:LEU:HA | 51:BZ:76:LEU:HD23 | 1.85 | 0.42 |
| 1:CA:1118:C:H1' | 1:CA:1179:A:C5 | 2.54 | 0.42 |
| 1:CA:1392:G:H2' | 1:CA:1393:U:H5' | 2.01 | 0.42 |
| 1:CA:1446:U:O2' | 1:CA:1447:A:H8 | 1.97 | 0.42 |
| 1:CA:1507:A:C2 | 1:CA:1508:G:C4 | 3.07 | 0.42 |
| 1:CA:24:U:O2' | 1:CA:25:C:H5' | 2.20 | 0.42 |
| 1:CA:282:A:N3 | 1:CA:282:A:H2' | 2.35 | 0.42 |
| 1:CA:355:C:N3 | 1:CA:356:A:C8 | 2.88 | 0.42 |
| 1:CA:375:U:C4 | 1:CA:376:G:N7 | 2.88 | 0.42 |
| 1:CA:430:A:C2' | 1:CA:431:A:H5' | 2.50 | 0.42 |
| 1:CA:452:A:N7 | 1:CA:480:U:O4 | 2.53 | 0.42 |
| 1:CA:724:G:C2 | 1:CA:725:G:C8 | 3.07 | 0.42 |
| 1:CA:73:G:N2 | 1:CA:76:C:C2 | 2.88 | 0.42 |
| 1:CA:867:G:N2 | 1:CA:868:C:C2 | 2.88 | 0.42 |
| 3:CC:100:ALA:O | 3:CC:101:LEU:HB2 | 2.20 | 0.42 |
| 4:CD:33:MET:HE1 | 4:CD:37:PRO:HA | 2.02 | 0.42 |
| 5:CE:100:VAL:HG13 | 5:CE:118:ILE:HG22 | 2.02 | 0.42 |
| 8:CH:113:SER:H | 8:CH:134:ILE:CG1 | 2.31 | 0.42 |
| 9:CI:46:ALA:HA | 9:CI:78:LYS:HZ1 | 1.85 | 0.42 |
| 10:CJ:62:HIS:CE1 | 14:CN:61:TRP:CH2 | 3.07 | 0.42 |
| 16:CP:49:LEU:O | 16:CP:50:LYS:HB2 | 2.19 | 0.42 |
| 17:CQ:27:PHE:CE1 | 17:CQ:36:ILE:HD11 | 2.54 | 0.42 |
| 18:CR:65:ILE:HG13 | 18:CR:65:ILE:H | 1.59 | 0.42 |
| 24:D2:32:LEU:C | 24:D2:32:LEU:HD12 | 2.40 | 0.42 |
| 30:D8:35:GLN:HB3 | 31:DA:2420:C:OP1 | 2.19 | 0.42 |
| 31:DA:1017:G:H2' | 31:DA:1018:C:H6 | 1.85 | 0.42 |
| 31:DA:1173:G:H5' | 31:DA:1174:A:P | 2.60 | 0.42 |
| 31:DA:1403:C:H2' | 31:DA:1404:C:O4' | 2.19 | 0.42 |
| 31:DA:141:A:H2' | 31:DA:1408:C:O2' | 2.20 | 0.42 |
| 31:DA:1636:C:H2' | 31:DA:1637:A:C8 | 2.54 | 0.42 |
| 31:DA:1648:C:C2' | 31:DA:1649:G:O5' | 2.68 | 0.42 |
| 31:DA:2189:U:H2' | 31:DA:2190:G:O4' | 2.20 | 0.42 |
| 31:DA:827:U:O2 | 31:DA:2246:G:H4' | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:2411:A:N3 | 31:DA:2411:A:H2' | 2.35 | 0.42 |
| 31:DA:2470:G:C6 | 31:DA:2471:C:C5 | 3.08 | 0.42 |
| 31:DA:2677:G:H2' | 31:DA:2678:C:C6 | 2.55 | 0.42 |
| 31:DA:494:G:H5'' | 31:DA:494:G:C8 | 2.52 | 0.42 |
| 31:DA:547:A:N3 | 31:DA:547:A:H2' | 2.34 | 0.42 |
| 31:DA:780:G:N2 | 31:DA:783:A:H62 | 2.08 | 0.42 |
| 31:DA:921:G:C6 | 31:DA:922:U:C4 | 3.07 | 0.42 |
| 31:DA:979:G:H3' | 31:DA:980:A:H5'' | 2.02 | 0.42 |
| 32:DB:73:A:H2' | 32:DB:73:A:N3 | 2.34 | 0.42 |
| 33:DD:10:THR:HB | 33:DD:11:PRO:HD2 | 2.02 | 0.42 |
| 33:DD:266:SER:O | 33:DD:267:SER:HB2 | 2.20 | 0.42 |
| 33:DD:35:LYS:HG2 | 33:DD:64:ILE:CA | 2.50 | 0.42 |
| 33:DD:85:ASP:OD1 | 33:DD:86:PRO:HD2 | 2.20 | 0.42 |
| 34:DE:78:LEU:HG | 34:DE:78:LEU:H | 1.56 | 0.42 |
| 35:DF:199:TRP:CZ3 | 35:DF:203:GLN:HG3 | 2.55 | 0.42 |
| 35:DF:53:THR:N | 35:DF:56:GLU:HB2 | 2.33 | 0.42 |
| 36:DG:16:ARG:HH11 | 36:DG:31:VAL:CG1 | 2.31 | 0.42 |
| 37:DH:85:LYS:HZ3 | 37:DH:145:ALA:CA | 2.32 | 0.42 |
| 39:DN:93:THR:O | 39:DN:94:HIS:C | 2.57 | 0.42 |
| 41:DP:59:LEU:CA | 41:DP:61:ARG:NH1 | 2.59 | 0.42 |
| 49:DX:8:ILE:N | 49:DX:8:ILE:HD12 | 2.34 | 0.42 |
| 50:DY:53:PRO:O | 50:DY:56:PRO:O | 2.37 | 0.42 |
| 1:AA:1090:U:N3 | 1:AA:1091:U:C5 | 2.87 | 0.42 |
| 1:AA:1091:U:H2' | 1:AA:1091:U:O2 | 2.19 | 0.42 |
| 1:AA:1099:G:H2' | 1:AA:1099:G:N3 | 2.35 | 0.42 |
| 1:AA:1163:C:C2 | 1:AA:1174:G:N2 | 2.88 | 0.42 |
| 1:AA:976:G:C8 | 1:AA:1362:C:N4 | 2.88 | 0.42 |
| 1:AA:1367:C:C4 | 1:AA:1368:G:N7 | 2.87 | 0.42 |
| 1:AA:156:G:C6 | 1:AA:166:G:N1 | 2.88 | 0.42 |
| 1:AA:191:G:N3 | 20:AT:103:GLY:O | 2.53 | 0.42 |
| 1:AA:355:C:H5' | 1:AA:389:A:OP2 | 2.19 | 0.42 |
| 1:AA:392:G:C4 | 1:AA:393:A:C8 | 3.07 | 0.42 |
| 1:AA:430:A:C2' | 1:AA:431:A:H5' | 2.50 | 0.42 |
| 1:AA:682:G:C6 | 1:AA:683:G:C5 | 3.08 | 0.42 |
| 1:AA:687:A:C2 | 1:AA:704:A:C6 | 3.07 | 0.42 |
| 1:AA:812:C:OP1 | 1:AA:903:G:H1' | 2.20 | 0.42 |
| 2:AB:15:VAL:H | 2:AB:16:HIS:HD1 | 1.66 | 0.42 |
| 2:AB:8:LYS:HZ2 | 2:AB:217:ARG:HH11 | 1.67 | 0.42 |
| 3:AC:66:VAL:O | 3:AC:66:VAL:HG12 | 2.19 | 0.42 |
| 3:AC:95:THR:HG22 | 3:AC:97:LYS:N | 2.33 | 0.42 |
| 4:AD:108:LEU:HD21 | 4:AD:183:GLY:HA3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AD:180:GLY:O | 4:AD:182:LYS:HG2 | 2.20 | 0.42 |
| 12:AL:70:ILE:HG13 | 12:AL:100:ILE:HD12 | 2.02 | 0.42 |
| 12:AL:35:GLY:O | 12:AL:83:VAL:HG12 | 2.20 | 0.42 |
| 13:AM:16:ASP:N | 13:AM:16:ASP:OD2 | 2.53 | 0.42 |
| 17:AQ:52:LYS:HD2 | 17:AQ:52:LYS:H | 1.84 | 0.42 |
| 22:B0:71:ASP:O | 22:B0:72:ARG:HG2 | 2.20 | 0.42 |
| 24:B2:32:LEU:HD13 | 24:B2:32:LEU:HA | 1.61 | 0.42 |
| 31:BA:1300:U:H2' | 31:BA:1626:G:N2 | 2.35 | 0.42 |
| 31:BA:1801:G:H3' | 31:BA:1802:A:H5' | 2.01 | 0.42 |
| 31:BA:2471:C:C4 | 31:BA:2472:G:C5 | 3.08 | 0.42 |
| 31:BA:2821:A:H2' | 31:BA:2822:G:H8 | 1.83 | 0.42 |
| 31:BA:394:A:C6 | 31:BA:395:U:C4 | 3.08 | 0.42 |
| 31:BA:417:C:H2' | 31:BA:417:C:O2 | 2.20 | 0.42 |
| 31:BA:701:G:N2 | 31:BA:732:C:C2 | 2.88 | 0.42 |
| 27:B5:2:ALA:N | 31:BA:747:U:C2 | 2.88 | 0.42 |
| 31:BA:909:A:H2' | 31:BA:912:C:H5 | 1.85 | 0.42 |
| 32:BB:86:G:H1 | 32:BB:91:C:N4 | 2.18 | 0.42 |
| 31:BA:745:G:OP2 | 34:BE:133:LYS:HE3 | 2.20 | 0.42 |
| 36:BG:111:LEU:HA | 36:BG:114:ILE:CG1 | 2.49 | 0.42 |
| 37:BH:41:MET:O | 37:BH:42:ARG:C | 2.58 | 0.42 |
| 39:BN:128:HIS:O | 39:BN:129:PRO:C | 2.58 | 0.42 |
| 41:BP:143:GLY:CA | 41:BP:145:PRO:HD3 | 2.49 | 0.42 |
| 41:BP:88:LEU:HA | 41:BP:88:LEU:HD12 | 1.76 | 0.42 |
| 44:BS:90:GLY:C | 44:BS:92:TYR:N | 2.72 | 0.42 |
| 45:BT:100:TYR:O | 45:BT:103:ARG:HG3 | 2.19 | 0.42 |
| 49:BX:28:PHE:N | 49:BX:28:PHE:CD1 | 2.88 | 0.42 |
| 49:BX:27:THR:OG1 | 49:BX:77:LYS:HA | 2.19 | 0.42 |
| 50:BY:8:LYS:CD | 50:BY:28:LYS:HZ3 | 2.33 | 0.42 |
| 1:CA:1090:U:N3 | 1:CA:1091:U:C5 | 2.88 | 0.42 |
| 1:CA:112:G:C2 | 1:CA:113:G:C8 | 3.08 | 0.42 |
| 1:CA:1158:C:C2 | 1:CA:1160:G:N7 | 2.88 | 0.42 |
| 1:CA:270:A:C5 | 1:CA:271:C:C4 | 3.08 | 0.42 |
| 1:CA:340:U:H2' | 1:CA:341:C:O4' | 2.20 | 0.42 |
| 1:CA:503:C:O5' | 1:CA:503:C:H6 | 2.02 | 0.42 |
| 1:CA:872:A:C2 | 1:CA:874:G:C6 | 3.07 | 0.42 |
| 1:CA:962:C:H2' | 1:CA:963:G:O4' | 2.20 | 0.42 |
| 1:CA:991:U:O4 | 1:CA:1212:U:O2' | 2.25 | 0.42 |
| 2:CB:158:LEU:HD12 | 2:CB:158:LEU:N | 2.35 | 0.42 |
| 1:CA:1071:C:O3' | 5:CE:49:PRO:HG2 | 2.19 | 0.42 |
| 11:CK:48:ILE:HG22 | 11:CK:49:GLY:N | 2.34 | 0.42 |
| 12:CL:69:TYR:HD2 | 12:CL:99:HIS:CD2 | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:CN:32:SER:O | 14:CN:40:CYS:HA | 2.19 | 0.42 |
| 16:CP:21:VAL:O | 16:CP:33:ILE:HB | 2.19 | 0.42 |
| 16:CP:39:TYR:CD1 | 16:CP:40:ASP:N | 2.88 | 0.42 |
| 26:D4:15:ILE:O | 26:D4:16:CYS:C | 2.58 | 0.42 |
| 27:D5:25:LEU:HD12 | 48:DW:19:LEU:C | 2.40 | 0.42 |
| 30:D8:60:LEU:HB3 | 30:D8:63:PRO:HG2 | 2.00 | 0.42 |
| 31:DA:108:U:C2 | 31:DA:109:G:C8 | 3.07 | 0.42 |
| 31:DA:1131:G:C2 | 31:DA:1132:A:C4 | 3.08 | 0.42 |
| 31:DA:1291:C:C2 | 31:DA:1292:U:C5 | 3.08 | 0.42 |
| 31:DA:1420:U:HO2' | 31:DA:1421:G:P | 2.42 | 0.42 |
| 31:DA:1476:C:H2' | 31:DA:1477:A:O5' | 2.20 | 0.42 |
| 31:DA:1722:A:H2 | 31:DA:1740:G:H2' | 1.85 | 0.42 |
| 31:DA:1980:G:O5' | 31:DA:1980:G:H2' | 2.19 | 0.42 |
| 31:DA:2070:G:H2' | 31:DA:2071:A:H8 | 1.85 | 0.42 |
| 31:DA:214:G:H21 | 31:DA:216:A:H1' | 1.85 | 0.42 |
| 31:DA:2287:A:C4 | 31:DA:2289:G:N7 | 2.87 | 0.42 |
| 31:DA:243:U:O2' | 31:DA:244:A:H5' | 2.20 | 0.42 |
| 31:DA:2508:G:O2' | 31:DA:2509:G:H5' | 2.20 | 0.42 |
| 31:DA:9:U:C4 | 31:DA:2629:A:C6 | 3.07 | 0.42 |
| 31:DA:2651:C:O2' | 31:DA:2652:C:H5' | 2.20 | 0.42 |
| 31:DA:2712:U:H1' | 31:DA:2712(A):A:H8 | 1.81 | 0.42 |
| 31:DA:2821:A:C2 | 31:DA:2822:G:C4 | 3.08 | 0.42 |
| 31:DA:292:C:H2' | 31:DA:293:U:C6 | 2.55 | 0.42 |
| 31:DA:906:G:H2' | 31:DA:907:U:O5' | 2.20 | 0.42 |
| 31:DA:951:C:C2' | 31:DA:952:G:H5' | 2.50 | 0.42 |
| 33:DD:159:ALA:C | 33:DD:161:THR:H | 2.22 | 0.42 |
| 33:DD:35:LYS:CD | 33:DD:64:ILE:N | 2.82 | 0.42 |
| 33:DD:85:ASP:HB2 | 33:DD:92:ILE:HG12 | 2.01 | 0.42 |
| 34:DE:7:VAL:HA | 34:DE:194:GLY:O | 2.20 | 0.42 |
| 34:DE:8:LYS:HG2 | 34:DE:192:ASN:HD22 | 1.85 | 0.42 |
| 41:DP:95:VAL:CG1 | 41:DP:123:LEU:HD11 | 2.50 | 0.42 |
| 41:DP:95:VAL:CG2 | 41:DP:125:VAL:HB | 2.47 | 0.42 |
| 42:DQ:86:GLY:C | 42:DQ:88:GLY:N | 2.72 | 0.42 |
| 45:DT:99:LEU:HB3 | 45:DT:101:PHE:CE1 | 2.54 | 0.42 |
| 47:DV:61:VAL:O | 47:DV:99:ILE:N | 2.37 | 0.42 |
| 49:DX:36:LYS:O | 49:DX:39:ILE:HG23 | 2.20 | 0.42 |
| 50:DY:79:CYS:SG | 50:DY:80:GLY:N | 2.92 | 0.42 |
| 51:DZ:44:PHE:CZ | 51:DZ:48:PHE:CD2 | 3.07 | 0.42 |
| 1:AA:1086:U:H2' | 1:AA:1087:G:C8 | 2.55 | 0.42 |
| 1:AA:25:C:H2' | 1:AA:26:A:H8 | 1.84 | 0.42 |
| 1:AA:595:G:H1' | 1:AA:596:C:H5 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:627:G:O2' | 1:AA:628:G:H5' | 2.19 | 0.42 |
| 1:AA:731:G:H2' | 1:AA:732:C:C6 | 2.55 | 0.42 |
| 1:AA:696:A:H1' | 1:AA:786:G:O2' | 2.19 | 0.42 |
| 2:AB:140:HIS:HA | 2:AB:143:GLU:HG3 | 2.01 | 0.42 |
| 3:AC:150:LYS:HG3 | 3:AC:169:ALA:HB2 | 2.02 | 0.42 |
| 4:AD:105:VAL:O | 4:AD:105:VAL:CG1 | 2.68 | 0.42 |
| 6:AF:14:LEU:HA | 6:AF:14:LEU:HD23 | 1.94 | 0.42 |
| 8:AH:11:THR:HA | 8:AH:14:ARG:NH1 | 2.34 | 0.42 |
| 1:AA:1048:G:H4' | 14:AN:2:ALA:N | 2.34 | 0.42 |
| 17:AQ:14:LYS:NZ | 17:AQ:14:LYS:HB2 | 2.34 | 0.42 |
| 18:AR:25:THR:O | 18:AR:26:LEU:HD23 | 2.19 | 0.42 |
| 18:AR:59:SER:H | 18:AR:62:GLU:CD | 2.23 | 0.42 |
| 22:B0:25:ARG:HB2 | 22:B0:37:LEU:HD23 | 2.01 | 0.42 |
| 22:B0:82:ARG:HA | 22:B0:83:PRO:HD2 | 1.89 | 0.42 |
| 27:B5:19:ARG:HD2 | 27:B5:19:ARG:HH11 | 1.67 | 0.42 |
| 27:B5:29:THR:O | 27:B5:30:LEU:HD23 | 2.20 | 0.42 |
| 29:B7:48:LYS:CD | 29:B7:48:LYS:N | 2.82 | 0.42 |
| 31:BA:1158:C:O5' | 31:BA:1158:C:H6 | 2.02 | 0.42 |
| 31:BA:1195:G:C2' | 31:BA:1196:C:H5' | 2.49 | 0.42 |
| 31:BA:1419:A:C8 | 31:BA:1421:G:C6 | 3.08 | 0.42 |
| 31:BA:1420:U:HO2' | 31:BA:1421:G:P | 2.43 | 0.42 |
| 31:BA:1866:C:O2 | 31:BA:1876:A:H1' | 2.20 | 0.42 |
| 31:BA:2275:C:H5' | 31:BA:2275:C:C6 | 2.54 | 0.42 |
| 31:BA:2292:C:C2' | 31:BA:2293:C:H5' | 2.50 | 0.42 |
| 31:BA:2476:A:C5 | 31:BA:2477:C:C5 | 3.08 | 0.42 |
| 32:BB:33:G:C2' | 32:BB:34:U:H5' | 2.50 | 0.42 |
| 33:BD:131:LEU:N | 33:BD:131:LEU:HD12 | 2.33 | 0.42 |
| 33:BD:35:LYS:HZ3 | 33:BD:104:TYR:HD1 | 1.67 | 0.42 |
| 34:BE:48:GLN:HG3 | 34:BE:78:LEU:HB3 | 2.01 | 0.42 |
| 35:BF:60:SER:OG | 35:BF:61:GLY:N | 2.51 | 0.42 |
| 37:BH:89:ILE:CD1 | 37:BH:90:LYS:N | 2.83 | 0.42 |
| 38:BI:9:LEU:N | 38:BI:13:GLY:HA2 | 2.31 | 0.42 |
| 38:BI:56:LYS:HA | 38:BI:59:ALA:CB | 2.49 | 0.42 |
| 39:BN:55:VAL:HG12 | 39:BN:126:PRO:HA | 2.02 | 0.42 |
| 39:BN:64:GLY:O | 39:BN:65:LYS:HE2 | 2.19 | 0.42 |
| 50:BY:23:ARG:O | 50:BY:24:VAL:HB | 2.20 | 0.42 |
| 50:BY:46:LYS:O | 50:BY:47:LYS:HE3 | 2.20 | 0.42 |
| 51:BZ:52:SER:OG | 51:BZ:53:ILE:N | 2.51 | 0.42 |
| 1:CA:1027:C:H6 | 1:CA:1027:C:O5' | 2.03 | 0.42 |
| 1:CA:1086:U:H2' | 1:CA:1087:G:C8 | 2.55 | 0.42 |
| 1:CA:1279:A:O2' | 1:CA:1282:C:N4 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1465:C:C4 | 1:CA:1466:C:C4 | 3.08 | 0.42 |
| 1:CA:816:A:OP2 | 1:CA:1527:C:H5' | 2.20 | 0.42 |
| 1:CA:382:A:N3 | 1:CA:383:A:C8 | 2.88 | 0.42 |
| 1:CA:718:G:C1' | 11:CK:116:HIS:HA | 2.50 | 0.42 |
| 1:CA:763:G:C5 | 1:CA:764:C:C5 | 3.08 | 0.42 |
| 1:CA:978:A:C5' | 1:CA:979:C:OP2 | 2.67 | 0.42 |
| 6:CF:12:PRO:HG3 | 6:CF:55:ASP:HB3 | 2.02 | 0.42 |
| 7:CG:149:ARG:HG2 | 7:CG:149:ARG:O | 2.20 | 0.42 |
| 8:CH:87:SER:HB2 | 8:CH:93:VAL:HB | 2.02 | 0.42 |
| 11:CK:30:VAL:HG21 | 11:CK:65:ALA:HA | 2.02 | 0.42 |
| 11:CK:69:ALA:O | 11:CK:73:MET:HG2 | 2.20 | 0.42 |
| 11:CK:99:GLN:OE1 | 11:CK:105:VAL:HG11 | 2.20 | 0.42 |
| 12:CL:39:VAL:HG12 | 12:CL:40:VAL:N | 2.35 | 0.42 |
| 17:CQ:22:LEU:HD12 | 17:CQ:23:VAL:H | 1.83 | 0.42 |
| 22:D0:42:GLY:HA3 | 31:DA:2331:G:O4' | 2.20 | 0.42 |
| 24:D2:33:MET:HG2 | 49:DX:11:PRO:CD | 2.39 | 0.42 |
| 28:D6:40:CYS:SG | 28:D6:45:LYS:CD | 3.08 | 0.42 |
| 30:D8:4:MET:HB2 | 30:D8:4:MET:HE2 | 1.81 | 0.42 |
| 30:D8:52:LYS:O | 30:D8:52:LYS:HG3 | 2.20 | 0.42 |
| 31:DA:1213:A:O2' | 31:DA:1214:A:H5' | 2.20 | 0.42 |
| 31:DA:1349:A:H2' | 31:DA:1350:C:OP1 | 2.20 | 0.42 |
| 31:DA:1486:A:C2' | 31:DA:1487:G:H5' | 2.50 | 0.42 |
| 31:DA:1614:A:N6 | 48:DW:87:PRO:HA | 2.35 | 0.42 |
| 31:DA:754:C:O4' | 31:DA:1618:A:H2 | 2.03 | 0.42 |
| 31:DA:1876:A:H2' | 31:DA:1877:A:C8 | 2.55 | 0.42 |
| 31:DA:2263:C:C6 | 31:DA:2263:C:H5' | 2.41 | 0.42 |
| 31:DA:2287:A:N1 | 31:DA:2346:A:C2 | 2.87 | 0.42 |
| 31:DA:2473:U:C4 | 31:DA:2474:C:C5 | 3.07 | 0.42 |
| 31:DA:2656:U:H2' | 31:DA:2657:A:C5' | 2.50 | 0.42 |
| 31:DA:2851:A:H2' | 31:DA:2852:G:O4' | 2.20 | 0.42 |
| 31:DA:2895:U:C5 | 31:DA:2896:C:C5 | 3.05 | 0.42 |
| 31:DA:719:C:C2 | 31:DA:720:C:C5 | 3.08 | 0.42 |
| 31:DA:950:G:C6 | 31:DA:951:C:C4 | 3.08 | 0.42 |
| 34:DE:2:LYS:HG2 | 34:DE:95:ILE:HG23 | 2.02 | 0.42 |
| 34:DE:3:GLY:HA3 | 34:DE:81:ILE:HG21 | 2.01 | 0.42 |
| 37:DH:46:GLU:O | 37:DH:47:GLU:HB2 | 2.20 | 0.42 |
| 37:DH:94:TYR:N | 37:DH:94:TYR:HD1 | 2.18 | 0.42 |
| 31:DA:2094:G:OP1 | 38:DI:22:LYS:HD3 | 2.20 | 0.42 |
| 44:DS:101:LEU:O | 44:DS:102:ALA:O | 2.37 | 0.42 |
| 45:DT:27:THR:OG1 | 45:DT:28:VAL:N | 2.53 | 0.42 |
| 45:DT:30:VAL:HG22 | 45:DT:84:GLN:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:DT:65:LYS:O | 45:DT:72:VAL:N | 2.36 | 0.42 |
| 46:DU:12:ARG:HA | 46:DU:15:LYS:HG2 | 2.01 | 0.42 |
| 49:DX:34:ALA:O | 49:DX:35:THR:C | 2.58 | 0.42 |
| 49:DX:5:TYR:O | 49:DX:7:VAL:N | 2.52 | 0.42 |
| 1:AA:1169:A:H2' | 1:AA:1170:A:O4' | 2.20 | 0.42 |
| 1:AA:1277:C:O2' | 1:AA:1279:A:H1' | 2.20 | 0.42 |
| 1:AA:1498:U:H1' | 1:AA:1499:A:OP2 | 2.20 | 0.42 |
| 1:AA:328:C:H4' | 1:AA:329:A:H5' | 2.01 | 0.42 |
| 1:AA:414:A:C4 | 1:AA:415:A:C8 | 3.08 | 0.42 |
| 1:AA:579:G:C6 | 1:AA:580:U:C4 | 3.08 | 0.42 |
| 1:AA:604:G:N7 | 1:AA:605:U:C5 | 2.88 | 0.42 |
| 1:AA:69:G:N2 | 1:AA:70:G:C4 | 2.87 | 0.42 |
| 1:AA:718:G:C1' | 11:AK:116:HIS:HA | 2.50 | 0.42 |
| 1:AA:923:A:H2' | 1:AA:924:C:O4' | 2.20 | 0.42 |
| 2:AB:193:ASP:HA | 2:AB:194:PRO:HD2 | 1.84 | 0.42 |
| 3:AC:69:HIS:N | 3:AC:69:HIS:CD2 | 2.87 | 0.42 |
| 6:AF:76:ALA:HB1 | 6:AF:80:ARG:NH2 | 2.33 | 0.42 |
| 7:AG:20:ASP:HB3 | 7:AG:23:VAL:HG23 | 2.02 | 0.42 |
| 8:AH:103:VAL:HG21 | 8:AH:110:ALA:HB2 | 2.01 | 0.42 |
| 12:AL:126:LYS:HD2 | 12:AL:127:GLU:H | 1.84 | 0.42 |
| 1:AA:523:A:N1 | 12:AL:92:ASP:HB2 | 2.35 | 0.42 |
| 1:AA:719:C:O2' | 18:AR:49:LYS:HB3 | 2.20 | 0.42 |
| 22:B0:72:ARG:NH2 | 22:B0:75:LEU:HD12 | 2.35 | 0.42 |
| 23:B1:85:LEU:CB | 23:B1:87:PRO:HD3 | 2.49 | 0.42 |
| 24:B2:25:VAL:HG13 | 24:B2:26:ARG:CD | 2.37 | 0.42 |
| 30:B8:36:LYS:O | 30:B8:37:SER:O | 2.38 | 0.42 |
| 30:B8:29:LYS:NZ | 30:B8:44:LYS:HB2 | 2.35 | 0.42 |
| 31:BA:1317:A:H2' | 31:BA:1318:C:H6 | 1.84 | 0.42 |
| 31:BA:154(A):C:O4' | 31:BA:154(A):C:O2 | 2.38 | 0.42 |
| 31:BA:1783:A:N1 | 31:BA:2587:A:C4 | 2.88 | 0.42 |
| 31:BA:1902:C:H4' | 33:BD:244:ARG:HB2 | 2.01 | 0.42 |
| 31:BA:1979:C:C2' | 31:BA:1980:G:H5' | 2.50 | 0.42 |
| 31:BA:1667:G:H1' | 31:BA:1991:U:O4 | 2.20 | 0.42 |
| 31:BA:2048:G:C6 | 31:BA:2049:G:C5 | 3.08 | 0.42 |
| 31:BA:2803:C:H3' | 31:BA:2803:C:OP2 | 2.19 | 0.42 |
| 31:BA:465:G:H2' | 31:BA:466:A:C8 | 2.54 | 0.42 |
| 31:BA:708:C:N4 | 31:BA:723:G:H1 | 2.17 | 0.42 |
| 35:BF:192:LEU:HD23 | 35:BF:193:VAL:H | 1.84 | 0.42 |
| 36:BG:181:ARG:HB2 | 36:BG:181:ARG:HE | 1.70 | 0.42 |
| 37:BH:20:ALA:O | 37:BH:21:PRO:C | 2.59 | 0.42 |
| 38:BI:2:LYS:HD2 | 38:BI:20:ASP:HB3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:814:C:H5 | 41:BP:27:HIS:CE1 | 2.36 | 0.42 |
| 41:BP:39:LYS:HE3 | 41:BP:42:SER:CB | 2.50 | 0.42 |
| 41:BP:91:PHE:CD2 | 41:BP:91:PHE:O | 2.73 | 0.42 |
| 42:BQ:76:LYS:N | 42:BQ:88:GLY:HA2 | 2.34 | 0.42 |
| 43:BR:74:LYS:HD2 | 43:BR:77:ARG:NH2 | 2.34 | 0.42 |
| 43:BR:87:TYR:HE1 | 43:BR:117:VAL:HG12 | 1.84 | 0.42 |
| 45:BT:98:LYS:HB3 | 45:BT:100:TYR:CE1 | 2.54 | 0.42 |
| 45:BT:27:THR:O | 45:BT:28:VAL:CG2 | 2.66 | 0.42 |
| 31:BA:2875:C:H4' | 45:BT:5:ALA:HB2 | 2.01 | 0.42 |
| 48:BW:2:GLU:CA | 48:BW:64:MET:HE1 | 2.47 | 0.42 |
| 51:BZ:69:THR:HG22 | 51:BZ:90:VAL:CA | 2.47 | 0.42 |
| 51:BZ:73:GLN:N | 51:BZ:87:ASP:OD1 | 2.53 | 0.42 |
| 1:CA:447:G:O6 | 1:CA:485:G:H1' | 2.20 | 0.42 |
| 1:CA:538:G:OP2 | 12:CL:115:LYS:CG | 2.68 | 0.42 |
| 1:CA:761:G:C5 | 1:CA:762:C:C5 | 3.08 | 0.42 |
| 1:CA:874:G:C2' | 1:CA:875:C:H5' | 2.50 | 0.42 |
| 1:CA:92:C:H2' | 1:CA:93:G:H8 | 1.82 | 0.42 |
| 2:CB:140:HIS:HA | 2:CB:143:GLU:HG3 | 2.01 | 0.42 |
| 4:CD:116:GLN:NE2 | 4:CD:157:LEU:HD21 | 2.35 | 0.42 |
| 4:CD:180:GLY:O | 4:CD:182:LYS:HG2 | 2.20 | 0.42 |
| 4:CD:79:PHE:CE1 | 4:CD:204:ILE:HA | 2.55 | 0.42 |
| 5:CE:137:GLU:O | 5:CE:141:GLN:HG3 | 2.19 | 0.42 |
| 10:CJ:54:PHE:HZ | 10:CJ:55:LYS:HZ2 | 1.67 | 0.42 |
| 10:CJ:51:ARG:H | 10:CJ:60:ARG:HA | 1.84 | 0.42 |
| 10:CJ:8:LEU:HB3 | 10:CJ:16:LEU:HD21 | 2.02 | 0.42 |
| 15:CO:78:TYR:O | 15:CO:82:ILE:HG22 | 2.20 | 0.42 |
| 17:CQ:99:SER:C | 17:CQ:100:LYS:HD3 | 2.39 | 0.42 |
| 18:CR:71:LYS:O | 18:CR:74:ARG:HB2 | 2.18 | 0.42 |
| 23:D1:94:LEU:CD2 | 23:D1:95:LEU:N | 2.81 | 0.42 |
| 30:D8:3:LYS:HE3 | 31:DA:242:G:O5' | 2.19 | 0.42 |
| 31:DA:1439:A:C2 | 31:DA:1553:A:C5 | 3.08 | 0.42 |
| 31:DA:1973:G:C4 | 31:DA:1974:C:C5 | 3.08 | 0.42 |
| 31:DA:2262:U:H4' | 31:DA:2328:A:C2 | 2.55 | 0.42 |
| 31:DA:2437:U:H2' | 31:DA:2438:U:H6 | 1.84 | 0.42 |
| 31:DA:755:C:H2' | 31:DA:756:C:H6 | 1.84 | 0.42 |
| 31:DA:832:G:O2' | 41:DP:52:GLU:HB3 | 2.19 | 0.42 |
| 31:DA:946:G:O2' | 31:DA:947:G:H5' | 2.19 | 0.42 |
| 33:DD:65:ILE:HD11 | 33:DD:67:PHE:CZ | 2.48 | 0.42 |
| 34:DE:101:ARG:CB | 34:DE:169:ASN:ND2 | 2.82 | 0.42 |
| 36:DG:111:LEU:HA | 36:DG:114:ILE:CG1 | 2.50 | 0.42 |
| 36:DG:54:GLU:O | 36:DG:57:ALA:HB3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 37:DH:33:LEU:HD11 | 37:DH:136:ILE:O | 2.20 | 0.42 |
| 37:DH:85:LYS:HZ3 | 37:DH:145:ALA:CB | 2.33 | 0.42 |
| 39:DN:46:VAL:HG13 | 39:DN:48:MET:HG3 | 2.01 | 0.42 |
| 39:DN:82:LEU:N | 39:DN:82:LEU:HD12 | 2.18 | 0.42 |
| 40:DO:10:VAL:CG2 | 40:DO:10:VAL:O | 2.64 | 0.42 |
| 40:DO:87:ILE:HD13 | 40:DO:87:ILE:HA | 1.60 | 0.42 |
| 30:D8:27:THR:CA | 41:DP:62:LEU:HD11 | 2.44 | 0.42 |
| 45:DT:28:VAL:HG13 | 45:DT:46:GLU:CB | 2.48 | 0.42 |
| 40:DO:104:ARG:NH1 | 45:DT:35:LYS:HD3 | 2.34 | 0.42 |
| 45:DT:90:GLN:NE2 | 45:DT:124:ASP:OD2 | 2.53 | 0.42 |
| 46:DU:84:LYS:C | 46:DU:86:ALA:H | 2.23 | 0.42 |
| 31:DA:814:C:C5' | 47:DV:86:GLY:HA3 | 2.50 | 0.42 |
| 48:DW:82:LEU:HA | 48:DW:82:LEU:HD12 | 1.77 | 0.42 |
| 49:DX:52:VAL:HB | 49:DX:80:ILE:CG2 | 2.50 | 0.42 |
| 50:DY:39:VAL:CG1 | 50:DY:40:GLU:H | 2.25 | 0.42 |
| 50:DY:45:VAL:HG22 | 50:DY:62:GLU:N | 2.34 | 0.42 |
| 50:DY:90:LEU:CD1 | 50:DY:91:GLU:HG2 | 2.50 | 0.42 |
| 51:DZ:11:GLU:HB2 | 51:DZ:13:GLU:OE2 | 2.20 | 0.42 |
| 51:DZ:151:HIS:CB | 51:DZ:170:THR:HA | 2.49 | 0.42 |
| 1:AA:1014:A:C2 | 1:AA:1219:U:O2 | 2.73 | 0.41 |
| 1:AA:1429:C:H2' | 1:AA:1430:C:C6 | 2.55 | 0.41 |
| 1:AA:1442:G:HO2' | 1:AA:1442(A):G:H5'' | 1.79 | 0.41 |
| 1:AA:253:U:H2' | 1:AA:254:G:H8 | 1.84 | 0.41 |
| 1:AA:376:G:N3 | 1:AA:389:A:C2 | 2.87 | 0.41 |
| 1:AA:434:U:H2' | 1:AA:435:C:C6 | 2.55 | 0.41 |
| 1:AA:579:G:C5 | 1:AA:580:U:C4 | 3.07 | 0.41 |
| 1:AA:69:G:N2 | 1:AA:70:G:C5 | 2.88 | 0.41 |
| 1:AA:785:G:H2' | 1:AA:786:G:H5' | 2.02 | 0.41 |
| 1:AA:963:G:H1 | 1:AA:972:C:N4 | 2.17 | 0.41 |
| 3:AC:106:VAL:HG12 | 3:AC:108:ASN:H | 1.85 | 0.41 |
| 4:AD:108:LEU:HG | 4:AD:110:PHE:HE1 | 1.85 | 0.41 |
| 4:AD:60:GLU:O | 4:AD:63:LYS:HB3 | 2.19 | 0.41 |
| 11:AK:69:ALA:O | 11:AK:73:MET:HG2 | 2.19 | 0.41 |
| 1:AA:1226:C:N4 | 13:AM:104:ARG:HB2 | 2.33 | 0.41 |
| 13:AM:72:ALA:O | 13:AM:75:ALA:HB3 | 2.19 | 0.41 |
| 17:AQ:45:HIS:ND1 | 17:AQ:65:ILE:HG21 | 2.35 | 0.41 |
| 1:AA:1319:A:OP1 | 19:AS:10:PHE:CD1 | 2.73 | 0.41 |
| 20:AT:76:ALA:O | 20:AT:77:ALA:C | 2.58 | 0.41 |
| 20:AT:75:ASN:CA | 20:AT:78:ALA:HB3 | 2.49 | 0.41 |
| 23:B1:10:LYS:HG2 | 23:B1:11:ARG:H | 1.84 | 0.41 |
| 24:B2:30:ARG:CG | 24:B2:30:ARG:NH1 | 2.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B3:26:LEU:HD23 | 25:B3:26:LEU:HA | 1.77 | 0.41 |
| 29:B7:24:THR:O | 29:B7:28:ARG:HG3 | 2.20 | 0.41 |
| 30:B8:25:MET:HB2 | 41:BP:62:LEU:HD21 | 2.00 | 0.41 |
| 30:B8:38:GLY:C | 30:B8:40:GLU:H | 2.22 | 0.41 |
| 31:BA:1034:G:H2' | 31:BA:1035:U:O4' | 2.20 | 0.41 |
| 31:BA:1379:A:C2' | 31:BA:1380:G:OP1 | 2.66 | 0.41 |
| 31:BA:139(A):G:N1 | 49:BX:44:GLU:OE1 | 2.52 | 0.41 |
| 31:BA:1434:A:C2' | 31:BA:1435:G:H5' | 2.50 | 0.41 |
| 31:BA:1467:C:C2 | 31:BA:1526:G:N2 | 2.88 | 0.41 |
| 31:BA:1628:G:O2' | 31:BA:1629:U:H5' | 2.19 | 0.41 |
| 31:BA:1856:G:C2' | 31:BA:1857:G:H5' | 2.50 | 0.41 |
| 31:BA:1904:G:H2' | 31:BA:1905:C:O4' | 2.20 | 0.41 |
| 31:BA:2296:U:H4' | 31:BA:2297:C:OP1 | 2.19 | 0.41 |
| 28:B6:19:ARG:HH12 | 31:BA:2400:G:H5' | 1.84 | 0.41 |
| 31:BA:2552:U:H2' | 31:BA:2554:U:OP2 | 2.20 | 0.41 |
| 31:BA:262:A:H2' | 31:BA:263:C:O4' | 2.20 | 0.41 |
| 31:BA:271(M):G:H2' | 31:BA:271(N):U:H5' | 2.01 | 0.41 |
| 31:BA:2762:G:C5' | 31:BA:2762:G:C8 | 3.02 | 0.41 |
| 31:BA:2870:C:O2' | 31:BA:2871:C:H5' | 2.20 | 0.41 |
| 31:BA:301:G:H1' | 31:BA:302:C:C6 | 2.55 | 0.41 |
| 31:BA:695:G:C4 | 31:BA:696:G:C8 | 3.08 | 0.41 |
| 31:BA:721:C:C2' | 31:BA:721:C:O2 | 2.67 | 0.41 |
| 31:BA:966:G:C6 | 31:BA:967:C:N4 | 2.88 | 0.41 |
| 32:BB:87:G:H2' | 32:BB:88:C:H5'' | 2.01 | 0.41 |
| 34:BE:101:ARG:CB | 34:BE:169:ASN:ND2 | 2.82 | 0.41 |
| 34:BE:179:GLU:O | 34:BE:180:ASN:HB2 | 2.20 | 0.41 |
| 36:BG:107:LEU:HD23 | 36:BG:111:LEU:HD12 | 2.02 | 0.41 |
| 36:BG:7:LEU:CD2 | 36:BG:176:LEU:HD22 | 2.50 | 0.41 |
| 38:BI:42:SER:O | 38:BI:43:ASN:C | 2.58 | 0.41 |
| 39:BN:5:VAL:HA | 39:BN:6:PRO:HD3 | 1.41 | 0.41 |
| 39:BN:22:THR:HA | 39:BN:61:ARG:O | 2.20 | 0.41 |
| 39:BN:95:PRO:HG2 | 39:BN:96:GLU:OE2 | 2.20 | 0.41 |
| 40:BO:10:VAL:HG21 | 40:BO:16:ALA:C | 2.38 | 0.41 |
| 41:BP:103:ALA:O | 41:BP:104:GLY:C | 2.58 | 0.41 |
| 41:BP:48:PRO:CG | 41:BP:49:ARG:H | 2.27 | 0.41 |
| 44:BS:59:LYS:NZ | 44:BS:68:GLN:NE2 | 2.68 | 0.41 |
| 45:BT:16:ARG:HD3 | 45:BT:16:ARG:HA | 1.52 | 0.41 |
| 39:BN:42:TRP:CB | 46:BU:64:ARG:NH1 | 2.69 | 0.41 |
| 47:BV:13:ARG:HH11 | 47:BV:13:ARG:HG2 | 1.85 | 0.41 |
| 49:BX:47:PHE:O | 49:BX:48:LYS:C | 2.58 | 0.41 |
| 49:BX:82:GLN:CD | 49:BX:83:VAL:HG22 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1004:A:N7 | 1:CA:1036:G:O6 | 2.52 | 0.41 |
| 1:CA:1277:C:O2' | 1:CA:1279:A:H1' | 2.19 | 0.41 |
| 1:CA:1490:C:O2' | 1:CA:1491:G:H5' | 2.20 | 0.41 |
| 1:CA:282:A:H5'' | 1:CA:283:C:OP2 | 2.20 | 0.41 |
| 1:CA:436:C:O2' | 1:CA:437:U:P | 2.78 | 0.41 |
| 1:CA:473:G:C2 | 1:CA:474:G:C5 | 3.07 | 0.41 |
| 1:CA:515:G:N2 | 1:CA:537:G:C4 | 2.88 | 0.41 |
| 1:CA:55:A:C4 | 1:CA:56:U:C5 | 3.08 | 0.41 |
| 1:CA:617:G:C2 | 1:CA:618:C:C6 | 3.08 | 0.41 |
| 1:CA:696:A:H1' | 1:CA:786:G:O2' | 2.20 | 0.41 |
| 1:CA:722:A:N6 | 1:CA:724:G:C2 | 2.88 | 0.41 |
| 1:CA:818:G:O2' | 1:CA:820:U:H6 | 2.03 | 0.41 |
| 1:CA:832:C:N3 | 1:CA:855:G:C2 | 2.87 | 0.41 |
| 1:CA:872:A:C5 | 1:CA:874:G:C8 | 3.08 | 0.41 |
| 2:CB:41:ILE:N | 2:CB:41:ILE:HD12 | 2.35 | 0.41 |
| 3:CC:11:ARG:O | 3:CC:13:GLY:N | 2.53 | 0.41 |
| 3:CC:122:GLU:O | 3:CC:126:ARG:HG3 | 2.20 | 0.41 |
| 3:CC:36:ASP:OD2 | 3:CC:57:ILE:HG21 | 2.20 | 0.41 |
| 4:CD:99:SER:O | 4:CD:140:VAL:HG23 | 2.20 | 0.41 |
| 4:CD:128:VAL:HA | 4:CD:145:GLU:O | 2.20 | 0.41 |
| 11:CK:73:MET:SD | 11:CK:103:LEU:CD2 | 3.08 | 0.41 |
| 16:CP:64:ALA:O | 16:CP:65:GLN:C | 2.56 | 0.41 |
| 17:CQ:67:LYS:O | 17:CQ:69:LYS:N | 2.53 | 0.41 |
| 17:CQ:59:ILE:HG21 | 17:CQ:71:PHE:HB3 | 1.97 | 0.41 |
| 20:CT:89:ARG:NH2 | 20:CT:104:LEU:HD21 | 2.34 | 0.41 |
| 23:D1:13:ILE:HG12 | 23:D1:14:VAL:CA | 2.50 | 0.41 |
| 24:D2:55:ARG:CG | 24:D2:55:ARG:O | 2.67 | 0.41 |
| 30:D8:29:LYS:HB2 | 30:D8:44:LYS:HG2 | 2.01 | 0.41 |
| 31:DA:1444:G:O6 | 31:DA:1466:G:C6 | 2.73 | 0.41 |
| 31:DA:1517:G:C6 | 31:DA:1518:U:N3 | 2.88 | 0.41 |
| 31:DA:1635:G:H2' | 31:DA:1636:C:C6 | 2.55 | 0.41 |
| 31:DA:1992:G:H8 | 31:DA:1992:G:OP1 | 2.03 | 0.41 |
| 31:DA:2270:G:H2' | 31:DA:2271:G:H5' | 2.02 | 0.41 |
| 31:DA:2308:G:O6 | 31:DA:2310:A:H2' | 2.20 | 0.41 |
| 31:DA:1759:A:H4' | 31:DA:2715:C:O4' | 2.20 | 0.41 |
| 31:DA:271(S):G:C5 | 31:DA:271(T):C:C5 | 3.08 | 0.41 |
| 31:DA:2743:C:H2' | 31:DA:2744:G:O4' | 2.20 | 0.41 |
| 31:DA:894:C:H2' | 31:DA:895:U:H5' | 2.02 | 0.41 |
| 31:DA:928:G:H8 | 31:DA:928:G:O5' | 2.02 | 0.41 |
| 32:DB:40:U:C2' | 32:DB:41:U:OP1 | 2.68 | 0.41 |
| 33:DD:35:LYS:HZ3 | 33:DD:104:TYR:HD1 | 1.65 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DD:35:LYS:HD2 | 33:DD:63:ARG:HB3 | 2.01 | 0.41 |
| 34:DE:11:MET:HB3 | 34:DE:24:THR:HA | 2.02 | 0.41 |
| 34:DE:34:VAL:HG23 | 34:DE:34:VAL:O | 2.19 | 0.41 |
| 35:DF:68:LYS:O | 35:DF:68:LYS:HG2 | 2.20 | 0.41 |
| 38:DI:15:VAL:C | 38:DI:17:GLN:H | 2.22 | 0.41 |
| 41:DP:113:LYS:HA | 41:DP:129:ALA:O | 2.20 | 0.41 |
| 42:DQ:70:PRO:HA | 42:DQ:94:VAL:O | 2.20 | 0.41 |
| 45:DT:27:THR:C | 45:DT:28:VAL:HG23 | 2.39 | 0.41 |
| 47:DV:2:PHE:HB3 | 47:DV:3:ALA:H | 1.12 | 0.41 |
| 47:DV:90:PRO:CD | 47:DV:91:TYR:H | 2.30 | 0.41 |
| 47:DV:96:ILE:HG23 | 47:DV:97:LYS:N | 2.34 | 0.41 |
| 49:DX:25:LYS:HG3 | 49:DX:26:TYR:CD1 | 2.54 | 0.41 |
| 49:DX:60:ARG:HH21 | 49:DX:74:PRO:CG | 2.33 | 0.41 |
| 50:DY:47:LYS:HB3 | 50:DY:47:LYS:HE3 | 1.35 | 0.41 |
| 50:DY:90:LEU:HG | 50:DY:91:GLU:N | 2.35 | 0.41 |
| 51:DZ:143:GLY:C | 51:DZ:144:LEU:HD22 | 2.41 | 0.41 |
| 51:DZ:151:HIS:ND1 | 51:DZ:170:THR:HG22 | 2.35 | 0.41 |
| 1:AA:355:C:H2' | 1:AA:356:A:C5' | 2.50 | 0.41 |
| 1:AA:734:G:C2 | 1:AA:735:C:C2 | 3.07 | 0.41 |
| 1:AA:788:U:C2' | 1:AA:789:U:H5' | 2.51 | 0.41 |
| 1:AA:791:G:H2' | 1:AA:792:A:H5' | 2.01 | 0.41 |
| 1:AA:939:G:H5'' | 7:AG:102:ARG:HH22 | 1.83 | 0.41 |
| 2:AB:88:ALA:O | 2:AB:90:MET:HG2 | 2.20 | 0.41 |
| 3:AC:6:HIS:CD2 | 3:AC:8:ILE:HB | 2.55 | 0.41 |
| 4:AD:14:ARG:HA | 4:AD:39:PRO:CG | 2.51 | 0.41 |
| 6:AF:40:VAL:O | 6:AF:40:VAL:HG13 | 2.19 | 0.41 |
| 7:AG:146:GLU:CA | 7:AG:149:ARG:HB2 | 2.43 | 0.41 |
| 8:AH:53:VAL:HG12 | 8:AH:53:VAL:O | 2.20 | 0.41 |
| 9:AI:126:SER:O | 9:AI:127:LYS:HB3 | 2.21 | 0.41 |
| 10:AJ:58:ASP:O | 10:AJ:59:SER:C | 2.58 | 0.41 |
| 12:AL:39:VAL:HG12 | 12:AL:40:VAL:N | 2.35 | 0.41 |
| 15:AO:4:THR:OG1 | 15:AO:7:GLU:HB2 | 2.20 | 0.41 |
| 17:AQ:22:LEU:HD12 | 17:AQ:40:LYS:O | 2.19 | 0.41 |
| 20:AT:33:ILE:HD13 | 20:AT:33:ILE:N | 2.35 | 0.41 |
| 24:B2:14:ARG:CZ | 24:B2:57:ILE:HG22 | 2.46 | 0.41 |
| 28:B6:48:VAL:O | 28:B6:48:VAL:CG2 | 2.67 | 0.41 |
| 29:B7:43:THR:O | 29:B7:44:PRO:C | 2.58 | 0.41 |
| 31:BA:1168:G:O2' | 31:BA:1169:G:H5' | 2.20 | 0.41 |
| 31:BA:128:C:C5' | 31:BA:128:C:H6 | 2.27 | 0.41 |
| 31:BA:1486:A:C2' | 31:BA:1487:G:H5' | 2.49 | 0.41 |
| 31:BA:1914:C:H2' | 31:BA:1915:U:O4' | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:2093:G:OP2 | 38:BI:22:LYS:HG2 | 2.20 | 0.41 |
| 31:BA:2484:G:C2 | 31:BA:2485:G:C8 | 3.08 | 0.41 |
| 31:BA:2510:C:C4 | 31:BA:2511:U:C4 | 3.08 | 0.41 |
| 31:BA:493:G:H2' | 31:BA:494:G:H5'' | 2.02 | 0.41 |
| 31:BA:646:A:H2' | 31:BA:647:G:O5' | 2.20 | 0.41 |
| 31:BA:675:A:C8 | 31:BA:804:A:N1 | 2.88 | 0.41 |
| 31:BA:825:C:C3' | 31:BA:825:C:C6 | 3.04 | 0.41 |
| 33:BD:11:PRO:C | 33:BD:13:ARG:H | 2.23 | 0.41 |
| 33:BD:237:GLU:HB3 | 33:BD:238:GLY:H | 1.63 | 0.41 |
| 34:BE:134:ILE:N | 34:BE:134:ILE:HD13 | 2.32 | 0.41 |
| 34:BE:47:VAL:HB | 34:BE:49:LEU:CD2 | 2.50 | 0.41 |
| 36:BG:43:LEU:N | 36:BG:43:LEU:HD22 | 2.35 | 0.41 |
| 36:BG:92:VAL:HG22 | 36:BG:93:THR:N | 2.34 | 0.41 |
| 39:BN:25:ARG:CG | 39:BN:25:ARG:NH1 | 2.81 | 0.41 |
| 44:BS:54:LEU:HD13 | 44:BS:57:LYS:O | 2.20 | 0.41 |
| 46:BU:28:ARG:NH1 | 46:BU:38:THR:OG1 | 2.42 | 0.41 |
| 31:BA:995:C:O2 | 46:BU:57:PHE:CD2 | 2.73 | 0.41 |
| 50:BY:79:CYS:O | 50:BY:80:GLY:O | 2.38 | 0.41 |
| 51:BZ:28:MET:HE2 | 51:BZ:59:LEU:HD12 | 2.00 | 0.41 |
| 1:CA:108:G:H5'' | 1:CA:109:A:C5' | 2.46 | 0.41 |
| 1:CA:116:A:C8 | 1:CA:116:A:OP2 | 2.73 | 0.41 |
| 1:CA:1320:C:H2' | 1:CA:1321:C:O4' | 2.20 | 0.41 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C5 | 2.52 | 0.41 |
| 1:CA:450:G:OP1 | 16:CP:43:LYS:NZ | 2.50 | 0.41 |
| 1:CA:563:A:C8 | 1:CA:567:G:C1' | 3.03 | 0.41 |
| 1:CA:664:G:P | 18:CR:64:ARG:HH21 | 2.42 | 0.41 |
| 1:CA:730:G:O2' | 1:CA:766:A:H5' | 2.20 | 0.41 |
| 1:CA:885:G:O2' | 1:CA:914:A:N1 | 2.41 | 0.41 |
| 2:CB:111:ARG:NH1 | 2:CB:111:ARG:CG | 2.63 | 0.41 |
| 2:CB:23:ARG:HG2 | 2:CB:23:ARG:O | 2.20 | 0.41 |
| 2:CB:25:ASN:O | 2:CB:27:LYS:N | 2.53 | 0.41 |
| 8:CH:77:GLU:CG | 8:CH:78:GLN:H | 2.33 | 0.41 |
| 10:CJ:48:THR:HG23 | 10:CJ:62:HIS:HB3 | 2.01 | 0.41 |
| 11:CK:31:THR:OG1 | 11:CK:42:TRP:HB3 | 2.20 | 0.41 |
| 11:CK:65:ALA:HB3 | 11:CK:97:ALA:CB | 2.50 | 0.41 |
| 13:CM:54:VAL:O | 13:CM:58:GLU:HB2 | 2.20 | 0.41 |
| 16:CP:8:ARG:O | 16:CP:9:PHE:CD2 | 2.73 | 0.41 |
| 17:CQ:62:SER:OG | 17:CQ:72:ARG:HB2 | 2.20 | 0.41 |
| 18:CR:66:LEU:HD11 | 18:CR:70:ILE:HD11 | 2.02 | 0.41 |
| 20:CT:24:LEU:C | 20:CT:24:LEU:HD13 | 2.41 | 0.41 |
| 23:D1:26:ARG:HD3 | 23:D1:34:THR:HB | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:D2:40:SER:O | 24:D2:41:ILE:O | 2.38 | 0.41 |
| 31:DA:1106:A:O2' | 31:DA:1107:G:O4' | 2.31 | 0.41 |
| 31:DA:1288:U:O2 | 31:DA:1327:C:C2 | 2.73 | 0.41 |
| 31:DA:1324:G:C2 | 31:DA:1328:G:N1 | 2.89 | 0.41 |
| 31:DA:770:G:N3 | 31:DA:1354:A:H2 | 2.18 | 0.41 |
| 31:DA:1478:G:C2 | 31:DA:1479:G:C8 | 3.07 | 0.41 |
| 31:DA:414:C:H4' | 31:DA:1879:C:O2 | 2.20 | 0.41 |
| 31:DA:1891:G:C5 | 31:DA:1892:C:C4 | 3.08 | 0.41 |
| 31:DA:945:A:C4 | 31:DA:2448:A:C2 | 3.07 | 0.41 |
| 31:DA:2446:G:N2 | 31:DA:2449:U:O2 | 2.52 | 0.41 |
| 31:DA:252:G:O2' | 31:DA:253:C:H5' | 2.20 | 0.41 |
| 31:DA:2592:G:C5 | 31:DA:2593:U:C5 | 3.08 | 0.41 |
| 31:DA:2758:A:C2 | 31:DA:2759:G:H1' | 2.55 | 0.41 |
| 31:DA:224:G:N7 | 31:DA:420:C:H4' | 2.35 | 0.41 |
| 31:DA:565:C:H2' | 31:DA:566:U:O4' | 2.19 | 0.41 |
| 31:DA:769:G:C2' | 31:DA:770:G:H5' | 2.49 | 0.41 |
| 31:DA:196:A:O2' | 31:DA:805:G:O6 | 2.28 | 0.41 |
| 31:DA:842:G:N2 | 31:DA:937:U:C2 | 2.88 | 0.41 |
| 31:DA:868:U:C4 | 31:DA:869:G:N7 | 2.88 | 0.41 |
| 31:DA:926:A:H5'' | 31:DA:926:A:H8 | 1.85 | 0.41 |
| 32:DB:41:U:H2' | 32:DB:42:C:OP1 | 2.20 | 0.41 |
| 33:DD:13:ARG:HA | 33:DD:16:MET:HE3 | 2.02 | 0.41 |
| 33:DD:33:LEU:O | 33:DD:35:LYS:N | 2.53 | 0.41 |
| 34:DE:1:MET:O | 34:DE:2:LYS:C | 2.59 | 0.41 |
| 35:DF:165:ARG:HA | 35:DF:168:ARG:HD3 | 2.03 | 0.41 |
| 35:DF:20:LEU:HB3 | 35:DF:23:ASP:HB2 | 2.02 | 0.41 |
| 35:DF:3:GLU:C | 35:DF:24:LEU:HG | 2.40 | 0.41 |
| 35:DF:31:HIS:O | 35:DF:34:TRP:HB3 | 2.20 | 0.41 |
| 36:DG:144:ILE:HA | 36:DG:144:ILE:HD12 | 1.90 | 0.41 |
| 39:DN:75:TYR:CE2 | 39:DN:83:LYS:NZ | 2.88 | 0.41 |
| 40:DO:75:SER:OG | 40:DO:76:ALA:N | 2.53 | 0.41 |
| 41:DP:115:LEU:HA | 41:DP:134:ALA:CB | 2.34 | 0.41 |
| 41:DP:131:SER:O | 41:DP:132:LYS:C | 2.58 | 0.41 |
| 43:DR:21:TYR:CZ | 43:DR:43:GLU:HG2 | 2.55 | 0.41 |
| 44:DS:19:LYS:CG | 44:DS:19:LYS:O | 2.67 | 0.41 |
| 44:DS:29:PHE:CD2 | 44:DS:30:ARG:N | 2.88 | 0.41 |
| 44:DS:28:VAL:HG21 | 44:DS:87:PHE:CZ | 2.55 | 0.41 |
| 46:DU:84:LYS:HG3 | 46:DU:85:LYS:N | 2.35 | 0.41 |
| 50:DY:23:ARG:O | 50:DY:24:VAL:O | 2.38 | 0.41 |
| 51:DZ:39:VAL:HG21 | 51:DZ:44:PHE:CD2 | 2.54 | 0.41 |
| 1:AA:1058:G:H1 | 1:AA:1199:U:H3 | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1158:C:C2 | 1:AA:1160:G:N7 | 2.88 | 0.41 |
| 1:AA:1052:U:O4 | 1:AA:1200:C:C2 | 2.74 | 0.41 |
| 1:AA:1379:G:C6 | 1:AA:1380:U:O4 | 2.72 | 0.41 |
| 1:AA:1452:C:O4' | 1:AA:1456:G:N1 | 2.53 | 0.41 |
| 1:AA:201:C:N4 | 1:AA:203:U:N1 | 2.69 | 0.41 |
| 1:AA:288:A:H2' | 1:AA:289:G:H4' | 2.01 | 0.41 |
| 1:AA:612:C:C2' | 1:AA:613:C:H5' | 2.50 | 0.41 |
| 1:AA:685:G:HO2' | 1:AA:686:U:H5' | 1.82 | 0.41 |
| 1:AA:734:G:C5 | 1:AA:735:C:C4 | 3.08 | 0.41 |
| 2:AB:15:VAL:HG21 | 2:AB:209:ARG:HH21 | 1.84 | 0.41 |
| 2:AB:69:LEU:HB2 | 2:AB:159:PRO:HG2 | 2.02 | 0.41 |
| 4:AD:11:LEU:C | 4:AD:13:ARG:N | 2.71 | 0.41 |
| 4:AD:79:PHE:CE1 | 4:AD:204:ILE:HA | 2.55 | 0.41 |
| 4:AD:36:ARG:HG2 | 4:AD:38:TYR:OH | 2.20 | 0.41 |
| 6:AF:30:LEU:CB | 6:AF:35:ALA:HB3 | 2.46 | 0.41 |
| 6:AF:67:MET:CB | 6:AF:68:PRO:HD2 | 2.49 | 0.41 |
| 6:AF:76:ALA:O | 6:AF:80:ARG:HG3 | 2.19 | 0.41 |
| 7:AG:18:TYR:CE2 | 7:AG:59:LEU:HB2 | 2.55 | 0.41 |
| 8:AH:86:ILE:CB | 8:AH:133:LEU:HD22 | 2.48 | 0.41 |
| 9:AI:79:LEU:HD13 | 9:AI:79:LEU:C | 2.41 | 0.41 |
| 10:AJ:35:SER:OG | 10:AJ:73:ASP:HB2 | 2.20 | 0.41 |
| 17:AQ:50:LYS:HG3 | 17:AQ:51:TYR:CD1 | 2.55 | 0.41 |
| 1:AA:664:G:P | 18:AR:64:ARG:HH21 | 2.43 | 0.41 |
| 18:AR:74:ARG:HE | 18:AR:81:PHE:HA | 1.85 | 0.41 |
| 20:AT:90:GLN:O | 20:AT:93:GLU:OE2 | 2.38 | 0.41 |
| 21:AU:22:ARG:N | 21:AU:23:PRO:HD3 | 2.35 | 0.41 |
| 23:B1:16:ASN:HB3 | 23:B1:46:LEU:HD11 | 1.99 | 0.41 |
| 23:B1:26:ARG:HB2 | 23:B1:34:THR:CA | 2.48 | 0.41 |
| 25:B3:52:HIS:CD2 | 32:BB:83:G:H5' | 2.55 | 0.41 |
| 28:B6:10:LEU:HD22 | 28:B6:10:LEU:N | 2.35 | 0.41 |
| 31:BA:1108:U:H2' | 31:BA:1109:C:C5' | 2.41 | 0.41 |
| 31:BA:1179:C:H2' | 31:BA:1179:C:O2 | 2.20 | 0.41 |
| 31:BA:1221:C:H2' | 31:BA:1221(A):C:H6 | 1.84 | 0.41 |
| 31:BA:1441:G:C2' | 31:BA:1442:G:H5' | 2.50 | 0.41 |
| 31:BA:1514:U:C2' | 31:BA:1515:G:H5' | 2.50 | 0.41 |
| 31:BA:1695:G:N2 | 31:BA:1696:G:C8 | 2.88 | 0.41 |
| 31:BA:1705:G:C6 | 31:BA:1706:U:C4 | 3.08 | 0.41 |
| 31:BA:204:A:O3' | 31:BA:205:G:H4' | 2.20 | 0.41 |
| 31:BA:2340:G:O2' | 31:BA:2341:G:H5' | 2.20 | 0.41 |
| 31:BA:2584:U:H6 | 31:BA:2585:U:C6 | 2.38 | 0.41 |
| 31:BA:2842:G:O2' | 31:BA:2843:G:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:BA:750:A:C2 | 31:BA:753:C:C6 | 3.08 | 0.41 |
| 31:BA:881:G:N2 | 31:BA:896:A:H62 | 2.18 | 0.41 |
| 31:BA:975(A):G:H1' | 31:BA:990:A:C2 | 2.55 | 0.41 |
| 34:BE:101:ARG:CG | 34:BE:169:ASN:ND2 | 2.84 | 0.41 |
| 35:BF:140:LEU:O | 35:BF:141:ALA:C | 2.57 | 0.41 |
| 36:BG:41:GLN:HG2 | 36:BG:155:MET:CB | 2.39 | 0.41 |
| 41:BP:14:LYS:H | 41:BP:14:LYS:HG3 | 1.53 | 0.41 |
| 43:BR:59:ASP:OD2 | 43:BR:59:ASP:N | 2.53 | 0.41 |
| 46:BU:88:ILE:CD1 | 46:BU:88:ILE:C | 2.89 | 0.41 |
| 47:BV:71:LEU:HD13 | 47:BV:72:VAL:HG23 | 2.01 | 0.41 |
| 1:CA:1026:G:H5' | 1:CA:1027:C:OP2 | 2.20 | 0.41 |
| 1:CA:955:U:C1' | 1:CA:1227:A:H61 | 2.23 | 0.41 |
| 1:CA:1246:C:H2' | 1:CA:1247:U:H6 | 1.85 | 0.41 |
| 1:CA:156:G:C6 | 1:CA:166:G:N1 | 2.88 | 0.41 |
| 1:CA:329:A:C2 | 1:CA:332:G:C4 | 3.08 | 0.41 |
| 1:CA:444:C:C2 | 1:CA:445:G:C8 | 3.08 | 0.41 |
| 1:CA:623:C:N4 | 1:CA:624:C:N4 | 2.68 | 0.41 |
| 1:CA:666:G:C5 | 1:CA:741:G:C6 | 3.09 | 0.41 |
| 1:CA:667:G:C2 | 1:CA:740:U:O2 | 2.74 | 0.41 |
| 1:CA:954:G:H21 | 1:CA:1227:A:N6 | 2.03 | 0.41 |
| 4:CD:36:ARG:C | 4:CD:38:TYR:H | 2.23 | 0.41 |
| 4:CD:43:HIS:CE1 | 4:CD:46:LYS:HZ2 | 2.36 | 0.41 |
| 5:CE:26:PHE:O | 5:CE:27:ARG:HB2 | 2.19 | 0.41 |
| 7:CG:92:SER:CB | 7:CG:94:ARG:HH21 | 2.33 | 0.41 |
| 8:CH:114:THR:HB | 8:CH:130:GLY:O | 2.19 | 0.41 |
| 9:CI:126:SER:O | 9:CI:127:LYS:HB3 | 2.20 | 0.41 |
| 13:CM:34:LEU:HD13 | 13:CM:41:PRO:CG | 2.42 | 0.41 |
| 1:CA:1048:G:H4' | 14:CN:2:ALA:N | 2.35 | 0.41 |
| 15:CO:4:THR:OG1 | 15:CO:7:GLU:HB2 | 2.20 | 0.41 |
| 26:D4:23:GLU:O | 26:D4:24:THR:CB | 2.68 | 0.41 |
| 27:D5:57:VAL:C | 27:D5:58:LEU:HD12 | 2.40 | 0.41 |
| 28:D6:44:ARG:HB3 | 28:D6:45:LYS:H | 1.56 | 0.41 |
| 31:DA:1044:G:N1 | 31:DA:1112:G:O6 | 2.53 | 0.41 |
| 31:DA:1047:G:C8 | 31:DA:1110:G:C6 | 3.09 | 0.41 |
| 31:DA:1126:A:H4' | 31:DA:1127:A:O5' | 2.20 | 0.41 |
| 31:DA:1204:A:N6 | 31:DA:1240:U:H2' | 2.34 | 0.41 |
| 31:DA:1816:G:H8 | 33:DD:62:TYR:CZ | 2.38 | 0.41 |
| 31:DA:1833:U:C2 | 31:DA:1834:U:C6 | 3.08 | 0.41 |
| 31:DA:2584:U:H2' | 31:DA:2585:U:C6 | 2.54 | 0.41 |
| 31:DA:2660:A:H5' | 31:DA:2661:G:N2 | 2.29 | 0.41 |
| 31:DA:2801:A:H4' | 31:DA:2801(A):A:O5' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:2834:G:N2 | 31:DA:2882:A:N6 | 2.69 | 0.41 |
| 31:DA:778:G:H2' | 31:DA:779:U:C6 | 2.55 | 0.41 |
| 32:DB:40:U:H1' | 32:DB:45:A:H61 | 1.85 | 0.41 |
| 33:DD:35:LYS:CE | 33:DD:65:ILE:HG22 | 2.50 | 0.41 |
| 34:DE:134:ILE:HD13 | 34:DE:134:ILE:N | 2.33 | 0.41 |
| 35:DF:143:ALA:HB1 | 35:DF:148:LEU:HB2 | 2.01 | 0.41 |
| 39:DN:56:ASN:H | 39:DN:125:GLY:N | 2.18 | 0.41 |
| 40:DO:13:ASN:ND2 | 40:DO:97:ARG:N | 2.64 | 0.41 |
| 40:DO:77:ILE:HG12 | 40:DO:78:ARG:N | 2.34 | 0.41 |
| 41:DP:66:GLY:O | 41:DP:67:MET:HB3 | 2.19 | 0.41 |
| 43:DR:34:ILE:HD12 | 43:DR:34:ILE:HA | 1.65 | 0.41 |
| 45:DT:67:SER:O | 45:DT:68:TYR:HB2 | 2.20 | 0.41 |
| 46:DU:92:ARG:HH22 | 47:DV:10:LYS:CA | 2.33 | 0.41 |
| 47:DV:4:ILE:HA | 47:DV:12:TYR:O | 2.21 | 0.41 |
| 49:DX:65:ARG:CA | 49:DX:65:ARG:NE | 2.83 | 0.41 |
| 51:DZ:133:ILE:HA | 51:DZ:134:PRO:HD2 | 1.90 | 0.41 |
| 1:AA:1030(C):G:H2' | 1:AA:1030(D):A:O4' | 2.19 | 0.41 |
| 1:AA:1216:G:H5'' | 14:AN:5:ALA:HB2 | 2.02 | 0.41 |
| 1:AA:1371:G:OP1 | 9:AI:11:LYS:HG2 | 2.20 | 0.41 |
| 1:AA:340:U:H2' | 1:AA:341:C:O4' | 2.20 | 0.41 |
| 1:AA:541:G:H2' | 1:AA:542:G:C8 | 2.55 | 0.41 |
| 1:AA:543:C:N3 | 1:AA:544:G:C8 | 2.88 | 0.41 |
| 1:AA:832:C:O2' | 1:AA:833:U:O5' | 2.34 | 0.41 |
| 1:AA:828:A:H5'' | 1:AA:859:A:N1 | 2.34 | 0.41 |
| 1:AA:92:C:C3' | 1:AA:93:G:H8 | 2.33 | 0.41 |
| 2:AB:68:ILE:HG13 | 2:AB:161:ALA:HB3 | 2.03 | 0.41 |
| 2:AB:19:HIS:CG | 2:AB:20:GLU:H | 2.37 | 0.41 |
| 18:AR:87:ARG:O | 18:AR:87:ARG:HG2 | 2.21 | 0.41 |
| 20:AT:59:ALA:O | 20:AT:62:LEU:N | 2.54 | 0.41 |
| 27:B5:57:VAL:C | 27:B5:58:LEU:CG | 2.88 | 0.41 |
| 30:B8:4:MET:HE2 | 30:B8:4:MET:HB2 | 1.83 | 0.41 |
| 31:BA:1028:A:H61 | 31:BA:1125:G:H2' | 1.86 | 0.41 |
| 31:BA:1276:A:C2 | 31:BA:1277:G:C8 | 3.09 | 0.41 |
| 31:BA:1312:U:OP2 | 49:BX:62:LYS:HE3 | 2.21 | 0.41 |
| 31:BA:1384:A:H1' | 31:BA:1405:U:O4' | 2.20 | 0.41 |
| 31:BA:1416:G:OP2 | 31:BA:1416:G:H4' | 2.20 | 0.41 |
| 31:BA:1449:A:O2' | 31:BA:1530:C:H5 | 2.04 | 0.41 |
| 31:BA:1501:C:H2' | 31:BA:1502:C:H6 | 1.85 | 0.41 |
| 31:BA:1349:A:N6 | 31:BA:1598:C:N4 | 2.68 | 0.41 |
| 31:BA:1843:C:H2' | 31:BA:1844:C:C6 | 2.56 | 0.41 |
| 31:BA:2276:G:C2' | 31:BA:2277:G:H5' | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:271(F):C:N3 | 31:BA:271(G):C:C5 | 2.89 | 0.41 |
| 31:BA:271(L):U:H4' | 31:BA:271(M):G:C6 | 2.53 | 0.41 |
| 31:BA:352:G:HO2' | 31:BA:353:G:P | 2.42 | 0.41 |
| 31:BA:557:U:O2' | 31:BA:558:G:H5' | 2.21 | 0.41 |
| 31:BA:587:C:C5 | 41:BP:33:ARG:CG | 2.94 | 0.41 |
| 31:BA:752:A:O2' | 31:BA:753:C:OP2 | 2.32 | 0.41 |
| 31:BA:775:G:C5 | 31:BA:794:G:C8 | 3.08 | 0.41 |
| 34:BE:119:ARG:HD2 | 34:BE:120:TRP:CE2 | 2.55 | 0.41 |
| 34:BE:31:CYS:SG | 34:BE:51:PHE:HD2 | 2.43 | 0.41 |
| 35:BF:22:ALA:HA | 35:BF:26:ALA:HA | 2.02 | 0.41 |
| 37:BH:100:GLY:C | 37:BH:102:ALA:H | 2.22 | 0.41 |
| 37:BH:163:TYR:HD1 | 37:BH:163:TYR:H | 1.69 | 0.41 |
| 38:BI:78:THR:OG1 | 38:BI:141:LYS:HD2 | 2.19 | 0.41 |
| 39:BN:131:GLN:CD | 39:BN:134:ARG:CB | 2.88 | 0.41 |
| 41:BP:65:ARG:C | 41:BP:66:GLY:O | 2.58 | 0.41 |
| 44:BS:106:ARG:HD2 | 44:BS:107:GLU:O | 2.20 | 0.41 |
| 45:BT:56:GLY:C | 45:BT:59:THR:HG22 | 2.41 | 0.41 |
| 46:BU:24:TYR:HB2 | 46:BU:29:SER:HB3 | 2.01 | 0.41 |
| 46:BU:69:CYS:O | 46:BU:74:LEU:HD12 | 2.19 | 0.41 |
| 47:BV:28:GLU:CB | 47:BV:29:PRO:HD3 | 2.51 | 0.41 |
| 49:BX:80:ILE:CG2 | 49:BX:81:VAL:N | 2.82 | 0.41 |
| 50:BY:37:VAL:HG22 | 50:BY:67:LEU:HB3 | 2.01 | 0.41 |
| 51:BZ:42:VAL:HG13 | 51:BZ:43:GLU:H | 1.85 | 0.41 |
| 1:CA:976:G:C8 | 1:CA:1362:C:N4 | 2.89 | 0.41 |
| 1:CA:439:A:C5 | 1:CA:441:A:H1' | 2.56 | 0.41 |
| 1:CA:665:A:C2 | 1:CA:732:C:C2 | 3.08 | 0.41 |
| 1:CA:833:U:C2 | 1:CA:834:C:C5 | 3.08 | 0.41 |
| 3:CC:22:TRP:HB2 | 3:CC:23:TYR:H | 1.73 | 0.41 |
| 4:CD:90:GLY:O | 4:CD:94:LEU:CD1 | 2.68 | 0.41 |
| 5:CE:7:GLU:O | 5:CE:8:GLU:HB3 | 2.20 | 0.41 |
| 6:CF:55:ASP:HA | 6:CF:56:PRO:HD2 | 1.95 | 0.41 |
| 13:CM:112:GLY:C | 13:CM:113:PRO:HG2 | 2.40 | 0.41 |
| 1:CA:976:G:P | 14:CN:32:SER:H | 2.41 | 0.41 |
| 15:CO:39:LEU:HD13 | 15:CO:39:LEU:C | 2.41 | 0.41 |
| 19:CS:19:VAL:O | 19:CS:19:VAL:HG12 | 2.20 | 0.41 |
| 20:CT:23:ARG:O | 20:CT:27:LYS:HB2 | 2.20 | 0.41 |
| 27:D5:36:CYS:CB | 27:D5:49:CYS:SG | 3.09 | 0.41 |
| 31:DA:1022:G:C5 | 31:DA:1140:C:C4 | 3.07 | 0.41 |
| 31:DA:1374:G:C6 | 31:DA:1375:C:C4 | 3.09 | 0.41 |
| 31:DA:2097:C:H2' | 31:DA:2098:U:C6 | 2.56 | 0.41 |
| 31:DA:2099:U:H2' | 31:DA:2099:U:O2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DA:2205:C:C2 | 31:DA:2220:G:N1 | 2.88 | 0.41 |
| 30:D8:5:LYS:NZ | 31:DA:253:C:OP2 | 2.48 | 0.41 |
| 31:DA:2626:C:O2' | 31:DA:2627:G:H5' | 2.21 | 0.41 |
| 31:DA:2659:G:H8 | 31:DA:2659:G:C5' | 2.33 | 0.41 |
| 31:DA:2668:G:O2' | 31:DA:2669:G:H5' | 2.20 | 0.41 |
| 31:DA:2842:G:O2' | 31:DA:2843:G:H5' | 2.20 | 0.41 |
| 31:DA:1709:U:O2' | 31:DA:2859:G:H1' | 2.20 | 0.41 |
| 31:DA:2862:G:H2' | 31:DA:2863:C:H6 | 1.85 | 0.41 |
| 31:DA:452:G:C2 | 31:DA:458:G:C5 | 3.08 | 0.41 |
| 31:DA:528:A:O2' | 31:DA:529:A:H5' | 2.20 | 0.41 |
| 31:DA:53:A:C8 | 31:DA:54:G:C8 | 3.09 | 0.41 |
| 31:DA:671:C:C5' | 31:DA:671:C:C6 | 2.99 | 0.41 |
| 31:DA:83:G:H22 | 31:DA:102:G:HO2' | 1.62 | 0.41 |
| 31:DA:893:C:H2' | 31:DA:894:C:O5' | 2.19 | 0.41 |
| 31:DA:958:U:C2' | 31:DA:959:A:OP1 | 2.68 | 0.41 |
| 32:DB:15:A:H1' | 32:DB:110:G:C8 | 2.55 | 0.41 |
| 32:DB:87:G:H2' | 32:DB:88:C:H5'' | 2.02 | 0.41 |
| 33:DD:79:VAL:HG21 | 33:DD:111:LEU:CD1 | 2.49 | 0.41 |
| 31:DA:2784:C:H1' | 34:DE:37:ARG:HH21 | 1.85 | 0.41 |
| 34:DE:47:VAL:HB | 34:DE:49:LEU:CD2 | 2.50 | 0.41 |
| 34:DE:51:PHE:CG | 34:DE:52:LEU:N | 2.88 | 0.41 |
| 34:DE:1:MET:HB2 | 34:DE:84:PHE:HB2 | 2.03 | 0.41 |
| 35:DF:13:SER:HA | 35:DF:14:PRO:HD3 | 1.84 | 0.41 |
| 35:DF:6:VAL:O | 35:DF:124:LEU:HD12 | 2.20 | 0.41 |
| 37:DH:83:TYR:HA | 37:DH:135:GLY:O | 2.20 | 0.41 |
| 37:DH:156:ALA:C | 37:DH:158:HIS:H | 2.23 | 0.41 |
| 43:DR:74:LYS:HD2 | 43:DR:77:ARG:NH2 | 2.31 | 0.41 |
| 44:DS:106:ARG:HD2 | 44:DS:107:GLU:O | 2.20 | 0.41 |
| 46:DU:83:LEU:HD12 | 46:DU:83:LEU:HA | 1.76 | 0.41 |
| 47:DV:25:LEU:H | 47:DV:94:LEU:HD12 | 1.82 | 0.41 |
| 47:DV:36:PRO:CG | 47:DV:62:LEU:HD11 | 2.50 | 0.41 |
| 48:DW:55:ALA:O | 48:DW:56:ALA:C | 2.56 | 0.41 |
| 49:DX:57:LEU:O | 49:DX:76:ARG:N | 2.49 | 0.41 |
| 50:DY:35:TYR:O | 50:DY:35:TYR:CD2 | 2.74 | 0.41 |
| 51:DZ:124:ILE:CG1 | 51:DZ:125:LEU:N | 2.83 | 0.41 |
| 51:DZ:139:VAL:HG12 | 51:DZ:141:VAL:H | 1.86 | 0.41 |
| 1:AA:1015:A:N6 | 1:AA:1016:A:C6 | 2.89 | 0.41 |
| 1:AA:1134:G:N2 | 1:AA:1141:C:C2 | 2.88 | 0.41 |
| 1:AA:1322:C:H5' | 13:AM:100:GLY:HA3 | 2.03 | 0.41 |
| 1:AA:1463:C:O2' | 1:AA:1464:G:H5' | 2.21 | 0.41 |
| 1:AA:1516:G:H2' | 1:AA:1518:A:OP2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:445:G:C6 | 1:AA:490:G:C6 | 3.08 | 0.41 |
| 1:AA:509:A:C2 | 1:AA:510:A:C2 | 3.08 | 0.41 |
| 1:AA:563:A:C8 | 1:AA:567:G:O4' | 2.73 | 0.41 |
| 1:AA:655:A:C2 | 1:AA:656:C:C2 | 3.08 | 0.41 |
| 1:AA:659:U:O2 | 1:AA:659:U:H2' | 2.19 | 0.41 |
| 1:AA:831:U:O2' | 1:AA:832:C:H5' | 2.21 | 0.41 |
| 1:AA:996:A:H2' | 1:AA:997:U:C6 | 2.56 | 0.41 |
| 2:AB:142:LEU:HD23 | 2:AB:142:LEU:O | 2.21 | 0.41 |
| 2:AB:163:PHE:HD2 | 2:AB:185:ILE:HB | 1.84 | 0.41 |
| 2:AB:35:GLU:HA | 2:AB:39:ILE:O | 2.20 | 0.41 |
| 2:AB:96:ARG:O | 2:AB:98:LEU:N | 2.53 | 0.41 |
| 2:AB:93:VAL:HG11 | 2:AB:97:TRP:HD1 | 1.86 | 0.41 |
| 4:AD:33:MET:HE1 | 4:AD:37:PRO:HA | 2.02 | 0.41 |
| 4:AD:78:LEU:O | 4:AD:81:GLU:HB3 | 2.20 | 0.41 |
| 6:AF:22:GLU:C | 6:AF:24:GLU:N | 2.73 | 0.41 |
| 9:AI:3:GLN:HB3 | 9:AI:20:ARG:NE | 2.35 | 0.41 |
| 9:AI:4:TYR:HA | 9:AI:88:TYR:CE1 | 2.55 | 0.41 |
| 12:AL:31:PRO:HB2 | 12:AL:32:PHE:CD2 | 2.55 | 0.41 |
| 12:AL:38:THR:HG23 | 12:AL:39:VAL:HG23 | 2.01 | 0.41 |
| 18:AR:63:GLN:OE1 | 18:AR:66:LEU:HD23 | 2.20 | 0.41 |
| 18:AR:84:LYS:HD3 | 18:AR:84:LYS:HA | 1.97 | 0.41 |
| 23:B1:83:GLU:C | 23:B1:85:LEU:H | 2.23 | 0.41 |
| 31:BA:1557:C:H5'' | 31:BA:1558:A:OP2 | 2.20 | 0.41 |
| 31:BA:1910:G:O2' | 31:BA:1911:U:H5' | 2.20 | 0.41 |
| 31:BA:2189:U:H2' | 31:BA:2190:G:O4' | 2.21 | 0.41 |
| 31:BA:2563:U:O2 | 31:BA:2565:A:H8 | 2.03 | 0.41 |
| 31:BA:2729:G:H2' | 31:BA:2730:C:C6 | 2.55 | 0.41 |
| 31:BA:363(A):A:H2' | 31:BA:363(A):A:N3 | 2.36 | 0.41 |
| 31:BA:753:C:O2' | 31:BA:754:C:H5' | 2.20 | 0.41 |
| 31:BA:828:U:H4' | 31:BA:831:G:C2 | 2.55 | 0.41 |
| 32:BB:24:G:N7 | 32:BB:56:G:H2' | 2.36 | 0.41 |
| 31:BA:2784:C:H1' | 34:BE:37:ARG:HH21 | 1.85 | 0.41 |
| 34:BE:56:PRO:C | 34:BE:58:ARG:N | 2.74 | 0.41 |
| 35:BF:18:ARG:CG | 35:BF:19:GLU:N | 2.75 | 0.41 |
| 36:BG:115:ARG:HB2 | 36:BG:116:ASP:H | 1.70 | 0.41 |
| 37:BH:40:GLU:O | 37:BH:41:MET:CB | 2.68 | 0.41 |
| 39:BN:42:TRP:HA | 39:BN:48:MET:CE | 2.34 | 0.41 |
| 40:BO:107:ARG:HE | 40:BO:107:ARG:HB2 | 1.69 | 0.41 |
| 41:BP:95:VAL:CG1 | 41:BP:123:LEU:HD11 | 2.51 | 0.41 |
| 42:BQ:35:VAL:CG1 | 42:BQ:130:LYS:HB3 | 2.41 | 0.41 |
| 42:BQ:78:PRO:C | 42:BQ:79:LEU:HG | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BQ:88:GLY:O | 42:BQ:89:ASN:HB2 | 2.21 | 0.41 |
| 45:BT:107:ASP:CG | 45:BT:109:GLU:H | 2.24 | 0.41 |
| 45:BT:24:PRO:HB3 | 45:BT:99:LEU:HD21 | 2.01 | 0.41 |
| 47:BV:72:VAL:CG1 | 47:BV:73:SER:N | 2.73 | 0.41 |
| 48:BW:57:ASN:O | 48:BW:58:ALA:C | 2.58 | 0.41 |
| 51:BZ:130:PRO:HA | 51:BZ:133:ILE:CD1 | 2.49 | 0.41 |
| 1:CA:1091:U:O2 | 1:CA:1093:A:C8 | 2.74 | 0.41 |
| 1:CA:129:U:H5' | 17:CQ:3:LYS:HZ1 | 1.86 | 0.41 |
| 1:CA:344:A:H4' | 1:CA:345:C:OP2 | 2.20 | 0.41 |
| 1:CA:392:G:O2' | 1:CA:393:A:H5' | 2.21 | 0.41 |
| 1:CA:685:G:N2 | 1:CA:686:U:O4 | 2.53 | 0.41 |
| 1:CA:731:G:C6 | 1:CA:732:C:N4 | 2.89 | 0.41 |
| 1:CA:741:G:H2' | 1:CA:742:G:C8 | 2.55 | 0.41 |
| 1:CA:972:C:H4' | 10:CJ:57:LYS:CG | 2.48 | 0.41 |
| 4:CD:109:GLY:C | 4:CD:111:ALA:N | 2.73 | 0.41 |
| 5:CE:143:ARG:NH1 | 8:CH:77:GLU:OE2 | 2.53 | 0.41 |
| 5:CE:31:LEU:CD1 | 5:CE:129:ILE:HA | 2.50 | 0.41 |
| 7:CG:87:VAL:HG22 | 7:CG:154:TYR:HB2 | 2.02 | 0.41 |
| 8:CH:44:PHE:HD1 | 8:CH:79:VAL:HG12 | 1.84 | 0.41 |
| 10:CJ:94:VAL:CG1 | 10:CJ:95:GLU:N | 2.83 | 0.41 |
| 14:CN:44:LEU:C | 14:CN:44:LEU:HD12 | 2.40 | 0.41 |
| 14:CN:46:GLU:O | 14:CN:50:LYS:HG3 | 2.20 | 0.41 |
| 15:CO:55:GLY:O | 15:CO:58:MET:N | 2.54 | 0.41 |
| 20:CT:26:ASN:HA | 20:CT:29:LYS:HG2 | 2.02 | 0.41 |
| 21:CU:22:ARG:N | 21:CU:23:PRO:HD3 | 2.35 | 0.41 |
| 23:D1:8:SER:N | 23:D1:46:LEU:CD1 | 2.83 | 0.41 |
| 26:D4:28:LYS:CB | 36:DG:113:ARG:HH22 | 2.33 | 0.41 |
| 27:D5:13:LYS:O | 27:D5:14:ALA:C | 2.58 | 0.41 |
| 27:D5:47:PRO:C | 27:D5:48:GLU:OE2 | 2.58 | 0.41 |
| 28:D6:19:ARG:HG3 | 28:D6:20:ASN:H | 1.85 | 0.41 |
| 29:D7:10:ARG:HG3 | 31:DA:125:G:C6 | 2.56 | 0.41 |
| 31:DA:1417:C:O2' | 31:DA:1418:G:H5' | 2.20 | 0.41 |
| 31:DA:145:G:C2' | 31:DA:146:G:C5' | 2.80 | 0.41 |
| 31:DA:1531:C:H5'' | 31:DA:1532:C:C6 | 2.49 | 0.41 |
| 31:DA:1778:U:C4 | 31:DA:1784:A:C4 | 3.08 | 0.41 |
| 31:DA:2199:A:C8 | 31:DA:2200:C:C5 | 3.08 | 0.41 |
| 31:DA:2602:A:H4' | 31:DA:2603:G:C5' | 2.51 | 0.41 |
| 31:DA:29:U:H2' | 31:DA:30:G:C8 | 2.56 | 0.41 |
| 31:DA:329:G:H4' | 31:DA:330:A:OP2 | 2.20 | 0.41 |
| 31:DA:362:U:C6 | 31:DA:362:U:C3' | 3.04 | 0.41 |
| 31:DA:363(C):G:C2 | 31:DA:363(D):G:C4 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:417:C:H2' | 31:DA:417:C:O2 | 2.21 | 0.41 |
| 31:DA:614:U:O2 | 31:DA:614:U:O4' | 2.37 | 0.41 |
| 31:DA:735:A:H3' | 31:DA:736:C:H6 | 1.85 | 0.41 |
| 22:D0:27:GLU:HB3 | 31:DA:856:C:C1' | 2.50 | 0.41 |
| 31:DA:880:G:N2 | 31:DA:898:C:C4 | 2.89 | 0.41 |
| 31:DA:909:A:H2' | 31:DA:912:C:H5 | 1.84 | 0.41 |
| 31:DA:921:G:O2' | 31:DA:922:U:H5' | 2.21 | 0.41 |
| 34:DE:28:ALA:HB3 | 34:DE:93:VAL:CG2 | 2.50 | 0.41 |
| 35:DF:158:THR:CG2 | 35:DF:160:ASN:H | 2.24 | 0.41 |
| 35:DF:153:SER:HA | 35:DF:172:TRP:O | 2.21 | 0.41 |
| 35:DF:18:ARG:CG | 35:DF:19:GLU:N | 2.75 | 0.41 |
| 35:DF:1:MET:O | 35:DF:2:LYS:O | 2.39 | 0.41 |
| 38:DI:114:LEU:O | 38:DI:115:ALA:HB3 | 2.21 | 0.41 |
| 38:DI:14:ASP:O | 38:DI:17:GLN:HB2 | 2.21 | 0.41 |
| 40:DO:13:ASN:H | 40:DO:13:ASN:HD22 | 1.67 | 0.41 |
| 41:DP:146:VAL:CG2 | 41:DP:147:LEU:N | 2.78 | 0.41 |
| 42:DQ:104:PHE:HE1 | 42:DQ:125:LEU:HD11 | 1.85 | 0.41 |
| 46:DU:98:LEU:O | 46:DU:101:ARG:O | 2.39 | 0.41 |
| 1:AA:1091:U:O2 | 1:AA:1093:A:C8 | 2.74 | 0.41 |
| 1:AA:1127:G:C2' | 1:AA:1147:C:H42 | 2.34 | 0.41 |
| 1:AA:1334:G:C8 | 1:AA:1334:G:OP2 | 2.74 | 0.41 |
| 1:AA:358:U:H2' | 1:AA:359:U:C6 | 2.54 | 0.41 |
| 1:AA:443:C:N3 | 1:AA:444:C:C5 | 2.88 | 0.41 |
| 1:AA:761:G:C5 | 1:AA:762:C:C5 | 3.08 | 0.41 |
| 1:AA:962:C:H2' | 1:AA:963:G:O4' | 2.20 | 0.41 |
| 1:AA:972:C:H4' | 10:AJ:57:LYS:CG | 2.49 | 0.41 |
| 3:AC:188:LEU:O | 3:AC:189:ALA:HB2 | 2.20 | 0.41 |
| 4:AD:109:GLY:C | 4:AD:111:ALA:N | 2.73 | 0.41 |
| 1:AA:1298:C:H2' | 7:AG:114:ARG:NH1 | 2.36 | 0.41 |
| 10:AJ:22:LYS:O | 10:AJ:22:LYS:HD2 | 2.20 | 0.41 |
| 10:AJ:44:VAL:HG12 | 10:AJ:45:ARG:N | 2.35 | 0.41 |
| 10:AJ:51:ARG:H | 10:AJ:60:ARG:HA | 1.84 | 0.41 |
| 10:AJ:62:HIS:O | 10:AJ:62:HIS:HD2 | 2.03 | 0.41 |
| 12:AL:102:ARG:NH1 | 12:AL:102:ARG:CG | 2.79 | 0.41 |
| 12:AL:115:LYS:HB3 | 12:AL:116:SER:H | 1.75 | 0.41 |
| 14:AN:51:GLY:C | 14:AN:53:LEU:N | 2.74 | 0.41 |
| 16:AP:8:ARG:O | 16:AP:9:PHE:CD2 | 2.74 | 0.41 |
| 20:AT:89:ARG:NH2 | 20:AT:104:LEU:HD21 | 2.33 | 0.41 |
| 23:B1:11:ARG:CG | 23:B1:61:ARG:O | 2.68 | 0.41 |
| 23:B1:85:LEU:HB3 | 23:B1:87:PRO:HD2 | 2.03 | 0.41 |
| 31:BA:1047:G:H4' | 31:BA:1047:G:OP1 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1047:G:C8 | 31:BA:1110:G:C6 | 3.09 | 0.41 |
| 31:BA:1157:G:H2' | 31:BA:1158:C:H5' | 2.01 | 0.41 |
| 31:BA:1264:G:H3' | 31:BA:1265:A:H5'' | 2.02 | 0.41 |
| 31:BA:1444:G:O6 | 31:BA:1466:G:C6 | 2.73 | 0.41 |
| 31:BA:1470:G:C6 | 31:BA:1519:G:N7 | 2.89 | 0.41 |
| 31:BA:1956:U:H2' | 31:BA:1957:C:H5' | 2.02 | 0.41 |
| 31:BA:2097:C:H2' | 31:BA:2098:U:C6 | 2.56 | 0.41 |
| 31:BA:2183:C:H2' | 31:BA:2184:G:C8 | 2.55 | 0.41 |
| 22:B0:36:ILE:HG23 | 31:BA:2354:G:O2' | 2.20 | 0.41 |
| 31:BA:2579:C:H2' | 31:BA:2580:U:O4' | 2.20 | 0.41 |
| 31:BA:271(A):A:C2 | 31:BA:272(D):G:N3 | 2.87 | 0.41 |
| 31:BA:32:C:O2' | 31:BA:33:U:H5' | 2.21 | 0.41 |
| 31:BA:354:G:C3' | 31:BA:354:G:C8 | 3.04 | 0.41 |
| 33:BD:149:PRO:O | 33:BD:150:LYS:HB2 | 2.20 | 0.41 |
| 34:BE:27:LEU:HD22 | 45:BT:1:MET:HE2 | 2.00 | 0.41 |
| 35:BF:160:ASN:ND2 | 35:BF:162:LEU:HB2 | 2.34 | 0.41 |
| 36:BG:108:ASN:O | 36:BG:112:PRO:HG2 | 2.20 | 0.41 |
| 36:BG:144:ILE:HD12 | 36:BG:144:ILE:HA | 1.91 | 0.41 |
| 37:BH:38:SER:HA | 37:BH:39:PRO:HD3 | 1.87 | 0.41 |
| 38:BI:8:PRO:O | 38:BI:9:LEU:HD23 | 2.20 | 0.41 |
| 40:BO:17:ARG:HD3 | 40:BO:17:ARG:HA | 1.62 | 0.41 |
| 41:BP:16:ARG:HG3 | 41:BP:18:ARG:H | 1.84 | 0.41 |
| 41:BP:85:LEU:CD2 | 41:BP:85:LEU:N | 2.76 | 0.41 |
| 42:BQ:81:VAL:C | 42:BQ:82:ARG:CG | 2.88 | 0.41 |
| 42:BQ:85:LYS:HG3 | 42:BQ:86:GLY:H | 1.85 | 0.41 |
| 43:BR:38:VAL:HG12 | 43:BR:42:LYS:HD2 | 2.02 | 0.41 |
| 46:BU:31:SER:C | 46:BU:33:ARG:N | 2.69 | 0.41 |
| 46:BU:34:LYS:HA | 46:BU:34:LYS:HE3 | 2.03 | 0.41 |
| 49:BX:55:ASN:HB2 | 49:BX:78:LYS:HD2 | 2.03 | 0.41 |
| 49:BX:60:ARG:HG2 | 49:BX:72:LYS:H | 1.85 | 0.41 |
| 50:BY:77:PRO:O | 50:BY:78:ALA:CB | 2.68 | 0.41 |
| 51:BZ:139:VAL:HG12 | 51:BZ:141:VAL:H | 1.85 | 0.41 |
| 51:BZ:151:HIS:CB | 51:BZ:170:THR:HA | 2.50 | 0.41 |
| 1:CA:1030(C):G:H2' | 1:CA:1030(D):A:O4' | 2.20 | 0.41 |
| 1:CA:1334:G:C8 | 1:CA:1334:G:OP2 | 2.73 | 0.41 |
| 1:CA:945:G:N1 | 1:CA:1337:G:C2 | 2.88 | 0.41 |
| 1:CA:1352:C:H2' | 1:CA:1353:G:C8 | 2.55 | 0.41 |
| 1:CA:1425:U:H2' | 1:CA:1426:C:C6 | 2.56 | 0.41 |
| 1:CA:36:C:C2' | 1:CA:37:U:H5' | 2.51 | 0.41 |
| 1:CA:673:G:N1 | 1:CA:674:G:C6 | 2.88 | 0.41 |
| 1:CA:811:C:H4' | 1:CA:900:A:N6 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:CA:93:G:H2' | 1:CA:96:U:C5' | 2.50 | 0.41 |
| 2:CB:111:ARG:HA | 2:CB:114:ARG:HB3 | 2.03 | 0.41 |
| 2:CB:83:MET:SD | 2:CB:234:PRO:HG2 | 2.60 | 0.41 |
| 3:CC:150:LYS:HG3 | 3:CC:169:ALA:HB2 | 2.03 | 0.41 |
| 3:CC:19:GLU:O | 3:CC:40:ARG:NH2 | 2.53 | 0.41 |
| 3:CC:69:HIS:N | 3:CC:69:HIS:CD2 | 2.87 | 0.41 |
| 6:CF:9:VAL:C | 6:CF:10:LEU:HD12 | 2.41 | 0.41 |
| 1:CA:1368:G:OP2 | 9:CI:112:LYS:CD | 2.69 | 0.41 |
| 9:CI:17:VAL:HG22 | 9:CI:63:ILE:CG1 | 2.50 | 0.41 |
| 10:CJ:22:LYS:O | 10:CJ:22:LYS:HD2 | 2.21 | 0.41 |
| 12:CL:102:ARG:HG3 | 12:CL:102:ARG:NH1 | 2.35 | 0.41 |
| 12:CL:64:TYR:O | 12:CL:65:GLU:HB2 | 2.21 | 0.41 |
| 17:CQ:33:GLY:O | 17:CQ:34:LYS:O | 2.39 | 0.41 |
| 31:DA:1153:C:OP1 | 46:DU:76:TYR:OH | 2.35 | 0.41 |
| 31:DA:1274:A:N3 | 31:DA:1297:C:H1' | 2.36 | 0.41 |
| 29:D7:10:ARG:NH2 | 31:DA:1378:A:OP1 | 2.53 | 0.41 |
| 31:DA:1502:C:H5'' | 31:DA:1502:C:C6 | 2.55 | 0.41 |
| 31:DA:1504:C:O2' | 31:DA:1505:C:C5' | 2.69 | 0.41 |
| 31:DA:1509(A):A:H2' | 31:DA:1509(B):A:C8 | 2.43 | 0.41 |
| 31:DA:1677:A:C2' | 31:DA:1678:G:O5' | 2.68 | 0.41 |
| 31:DA:2226:C:H6 | 31:DA:2226:C:O5' | 2.03 | 0.41 |
| 31:DA:2261:C:O2' | 31:DA:2262:U:H5' | 2.21 | 0.41 |
| 31:DA:245:G:C5 | 31:DA:246:C:C5 | 3.08 | 0.41 |
| 31:DA:2526:G:C6 | 31:DA:2527:C:C4 | 3.09 | 0.41 |
| 31:DA:576:U:O2' | 31:DA:577:G:H5' | 2.21 | 0.41 |
| 31:DA:975:C:H4' | 31:DA:975:C:OP2 | 2.20 | 0.41 |
| 36:DG:38:VAL:HG22 | 36:DG:93:THR:HG23 | 2.02 | 0.41 |
| 39:DN:15:LEU:HD23 | 39:DN:53:VAL:HB | 2.03 | 0.41 |
| 47:DV:19:LYS:HG2 | 47:DV:96:ILE:CG2 | 2.51 | 0.41 |
| 51:DZ:10:ARG:NH2 | 51:DZ:26:GLY:O | 2.53 | 0.41 |
| 1:AA:1057:G:C4 | 1:AA:1204:A:C2 | 3.09 | 0.41 |
| 1:AA:112:G:C2 | 1:AA:113:G:C8 | 3.09 | 0.41 |
| 1:AA:174:C:O5' | 1:AA:174:C:H6 | 2.03 | 0.41 |
| 1:AA:17:U:H2' | 1:AA:18:C:H6 | 1.77 | 0.41 |
| 1:AA:193:C:O2' | 1:AA:194:C:H5' | 2.21 | 0.41 |
| 1:AA:236:G:C5 | 1:AA:237:C:C5 | 3.08 | 0.41 |
| 1:AA:274:A:H4' | 1:AA:275:G:OP1 | 2.20 | 0.41 |
| 1:AA:318:G:C2 | 1:AA:319:G:C5 | 3.09 | 0.41 |
| 1:AA:49:U:C2 | 1:AA:361:G:N2 | 2.89 | 0.41 |
| 1:AA:628:G:C2 | 1:AA:629:G:C4 | 3.09 | 0.41 |
| 1:AA:639:G:O2' | 1:AA:640:A:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:658:G:N3 | 1:AA:659:U:C6 | 2.89 | 0.41 |
| 1:AA:692:U:O2' | 1:AA:694:A:N7 | 2.46 | 0.41 |
| 4:AD:173:TRP:HA | 4:AD:187:ARG:NH1 | 2.35 | 0.41 |
| 1:AA:508:C:OP1 | 4:AD:209:ARG:NH2 | 2.54 | 0.41 |
| 4:AD:8:VAL:CB | 4:AD:21:LEU:HD12 | 2.35 | 0.41 |
| 4:AD:59:ARG:HA | 4:AD:59:ARG:NE | 2.36 | 0.41 |
| 4:AD:67:ILE:HG22 | 4:AD:68:TYR:HD1 | 1.85 | 0.41 |
| 5:AE:102:ALA:HB2 | 5:AE:120:THR:OG1 | 2.20 | 0.41 |
| 5:AE:77:PRO:HB2 | 5:AE:143:ARG:O | 2.20 | 0.41 |
| 5:AE:7:GLU:HB3 | 5:AE:112:LEU:HD13 | 2.03 | 0.41 |
| 11:AK:117:ASN:HD22 | 11:AK:117:ASN:HA | 1.61 | 0.41 |
| 11:AK:34:ASP:HB2 | 11:AK:35:PRO:CD | 2.50 | 0.41 |
| 12:AL:102:ARG:HG3 | 12:AL:102:ARG:NH1 | 2.35 | 0.41 |
| 16:AP:82:GLN:N | 16:AP:82:GLN:HE21 | 2.19 | 0.41 |
| 20:AT:13:LEU:CD1 | 20:AT:13:LEU:H | 2.29 | 0.41 |
| 23:B1:30:VAL:O | 23:B1:30:VAL:CG1 | 2.68 | 0.41 |
| 27:B5:31:VAL:O | 27:B5:39:MET:HA | 2.20 | 0.41 |
| 31:BA:9:U:O2' | 31:BA:10:G:P | 2.79 | 0.41 |
| 31:BA:1299:G:H5'' | 31:BA:1300:U:OP1 | 2.21 | 0.41 |
| 31:BA:1317:A:H2' | 31:BA:1318:C:C6 | 2.56 | 0.41 |
| 31:BA:1509(A):A:H2' | 31:BA:1509(B):A:C8 | 2.45 | 0.41 |
| 31:BA:1531:C:C3' | 31:BA:1532:C:C5' | 2.97 | 0.41 |
| 31:BA:1648:C:C2' | 31:BA:1649:G:O5' | 2.69 | 0.41 |
| 23:B1:37:ILE:HG23 | 31:BA:2080:G:O5' | 2.21 | 0.41 |
| 31:BA:2273:A:H2' | 31:BA:2274:A:C8 | 2.56 | 0.41 |
| 31:BA:2274:A:O5' | 31:BA:2275:C:OP2 | 2.38 | 0.41 |
| 31:BA:2304:G:H22 | 31:BA:2312:U:H3 | 1.68 | 0.41 |
| 22:B0:43:THR:N | 31:BA:2331:G:H4' | 2.28 | 0.41 |
| 31:BA:2471:C:O2 | 31:BA:2471:C:H2' | 2.19 | 0.41 |
| 31:BA:272(G):C:N4 | 31:BA:363(C):G:H1 | 2.19 | 0.41 |
| 31:BA:416:C:C2 | 31:BA:417:C:C6 | 3.09 | 0.41 |
| 31:BA:540:C:H2' | 31:BA:541:C:C6 | 2.56 | 0.41 |
| 31:BA:543:C:C5 | 31:BA:547:A:N7 | 2.89 | 0.41 |
| 31:BA:908:C:O2' | 31:BA:909:A:H5' | 2.21 | 0.41 |
| 31:BA:910:A:C6 | 31:BA:911:A:C6 | 3.08 | 0.41 |
| 33:BD:44:ASN:HB3 | 33:BD:48:ARG:C | 2.41 | 0.41 |
| 36:BG:86:MET:O | 36:BG:87:PRO:C | 2.58 | 0.41 |
| 40:BO:68:GLU:HB3 | 40:BO:78:ARG:HH11 | 1.85 | 0.41 |
| 40:BO:75:SER:OG | 40:BO:76:ALA:N | 2.53 | 0.41 |
| 40:BO:77:ILE:HG12 | 40:BO:78:ARG:N | 2.35 | 0.41 |
| 31:BA:2334:G:H5' | 44:BS:13:ARG:HB3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:BS:33:LYS:HA | 44:BS:33:LYS:HD3 | 1.66 | 0.41 |
| 47:BV:23:GLU:O | 47:BV:24:LYS:C | 2.59 | 0.41 |
| 50:BY:31:LEU:HD13 | 50:BY:31:LEU:HA | 1.54 | 0.41 |
| 50:BY:81:LYS:CE | 50:BY:97:ARG:HG2 | 2.51 | 0.41 |
| 1:CA:102:G:C6 | 1:CA:103:C:N4 | 2.89 | 0.41 |
| 1:CA:1191:A:H5'' | 3:CC:4:LYS:HZ2 | 1.86 | 0.41 |
| 1:CA:1412:C:H42 | 1:CA:1488:G:H1 | 1.69 | 0.41 |
| 1:CA:66:G:C4' | 1:CA:173:U:C5 | 3.00 | 0.41 |
| 1:CA:318:G:C2 | 1:CA:319:G:C5 | 3.09 | 0.41 |
| 1:CA:389:A:H2' | 1:CA:390:C:C5' | 2.50 | 0.41 |
| 1:CA:405:U:H5'' | 1:CA:406:G:O4' | 2.21 | 0.41 |
| 1:CA:543:C:N3 | 1:CA:544:G:N7 | 2.69 | 0.41 |
| 1:CA:707:C:C2 | 1:CA:708:C:C5 | 3.09 | 0.41 |
| 1:CA:782:A:C8 | 1:CA:783:C:C5 | 3.09 | 0.41 |
| 1:CA:836:G:C6 | 1:CA:851:G:C5 | 3.08 | 0.41 |
| 2:CB:190:THR:C | 2:CB:192:SER:H | 2.23 | 0.41 |
| 3:CC:186:PHE:CD1 | 3:CC:198:VAL:O | 2.73 | 0.41 |
| 4:CD:121:VAL:O | 4:CD:134:ASP:HA | 2.20 | 0.41 |
| 4:CD:23:GLY:O | 4:CD:27:TYR:CD1 | 2.73 | 0.41 |
| 4:CD:79:PHE:CD1 | 4:CD:207:TYR:CD1 | 3.08 | 0.41 |
| 5:CE:107:ARG:O | 5:CE:108:ALA:C | 2.59 | 0.41 |
| 1:CA:1298:C:H2' | 7:CG:114:ARG:NH1 | 2.35 | 0.41 |
| 10:CJ:24:VAL:O | 10:CJ:28:ARG:HG3 | 2.20 | 0.41 |
| 12:CL:38:THR:HG23 | 12:CL:39:VAL:N | 2.36 | 0.41 |
| 1:CA:521:G:H4' | 12:CL:73:GLU:HG2 | 2.02 | 0.41 |
| 16:CP:21:VAL:HG23 | 16:CP:21:VAL:O | 2.21 | 0.41 |
| 18:CR:37:VAL:HG23 | 18:CR:38:GLU:H | 1.86 | 0.41 |
| 23:D1:10:LYS:HG2 | 23:D1:11:ARG:H | 1.86 | 0.41 |
| 23:D1:44:PRO:HA | 31:DA:2231:C:OP1 | 2.20 | 0.41 |
| 27:D5:57:VAL:C | 27:D5:58:LEU:CG | 2.89 | 0.41 |
| 31:DA:1336:A:O2' | 31:DA:1337:G:H5' | 2.21 | 0.41 |
| 31:DA:1416:G:O2' | 31:DA:1417:C:C6 | 2.71 | 0.41 |
| 31:DA:1502:C:O2 | 31:DA:1502:C:C2' | 2.69 | 0.41 |
| 31:DA:1812:A:C2 | 31:DA:1813:G:C5 | 3.09 | 0.41 |
| 31:DA:1858:G:H1' | 31:DA:1884:A:H61 | 1.86 | 0.41 |
| 31:DA:1879:C:C2' | 31:DA:1880:C:H5' | 2.50 | 0.41 |
| 23:D1:41:ARG:NH2 | 31:DA:205:G:O6 | 2.53 | 0.41 |
| 31:DA:2061:G:C2 | 31:DA:2063:C:C4 | 3.09 | 0.41 |
| 31:DA:2444:G:OP2 | 35:DF:68:LYS:HE2 | 2.20 | 0.41 |
| 31:DA:2689:U:H5'' | 31:DA:2690:C:H5' | 2.01 | 0.41 |
| 31:DA:271(F):C:N3 | 31:DA:271(G):C:C5 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:D7:37:LYS:HE2 | 31:DA:469:G:O6 | 2.21 | 0.41 |
| 31:DA:614(C):A:C4 | 35:DF:180:GLY:CA | 3.04 | 0.41 |
| 31:DA:61:G:H1 | 31:DA:94:C:N4 | 2.17 | 0.41 |
| 31:DA:664:C:H2' | 31:DA:665:C:H6 | 1.85 | 0.41 |
| 33:DD:266:SER:O | 33:DD:267:SER:OG | 2.35 | 0.41 |
| 35:DF:50:SER:HB2 | 35:DF:94:PRO:HD3 | 2.02 | 0.41 |
| 35:DF:81:PRO:HB3 | 35:DF:87:GLY:O | 2.21 | 0.41 |
| 37:DH:117:PRO:HB3 | 37:DH:123:PHE:HD1 | 1.85 | 0.41 |
| 37:DH:156:ALA:O | 37:DH:157:TYR:C | 2.58 | 0.41 |
| 37:DH:40:GLU:O | 37:DH:41:MET:CB | 2.69 | 0.41 |
| 39:DN:78:TYR:CD1 | 39:DN:79:PRO:CG | 3.04 | 0.41 |
| 40:DO:1:MET:HB2 | 40:DO:32:TYR:HB3 | 2.03 | 0.41 |
| 41:DP:16:ARG:CB | 41:DP:16:ARG:CZ | 2.97 | 0.41 |
| 41:DP:16:ARG:NH1 | 41:DP:18:ARG:HG2 | 2.36 | 0.41 |
| 43:DR:74:LYS:CE | 43:DR:77:ARG:HH21 | 2.33 | 0.41 |
| 46:DU:39:LEU:HA | 46:DU:39:LEU:HD23 | 1.75 | 0.41 |
| 47:DV:21:ARG:H | 47:DV:21:ARG:CD | 2.33 | 0.41 |
| 51:DZ:28:MET:HG3 | 51:DZ:35:ARG:HB2 | 2.01 | 0.41 |
| 1:AA:1141:C:H6 | 1:AA:1141:C:H3' | 1.85 | 0.41 |
| 1:AA:1378:C:N4 | 1:AA:1379:G:C2 | 2.89 | 0.41 |
| 1:AA:1386:G:N3 | 1:AA:1387:G:C8 | 2.88 | 0.41 |
| 1:AA:1469:G:H2' | 1:AA:1470:G:H8 | 1.86 | 0.41 |
| 1:AA:560:U:H6 | 1:AA:560:U:H2' | 1.60 | 0.41 |
| 1:AA:625:G:H2' | 1:AA:626:U:C6 | 2.56 | 0.41 |
| 1:AA:741:G:H2' | 1:AA:742:G:C8 | 2.56 | 0.41 |
| 1:AA:775:G:O2' | 1:AA:776:G:H5' | 2.21 | 0.41 |
| 2:AB:93:VAL:HG11 | 2:AB:97:TRP:CD1 | 2.56 | 0.41 |
| 3:AC:36:ASP:OD2 | 3:AC:57:ILE:HG21 | 2.21 | 0.41 |
| 10:AJ:51:ARG:CG | 10:AJ:61:GLU:HB2 | 2.50 | 0.41 |
| 12:AL:92:ASP:O | 12:AL:93:LEU:HD23 | 2.21 | 0.41 |
| 16:AP:32:TYR:O | 16:AP:32:TYR:HD2 | 2.02 | 0.41 |
| 20:AT:84:LEU:O | 20:AT:88:VAL:HG23 | 2.20 | 0.41 |
| 25:B3:46:ASN:HA | 25:B3:46:ASN:HD22 | 1.63 | 0.41 |
| 31:BA:1022:G:C5 | 31:BA:1140:C:N4 | 2.89 | 0.41 |
| 31:BA:1410:G:H1 | 31:BA:1592:C:N4 | 2.18 | 0.41 |
| 31:BA:442:G:O4' | 35:BF:46:ARG:HD3 | 2.21 | 0.41 |
| 31:BA:900:A:C4 | 31:BA:901:A:C8 | 3.09 | 0.41 |
| 33:BD:183:ARG:HG2 | 33:BD:183:ARG:HH11 | 1.85 | 0.41 |
| 33:BD:83:GLU:OE1 | 33:BD:104:TYR:CE2 | 2.74 | 0.41 |
| 31:BA:1673:U:C5 | 34:BE:129:HIS:HD2 | 2.38 | 0.41 |
| 34:BE:21:VAL:O | 34:BE:23:VAL:HG22 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BF:142:TRP:CE3 | 35:BF:143:ALA:N | 2.89 | 0.41 |
| 36:BG:116:ASP:O | 36:BG:117:PHE:HB3 | 2.21 | 0.41 |
| 36:BG:15:VAL:HG13 | 36:BG:175:LEU:CD1 | 2.51 | 0.41 |
| 37:BH:150:ALA:O | 37:BH:151:ILE:C | 2.59 | 0.41 |
| 37:BH:89:ILE:HB | 37:BH:90:LYS:H | 1.60 | 0.41 |
| 38:BI:132:PRO:HG2 | 38:BI:133:HIS:HD2 | 1.86 | 0.41 |
| 38:BI:45:LYS:O | 38:BI:48:GLU:N | 2.54 | 0.41 |
| 38:BI:5:LEU:HA | 38:BI:36:ALA:HB2 | 2.02 | 0.41 |
| 41:BP:114:ILE:HG13 | 41:BP:115:LEU:N | 2.32 | 0.41 |
| 30:B8:58:ILE:CG2 | 41:BP:49:ARG:HD3 | 2.51 | 0.41 |
| 42:BQ:20:ALA:CB | 42:BQ:98:LYS:HB3 | 2.51 | 0.41 |
| 44:BS:58:LEU:O | 44:BS:59:LYS:O | 2.37 | 0.41 |
| 45:BT:29:ARG:HG3 | 45:BT:30:VAL:H | 1.85 | 0.41 |
| 45:BT:90:GLN:NE2 | 45:BT:124:ASP:OD2 | 2.54 | 0.41 |
| 47:BV:71:LEU:HD13 | 47:BV:72:VAL:HB | 2.02 | 0.41 |
| 48:BW:55:ALA:O | 48:BW:56:ALA:C | 2.59 | 0.41 |
| 49:BX:5:TYR:O | 49:BX:7:VAL:N | 2.53 | 0.41 |
| 51:BZ:44:PHE:C | 51:BZ:44:PHE:CD1 | 2.93 | 0.41 |
| 1:CA:102:G:C6 | 1:CA:103:C:C5 | 3.08 | 0.41 |
| 1:CA:11:G:C5 | 1:CA:12:U:C5 | 3.09 | 0.41 |
| 1:CA:185:A:N6 | 1:CA:186:C:N4 | 2.69 | 0.41 |
| 1:CA:234:C:H2' | 1:CA:235:C:C6 | 2.54 | 0.41 |
| 1:CA:577:G:C2 | 1:CA:578:C:C5 | 3.08 | 0.41 |
| 1:CA:66:G:O4' | 1:CA:173:U:C4 | 2.74 | 0.41 |
| 1:CA:673:G:H5'' | 6:CF:87:ARG:CZ | 2.51 | 0.41 |
| 1:CA:731:G:H2' | 1:CA:732:C:C6 | 2.56 | 0.41 |
| 1:CA:90:U:H6 | 1:CA:90:U:H3' | 1.86 | 0.41 |
| 3:CC:134:ILE:HG22 | 3:CC:168:ALA:HB3 | 2.02 | 0.41 |
| 4:CD:206:PHE:CD2 | 4:CD:207:TYR:CE2 | 3.09 | 0.41 |
| 4:CD:56:VAL:HG12 | 4:CD:202:LEU:CD1 | 2.50 | 0.41 |
| 5:CE:77:PRO:HB2 | 5:CE:143:ARG:O | 2.21 | 0.41 |
| 5:CE:15:ARG:CZ | 5:CE:26:PHE:CE2 | 3.04 | 0.41 |
| 5:CE:11:ILE:HB | 5:CE:31:LEU:O | 2.21 | 0.41 |
| 8:CH:41:ARG:O | 8:CH:41:ARG:HG2 | 2.21 | 0.41 |
| 8:CH:44:PHE:CD1 | 8:CH:79:VAL:HG12 | 2.56 | 0.41 |
| 12:CL:38:THR:HG23 | 12:CL:39:VAL:HG23 | 2.02 | 0.41 |
| 10:CJ:49:VAL:HG22 | 14:CN:41:ARG:HB2 | 2.03 | 0.41 |
| 14:CN:51:GLY:C | 14:CN:53:LEU:N | 2.73 | 0.41 |
| 18:CR:71:LYS:O | 18:CR:72:ARG:C | 2.59 | 0.41 |
| 20:CT:30:LYS:C | 20:CT:30:LYS:HD2 | 2.41 | 0.41 |
| 20:CT:33:ILE:HD13 | 20:CT:33:ILE:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:CT:61:SER:OG | 20:CT:65:LYS:HE3 | 2.21 | 0.41 |
| 25:D3:10:LYS:HB3 | 25:D3:53:LEU:HA | 2.02 | 0.41 |
| 31:DA:1038:C:H2' | 31:DA:1038:C:O2 | 2.21 | 0.41 |
| 31:DA:1028:A:H61 | 31:DA:1125:G:H2' | 1.84 | 0.41 |
| 31:DA:1179:C:O2 | 31:DA:1179:C:H2' | 2.21 | 0.41 |
| 31:DA:1245:G:OP1 | 41:DP:16:ARG:CD | 2.68 | 0.41 |
| 31:DA:1414:G:C6 | 31:DA:1415:U:C4 | 3.09 | 0.41 |
| 31:DA:1444:G:C2 | 31:DA:1548:C:N3 | 2.89 | 0.41 |
| 31:DA:1685:C:O2' | 31:DA:1686:C:H5' | 2.21 | 0.41 |
| 31:DA:1721:G:N2 | 31:DA:1739:U:OP2 | 2.54 | 0.41 |
| 31:DA:1741:A:N7 | 31:DA:1742:G:N1 | 2.69 | 0.41 |
| 31:DA:1946:U:C2 | 31:DA:1947:C:C5 | 3.09 | 0.41 |
| 31:DA:2093:G:N7 | 31:DA:2225:A:H2' | 2.36 | 0.41 |
| 31:DA:2275:C:H5' | 31:DA:2275:C:C6 | 2.55 | 0.41 |
| 31:DA:2280:G:H2' | 31:DA:2281:C:H5' | 2.03 | 0.41 |
| 31:DA:2721:A:H1' | 31:DA:2873:A:O2' | 2.20 | 0.41 |
| 31:DA:353:G:C2' | 31:DA:354:G:O5' | 2.69 | 0.41 |
| 31:DA:445:C:O2' | 31:DA:446:G:H5' | 2.21 | 0.41 |
| 31:DA:729:G:C5 | 33:DD:208:LYS:HB2 | 2.56 | 0.41 |
| 31:DA:83:G:N1 | 31:DA:102:G:H2' | 2.33 | 0.41 |
| 24:D2:41:ILE:CG1 | 31:DA:94(A):G:N2 | 2.83 | 0.41 |
| 31:DA:973:A:H5' | 31:DA:1188:U:H1' | 2.02 | 0.41 |
| 32:DB:40:U:H1' | 32:DB:45:A:N6 | 2.35 | 0.41 |
| 33:DD:5:LYS:N | 33:DD:5:LYS:HD2 | 2.36 | 0.41 |
| 35:DF:7:TYR:HB3 | 35:DF:16:GLY:CA | 2.51 | 0.41 |
| 35:DF:176:LEU:HD21 | 35:DF:180:GLY:O | 2.21 | 0.41 |
| 35:DF:9:ILE:HG12 | 35:DF:14:PRO:HA | 2.02 | 0.41 |
| 36:DG:60:LEU:HD22 | 36:DG:63:ILE:HG13 | 2.03 | 0.41 |
| 37:DH:158:HIS:NE2 | 37:DH:169:VAL:C | 2.74 | 0.41 |
| 38:DI:88:ILE:HG13 | 38:DI:122:GLU:N | 2.36 | 0.41 |
| 39:DN:91:LEU:HA | 39:DN:95:PRO:HB3 | 2.02 | 0.41 |
| 41:DP:111:ARG:HG3 | 41:DP:128:HIS:CG | 2.56 | 0.41 |
| 41:DP:114:ILE:HG13 | 41:DP:115:LEU:N | 2.30 | 0.41 |
| 42:DQ:118:LEU:HA | 42:DQ:118:LEU:HD23 | 1.77 | 0.41 |
| 43:DR:56:LYS:HE2 | 43:DR:87:TYR:HB3 | 2.03 | 0.41 |
| 1:CA:1442(B):A:C2 | 45:DT:118:ARG:CZ | 3.04 | 0.41 |
| 48:DW:51:LEU:O | 48:DW:51:LEU:HD22 | 2.20 | 0.41 |
| 49:DX:36:LYS:O | 49:DX:38:GLU:N | 2.54 | 0.41 |
| 50:DY:13:VAL:HG12 | 50:DY:73:ARG:O | 2.20 | 0.41 |
| 1:AA:1084:G:OP1 | 1:AA:1086:U:C5 | 2.74 | 0.41 |
| 1:AA:1194:U:H4' | 5:AE:22:GLY:CA | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1264:C:H2' | 1:AA:1265:G:C8 | 2.52 | 0.41 |
| 1:AA:155:C:H2' | 1:AA:156:G:H8 | 1.86 | 0.41 |
| 1:AA:349:A:C2' | 1:AA:350:G:H5' | 2.50 | 0.41 |
| 1:AA:390:C:H3' | 1:AA:390:C:H6 | 1.85 | 0.41 |
| 1:AA:689:C:O2' | 1:AA:690:G:H5' | 2.20 | 0.41 |
| 2:AB:178:ARG:HG3 | 8:AH:72:PRO:HA | 2.01 | 0.41 |
| 4:AD:111:ALA:HB2 | 4:AD:120:LEU:HD12 | 2.02 | 0.41 |
| 5:AE:63:ARG:HA | 5:AE:66:MET:SD | 2.60 | 0.41 |
| 5:AE:87:SER:HB3 | 5:AE:125:SER:O | 2.20 | 0.41 |
| 7:AG:92:SER:CB | 7:AG:94:ARG:HH21 | 2.34 | 0.41 |
| 8:AH:1:MET:N | 8:AH:1:MET:HE2 | 2.33 | 0.41 |
| 9:AI:77:ILE:O | 9:AI:81:ILE:HG12 | 2.20 | 0.41 |
| 9:AI:114:TYR:CE1 | 10:AJ:60:ARG:O | 2.73 | 0.41 |
| 12:AL:69:TYR:HD2 | 12:AL:99:HIS:CD2 | 2.39 | 0.41 |
| 13:AM:40:ASN:HA | 13:AM:41:PRO:HD3 | 1.79 | 0.41 |
| 15:AO:67:LEU:CD2 | 15:AO:78:TYR:CE1 | 3.03 | 0.41 |
| 18:AR:79:LEU:HA | 18:AR:80:PRO:HD3 | 1.91 | 0.41 |
| 20:AT:23:ARG:O | 20:AT:27:LYS:HB2 | 2.20 | 0.41 |
| 27:B5:42:PRO:CB | 27:B5:43:HIS:HD2 | 2.34 | 0.41 |
| 31:BA:1245:G:OP1 | 41:BP:16:ARG:CD | 2.69 | 0.41 |
| 31:BA:1614:A:H62 | 48:BW:87:PRO:HA | 1.86 | 0.41 |
| 31:BA:1709:U:O2' | 31:BA:2859:G:H1' | 2.20 | 0.41 |
| 31:BA:151:C:C2 | 31:BA:176:G:N2 | 2.89 | 0.41 |
| 23:B1:18:ILE:HD13 | 31:BA:188:G:OP1 | 2.20 | 0.41 |
| 31:BA:1956:U:C2' | 31:BA:1957:C:H5' | 2.51 | 0.41 |
| 31:BA:2559:C:O2' | 31:BA:2560:C:H5' | 2.21 | 0.41 |
| 31:BA:506:G:O3' | 31:BA:507:A:H8 | 2.03 | 0.41 |
| 31:BA:565:C:H2' | 31:BA:566:U:O4' | 2.20 | 0.41 |
| 31:BA:716:A:C2' | 31:BA:717:G:O5' | 2.69 | 0.41 |
| 24:B2:49:LYS:HD3 | 31:BA:76:C:H5'' | 2.02 | 0.41 |
| 31:BA:861:A:H2' | 31:BA:862:G:O4' | 2.20 | 0.41 |
| 24:B2:41:ILE:HG13 | 31:BA:94(A):G:H22 | 1.86 | 0.41 |
| 33:BD:182:LEU:O | 33:BD:271:ILE:HD12 | 2.21 | 0.41 |
| 34:BE:82:ARG:HG3 | 34:BE:83:ASP:N | 2.36 | 0.41 |
| 35:BF:154:VAL:HB | 35:BF:173:VAL:HG22 | 2.03 | 0.41 |
| 37:BH:115:VAL:HG11 | 37:BH:148:ILE:CD1 | 2.51 | 0.41 |
| 37:BH:157:TYR:O | 37:BH:158:HIS:HB2 | 2.19 | 0.41 |
| 38:BI:27:ARG:NH1 | 38:BI:27:ARG:CG | 2.84 | 0.41 |
| 39:BN:3:THR:O | 39:BN:4:TYR:CG | 2.74 | 0.41 |
| 42:BQ:36:ALA:O | 42:BQ:100:GLY:N | 2.52 | 0.41 |
| 44:BS:24:LEU:HA | 44:BS:24:LEU:HD23 | 1.80 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:BT:30:VAL:HG22 | 45:BT:84:GLN:O | 2.20 | 0.41 |
| 1:CA:1030(D):A:N7 | 1:CA:1031:G:N3 | 2.68 | 0.41 |
| 1:CA:1076:C:C2 | 1:CA:1082:G:N2 | 2.89 | 0.41 |
| 1:CA:1128:C:O2 | 1:CA:1130:A:N7 | 2.54 | 0.41 |
| 1:CA:1273:G:H3' | 1:CA:1274:G:H8 | 1.86 | 0.41 |
| 1:CA:1385:G:O2' | 1:CA:1386:G:H5' | 2.21 | 0.41 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:C6 | 2.56 | 0.41 |
| 1:CA:236:G:C6 | 1:CA:237:C:C4 | 3.09 | 0.41 |
| 1:CA:431:A:H2' | 1:CA:432:A:O4' | 2.21 | 0.41 |
| 1:CA:563:A:H2 | 12:CL:15:ARG:NH1 | 2.18 | 0.41 |
| 1:CA:579:G:H2' | 1:CA:580:U:H6 | 1.85 | 0.41 |
| 1:CA:602:A:C2 | 1:CA:603:U:C2 | 3.09 | 0.41 |
| 1:CA:682:G:C6 | 1:CA:683:G:C5 | 3.08 | 0.41 |
| 1:CA:892:A:C6 | 1:CA:893:C:C4 | 3.08 | 0.41 |
| 2:CB:179:LYS:HG2 | 2:CB:179:LYS:O | 2.20 | 0.41 |
| 2:CB:69:LEU:HD11 | 2:CB:93:VAL:HG23 | 2.01 | 0.41 |
| 3:CC:159:GLY:HA2 | 3:CC:193:TYR:CD1 | 2.56 | 0.41 |
| 4:CD:141:ARG:HB3 | 4:CD:142:PRO:HD2 | 2.02 | 0.41 |
| 4:CD:31:CYS:O | 4:CD:32:ALA:HB3 | 2.21 | 0.41 |
| 12:CL:55:VAL:HA | 12:CL:70:ILE:HD13 | 2.02 | 0.41 |
| 16:CP:55:ARG:HE | 16:CP:55:ARG:HA | 1.85 | 0.41 |
| 16:CP:39:TYR:HD2 | 16:CP:73:LEU:HD13 | 1.84 | 0.41 |
| 18:CR:36:ASN:O | 18:CR:39:VAL:HB | 2.21 | 0.41 |
| 1:CA:191:G:N3 | 20:CT:103:GLY:O | 2.54 | 0.41 |
| 26:D4:14:ILE:HA | 36:DG:5:VAL:HG13 | 2.02 | 0.41 |
| 28:D6:26:ASN:HB3 | 28:D6:32:ASN:ND2 | 2.36 | 0.41 |
| 31:DA:1341:U:O4 | 49:DX:16:LYS:HE2 | 2.21 | 0.41 |
| 31:DA:1405:U:C2 | 31:DA:1406:U:C5 | 3.08 | 0.41 |
| 31:DA:1416:G:O2' | 31:DA:1417:C:OP2 | 2.39 | 0.41 |
| 31:DA:1493:C:O2 | 31:DA:1493:C:C2' | 2.68 | 0.41 |
| 31:DA:1517:G:O2' | 31:DA:1518:U:H5' | 2.21 | 0.41 |
| 31:DA:1605:C:H1' | 31:DA:1610:A:C4 | 2.56 | 0.41 |
| 31:DA:17:G:H2' | 31:DA:18:C:H6 | 1.85 | 0.41 |
| 31:DA:1850:G:C6 | 31:DA:1851:U:C4 | 3.09 | 0.41 |
| 31:DA:2036:C:H6 | 31:DA:2036:C:C5' | 2.22 | 0.41 |
| 31:DA:2070:G:H2' | 31:DA:2071:A:C8 | 2.56 | 0.41 |
| 31:DA:2399:G:C6 | 31:DA:2400:G:C5 | 3.08 | 0.41 |
| 31:DA:253:C:H2' | 31:DA:254:G:O4' | 2.20 | 0.41 |
| 31:DA:2802:G:OP2 | 31:DA:2803:C:OP2 | 2.38 | 0.41 |
| 31:DA:2811:G:OP1 | 34:DE:60:ASN:HB3 | 2.21 | 0.41 |
| 31:DA:2893:G:H4' | 31:DA:2894:G:H8 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DA:552:G:C2' | 31:DA:553:G:H5' | 2.51 | 0.41 |
| 31:DA:633:A:H2' | 31:DA:634:C:H5' | 2.03 | 0.41 |
| 29:D7:12:ARG:HG3 | 31:DA:686:G:O6 | 2.21 | 0.41 |
| 31:DA:738:G:C6 | 31:DA:739:G:C2 | 3.08 | 0.41 |
| 31:DA:744:G:H2' | 31:DA:745:G:O5' | 2.21 | 0.41 |
| 31:DA:981:A:C2 | 31:DA:2027:G:N3 | 2.89 | 0.41 |
| 33:DD:198:ASN:HD22 | 33:DD:198:ASN:C | 2.24 | 0.41 |
| 31:DA:2599:G:P | 33:DD:236:GLY:H | 2.44 | 0.41 |
| 36:DG:63:ILE:HD13 | 36:DG:141:PHE:CZ | 2.55 | 0.41 |
| 38:DI:77:LEU:O | 38:DI:78:THR:O | 2.38 | 0.41 |
| 39:DN:43:THR:HG22 | 39:DN:45:ASN:HD21 | 1.84 | 0.41 |
| 39:DN:46:VAL:CG1 | 39:DN:48:MET:HG3 | 2.50 | 0.41 |
| 42:DQ:48:GLU:O | 42:DQ:52:VAL:CG1 | 2.69 | 0.41 |
| 42:DQ:69:PHE:CG | 42:DQ:70:PRO:HD2 | 2.56 | 0.41 |
| 43:DR:41:ALA:C | 43:DR:43:GLU:N | 2.74 | 0.41 |
| 45:DT:56:GLY:C | 45:DT:59:THR:HG22 | 2.41 | 0.41 |
| 47:DV:28:GLU:CB | 47:DV:29:PRO:HD3 | 2.51 | 0.41 |
| 48:DW:62:HIS:O | 48:DW:63:ASP:C | 2.58 | 0.41 |
| 50:DY:45:VAL:HG13 | 50:DY:62:GLU:OE2 | 2.21 | 0.41 |
| 1:AA:1064:G:C8 | 1:AA:1066:C:C2 | 3.09 | 0.41 |
| 1:AA:1067:A:H1' | 1:AA:1068:G:C8 | 2.56 | 0.41 |
| 1:AA:1105:A:H2' | 1:AA:1106:G:H8 | 1.86 | 0.41 |
| 1:AA:1128:C:O2 | 1:AA:1130:A:N7 | 2.54 | 0.41 |
| 1:AA:1273:G:H3' | 1:AA:1274:G:H8 | 1.86 | 0.41 |
| 1:AA:1302:U:C5 | 13:AM:17:VAL:HG21 | 2.56 | 0.41 |
| 1:AA:1502:A:C2 | 1:AA:1504:G:C2 | 3.09 | 0.41 |
| 1:AA:1392:G:H21 | 1:AA:1502:A:H8 | 1.68 | 0.41 |
| 1:AA:473:G:C2 | 1:AA:474:G:C5 | 3.09 | 0.41 |
| 1:AA:533:A:C4' | 1:AA:534:U:OP1 | 2.69 | 0.41 |
| 1:AA:950:U:H3' | 13:AM:102:ARG:NH1 | 2.30 | 0.41 |
| 1:AA:987:G:N2 | 1:AA:1219:U:N3 | 2.69 | 0.41 |
| 2:AB:42:ILE:HG12 | 2:AB:43:ASP:N | 2.36 | 0.41 |
| 3:AC:134:ILE:HG22 | 3:AC:168:ALA:HB3 | 2.03 | 0.41 |
| 1:AA:438:G:OP1 | 4:AD:125:HIS:HE1 | 2.04 | 0.41 |
| 4:AD:141:ARG:HB3 | 4:AD:142:PRO:HD2 | 2.03 | 0.41 |
| 4:AD:116:GLN:NE2 | 4:AD:157:LEU:HD21 | 2.35 | 0.41 |
| 4:AD:76:ARG:HD2 | 4:AD:207:TYR:CE1 | 2.55 | 0.41 |
| 7:AG:103:TRP:HA | 7:AG:106:GLN:HE21 | 1.84 | 0.41 |
| 7:AG:26:PHE:CG | 7:AG:62:PHE:CE1 | 3.08 | 0.41 |
| 8:AH:44:PHE:HD1 | 8:AH:79:VAL:HG12 | 1.85 | 0.41 |
| 9:AI:53:VAL:C | 9:AI:54:ASP:HB2 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:AO:43:LEU:HD23 | 15:AO:43:LEU:HA | 1.92 | 0.41 |
| 20:AT:89:ARG:HB2 | 20:AT:104:LEU:CD1 | 2.45 | 0.41 |
| 22:B0:14:ARG:HG2 | 31:BA:2279:G:O6 | 2.21 | 0.41 |
| 23:B1:67:ILE:N | 23:B1:68:PRO:CD | 2.84 | 0.41 |
| 24:B2:59:ARG:HA | 24:B2:59:ARG:HD2 | 1.87 | 0.41 |
| 31:BA:1175:U:C4' | 31:BA:1176:G:H2' | 2.51 | 0.41 |
| 31:BA:1313:U:H2' | 31:BA:1610:A:C2 | 2.56 | 0.41 |
| 31:BA:1403:C:H2' | 31:BA:1404:C:O4' | 2.20 | 0.41 |
| 31:BA:1495:A:C5' | 31:BA:1496:A:OP2 | 2.69 | 0.41 |
| 31:BA:1636:C:H2' | 31:BA:1637:A:C8 | 2.56 | 0.41 |
| 31:BA:1642:G:O2' | 31:BA:1643:G:H5' | 2.21 | 0.41 |
| 31:BA:1655:A:H1' | 34:BE:113:PHE:CD2 | 2.56 | 0.41 |
| 31:BA:1740:G:H4' | 31:BA:1741:A:OP1 | 2.17 | 0.41 |
| 31:BA:1879:C:C2' | 31:BA:1880:C:H5' | 2.51 | 0.41 |
| 31:BA:2208:A:O2' | 31:BA:2219:G:C8 | 2.69 | 0.41 |
| 31:BA:287:C:C2' | 31:BA:288:C:O5' | 2.68 | 0.41 |
| 31:BA:28:A:O2' | 31:BA:583:G:H5' | 2.21 | 0.41 |
| 31:BA:528:A:H3' | 31:BA:528:A:H8 | 1.86 | 0.41 |
| 31:BA:466:A:H2 | 31:BA:795:C:O2 | 2.03 | 0.41 |
| 31:BA:833:U:H2' | 31:BA:834:C:C6 | 2.56 | 0.41 |
| 31:BA:880:G:N2 | 31:BA:898:C:C4 | 2.89 | 0.41 |
| 32:BB:102:A:H8 | 32:BB:102:A:OP2 | 2.04 | 0.41 |
| 32:BB:45:A:C2' | 32:BB:46:A:H5' | 2.51 | 0.41 |
| 33:BD:125:ILE:HG13 | 33:BD:137:PRO:HD3 | 2.03 | 0.41 |
| 31:BA:443:A:N7 | 35:BF:45:ARG:HG2 | 2.35 | 0.41 |
| 26:B4:28:LYS:CB | 36:BG:113:ARG:HH22 | 2.34 | 0.41 |
| 36:BG:64:THR:HG23 | 36:BG:65:GLY:H | 1.84 | 0.41 |
| 36:BG:89:GLY:O | 36:BG:90:LEU:C | 2.59 | 0.41 |
| 37:BH:158:HIS:CD2 | 37:BH:170:ARG:O | 2.74 | 0.41 |
| 37:BH:61:HIS:O | 37:BH:62:LYS:C | 2.59 | 0.41 |
| 38:BI:79:ILE:HG12 | 38:BI:140:LEU:HD11 | 2.03 | 0.41 |
| 39:BN:99:LEU:O | 39:BN:103:VAL:HG23 | 2.21 | 0.41 |
| 39:BN:99:LEU:HA | 39:BN:99:LEU:HD22 | 1.58 | 0.41 |
| 41:BP:140:ALA:O | 41:BP:141:ALA:HB3 | 2.21 | 0.41 |
| 41:BP:126:VAL:HA | 41:BP:145:PRO:HB2 | 2.02 | 0.41 |
| 43:BR:3:HIS:O | 43:BR:4:LEU:CB | 2.68 | 0.41 |
| 43:BR:51:LEU:HD23 | 43:BR:51:LEU:HA | 1.74 | 0.41 |
| 46:BU:46:ALA:O | 46:BU:50:ARG:HB2 | 2.21 | 0.41 |
| 47:BV:4:ILE:HA | 47:BV:12:TYR:O | 2.20 | 0.41 |
| 47:BV:36:PRO:CG | 47:BV:62:LEU:HD11 | 2.48 | 0.41 |
| 49:BX:24:GLY:HA3 | 49:BX:80:ILE:HG12 | 2.00 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:BX:60:ARG:HB2 | 49:BX:74:PRO:CD | 2.48 | 0.41 |
| 50:BY:100:ALA:O | 50:BY:101:LYS:HB2 | 2.21 | 0.41 |
| 50:BY:10:GLY:C | 50:BY:27:VAL:HG22 | 2.42 | 0.41 |
| 50:BY:96:ILE:CG2 | 50:BY:97:ARG:N | 2.81 | 0.41 |
| 42:BQ:137:TYR:CE2 | 51:BZ:74:VAL:O | 2.72 | 0.41 |
| 1:CA:1058:G:H1 | 1:CA:1199:U:H3 | 1.67 | 0.41 |
| 1:CA:461:A:C5 | 1:CA:471:G:C6 | 3.09 | 0.41 |
| 1:CA:509:A:OP2 | 1:CA:509:A:H3' | 2.21 | 0.41 |
| 1:CA:293:G:H4' | 1:CA:609:A:N1 | 2.36 | 0.41 |
| 1:CA:909:A:H2' | 1:CA:910:C:O4' | 2.21 | 0.41 |
| 1:CA:987:G:N2 | 1:CA:1219:U:N3 | 2.69 | 0.41 |
| 2:CB:12:GLU:H | 2:CB:12:GLU:HG3 | 1.64 | 0.41 |
| 2:CB:55:PHE:HE1 | 2:CB:218:ALA:HA | 1.86 | 0.41 |
| 2:CB:70:PHE:O | 2:CB:92:TYR:HA | 2.21 | 0.41 |
| 3:CC:22:TRP:HE3 | 3:CC:23:TYR:O | 2.03 | 0.41 |
| 3:CC:95:THR:HG22 | 3:CC:97:LYS:N | 2.35 | 0.41 |
| 4:CD:155:LEU:O | 4:CD:159:ARG:HG2 | 2.21 | 0.41 |
| 4:CD:2:GLY:O | 4:CD:4:TYR:N | 2.53 | 0.41 |
| 4:CD:60:GLU:O | 4:CD:63:LYS:HB3 | 2.21 | 0.41 |
| 1:CA:922:G:H1' | 5:CE:19:MET:HB2 | 2.02 | 0.41 |
| 8:CH:10:LEU:CD2 | 8:CH:10:LEU:N | 2.84 | 0.41 |
| 5:CE:143:ARG:NH1 | 8:CH:77:GLU:OE1 | 2.52 | 0.41 |
| 13:CM:9:ILE:N | 13:CM:9:ILE:HD12 | 2.35 | 0.41 |
| 16:CP:75:ARG:O | 16:CP:77:ALA:N | 2.48 | 0.41 |
| 23:D1:66:HIS:O | 23:D1:67:ILE:C | 2.59 | 0.41 |
| 24:D2:37:PHE:HE2 | 24:D2:39:ALA:O | 2.02 | 0.41 |
| 24:D2:44:LEU:HD13 | 24:D2:44:LEU:HA | 1.57 | 0.41 |
| 31:DA:1227:G:C2' | 31:DA:1228:G:H5' | 2.51 | 0.41 |
| 31:DA:1510:G:C2 | 31:DA:1511:C:C2 | 3.09 | 0.41 |
| 31:DA:1719:G:O2' | 31:DA:1720:U:H5' | 2.20 | 0.41 |
| 31:DA:1926:U:H2' | 31:DA:1928:A:OP2 | 2.20 | 0.41 |
| 31:DA:529:A:N6 | 31:DA:2041:U:N3 | 2.61 | 0.41 |
| 31:DA:2282:G:H4' | 31:DA:2389:G:O2' | 2.20 | 0.41 |
| 31:DA:2576:G:H3' | 31:DA:2576:G:OP1 | 2.21 | 0.41 |
| 31:DA:2615:U:H2' | 31:DA:2616:C:C6 | 2.56 | 0.41 |
| 31:DA:2808:U:C4 | 31:DA:2809:A:N7 | 2.89 | 0.41 |
| 31:DA:330:A:H2 | 31:DA:1210:A:HO2' | 1.65 | 0.41 |
| 31:DA:538:G:H2' | 31:DA:539:G:H8 | 1.84 | 0.41 |
| 31:DA:609:A:H2' | 31:DA:610:G:O5' | 2.21 | 0.41 |
| 31:DA:69:C:O2 | 31:DA:69:C:H2' | 2.21 | 0.41 |
| 31:DA:855:G:C6 | 31:DA:856:C:N4 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:958:U:HO2' | 31:DA:959:A:P | 2.42 | 0.41 |
| 31:DA:994:C:O2' | 31:DA:996:A:OP1 | 2.26 | 0.41 |
| 32:DB:38:C:C2 | 32:DB:39:A:C8 | 3.08 | 0.41 |
| 33:DD:248:SER:C | 33:DD:250:TRP:N | 2.73 | 0.41 |
| 31:DA:2052:G:O4' | 34:DE:142:GLY:HA3 | 2.21 | 0.41 |
| 36:DG:16:ARG:HB2 | 36:DG:17:PRO:CD | 2.51 | 0.41 |
| 44:DS:53:SER:C | 44:DS:55:ALA:N | 2.74 | 0.41 |
| 44:DS:54:LEU:HD13 | 44:DS:57:LYS:O | 2.21 | 0.41 |
| 45:DT:28:VAL:CG1 | 45:DT:46:GLU:HB2 | 2.51 | 0.41 |
| 31:DA:1216:G:OP1 | 46:DU:8:VAL:HG22 | 2.21 | 0.41 |
| 47:DV:2:PHE:O | 47:DV:14:VAL:O | 2.39 | 0.41 |
| 47:DV:25:LEU:CB | 47:DV:94:LEU:HD13 | 2.47 | 0.41 |
| 49:DX:18:TYR:O | 49:DX:20:GLY:N | 2.54 | 0.41 |
| 50:DY:8:LYS:HB2 | 50:DY:28:LYS:HZ3 | 1.86 | 0.41 |
| 50:DY:45:VAL:HG21 | 50:DY:62:GLU:N | 2.35 | 0.41 |
| 1:AA:1010:G:N2 | 1:AA:1020:U:C2 | 2.88 | 0.41 |
| 1:AA:1027:C:O5' | 1:AA:1027:C:H6 | 2.04 | 0.41 |
| 1:AA:1118:C:H1' | 1:AA:1179:A:C5 | 2.56 | 0.41 |
| 1:AA:1276:G:O2' | 1:AA:1282:C:H1' | 2.21 | 0.41 |
| 1:AA:1411:C:O2' | 1:AA:1412:C:H5' | 2.21 | 0.41 |
| 1:AA:1508:G:H2' | 1:AA:1509:C:O4' | 2.21 | 0.41 |
| 1:AA:35:G:C2 | 1:AA:550:G:C2 | 3.09 | 0.41 |
| 1:AA:461:A:C5 | 1:AA:471:G:C6 | 3.08 | 0.41 |
| 1:AA:518:C:C2 | 1:AA:530:G:C6 | 3.09 | 0.41 |
| 1:AA:617:G:C6 | 1:AA:618:C:C5 | 3.09 | 0.41 |
| 1:AA:628:G:O2' | 1:AA:629:G:H5' | 2.21 | 0.41 |
| 1:AA:727:G:C6 | 1:AA:731:G:C6 | 3.09 | 0.41 |
| 2:AB:22:LYS:HA | 2:AB:22:LYS:HZ2 | 1.80 | 0.41 |
| 2:AB:52:GLU:HG2 | 2:AB:53:ARG:N | 2.35 | 0.41 |
| 4:AD:28:SER:C | 4:AD:30:LYS:H | 2.24 | 0.41 |
| 4:AD:57:ARG:NH2 | 4:AD:205:GLU:OE2 | 2.54 | 0.41 |
| 1:AA:939:G:C5' | 7:AG:102:ARG:HH22 | 2.34 | 0.41 |
| 9:AI:105:ASP:C | 9:AI:107:ARG:H | 2.24 | 0.41 |
| 10:AJ:40:LEU:HB2 | 10:AJ:41:PRO:CD | 2.38 | 0.41 |
| 11:AK:81:ASP:OD2 | 11:AK:106:LYS:HG2 | 2.21 | 0.41 |
| 11:AK:38:ASN:HA | 11:AK:39:PRO:HD3 | 1.88 | 0.41 |
| 16:AP:55:ARG:HE | 16:AP:55:ARG:HA | 1.86 | 0.41 |
| 17:AQ:65:ILE:N | 17:AQ:65:ILE:HD12 | 2.35 | 0.41 |
| 23:B1:87:PRO:O | 23:B1:91:LYS:N | 2.28 | 0.41 |
| 25:B3:59:VAL:O | 25:B3:59:VAL:HG12 | 2.20 | 0.41 |
| 28:B6:15:GLU:OE1 | 28:B6:18:ARG:CG | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:B8:44:LYS:N | 30:B8:44:LYS:HD2 | 2.36 | 0.41 |
| 31:BA:1012:U:OP1 | 46:BU:75:ASN:OD1 | 2.38 | 0.41 |
| 31:BA:1234:U:O2' | 31:BA:1235:G:H5' | 2.21 | 0.41 |
| 31:BA:577:G:O2' | 31:BA:1254:A:OP1 | 2.36 | 0.41 |
| 31:BA:1269:A:H2' | 31:BA:1270:C:C6 | 2.56 | 0.41 |
| 31:BA:1406:U:H2' | 31:BA:1407:C:H6 | 1.86 | 0.41 |
| 31:BA:1445(A):C:C2 | 31:BA:1446:C:C5 | 3.09 | 0.41 |
| 31:BA:1476:C:C2' | 31:BA:1477:A:O5' | 2.67 | 0.41 |
| 31:BA:1476:C:H2' | 31:BA:1477:A:O5' | 2.21 | 0.41 |
| 31:BA:1485:G:N2 | 31:BA:1505:C:C5 | 2.89 | 0.41 |
| 31:BA:1677:A:C2' | 31:BA:1678:G:O5' | 2.69 | 0.41 |
| 31:BA:195:A:H61 | 31:BA:198:C:H3' | 1.85 | 0.41 |
| 31:BA:2070:G:C2 | 31:BA:2442:C:C2 | 3.09 | 0.41 |
| 31:BA:2103:C:O2 | 31:BA:2187:G:C2 | 2.74 | 0.41 |
| 31:BA:2236:C:C2' | 31:BA:2237:G:H5' | 2.51 | 0.41 |
| 31:BA:2287:A:N1 | 31:BA:2346:A:C2 | 2.89 | 0.41 |
| 31:BA:2409:G:C6 | 31:BA:2410:G:C5 | 3.09 | 0.41 |
| 31:BA:271(E):U:C2 | 31:BA:271(F):C:C5 | 3.09 | 0.41 |
| 31:BA:2721:A:H1' | 31:BA:2873:A:O2' | 2.21 | 0.41 |
| 31:BA:817:C:C2 | 31:BA:818:G:C8 | 3.09 | 0.41 |
| 31:BA:855:G:H2' | 31:BA:856:C:C6 | 2.56 | 0.41 |
| 33:BD:211:ARG:O | 33:BD:215:LEU:HG | 2.21 | 0.41 |
| 33:BD:5:LYS:HD2 | 33:BD:5:LYS:N | 2.36 | 0.41 |
| 33:BD:92:ILE:HD13 | 33:BD:104:TYR:CD2 | 2.55 | 0.41 |
| 34:BE:21:VAL:CG2 | 34:BE:21:VAL:O | 2.69 | 0.41 |
| 35:BF:29:ASN:O | 35:BF:30:PRO:C | 2.59 | 0.41 |
| 39:BN:65:LYS:O | 39:BN:69:GLN:HB2 | 2.21 | 0.41 |
| 41:BP:95:VAL:CG2 | 41:BP:125:VAL:HB | 2.47 | 0.41 |
| 41:BP:88:LEU:C | 41:BP:90:ARG:N | 2.75 | 0.41 |
| 41:BP:91:PHE:HE2 | 41:BP:95:VAL:HG12 | 1.85 | 0.41 |
| 42:BQ:110:THR:HG1 | 42:BQ:113:GLN:HG3 | 1.79 | 0.41 |
| 44:BS:58:LEU:HA | 44:BS:58:LEU:HD12 | 1.79 | 0.41 |
| 46:BU:69:CYS:HG | 46:BU:79:PHE:HD1 | 1.69 | 0.41 |
| 46:BU:95:LEU:HD22 | 47:BV:4:ILE:CD1 | 2.48 | 0.41 |
| 47:BV:69:LYS:C | 47:BV:70:ILE:HG23 | 2.42 | 0.41 |
| 47:BV:75:PHE:N | 47:BV:75:PHE:CD1 | 2.89 | 0.41 |
| 48:BW:8:ARG:HA | 48:BW:102:HIS:HD2 | 1.85 | 0.41 |
| 50:BY:9:LYS:HB2 | 50:BY:10:GLY:H | 1.73 | 0.41 |
| 50:BY:27:VAL:CB | 50:BY:29:GLU:OE1 | 2.69 | 0.41 |
| 51:BZ:104:PHE:HA | 51:BZ:139:VAL:HB | 2.02 | 0.41 |
| 1:CA:1379:G:C6 | 1:CA:1380:U:O4 | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1474:G:H4' | 31:DA:1701:A:N3 | 2.35 | 0.41 |
| 1:CA:340:U:O2' | 1:CA:341:C:H5' | 2.21 | 0.41 |
| 1:CA:503:C:O2 | 1:CA:510:A:H2 | 2.04 | 0.41 |
| 1:CA:616:G:N2 | 1:CA:617:G:C8 | 2.89 | 0.41 |
| 1:CA:646:U:O5' | 1:CA:646:U:H6 | 2.04 | 0.41 |
| 1:CA:707:C:O2 | 1:CA:707:C:H2' | 2.21 | 0.41 |
| 1:CA:734:G:C2 | 1:CA:735:C:C2 | 3.09 | 0.41 |
| 2:CB:219:VAL:HA | 2:CB:222:ILE:HD12 | 2.02 | 0.41 |
| 3:CC:15:THR:CG2 | 3:CC:181:ASN:HA | 2.50 | 0.41 |
| 4:CD:38:TYR:HA | 4:CD:39:PRO:HD3 | 1.93 | 0.41 |
| 5:CE:127:ASN:O | 5:CE:128:PRO:C | 2.59 | 0.41 |
| 5:CE:18:ARG:NE | 5:CE:25:ARG:HB3 | 2.36 | 0.41 |
| 9:CI:118:LYS:O | 9:CI:119:ALA:HB3 | 2.21 | 0.41 |
| 11:CK:41:THR:HG22 | 11:CK:42:TRP:H | 1.84 | 0.41 |
| 11:CK:72:ALA:O | 11:CK:77:MET:HB3 | 2.21 | 0.41 |
| 1:CA:1226:C:N4 | 13:CM:104:ARG:HB2 | 2.34 | 0.41 |
| 13:CM:16:ASP:OD2 | 13:CM:16:ASP:N | 2.54 | 0.41 |
| 16:CP:32:TYR:O | 16:CP:32:TYR:CD2 | 2.74 | 0.41 |
| 1:CA:375:U:H5'' | 16:CP:6:LEU:HD22 | 2.02 | 0.41 |
| 18:CR:74:ARG:HE | 18:CR:81:PHE:HA | 1.86 | 0.41 |
| 20:CT:59:ALA:O | 20:CT:60:GLU:C | 2.60 | 0.41 |
| 30:D8:39:LYS:HG2 | 30:D8:39:LYS:O | 2.22 | 0.41 |
| 31:DA:1260:G:C6 | 31:DA:1261:C:C4 | 3.08 | 0.41 |
| 31:DA:142:A:C5' | 31:DA:142(A):C:C5 | 3.04 | 0.41 |
| 31:DA:528:A:C2 | 31:DA:2042:A:H2' | 2.56 | 0.41 |
| 31:DA:204:A:O3' | 31:DA:205:G:H4' | 2.21 | 0.41 |
| 31:DA:2263:C:O2' | 31:DA:2264:C:H5' | 2.20 | 0.41 |
| 31:DA:2290:G:C2 | 31:DA:2343:C:O2 | 2.74 | 0.41 |
| 31:DA:2507:C:H5'' | 31:DA:2573:C:N4 | 2.36 | 0.41 |
| 31:DA:2580:U:H2' | 31:DA:2580:U:O2 | 2.19 | 0.41 |
| 31:DA:2663:G:C6 | 31:DA:2664:G:C5 | 3.09 | 0.41 |
| 31:DA:2728:U:C2' | 31:DA:2729:G:H5' | 2.50 | 0.41 |
| 31:DA:2785:C:H2' | 31:DA:2786:U:O4' | 2.20 | 0.41 |
| 31:DA:311:A:C2 | 31:DA:331:A:H3' | 2.56 | 0.41 |
| 31:DA:359:A:H2' | 31:DA:360:G:O4' | 2.21 | 0.41 |
| 31:DA:745:G:H5'' | 31:DA:746:A:OP2 | 2.21 | 0.41 |
| 31:DA:768:G:C4 | 31:DA:769:G:C8 | 3.09 | 0.41 |
| 32:DB:39:A:H2' | 32:DB:39:A:N3 | 2.35 | 0.41 |
| 32:DB:46:A:H2' | 32:DB:47:C:O5' | 2.22 | 0.41 |
| 32:DB:71:C:C2' | 32:DB:71:C:O2 | 2.67 | 0.41 |
| 33:DD:218:ARG:HB3 | 33:DD:219:PRO:HD2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 35:DF:126:VAL:HG21 | 35:DF:129:PHE:CZ | 2.56 | 0.41 |
| 36:DG:116:ASP:O | 36:DG:117:PHE:HB3 | 2.21 | 0.41 |
| 38:DI:48:GLU:O | 38:DI:52:ARG:HG2 | 2.21 | 0.41 |
| 31:DA:637:A:OP1 | 41:DP:133:SER:CB | 2.69 | 0.41 |
| 42:DQ:20:ALA:HB2 | 42:DQ:99:PRO:CG | 2.49 | 0.41 |
| 45:DT:64:ARG:NH1 | 45:DT:103:ARG:HA | 2.35 | 0.41 |
| 46:DU:34:LYS:HA | 46:DU:34:LYS:HE3 | 2.03 | 0.41 |
| 47:DV:2:PHE:O | 47:DV:3:ALA:HB3 | 2.21 | 0.41 |
| 51:DZ:56:VAL:HA | 51:DZ:70:LEU:CD2 | 2.50 | 0.41 |
| 1:AA:1126:U:C2' | 1:AA:1127:G:O5' | 2.69 | 0.40 |
| 1:AA:1118:C:H1' | 1:AA:1179:A:C4 | 2.56 | 0.40 |
| 1:AA:117:G:C2' | 1:AA:118:U:H5' | 2.51 | 0.40 |
| 1:AA:1327:C:OP1 | 21:AU:20:LYS:HB3 | 2.20 | 0.40 |
| 1:AA:102:G:O2' | 1:AA:151:A:N3 | 2.43 | 0.40 |
| 1:AA:286:G:C5 | 1:AA:287:U:C5 | 3.09 | 0.40 |
| 1:AA:673:G:C2 | 1:AA:674:G:C5 | 3.08 | 0.40 |
| 1:AA:70:G:H2' | 1:AA:71:C:H6 | 1.86 | 0.40 |
| 1:AA:719:C:C5 | 1:AA:720:C:C5 | 3.08 | 0.40 |
| 1:AA:722:A:N6 | 1:AA:724:G:C2 | 2.89 | 0.40 |
| 2:AB:41:ILE:HD12 | 2:AB:41:ILE:N | 2.36 | 0.40 |
| 4:AD:79:PHE:CD1 | 4:AD:207:TYR:CD1 | 3.09 | 0.40 |
| 4:AD:23:GLY:O | 4:AD:27:TYR:CD1 | 2.73 | 0.40 |
| 4:AD:43:HIS:ND1 | 4:AD:46:LYS:NZ | 2.59 | 0.40 |
| 6:AF:8:ILE:HD12 | 6:AF:26:ILE:HD13 | 2.03 | 0.40 |
| 12:AL:27:LEU:HG | 12:AL:62:SER:OG | 2.20 | 0.40 |
| 10:AJ:49:VAL:HG22 | 14:AN:41:ARG:HB2 | 2.03 | 0.40 |
| 24:B2:18:PRO:C | 24:B2:20:GLU:N | 2.73 | 0.40 |
| 27:B5:46:CYS:O | 27:B5:48:GLU:N | 2.54 | 0.40 |
| 28:B6:19:ARG:CG | 28:B6:20:ASN:H | 2.29 | 0.40 |
| 30:B8:62:LEU:C | 30:B8:64:TYR:H | 2.24 | 0.40 |
| 31:BA:1049:C:O2 | 31:BA:1050:A:C8 | 2.74 | 0.40 |
| 31:BA:1122:G:C2 | 31:BA:1123:C:C6 | 3.09 | 0.40 |
| 31:BA:1438:U:C2' | 31:BA:1439:A:H5' | 2.51 | 0.40 |
| 31:BA:1509(B):A:H2' | 31:BA:1510:G:C8 | 2.56 | 0.40 |
| 31:BA:154(A):C:H5 | 31:BA:171:G:H1 | 1.66 | 0.40 |
| 31:BA:1578:U:C2' | 31:BA:1579:A:H5' | 2.52 | 0.40 |
| 31:BA:1655:A:H3' | 31:BA:1656:C:C6 | 2.56 | 0.40 |
| 31:BA:1947:C:C2' | 31:BA:1948:G:H5'' | 2.50 | 0.40 |
| 31:BA:2272:U:C5' | 31:BA:2273:A:OP1 | 2.69 | 0.40 |
| 31:BA:2409:G:H2' | 31:BA:2410:G:O4' | 2.20 | 0.40 |
| 31:BA:2660:A:O2' | 31:BA:2661:G:P | 2.80 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:271(M):G:N7 | 31:BA:271(O):C:N4 | 2.68 | 0.40 |
| 31:BA:271(P):C:C2' | 31:BA:271(Q):G:O5' | 2.69 | 0.40 |
| 31:BA:425:G:C2 | 31:BA:426:C:C6 | 3.09 | 0.40 |
| 31:BA:42:G:H2' | 31:BA:43:A:O4' | 2.21 | 0.40 |
| 31:BA:13:A:N1 | 31:BA:525:U:H2' | 2.36 | 0.40 |
| 31:BA:828:U:O2 | 31:BA:828:U:C2' | 2.68 | 0.40 |
| 32:BB:8:U:H5' | 32:BB:9:G:OP2 | 2.21 | 0.40 |
| 31:BA:764:A:OP1 | 33:BD:208:LYS:HE2 | 2.22 | 0.40 |
| 33:BD:254:THR:N | 33:BD:255:LYS:HZ1 | 2.20 | 0.40 |
| 33:BD:30:GLU:CG | 33:BD:63:ARG:NE | 2.82 | 0.40 |
| 36:BG:111:LEU:HB3 | 36:BG:117:PHE:CE1 | 2.55 | 0.40 |
| 36:BG:71:THR:CG2 | 36:BG:72:ARG:N | 2.81 | 0.40 |
| 38:BI:29:TYR:CD2 | 38:BI:30:LEU:HD23 | 2.51 | 0.40 |
| 43:BR:52:ILE:H | 43:BR:52:ILE:HG12 | 1.66 | 0.40 |
| 45:BT:67:SER:O | 45:BT:68:TYR:HB2 | 2.21 | 0.40 |
| 50:BY:44:ILE:N | 50:BY:44:ILE:HD12 | 2.27 | 0.40 |
| 51:BZ:150:LEU:HA | 51:BZ:151:HIS:HD2 | 1.85 | 0.40 |
| 51:BZ:14:LYS:HB2 | 51:BZ:17:ALA:HB3 | 2.02 | 0.40 |
| 1:CA:1280:A:O4' | 10:CJ:41:PRO:HG3 | 2.21 | 0.40 |
| 1:CA:1486:G:H2' | 1:CA:1487:G:O4' | 2.22 | 0.40 |
| 1:CA:323:U:O3' | 20:CT:22:ARG:HD3 | 2.21 | 0.40 |
| 1:CA:350:G:O2' | 1:CA:351:G:H5' | 2.21 | 0.40 |
| 1:CA:658:G:N3 | 1:CA:659:U:C6 | 2.89 | 0.40 |
| 1:CA:727:G:C6 | 1:CA:731:G:C6 | 3.10 | 0.40 |
| 1:CA:734:G:C6 | 1:CA:735:C:C4 | 3.09 | 0.40 |
| 1:CA:84:U:H3' | 1:CA:84:U:H6 | 1.85 | 0.40 |
| 1:CA:837:G:C2 | 1:CA:850:U:O2 | 2.74 | 0.40 |
| 1:CA:922:G:H2' | 1:CA:923:A:C8 | 2.56 | 0.40 |
| 1:CA:977:A:HO2' | 1:CA:981:U:H3 | 1.69 | 0.40 |
| 4:CD:192:GLU:H | 4:CD:192:GLU:CD | 2.23 | 0.40 |
| 1:CA:425:G:O3' | 4:CD:45:GLN:NE2 | 2.54 | 0.40 |
| 8:CH:97:VAL:HA | 8:CH:100:ILE:HD11 | 2.03 | 0.40 |
| 9:CI:83:ARG:HH21 | 9:CI:102:LEU:HD23 | 1.86 | 0.40 |
| 9:CI:4:TYR:HA | 9:CI:88:TYR:CE1 | 2.56 | 0.40 |
| 17:CQ:65:ILE:HD12 | 17:CQ:65:ILE:N | 2.36 | 0.40 |
| 17:CQ:8:GLY:HA3 | 17:CQ:22:LEU:O | 2.21 | 0.40 |
| 20:CT:16:HIS:O | 20:CT:19:SER:N | 2.54 | 0.40 |
| 23:D1:83:GLU:C | 23:D1:85:LEU:H | 2.25 | 0.40 |
| 41:BP:121:LYS:CD | 25:D3:2:PRO:HD3 | 2.50 | 0.40 |
| 28:D6:28:ARG:HA | 28:D6:32:ASN:ND2 | 2.21 | 0.40 |
| 28:D6:44:ARG:O | 28:D6:45:LYS:CG | 2.65 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DA:1175:U:C4' | 31:DA:1176:G:H2' | 2.51 | 0.40 |
| 31:DA:1346:G:C5 | 31:DA:1347:G:N7 | 2.89 | 0.40 |
| 31:DA:1379:A:C2' | 31:DA:1380:G:OP1 | 2.69 | 0.40 |
| 31:DA:1553:A:C5 | 31:DA:1555:G:C5 | 3.09 | 0.40 |
| 31:DA:1747:G:H2' | 31:DA:1747(A):G:H8 | 1.86 | 0.40 |
| 31:DA:1667:G:H1' | 31:DA:1991:U:O4 | 2.21 | 0.40 |
| 31:DA:2106:G:H1' | 31:DA:2184:G:H22 | 1.85 | 0.40 |
| 31:DA:2197:U:C5 | 31:DA:2224:G:C6 | 3.09 | 0.40 |
| 31:DA:2395:C:H2' | 31:DA:2396:G:O4' | 2.21 | 0.40 |
| 31:DA:2599:G:O2' | 31:DA:2600:A:H5' | 2.20 | 0.40 |
| 31:DA:2603:G:C5 | 31:DA:2604:U:C5 | 3.09 | 0.40 |
| 31:DA:1462:C:H4' | 31:DA:2703:C:H5' | 2.02 | 0.40 |
| 31:DA:460:A:C2 | 31:DA:470:A:C4 | 3.09 | 0.40 |
| 31:DA:879:G:H1 | 31:DA:898:C:H42 | 1.69 | 0.40 |
| 31:DA:995:C:C2 | 39:DN:4:TYR:CZ | 3.08 | 0.40 |
| 32:DB:66:A:C4 | 32:DB:109:C:N4 | 2.89 | 0.40 |
| 33:DD:69:ARG:HH12 | 33:DD:117:VAL:HG13 | 1.86 | 0.40 |
| 33:DD:44:ASN:HB3 | 33:DD:49:ILE:N | 2.36 | 0.40 |
| 34:DE:37:ARG:O | 34:DE:45:THR:N | 2.48 | 0.40 |
| 31:DA:2632:A:O2' | 34:DE:61:ARG:NH2 | 2.54 | 0.40 |
| 35:DF:127:GLU:OE1 | 35:DF:127:GLU:HA | 2.12 | 0.40 |
| 35:DF:70:THR:CG2 | 35:DF:72:ARG:HB2 | 2.51 | 0.40 |
| 36:DG:60:LEU:O | 36:DG:63:ILE:HG13 | 2.21 | 0.40 |
| 36:DG:73:ALA:O | 36:DG:85:GLY:HA2 | 2.21 | 0.40 |
| 37:DH:54:ARG:HB3 | 37:DH:65:HIS:HD2 | 1.83 | 0.40 |
| 39:DN:128:HIS:HE1 | 39:DN:134:ARG:HH11 | 1.70 | 0.40 |
| 40:DO:9:GLU:OE1 | 40:DO:9:GLU:HA | 2.21 | 0.40 |
| 43:DR:44:LEU:HD22 | 43:DR:48:VAL:HG23 | 2.02 | 0.40 |
| 43:DR:8:ARG:HB3 | 43:DR:9:LYS:H | 1.57 | 0.40 |
| 45:DT:68:TYR:O | 45:DT:70:VAL:N | 2.54 | 0.40 |
| 45:DT:29:ARG:CG | 45:DT:85:LYS:HA | 2.51 | 0.40 |
| 47:DV:45:THR:O | 47:DV:45:THR:HG22 | 2.21 | 0.40 |
| 47:DV:75:PHE:CD1 | 47:DV:75:PHE:N | 2.89 | 0.40 |
| 49:DX:18:TYR:C | 49:DX:20:GLY:N | 2.72 | 0.40 |
| 50:DY:68:HIS:N | 50:DY:71:LYS:NZ | 2.68 | 0.40 |
| 51:DZ:30:ASN:OD1 | 51:DZ:90:VAL:HB | 2.21 | 0.40 |
| 1:AA:1207:G:H2' | 1:AA:1208:C:C6 | 2.57 | 0.40 |
| 1:AA:1410:G:C6 | 1:AA:1411:C:C4 | 3.09 | 0.40 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C5 | 2.56 | 0.40 |
| 1:AA:149:A:N3 | 1:AA:150:C:C6 | 2.89 | 0.40 |
| 1:AA:152:A:C8 | 1:AA:153:C:C5 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:542:G:OP1 | 4:AD:10:ARG:NH2 | 2.48 | 0.40 |
| 1:AA:581:G:N2 | 1:AA:582:U:C4 | 2.90 | 0.40 |
| 1:AA:698:G:C6 | 1:AA:699:C:C4 | 3.10 | 0.40 |
| 2:AB:102:LEU:O | 2:AB:105:PHE:HB2 | 2.21 | 0.40 |
| 2:AB:69:LEU:HD11 | 2:AB:93:VAL:HG23 | 2.02 | 0.40 |
| 3:AC:15:THR:CG2 | 3:AC:181:ASN:HA | 2.51 | 0.40 |
| 5:AE:12:LEU:HD13 | 5:AE:12:LEU:O | 2.21 | 0.40 |
| 6:AF:48:LEU:HD22 | 18:AR:77:GLY:HA3 | 2.03 | 0.40 |
| 8:AH:26:VAL:O | 8:AH:26:VAL:HG22 | 2.19 | 0.40 |
| 10:AJ:48:THR:HA | 10:AJ:62:HIS:CB | 2.50 | 0.40 |
| 11:AK:31:THR:OG1 | 11:AK:42:TRP:HB3 | 2.21 | 0.40 |
| 14:AN:44:LEU:C | 14:AN:44:LEU:HD12 | 2.40 | 0.40 |
| 17:AQ:76:LEU:HD12 | 17:AQ:77:VAL:N | 2.36 | 0.40 |
| 18:AR:40:LEU:O | 18:AR:43:PHE:HB2 | 2.20 | 0.40 |
| 30:B8:30:ARG:HA | 30:B8:30:ARG:HD3 | 1.93 | 0.40 |
| 30:B8:32:LEU:HB3 | 30:B8:35:GLN:H | 1.78 | 0.40 |
| 31:BA:1412:A:O2' | 31:BA:1413:G:H5' | 2.21 | 0.40 |
| 31:BA:1416:G:O2' | 31:BA:1417:C:OP2 | 2.39 | 0.40 |
| 31:BA:142:A:C5' | 31:BA:142(A):C:H5 | 2.35 | 0.40 |
| 31:BA:1464:C:O2' | 31:BA:1528:A:C8 | 2.51 | 0.40 |
| 31:BA:1994:C:O2' | 31:BA:1995:U:H5' | 2.20 | 0.40 |
| 31:BA:2540:C:C2' | 31:BA:2541:A:H5' | 2.51 | 0.40 |
| 31:BA:2583:G:H2' | 31:BA:2584:U:O2 | 2.21 | 0.40 |
| 31:BA:2762:G:H8 | 31:BA:2762:G:H5' | 1.86 | 0.40 |
| 31:BA:2813:A:H2' | 31:BA:2814:C:O4' | 2.21 | 0.40 |
| 31:BA:272(J):C:N4 | 31:BA:363(A):A:N6 | 2.65 | 0.40 |
| 31:BA:844:C:O2' | 31:BA:845:G:H5' | 2.21 | 0.40 |
| 31:BA:901:A:H3' | 31:BA:902:C:H6 | 1.86 | 0.40 |
| 31:BA:866:A:N1 | 31:BA:914:C:C5 | 2.89 | 0.40 |
| 31:BA:917:A:H2' | 31:BA:918:A:O4' | 2.20 | 0.40 |
| 31:BA:950:G:C5 | 31:BA:951:C:C4 | 3.10 | 0.40 |
| 31:BA:979:G:H3' | 31:BA:980:A:H5'' | 2.03 | 0.40 |
| 33:BD:92:ILE:HD13 | 33:BD:104:TYR:CE2 | 2.56 | 0.40 |
| 33:BD:31:LYS:HG3 | 33:BD:31:LYS:O | 2.20 | 0.40 |
| 34:BE:37:ARG:O | 34:BE:45:THR:N | 2.46 | 0.40 |
| 34:BE:55:ASN:H | 34:BE:72:VAL:HG11 | 1.86 | 0.40 |
| 38:BI:62:LYS:HE2 | 38:BI:134:PRO:HG3 | 2.01 | 0.40 |
| 39:BN:128:HIS:HE1 | 39:BN:134:ARG:HH11 | 1.69 | 0.40 |
| 41:BP:62:LEU:HD23 | 41:BP:62:LEU:O | 2.21 | 0.40 |
| 43:BR:23:ASN:ND2 | 43:BR:23:ASN:N | 2.69 | 0.40 |
| 44:BS:14:VAL:O | 44:BS:15:ARG:C | 2.60 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 46:BU:108:GLU:O | 46:BU:111:GLU:N | 2.54 | 0.40 |
| 47:BV:94:LEU:C | 47:BV:94:LEU:HD23 | 2.42 | 0.40 |
| 50:BY:47:LYS:N | 50:BY:47:LYS:CD | 2.85 | 0.40 |
| 31:BA:84:A:C5' | 50:BY:9:LYS:HD3 | 2.51 | 0.40 |
| 51:BZ:161:VAL:O | 51:BZ:161:VAL:HG12 | 2.21 | 0.40 |
| 1:CA:1090:U:C2 | 1:CA:1091:U:C6 | 3.09 | 0.40 |
| 1:CA:1163:C:C2 | 1:CA:1174:G:N2 | 2.89 | 0.40 |
| 1:CA:1272:G:C6 | 1:CA:1273:G:C5 | 3.09 | 0.40 |
| 1:CA:145:G:N2 | 1:CA:146:G:H1' | 2.37 | 0.40 |
| 1:CA:193:C:O2' | 1:CA:194:C:H5' | 2.21 | 0.40 |
| 1:CA:828:A:H5'' | 1:CA:859:A:N1 | 2.36 | 0.40 |
| 2:CB:142:LEU:O | 2:CB:142:LEU:HD23 | 2.22 | 0.40 |
| 3:CC:125:GLU:CD | 3:CC:189:ALA:HA | 2.41 | 0.40 |
| 3:CC:27:LYS:HA | 3:CC:27:LYS:NZ | 2.36 | 0.40 |
| 4:CD:108:LEU:HD21 | 4:CD:183:GLY:HA3 | 2.03 | 0.40 |
| 6:CF:15:ASP:HB2 | 6:CF:16:GLN:H | 1.58 | 0.40 |
| 7:CG:124:LEU:HA | 7:CG:124:LEU:HD23 | 1.82 | 0.40 |
| 9:CI:105:ASP:C | 9:CI:107:ARG:H | 2.24 | 0.40 |
| 10:CJ:58:ASP:O | 10:CJ:59:SER:C | 2.60 | 0.40 |
| 16:CP:26:ARG:HD2 | 16:CP:31:LYS:O | 2.21 | 0.40 |
| 17:CQ:14:LYS:HB2 | 17:CQ:14:LYS:NZ | 2.36 | 0.40 |
| 19:CS:29:ARG:HB2 | 19:CS:48:THR:H | 1.86 | 0.40 |
| 31:DA:1043:C:OP2 | 31:DA:1043:C:H6 | 2.04 | 0.40 |
| 31:DA:9:U:O2' | 31:DA:10:G:P | 2.79 | 0.40 |
| 31:DA:1252:G:H8 | 31:DA:1252:G:OP1 | 2.04 | 0.40 |
| 31:DA:1373:A:C6 | 31:DA:1374:G:C4 | 3.09 | 0.40 |
| 31:DA:1553:A:C5 | 31:DA:1555:G:C4 | 3.09 | 0.40 |
| 31:DA:1809:A:C6 | 31:DA:1810:A:N1 | 2.89 | 0.40 |
| 31:DA:1899:G:O2' | 31:DA:1900:A:H5'' | 2.20 | 0.40 |
| 31:DA:1995:U:H3' | 31:DA:1996:C:H2' | 2.03 | 0.40 |
| 31:DA:573:G:O6 | 31:DA:2030:A:H3' | 2.21 | 0.40 |
| 31:DA:2031:A:C6 | 31:DA:2498:C:H1' | 2.56 | 0.40 |
| 31:DA:2223:G:OP1 | 33:DD:172:TYR:OH | 2.30 | 0.40 |
| 31:DA:2246:G:H1' | 31:DA:2426:A:C2 | 2.56 | 0.40 |
| 31:DA:271(J):C:C3' | 31:DA:271(K):U:H5'' | 2.51 | 0.40 |
| 55:DA:3330:ERY:H312 | 55:DA:3330:ERY:H2 | 1.88 | 0.40 |
| 31:DA:479:A:HO2' | 31:DA:481:G:H8 | 1.67 | 0.40 |
| 31:DA:590:A:H2' | 31:DA:591:C:C6 | 2.57 | 0.40 |
| 33:DD:155:LEU:HD23 | 33:DD:177:LEU:HD22 | 2.02 | 0.40 |
| 33:DD:213:ARG:HA | 33:DD:213:ARG:HD2 | 1.61 | 0.40 |
| 33:DD:25:THR:HG22 | 33:DD:82:ILE:C | 2.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DE:111:ARG:NH1 | 43:DR:2:ARG:NH2 | 2.50 | 0.40 |
| 34:DE:53:PRO:HB2 | 34:DE:54:GLN:H | 1.42 | 0.40 |
| 35:DF:126:VAL:HB | 35:DF:127:GLU:H | 1.73 | 0.40 |
| 36:DG:67:LYS:HD2 | 36:DG:67:LYS:N | 2.36 | 0.40 |
| 37:DH:103:LEU:HG | 37:DH:104:GLU:N | 2.37 | 0.40 |
| 37:DH:105:LEU:HD22 | 37:DH:105:LEU:N | 2.33 | 0.40 |
| 41:DP:98:GLU:H | 41:DP:101:VAL:HG12 | 1.86 | 0.40 |
| 42:DQ:133:ARG:O | 42:DQ:134:ARG:HB2 | 2.21 | 0.40 |
| 42:DQ:48:GLU:O | 42:DQ:52:VAL:HG13 | 2.21 | 0.40 |
| 44:DS:59:LYS:CE | 44:DS:68:GLN:HE22 | 2.33 | 0.40 |
| 48:DW:107:LEU:HA | 48:DW:107:LEU:HD12 | 1.70 | 0.40 |
| 50:DY:88:LYS:O | 50:DY:89:PHE:CB | 2.68 | 0.40 |
| 1:AA:1006:C:N4 | 1:AA:1024:G:H21 | 2.19 | 0.40 |
| 1:AA:1030(D):A:N7 | 1:AA:1031:G:N3 | 2.69 | 0.40 |
| 1:AA:1063:C:C5 | 1:AA:1064:G:C4 | 3.08 | 0.40 |
| 1:AA:1207:G:C2 | 1:AA:1208:C:C2 | 3.09 | 0.40 |
| 1:AA:1399:C:H4' | 1:AA:1400:C:C5' | 2.51 | 0.40 |
| 1:AA:234:C:O2 | 1:AA:235:C:C6 | 2.75 | 0.40 |
| 1:AA:330:C:C2' | 1:AA:331:G:H5' | 2.51 | 0.40 |
| 1:AA:515:G:C2' | 1:AA:516:U:H5' | 2.52 | 0.40 |
| 1:AA:655:A:C2 | 1:AA:754:C:N4 | 2.89 | 0.40 |
| 1:AA:734:G:H2' | 1:AA:735:C:C6 | 2.57 | 0.40 |
| 1:AA:764:C:C2' | 1:AA:765:G:O5' | 2.69 | 0.40 |
| 1:AA:78:G:H22 | 1:AA:91:C:H42 | 1.69 | 0.40 |
| 1:AA:827:U:C4 | 1:AA:870:U:C4 | 3.09 | 0.40 |
| 2:AB:161:ALA:HB1 | 2:AB:185:ILE:HD11 | 2.03 | 0.40 |
| 3:AC:125:GLU:CD | 3:AC:189:ALA:HA | 2.42 | 0.40 |
| 4:AD:78:LEU:HA | 4:AD:78:LEU:HD23 | 1.89 | 0.40 |
| 5:AE:67:VAL:HG22 | 5:AE:68:GLU:N | 2.36 | 0.40 |
| 9:AI:10:ARG:HD3 | 9:AI:75:ASP:HB3 | 2.03 | 0.40 |
| 1:AA:1350:A:OP1 | 9:AI:121:ARG:HG3 | 2.21 | 0.40 |
| 9:AI:99:LEU:O | 9:AI:100:GLY:C | 2.60 | 0.40 |
| 10:AJ:94:VAL:CG1 | 10:AJ:95:GLU:N | 2.84 | 0.40 |
| 17:AQ:27:PHE:CE1 | 17:AQ:36:ILE:HD11 | 2.56 | 0.40 |
| 1:AA:127:G:H4' | 17:AQ:2:PRO:HD2 | 2.03 | 0.40 |
| 18:AR:37:VAL:HG23 | 18:AR:38:GLU:H | 1.86 | 0.40 |
| 18:AR:45:SER:N | 18:AR:51:LEU:HD21 | 2.36 | 0.40 |
| 22:B0:27:GLU:HB3 | 31:BA:856:C:C1' | 2.51 | 0.40 |
| 25:B3:46:ASN:ND2 | 31:BA:851:U:C4' | 2.84 | 0.40 |
| 30:B8:4:MET:CE | 31:BA:593:G:O4' | 2.70 | 0.40 |
| 30:B8:4:MET:HE1 | 31:BA:593:G:O4' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:1397:U:O2' | 31:BA:1398:C:P | 2.80 | 0.40 |
| 31:BA:1794:U:O2' | 31:BA:1795:C:H5' | 2.20 | 0.40 |
| 31:BA:1899:G:O2' | 31:BA:1900:A:H5'' | 2.22 | 0.40 |
| 31:BA:526:A:N3 | 31:BA:2044:C:H1' | 2.36 | 0.40 |
| 31:BA:858:U:O2 | 31:BA:2268:A:H2' | 2.21 | 0.40 |
| 31:BA:2406:U:O5' | 31:BA:2406:U:H2' | 2.21 | 0.40 |
| 31:BA:2542:A:H8 | 31:BA:2544:G:O6 | 2.05 | 0.40 |
| 27:B5:7:PRO:HA | 31:BA:2615:U:N1 | 2.37 | 0.40 |
| 31:BA:2772:C:H2' | 31:BA:2773:C:C6 | 2.56 | 0.40 |
| 32:BB:65:C:N4 | 32:BB:109:C:C2 | 2.90 | 0.40 |
| 33:BD:186:HIS:CD2 | 33:BD:188:GLU:N | 2.63 | 0.40 |
| 33:BD:246:PRO:O | 33:BD:254:THR:HG22 | 2.21 | 0.40 |
| 35:BF:20:LEU:HB3 | 35:BF:23:ASP:HB2 | 2.03 | 0.40 |
| 36:BG:88:ILE:HG22 | 36:BG:89:GLY:N | 2.36 | 0.40 |
| 37:BH:100:GLY:C | 37:BH:102:ALA:N | 2.73 | 0.40 |
| 37:BH:158:HIS:NE2 | 37:BH:169:VAL:C | 2.74 | 0.40 |
| 37:BH:20:ALA:HB1 | 37:BH:21:PRO:CD | 2.44 | 0.40 |
| 41:BP:125:VAL:O | 41:BP:145:PRO:HD2 | 2.22 | 0.40 |
| 41:BP:33:ARG:O | 41:BP:35:HIS:O | 2.40 | 0.40 |
| 41:BP:91:PHE:CE2 | 41:BP:95:VAL:HG12 | 2.57 | 0.40 |
| 41:BP:97:PRO:O | 41:BP:98:GLU:CB | 2.49 | 0.40 |
| 45:BT:51:ARG:HG3 | 45:BT:98:LYS:HG3 | 2.04 | 0.40 |
| 45:BT:51:ARG:HD2 | 45:BT:62:THR:CG2 | 2.52 | 0.40 |
| 47:BV:4:ILE:O | 47:BV:4:ILE:HG22 | 2.21 | 0.40 |
| 1:CA:1099:G:C5 | 1:CA:1100:C:C4 | 3.09 | 0.40 |
| 1:CA:1169:A:H2' | 1:CA:1170:A:O4' | 2.21 | 0.40 |
| 1:CA:1244:C:H2' | 1:CA:1245:A:H8 | 1.84 | 0.40 |
| 1:CA:1407:C:H6 | 1:CA:1407:C:O5' | 2.03 | 0.40 |
| 1:CA:66:G:H5' | 1:CA:173:U:O4 | 2.21 | 0.40 |
| 1:CA:708:C:O2' | 1:CA:709:G:H5' | 2.20 | 0.40 |
| 1:CA:779:C:O2' | 1:CA:780:A:H5' | 2.21 | 0.40 |
| 2:CB:178:ARG:HG3 | 8:CH:72:PRO:HA | 2.03 | 0.40 |
| 2:CB:29:ALA:C | 2:CB:31:TYR:N | 2.74 | 0.40 |
| 2:CB:32:ILE:HA | 2:CB:42:ILE:HA | 2.03 | 0.40 |
| 2:CB:96:ARG:O | 2:CB:98:LEU:N | 2.55 | 0.40 |
| 5:CE:33:VAL:HG12 | 5:CE:34:VAL:H | 1.85 | 0.40 |
| 1:CA:970:C:N4 | 9:CI:128:ARG:OXT | 2.52 | 0.40 |
| 9:CI:3:GLN:HB3 | 9:CI:20:ARG:NE | 2.36 | 0.40 |
| 10:CJ:51:ARG:CG | 10:CJ:61:GLU:HB2 | 2.51 | 0.40 |
| 12:CL:22:SER:C | 12:CL:24:VAL:N | 2.74 | 0.40 |
| 13:CM:36:LYS:HB2 | 13:CM:59:TYR:CZ | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:CQ:50:LYS:HE3 | 17:CQ:51:TYR:HE1 | 1.86 | 0.40 |
| 17:CQ:67:LYS:CA | 17:CQ:70:ARG:HH12 | 2.28 | 0.40 |
| 18:CR:25:THR:O | 18:CR:25:THR:HG22 | 2.22 | 0.40 |
| 19:CS:49:ILE:HD12 | 19:CS:49:ILE:H | 1.87 | 0.40 |
| 19:CS:50:ALA:HA | 19:CS:58:VAL:O | 2.22 | 0.40 |
| 20:CT:89:ARG:HH21 | 20:CT:104:LEU:CD2 | 2.34 | 0.40 |
| 23:D1:47:GLN:O | 23:D1:48:LYS:O | 2.40 | 0.40 |
| 28:D6:37:ARG:HB3 | 31:DA:2344:U:O2' | 2.21 | 0.40 |
| 31:DA:1112:G:N2 | 31:DA:1113:U:O2 | 2.54 | 0.40 |
| 31:DA:1573:G:H2' | 31:DA:1574:C:H5' | 2.04 | 0.40 |
| 31:DA:1696:G:C5 | 31:DA:1697:G:N7 | 2.89 | 0.40 |
| 31:DA:1833:U:H2' | 31:DA:1834:U:O4' | 2.22 | 0.40 |
| 31:DA:1891:G:C6 | 31:DA:1892:C:C4 | 3.08 | 0.40 |
| 31:DA:2309:A:N3 | 31:DA:2310:A:C2 | 2.84 | 0.40 |
| 31:DA:2406:U:N3 | 41:DP:72:PRO:HG2 | 2.36 | 0.40 |
| 31:DA:2510:C:H2' | 31:DA:2511:U:O4' | 2.21 | 0.40 |
| 31:DA:2600:A:C6 | 31:DA:2601:C:N4 | 2.90 | 0.40 |
| 31:DA:353:G:H2' | 31:DA:354:G:O5' | 2.21 | 0.40 |
| 31:DA:475:U:C4 | 31:DA:481:G:O6 | 2.75 | 0.40 |
| 31:DA:528:A:C3' | 31:DA:528:A:C8 | 3.04 | 0.40 |
| 31:DA:774:A:H2 | 31:DA:787:U:O2' | 1.99 | 0.40 |
| 31:DA:844:C:O2' | 31:DA:845:G:H5' | 2.22 | 0.40 |
| 31:DA:862:G:H2' | 31:DA:863:A:O4' | 2.21 | 0.40 |
| 31:DA:911:A:C4 | 42:DQ:9:TYR:OH | 2.67 | 0.40 |
| 31:DA:917:A:H5' | 31:DA:917:A:C8 | 2.57 | 0.40 |
| 31:DA:987:G:H2' | 31:DA:988:A:O4' | 2.21 | 0.40 |
| 33:DD:61:LEU:HD13 | 33:DD:61:LEU:HA | 1.78 | 0.40 |
| 34:DE:56:PRO:C | 34:DE:58:ARG:H | 2.25 | 0.40 |
| 36:DG:148:MET:CE | 36:DG:148:MET:HA | 2.51 | 0.40 |
| 36:DG:6:ALA:O | 36:DG:10:LYS:HG3 | 2.21 | 0.40 |
| 37:DH:117:PRO:HA | 37:DH:118:PRO:HD2 | 2.01 | 0.40 |
| 37:DH:145:ALA:O | 37:DH:148:ILE:N | 2.55 | 0.40 |
| 37:DH:54:ARG:CB | 37:DH:65:HIS:HD2 | 2.34 | 0.40 |
| 39:DN:125:GLY:CA | 39:DN:126:PRO:O | 2.66 | 0.40 |
| 39:DN:129:PRO:O | 39:DN:130:HIS:CB | 2.69 | 0.40 |
| 41:DP:32:THR:HG21 | 41:DP:37:GLY:HA2 | 2.03 | 0.40 |
| 42:DQ:17:LEU:HD21 | 42:DQ:41:TRP:HE1 | 1.87 | 0.40 |
| 42:DQ:8:LYS:CD | 42:DQ:9:TYR:H | 2.34 | 0.40 |
| 45:DT:31:SER:OG | 45:DT:43:GLN:N | 2.54 | 0.40 |
| 47:DV:16:PRO:O | 47:DV:98:GLU:OE2 | 2.40 | 0.40 |
| 47:DV:50:PRO:HB2 | 47:DV:51:VAL:H | 1.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:DA:139(A):G:C2 | 49:DX:44:GLU:OE1 | 2.74 | 0.40 |
| 49:DX:82:GLN:CD | 49:DX:83:VAL:HG22 | 2.42 | 0.40 |
| 50:DY:72:VAL:C | 50:DY:73:ARG:HG3 | 2.41 | 0.40 |
| 51:DZ:5:LEU:HD12 | 51:DZ:47:VAL:CG2 | 2.51 | 0.40 |
| 1:AA:1004:A:N7 | 1:AA:1036:G:O6 | 2.54 | 0.40 |
| 1:AA:106:C:H2' | 1:AA:107:G:C8 | 2.56 | 0.40 |
| 1:AA:1187:G:C2 | 1:AA:1188:A:C4 | 3.10 | 0.40 |
| 1:AA:1422:G:H4' | 40:BO:49:ARG:HH12 | 1.85 | 0.40 |
| 1:AA:1442:G:N7 | 1:AA:1442(B):A:C2 | 2.89 | 0.40 |
| 1:AA:1486:G:H2' | 1:AA:1487:G:O4' | 2.21 | 0.40 |
| 1:AA:173:U:C6 | 1:AA:197:A:C2 | 3.09 | 0.40 |
| 1:AA:189:G:O6 | 1:AA:189(L):G:O6 | 2.39 | 0.40 |
| 1:AA:340:U:O2' | 1:AA:341:C:H5' | 2.21 | 0.40 |
| 1:AA:501:C:O4' | 1:AA:548:G:N2 | 2.55 | 0.40 |
| 1:AA:758:G:H4' | 1:AA:880:C:H4' | 2.03 | 0.40 |
| 1:AA:855:G:C2 | 1:AA:856:C:C2 | 3.09 | 0.40 |
| 2:AB:160:ASP:O | 2:AB:183:PRO:HD2 | 2.21 | 0.40 |
| 5:AE:31:LEU:CD1 | 5:AE:129:ILE:HA | 2.52 | 0.40 |
| 6:AF:89:MET:HG2 | 6:AF:89:MET:O | 2.21 | 0.40 |
| 9:AI:63:ILE:HG22 | 9:AI:64:THR:N | 2.37 | 0.40 |
| 14:AN:41:ARG:HG3 | 14:AN:42:ILE:N | 2.36 | 0.40 |
| 16:AP:39:TYR:HE1 | 16:AP:41:PRO:HA | 1.85 | 0.40 |
| 18:AR:41:LYS:C | 18:AR:43:PHE:H | 2.25 | 0.40 |
| 19:AS:10:PHE:HZ | 19:AS:70:LYS:HE2 | 1.87 | 0.40 |
| 20:AT:100:ILE:O | 20:AT:102:GLY:N | 2.55 | 0.40 |
| 20:AT:67:ALA:HB2 | 20:AT:77:ALA:HB2 | 2.04 | 0.40 |
| 26:B4:19:GLY:O | 26:B4:21:VAL:N | 2.53 | 0.40 |
| 28:B6:22:ALA:HB2 | 28:B6:39:TYR:CZ | 2.55 | 0.40 |
| 31:BA:1444:G:C2 | 31:BA:1548:C:C2 | 3.09 | 0.40 |
| 31:BA:1458:C:H4' | 31:BA:1459:G:C4 | 2.57 | 0.40 |
| 31:BA:1487:G:C2' | 31:BA:1488:G:O5' | 2.70 | 0.40 |
| 31:BA:1741:A:C5 | 31:BA:1742:G:N2 | 2.89 | 0.40 |
| 31:BA:2057:A:H2' | 31:BA:2058:A:C8 | 2.56 | 0.40 |
| 31:BA:2205:C:C2 | 31:BA:2220:G:N1 | 2.90 | 0.40 |
| 31:BA:2400:G:C5 | 31:BA:2401:U:C5 | 3.10 | 0.40 |
| 31:BA:2473:U:O2 | 31:BA:2473:U:H2' | 2.21 | 0.40 |
| 31:BA:250:G:C6 | 31:BA:251:A:C6 | 3.10 | 0.40 |
| 31:BA:2602:A:H4' | 31:BA:2603:G:C5' | 2.52 | 0.40 |
| 31:BA:2603:G:C5 | 31:BA:2604:U:C5 | 3.10 | 0.40 |
| 31:BA:271(J):C:C3' | 31:BA:271(K):U:H5'' | 2.51 | 0.40 |
| 31:BA:271(T):C:O2 | 31:BA:271(T):C:C2' | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:BA:2808:U:C2' | 31:BA:2809:A:O5' | 2.69 | 0.40 |
| 31:BA:301:G:C6 | 31:BA:317:G:C6 | 3.10 | 0.40 |
| 31:BA:363(C):G:H2' | 31:BA:363(D):G:C8 | 2.55 | 0.40 |
| 31:BA:692:C:O2' | 31:BA:693:C:H5' | 2.21 | 0.40 |
| 31:BA:879:G:H1 | 31:BA:898:C:H42 | 1.69 | 0.40 |
| 31:BA:943:U:O2' | 31:BA:944:G:H5' | 2.21 | 0.40 |
| 32:BB:40:U:H1' | 32:BB:45:A:H61 | 1.87 | 0.40 |
| 32:BB:40:U:H1' | 32:BB:45:A:N6 | 2.35 | 0.40 |
| 32:BB:46:A:H2' | 32:BB:47:C:O5' | 2.21 | 0.40 |
| 33:BD:232:PRO:HG2 | 33:BD:248:SER:O | 2.21 | 0.40 |
| 35:BF:132:VAL:C | 35:BF:134:GLY:H | 2.25 | 0.40 |
| 35:BF:203:GLN:O | 35:BF:206:ILE:O | 2.39 | 0.40 |
| 35:BF:50:SER:HB2 | 35:BF:94:PRO:HD3 | 2.03 | 0.40 |
| 36:BG:60:LEU:HD22 | 36:BG:63:ILE:HG13 | 2.03 | 0.40 |
| 31:BA:2094:G:H5' | 38:BI:25:TYR:CD2 | 2.57 | 0.40 |
| 38:BI:62:LYS:HE2 | 38:BI:134:PRO:HG2 | 2.03 | 0.40 |
| 40:BO:47:ILE:HG23 | 40:BO:48:PRO:HD2 | 2.04 | 0.40 |
| 31:BA:631:A:HO2' | 41:BP:67:MET:HB3 | 1.87 | 0.40 |
| 44:BS:89:ARG:HE | 44:BS:90:GLY:N | 2.17 | 0.40 |
| 45:BT:99:LEU:HB3 | 45:BT:101:PHE:CE1 | 2.57 | 0.40 |
| 31:BA:751:A:C5' | 48:BW:90:ARG:HA | 2.44 | 0.40 |
| 50:BY:96:ILE:CG2 | 50:BY:99:CYS:SG | 3.00 | 0.40 |
| 42:BQ:141:GLN:N | 51:BZ:53:ILE:HB | 2.37 | 0.40 |
| 1:CA:1367:C:N3 | 1:CA:1368:G:C8 | 2.90 | 0.40 |
| 1:CA:149:A:O2' | 1:CA:150:C:H6 | 2.04 | 0.40 |
| 1:CA:15:G:H4' | 5:CE:24:ARG:HH12 | 1.87 | 0.40 |
| 1:CA:185:A:C6 | 1:CA:186:C:N4 | 2.89 | 0.40 |
| 1:CA:136:C:N4 | 1:CA:227:G:H1 | 2.20 | 0.40 |
| 1:CA:36:C:O2' | 1:CA:37:U:H5' | 2.21 | 0.40 |
| 1:CA:460:G:N2 | 1:CA:471:G:C8 | 2.89 | 0.40 |
| 1:CA:451:A:N7 | 1:CA:481:G:N1 | 2.70 | 0.40 |
| 1:CA:615:C:C2 | 1:CA:616:G:C8 | 3.10 | 0.40 |
| 1:CA:626:U:N3 | 1:CA:627:G:N7 | 2.69 | 0.40 |
| 1:CA:775:G:O2' | 1:CA:776:G:H5' | 2.22 | 0.40 |
| 1:CA:92:C:C3' | 1:CA:93:G:H8 | 2.34 | 0.40 |
| 1:CA:994:A:H2' | 1:CA:994:A:N3 | 2.37 | 0.40 |
| 2:CB:15:VAL:H | 2:CB:16:HIS:HD1 | 1.67 | 0.40 |
| 3:CC:188:LEU:O | 3:CC:189:ALA:HB2 | 2.20 | 0.40 |
| 4:CD:172:PRO:O | 4:CD:187:ARG:NH2 | 2.51 | 0.40 |
| 4:CD:206:PHE:HD2 | 4:CD:207:TYR:CD2 | 2.40 | 0.40 |
| 5:CE:78:HIS:HE1 | 5:CE:142:LEU:HD23 | 1.81 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:CE:6:PHE:HB2 | 5:CE:34:VAL:HG13 | 2.02 | 0.40 |
| 6:CF:40:VAL:HG13 | 6:CF:40:VAL:O | 2.22 | 0.40 |
| 6:CF:53:ALA:O | 6:CF:54:LYS:HB2 | 2.21 | 0.40 |
| 7:CG:103:TRP:HA | 7:CG:106:GLN:HE21 | 1.86 | 0.40 |
| 1:CA:1350:A:OP1 | 9:CI:121:ARG:HG3 | 2.21 | 0.40 |
| 12:CL:21:LYS:N | 12:CL:21:LYS:HD2 | 2.36 | 0.40 |
| 12:CL:27:LEU:HG | 12:CL:62:SER:OG | 2.21 | 0.40 |
| 13:CM:79:LYS:O | 13:CM:82:MET:HB3 | 2.22 | 0.40 |
| 17:CQ:29:HIS:HA | 17:CQ:30:PRO:HD2 | 1.78 | 0.40 |
| 22:D0:24:LYS:HG3 | 22:D0:36:ILE:HD11 | 2.04 | 0.40 |
| 28:D6:11:LEU:O | 28:D6:23:THR:HA | 2.22 | 0.40 |
| 31:DA:996:A:N6 | 31:DA:1160:G:C6 | 2.90 | 0.40 |
| 31:DA:1170:G:OP2 | 31:DA:1170:G:H8 | 2.04 | 0.40 |
| 31:DA:1421:G:C2 | 31:DA:1422:G:C8 | 3.10 | 0.40 |
| 31:DA:1445(A):C:N3 | 31:DA:1446:C:C5 | 2.90 | 0.40 |
| 31:DA:1349:A:N6 | 31:DA:1598:C:N4 | 2.69 | 0.40 |
| 31:DA:1655:A:C4 | 31:DA:1656:C:C6 | 3.09 | 0.40 |
| 31:DA:1815:A:H8 | 31:DA:1815:A:OP1 | 2.05 | 0.40 |
| 31:DA:1821:A:C2' | 31:DA:1822:G:C5' | 2.84 | 0.40 |
| 31:DA:2402:C:C2' | 31:DA:2403:C:H5' | 2.50 | 0.40 |
| 31:DA:251:A:C5 | 31:DA:252:G:H1' | 2.56 | 0.40 |
| 31:DA:281:G:H21 | 31:DA:358:U:H5 | 1.69 | 0.40 |
| 31:DA:577:G:H8 | 31:DA:577:G:O5' | 2.05 | 0.40 |
| 31:DA:610:G:H2' | 31:DA:611:C:C6 | 2.57 | 0.40 |
| 31:DA:622:G:O2' | 31:DA:623:G:H5' | 2.21 | 0.40 |
| 31:DA:714:U:O2 | 31:DA:716:A:C8 | 2.74 | 0.40 |
| 31:DA:902:C:O2' | 31:DA:903:C:H5' | 2.22 | 0.40 |
| 33:DD:35:LYS:NZ | 33:DD:104:TYR:HD1 | 2.19 | 0.40 |
| 33:DD:246:PRO:HG2 | 33:DD:255:LYS:HG2 | 2.03 | 0.40 |
| 33:DD:30:GLU:CD | 33:DD:63:ARG:NE | 2.74 | 0.40 |
| 33:DD:44:ASN:HB3 | 33:DD:48:ARG:C | 2.42 | 0.40 |
| 33:DD:4:LYS:HB2 | 33:DD:18:VAL:CG1 | 2.51 | 0.40 |
| 35:DF:36:VAL:O | 35:DF:39:TRP:HB3 | 2.21 | 0.40 |
| 36:DG:108:ASN:O | 36:DG:112:PRO:HG2 | 2.21 | 0.40 |
| 37:DH:38:SER:HA | 37:DH:39:PRO:HD3 | 1.87 | 0.40 |
| 38:DI:116:LEU:HD21 | 38:DI:119:PRO:HA | 2.02 | 0.40 |
| 39:DN:15:LEU:HD22 | 39:DN:16:ILE:N | 2.35 | 0.40 |
| 43:DR:111:LEU:HD23 | 43:DR:111:LEU:HA | 1.91 | 0.40 |
| 44:DS:59:LYS:NZ | 44:DS:68:GLN:NE2 | 2.70 | 0.40 |
| 50:DY:31:LEU:HD22 | 50:DY:31:LEU:N | 2.35 | 0.40 |
| 50:DY:45:VAL:CG1 | 50:DY:62:GLU:OE2 | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:DY:6:HIS:N | 50:DY:6:HIS:ND1 | 2.68 | 0.40 |
| 50:DY:80:GLY:O | 50:DY:81:LYS:HB2 | 2.22 | 0.40 |
| 1:AA:1063:C:OP2 | 1:AA:1064:G:O2' | 2.39 | 0.40 |
| 1:AA:111:G:C5 | 1:AA:112:U:C5 | 3.09 | 0.40 |
| 1:AA:1446:U:O2' | 1:AA:1447:A:H8 | 1.97 | 0.40 |
| 1:AA:1493:A:H5'' | 1:AA:1494:G:OP2 | 2.21 | 0.40 |
| 1:AA:282:A:N3 | 1:AA:282:A:H2' | 2.37 | 0.40 |
| 1:AA:357:G:C2 | 1:AA:358:U:C5 | 3.09 | 0.40 |
| 1:AA:391:G:C6 | 1:AA:392:G:C5 | 3.09 | 0.40 |
| 1:AA:51:A:C6 | 1:AA:353:A:C2 | 3.09 | 0.40 |
| 1:AA:638:G:O2' | 1:AA:639:G:H5' | 2.22 | 0.40 |
| 1:AA:830:G:H2' | 1:AA:831:U:C6 | 2.51 | 0.40 |
| 1:AA:992:U:H4' | 1:AA:993:G:O5' | 2.22 | 0.40 |
| 2:AB:47:THR:O | 2:AB:51:LEU:N | 2.49 | 0.40 |
| 2:AB:55:PHE:HE1 | 2:AB:218:ALA:HA | 1.85 | 0.40 |
| 9:AI:104:ARG:O | 9:AI:104:ARG:HG2 | 2.21 | 0.40 |
| 10:AJ:82:ILE:O | 10:AJ:82:ILE:HG22 | 2.22 | 0.40 |
| 13:AM:36:LYS:HB2 | 13:AM:59:TYR:CZ | 2.56 | 0.40 |
| 15:AO:18:PHE:O | 15:AO:19:PRO:C | 2.58 | 0.40 |
| 15:AO:18:PHE:CE1 | 15:AO:21:ASP:HB2 | 2.57 | 0.40 |
| 17:AQ:50:LYS:HE3 | 17:AQ:51:TYR:CE1 | 2.56 | 0.40 |
| 20:AT:100:ILE:HD12 | 20:AT:100:ILE:N | 2.36 | 0.40 |
| 23:B1:65:SER:N | 23:B1:67:ILE:HD11 | 2.36 | 0.40 |
| 25:B3:12:PRO:HA | 25:B3:15:TYR:HD1 | 1.86 | 0.40 |
| 26:B4:15:ILE:O | 26:B4:16:CYS:C | 2.59 | 0.40 |
| 26:B4:17:GLY:C | 26:B4:19:GLY:H | 2.25 | 0.40 |
| 27:B5:49:CYS:O | 27:B5:50:GLY:C | 2.60 | 0.40 |
| 28:B6:19:ARG:HB3 | 28:B6:19:ARG:NH1 | 2.37 | 0.40 |
| 31:BA:1216:G:OP1 | 46:BU:8:VAL:HG22 | 2.22 | 0.40 |
| 31:BA:1276:A:O2' | 43:BR:16:HIS:CE1 | 2.72 | 0.40 |
| 31:BA:1465:G:C2 | 31:BA:1466:G:C4 | 3.09 | 0.40 |
| 31:BA:1952:A:C5 | 40:BO:22:ILE:CD1 | 3.04 | 0.40 |
| 31:BA:1952:A:C6 | 40:BO:22:ILE:CD1 | 3.04 | 0.40 |
| 31:BA:2205:C:O2 | 31:BA:2220:G:N1 | 2.54 | 0.40 |
| 31:BA:2259:G:C2 | 31:BA:2282:G:C6 | 3.09 | 0.40 |
| 31:BA:243:U:C2' | 31:BA:244:A:H5' | 2.51 | 0.40 |
| 31:BA:2619:C:H2' | 31:BA:2620:C:C6 | 2.56 | 0.40 |
| 31:BA:28:A:C5 | 31:BA:29:U:C5 | 3.09 | 0.40 |
| 31:BA:422:A:C6 | 31:BA:423:A:C6 | 3.09 | 0.40 |
| 24:B2:40:SER:HB2 | 31:BA:61:G:H1' | 2.03 | 0.40 |
| 33:BD:118:VAL:CG2 | 33:BD:119:ALA:N | 2.81 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BD:238:GLY:O | 33:BD:239:ARG:HB2 | 2.21 | 0.40 |
| 33:BD:65:ILE:HD13 | 33:BD:65:ILE:O | 2.21 | 0.40 |
| 34:BE:76:ARG:CG | 34:BE:195:LEU:HD22 | 2.50 | 0.40 |
| 34:BE:1:MET:O | 34:BE:2:LYS:C | 2.59 | 0.40 |
| 34:BE:77:ILE:CG2 | 34:BE:78:LEU:N | 2.85 | 0.40 |
| 35:BF:143:ALA:HB1 | 35:BF:148:LEU:HB2 | 2.03 | 0.40 |
| 35:BF:165:ARG:HA | 35:BF:168:ARG:HD3 | 2.04 | 0.40 |
| 35:BF:52:LYS:HG2 | 35:BF:56:GLU:HB3 | 2.03 | 0.40 |
| 26:B4:14:ILE:HA | 36:BG:5:VAL:HG13 | 2.03 | 0.40 |
| 36:BG:60:LEU:O | 36:BG:63:ILE:HG13 | 2.21 | 0.40 |
| 38:BI:13:GLY:O | 38:BI:15:VAL:N | 2.54 | 0.40 |
| 38:BI:56:LYS:HZ2 | 38:BI:57:ARG:N | 2.20 | 0.40 |
| 41:BP:51:PHE:HB3 | 41:BP:52:GLU:HG2 | 2.03 | 0.40 |
| 42:BQ:54:MET:HB3 | 42:BQ:64:ILE:HD11 | 2.04 | 0.40 |
| 46:BU:22:LYS:HD3 | 46:BU:22:LYS:HA | 1.81 | 0.40 |
| 47:BV:73:SER:OG | 47:BV:75:PHE:HE1 | 2.00 | 0.40 |
| 48:BW:27:LYS:O | 48:BW:28:SER:C | 2.60 | 0.40 |
| 49:BX:38:GLU:CD | 49:BX:38:GLU:N | 2.70 | 0.40 |
| 50:BY:71:LYS:CB | 50:BY:71:LYS:HZ3 | 2.31 | 0.40 |
| 51:BZ:120:ILE:O | 51:BZ:120:ILE:HG22 | 2.21 | 0.40 |
| 51:BZ:28:MET:HG3 | 51:BZ:35:ARG:HB2 | 2.02 | 0.40 |
| 1:CA:1064:G:C8 | 1:CA:1066:C:C2 | 3.10 | 0.40 |
| 1:CA:1091:U:H2' | 1:CA:1091:U:O2 | 2.21 | 0.40 |
| 1:CA:1500:A:OP2 | 1:CA:1505:G:OP1 | 2.39 | 0.40 |
| 1:CA:262:A:N6 | 1:CA:263:A:N6 | 2.69 | 0.40 |
| 1:CA:271:C:O2' | 1:CA:272:C:H5' | 2.21 | 0.40 |
| 1:CA:358:U:H2' | 1:CA:359:U:C6 | 2.56 | 0.40 |
| 1:CA:456:C:H2' | 1:CA:457:C:C6 | 2.57 | 0.40 |
| 1:CA:580:U:H2' | 1:CA:581:G:O4' | 2.22 | 0.40 |
| 1:CA:698:G:C6 | 1:CA:699:C:C4 | 3.09 | 0.40 |
| 1:CA:945:G:O6 | 1:CA:1337:G:C6 | 2.75 | 0.40 |
| 2:CB:174:VAL:O | 2:CB:178:ARG:HB2 | 2.21 | 0.40 |
| 4:CD:203:VAL:O | 4:CD:204:ILE:C | 2.59 | 0.40 |
| 4:CD:4:TYR:HE2 | 4:CD:7:PRO:O | 2.05 | 0.40 |
| 5:CE:87:SER:HB3 | 5:CE:131:ILE:HD13 | 2.03 | 0.40 |
| 9:CI:49:PRO:HA | 9:CI:101:PHE:CE1 | 2.56 | 0.40 |
| 14:CN:3:ARG:O | 14:CN:7:ILE:HG23 | 2.21 | 0.40 |
| 23:D1:19:GLN:CD | 23:D1:44:PRO:CB | 2.89 | 0.40 |
| 23:D1:37:ILE:HG23 | 31:DA:2080:G:O5' | 2.22 | 0.40 |
| 30:D8:16:ILE:CD1 | 30:D8:57:ARG:HG2 | 2.52 | 0.40 |
| 30:D8:51:ALA:C | 30:D8:53:PRO:HD2 | 2.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DA:1157:G:N1 | 31:DA:1158:C:C4 | 2.90 | 0.40 |
| 31:DA:1410:G:H1 | 31:DA:1592:C:N4 | 2.19 | 0.40 |
| 31:DA:1465:G:C2 | 31:DA:1466:G:C8 | 3.10 | 0.40 |
| 31:DA:1480:G:C6 | 31:DA:1481:U:N3 | 2.90 | 0.40 |
| 31:DA:1487:G:C2' | 31:DA:1488:G:O5' | 2.69 | 0.40 |
| 31:DA:1623:G:C2 | 31:DA:1624:G:C8 | 3.10 | 0.40 |
| 31:DA:2205:C:O2 | 31:DA:2220:G:N1 | 2.54 | 0.40 |
| 31:DA:2400:G:C6 | 31:DA:2401:U:C4 | 3.09 | 0.40 |
| 31:DA:2702:U:C2 | 31:DA:2702:U:OP1 | 2.74 | 0.40 |
| 31:DA:2813:A:C6 | 31:DA:2814:C:C4 | 3.08 | 0.40 |
| 31:DA:2889:C:H2' | 31:DA:2891:G:O4' | 2.21 | 0.40 |
| 31:DA:336:C:H5'' | 50:DY:7:VAL:CG1 | 2.51 | 0.40 |
| 31:DA:415:A:H2' | 31:DA:416:C:C6 | 2.57 | 0.40 |
| 31:DA:428:A:H8 | 31:DA:428:A:OP2 | 2.04 | 0.40 |
| 31:DA:604:G:C6 | 31:DA:605:C:C4 | 3.10 | 0.40 |
| 31:DA:814:C:O2' | 31:DA:815:C:H5' | 2.21 | 0.40 |
| 31:DA:826:U:H2' | 31:DA:828:U:O4' | 2.21 | 0.40 |
| 31:DA:861:A:H2' | 31:DA:862:G:O4' | 2.21 | 0.40 |
| 31:DA:942:G:C6 | 31:DA:943:U:C4 | 3.09 | 0.40 |
| 32:DB:92:C:H5'' | 51:DZ:79:ARG:HH22 | 1.86 | 0.40 |
| 33:DD:70:TRP:CZ3 | 33:DD:146:GLU:OE2 | 2.72 | 0.40 |
| 31:DA:764:A:OP1 | 33:DD:208:LYS:HE2 | 2.21 | 0.40 |
| 35:DF:115:ALA:O | 35:DF:116:ASP:C | 2.60 | 0.40 |
| 35:DF:132:VAL:O | 35:DF:134:GLY:N | 2.55 | 0.40 |
| 35:DF:53:THR:C | 35:DF:55:GLY:N | 2.74 | 0.40 |
| 37:DH:86:GLU:HA | 37:DH:132:ARG:HA | 2.04 | 0.40 |
| 38:DI:105:HIS:CD2 | 38:DI:105:HIS:N | 2.89 | 0.40 |
| 45:DT:51:ARG:HG3 | 45:DT:98:LYS:HG3 | 2.04 | 0.40 |
| 45:DT:58:ASN:HD22 | 45:DT:59:THR:N | 2.20 | 0.40 |
| 45:DT:91:ARG:HB2 | 45:DT:92:GLY:H | 1.49 | 0.40 |
| 46:DU:24:TYR:HB2 | 46:DU:29:SER:HB3 | 2.04 | 0.40 |
| 49:DX:40:LYS:C | 49:DX:42:ALA:N | 2.74 | 0.40 |
| 49:DX:77:LYS:CD | 49:DX:78:LYS:HG3 | 2.50 | 0.40 |
| 50:DY:16:ALA:HA | 50:DY:21:LYS:HD2 | 2.03 | 0.40 |
| 50:DY:27:VAL:HG12 | 50:DY:29:GLU:N | 2.13 | 0.40 |
| 50:DY:77:PRO:O | 50:DY:78:ALA:CB | 2.68 | 0.40 |
| 50:DY:76:CYS:HB3 | 50:DY:96:ILE:HD11 | 2.04 | 0.40 |
| 51:DZ:158:PRO:O | 51:DZ:161:VAL:HB | 2.22 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | AB | 233/256 (91%) | 165 (71%) | 51 (22%) | 17 (7%) | 1 | 5 |
| 2 | CB | 233/256 (91%) | 165 (71%) | 51 (22%) | 17 (7%) | 1 | 5 |
| 3 | AC | 205/239 (86%) | 156 (76%) | 35 (17%) | 14 (7%) | 1 | 6 |
| 3 | CC | 205/239 (86%) | 156 (76%) | 35 (17%) | 14 (7%) | 1 | 6 |
| 4 | AD | 206/209 (99%) | 128 (62%) | 59 (29%) | 19 (9%) | 1 | 3 |
| 4 | CD | 206/209 (99%) | 128 (62%) | 59 (29%) | 19 (9%) | 1 | 3 |
| 5 | AE | 149/160 (93%) | 106 (71%) | 31 (21%) | 12 (8%) | 1 | 4 |
| 5 | CE | 149/160 (93%) | 104 (70%) | 33 (22%) | 12 (8%) | 1 | 4 |
| 6 | AF | 99/101 (98%) | 76 (77%) | 18 (18%) | 5 (5%) | 2 | 12 |
| 6 | CF | 99/101 (98%) | 77 (78%) | 17 (17%) | 5 (5%) | 2 | 12 |
| 7 | AG | 153/156 (98%) | 132 (86%) | 17 (11%) | 4 (3%) | 5 | 27 |
| 7 | CG | 153/156 (98%) | 132 (86%) | 17 (11%) | 4 (3%) | 5 | 27 |
| 8 | AH | 136/138 (99%) | 105 (77%) | 24 (18%) | 7 (5%) | 2 | 12 |
| 8 | CH | 136/138 (99%) | 106 (78%) | 23 (17%) | 7 (5%) | 2 | 12 |
| 9 | AI | 123/128 (96%) | 93 (76%) | 21 (17%) | 9 (7%) | 1 | 5 |
| 9 | CI | 123/128 (96%) | 93 (76%) | 21 (17%) | 9 (7%) | 1 | 5 |
| 10 | AJ | 97/105 (92%) | 80 (82%) | 13 (13%) | 4 (4%) | 3 | 16 |
| 10 | CJ | 97/105 (92%) | 80 (82%) | 13 (13%) | 4 (4%) | 3 | 16 |
| 11 | AK | 117/129 (91%) | 92 (79%) | 20 (17%) | 5 (4%) | 2 | 15 |
| 11 | CK | 117/129 (91%) | 94 (80%) | 18 (15%) | 5 (4%) | 2 | 15 |
| 12 | AL | 123/135 (91%) | 85 (69%) | 24 (20%) | 14 (11%) | 0 | 2 |
| 12 | CL | 123/135 (91%) | 86 (70%) | 23 (19%) | 14 (11%) | 0 | 2 |
| 13 | AM | 107/126 (85%) | 85 (79%) | 17 (16%) | 5 (5%) | 2 | 14 |
| 13 | CM | 107/126 (85%) | 84 (78%) | 18 (17%) | 5 (5%) | 2 | 14 |
| 14 | AN | 58/61 (95%) | 51 (88%) | 5 (9%) | 2 (3%) | 3 | 20 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|--------------|----------|----------|----------|-------------|-----|
| 14 | CN | 58/61 (95%) | 50 (86%) | 6 (10%) | 2 (3%) | 3 | 20 |
| 15 | AO | 86/89 (97%) | 68 (79%) | 15 (17%) | 3 (4%) | 3 | 20 |
| 15 | CO | 86/89 (97%) | 67 (78%) | 16 (19%) | 3 (4%) | 3 | 20 |
| 16 | AP | 82/88 (93%) | 49 (60%) | 23 (28%) | 10 (12%) | 0 | 1 |
| 16 | CP | 82/88 (93%) | 48 (58%) | 24 (29%) | 10 (12%) | 0 | 1 |
| 17 | AQ | 98/105 (93%) | 77 (79%) | 15 (15%) | 6 (6%) | 1 | 8 |
| 17 | CQ | 98/105 (93%) | 76 (78%) | 16 (16%) | 6 (6%) | 1 | 8 |
| 18 | AR | 68/88 (77%) | 43 (63%) | 21 (31%) | 4 (6%) | 1 | 9 |
| 18 | CR | 68/88 (77%) | 40 (59%) | 22 (32%) | 6 (9%) | 1 | 3 |
| 19 | AS | 77/93 (83%) | 59 (77%) | 11 (14%) | 7 (9%) | 1 | 3 |
| 19 | CS | 77/93 (83%) | 59 (77%) | 11 (14%) | 7 (9%) | 1 | 3 |
| 20 | AT | 97/106 (92%) | 64 (66%) | 25 (26%) | 8 (8%) | 1 | 4 |
| 20 | CT | 97/106 (92%) | 61 (63%) | 29 (30%) | 7 (7%) | 1 | 5 |
| 21 | AU | 23/27 (85%) | 18 (78%) | 4 (17%) | 1 (4%) | 2 | 15 |
| 21 | CU | 23/27 (85%) | 18 (78%) | 4 (17%) | 1 (4%) | 2 | 15 |
| 22 | B0 | 83/85 (98%) | 68 (82%) | 11 (13%) | 4 (5%) | 2 | 13 |
| 22 | D0 | 83/85 (98%) | 70 (84%) | 9 (11%) | 4 (5%) | 2 | 13 |
| 23 | B1 | 87/98 (89%) | 52 (60%) | 17 (20%) | 18 (21%) | 0 | 0 |
| 23 | D1 | 87/98 (89%) | 52 (60%) | 18 (21%) | 17 (20%) | 0 | 0 |
| 24 | B2 | 49/72 (68%) | 22 (45%) | 17 (35%) | 10 (20%) | 0 | 0 |
| 24 | D2 | 49/72 (68%) | 24 (49%) | 13 (26%) | 12 (24%) | 0 | 0 |
| 25 | B3 | 58/60 (97%) | 50 (86%) | 6 (10%) | 2 (3%) | 3 | 20 |
| 25 | D3 | 58/60 (97%) | 51 (88%) | 4 (7%) | 3 (5%) | 2 | 12 |
| 26 | B4 | 30/71 (42%) | 4 (13%) | 11 (37%) | 15 (50%) | 0 | 0 |
| 26 | D4 | 30/71 (42%) | 4 (13%) | 11 (37%) | 15 (50%) | 0 | 0 |
| 27 | B5 | 57/60 (95%) | 41 (72%) | 7 (12%) | 9 (16%) | 0 | 1 |
| 27 | D5 | 57/60 (95%) | 42 (74%) | 6 (10%) | 9 (16%) | 0 | 1 |
| 28 | B6 | 41/54 (76%) | 21 (51%) | 7 (17%) | 13 (32%) | 0 | 0 |
| 28 | D6 | 41/54 (76%) | 21 (51%) | 7 (17%) | 13 (32%) | 0 | 0 |
| 29 | B7 | 47/49 (96%) | 43 (92%) | 4 (8%) | 0 | 100 | 100 |
| 29 | D7 | 47/49 (96%) | 44 (94%) | 3 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 30 | B8 | 62/65 (95%) | 42 (68%) | 8 (13%) | 12 (19%) | 0 | 0 |
| 30 | D8 | 62/65 (95%) | 44 (71%) | 6 (10%) | 12 (19%) | 0 | 0 |
| 33 | BD | 270/276 (98%) | 217 (80%) | 40 (15%) | 13 (5%) | 2 | 13 |
| 33 | DD | 270/276 (98%) | 214 (79%) | 42 (16%) | 14 (5%) | 2 | 12 |
| 34 | BE | 203/206 (98%) | 153 (75%) | 28 (14%) | 22 (11%) | 0 | 2 |
| 34 | DE | 203/206 (98%) | 151 (74%) | 29 (14%) | 23 (11%) | 0 | 2 |
| 35 | BF | 206/210 (98%) | 155 (75%) | 37 (18%) | 14 (7%) | 1 | 6 |
| 35 | DF | 206/210 (98%) | 151 (73%) | 42 (20%) | 13 (6%) | 1 | 7 |
| 36 | BG | 177/182 (97%) | 123 (70%) | 35 (20%) | 19 (11%) | 0 | 2 |
| 36 | DG | 177/182 (97%) | 125 (71%) | 32 (18%) | 20 (11%) | 0 | 2 |
| 37 | BH | 158/180 (88%) | 103 (65%) | 28 (18%) | 27 (17%) | 0 | 0 |
| 37 | DH | 158/180 (88%) | 103 (65%) | 30 (19%) | 25 (16%) | 0 | 1 |
| 38 | BI | 144/148 (97%) | 89 (62%) | 38 (26%) | 17 (12%) | 0 | 1 |
| 38 | DI | 144/148 (97%) | 89 (62%) | 39 (27%) | 16 (11%) | 0 | 2 |
| 39 | BN | 137/140 (98%) | 96 (70%) | 25 (18%) | 16 (12%) | 0 | 1 |
| 39 | DN | 137/140 (98%) | 94 (69%) | 26 (19%) | 17 (12%) | 0 | 1 |
| 40 | BO | 120/122 (98%) | 107 (89%) | 10 (8%) | 3 (2%) | 5 | 28 |
| 40 | DO | 120/122 (98%) | 103 (86%) | 15 (12%) | 2 (2%) | 9 | 39 |
| 41 | BP | 144/150 (96%) | 80 (56%) | 23 (16%) | 41 (28%) | 0 | 0 |
| 41 | DP | 144/150 (96%) | 80 (56%) | 24 (17%) | 40 (28%) | 0 | 0 |
| 42 | BQ | 134/141 (95%) | 95 (71%) | 23 (17%) | 16 (12%) | 0 | 1 |
| 42 | DQ | 134/141 (95%) | 94 (70%) | 25 (19%) | 15 (11%) | 0 | 2 |
| 43 | BR | 115/118 (98%) | 87 (76%) | 19 (16%) | 9 (8%) | 1 | 4 |
| 43 | DR | 115/118 (98%) | 84 (73%) | 21 (18%) | 10 (9%) | 1 | 3 |
| 44 | BS | 97/112 (87%) | 54 (56%) | 19 (20%) | 24 (25%) | 0 | 0 |
| 44 | DS | 97/112 (87%) | 53 (55%) | 21 (22%) | 23 (24%) | 0 | 0 |
| 45 | BT | 130/146 (89%) | 93 (72%) | 20 (15%) | 17 (13%) | 0 | 1 |
| 45 | DT | 130/146 (89%) | 92 (71%) | 22 (17%) | 16 (12%) | 0 | 1 |
| 46 | BU | 115/118 (98%) | 90 (78%) | 17 (15%) | 8 (7%) | 1 | 6 |
| 46 | DU | 115/118 (98%) | 85 (74%) | 22 (19%) | 8 (7%) | 1 | 6 |
| 47 | BV | 99/101 (98%) | 57 (58%) | 15 (15%) | 27 (27%) | 0 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|---|
| 47 | DV | 99/101 (98%) | 56 (57%) | 15 (15%) | 28 (28%) | 0 | 0 |
| 48 | BW | 111/113 (98%) | 88 (79%) | 14 (13%) | 9 (8%) | 1 | 4 |
| 48 | DW | 111/113 (98%) | 85 (77%) | 18 (16%) | 8 (7%) | 1 | 5 |
| 49 | BX | 91/96 (95%) | 52 (57%) | 16 (18%) | 23 (25%) | 0 | 0 |
| 49 | DX | 91/96 (95%) | 50 (55%) | 18 (20%) | 23 (25%) | 0 | 0 |
| 50 | BY | 99/110 (90%) | 49 (50%) | 21 (21%) | 29 (29%) | 0 | 0 |
| 50 | DY | 99/110 (90%) | 47 (48%) | 23 (23%) | 29 (29%) | 0 | 0 |
| 51 | BZ | 175/206 (85%) | 115 (66%) | 44 (25%) | 16 (9%) | 1 | 3 |
| 51 | DZ | 175/206 (85%) | 115 (66%) | 41 (23%) | 19 (11%) | 0 | 2 |
| All | All | 11152/12056 (92%) | 7925 (71%) | 2047 (18%) | 1180 (11%) | 0 | 2 |

All (1180) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 15 | VAL |
| 2 | AB | 154 | LEU |
| 2 | AB | 165 | VAL |
| 2 | AB | 194 | PRO |
| 2 | AB | 195 | ASP |
| 3 | AC | 47 | LEU |
| 3 | AC | 189 | ALA |
| 4 | AD | 3 | ARG |
| 4 | AD | 13 | ARG |
| 4 | AD | 14 | ARG |
| 4 | AD | 44 | GLY |
| 4 | AD | 129 | ASN |
| 4 | AD | 163 | GLU |
| 5 | AE | 37 | ARG |
| 5 | AE | 115 | VAL |
| 6 | AF | 15 | ASP |
| 6 | AF | 40 | VAL |
| 6 | AF | 81 | ILE |
| 7 | AG | 33 | ASP |
| 8 | AH | 2 | LEU |
| 8 | AH | 54 | ASP |
| 9 | AI | 124 | GLN |
| 9 | AI | 125 | TYR |
| 10 | AJ | 59 | SER |
| 12 | AL | 27 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | AL | 47 | LYS |
| 12 | AL | 65 | GLU |
| 12 | AL | 91 | LYS |
| 12 | AL | 115 | LYS |
| 13 | AM | 12 | ASN |
| 13 | AM | 83 | ASP |
| 13 | AM | 106 | ASN |
| 17 | AQ | 34 | LYS |
| 18 | AR | 20 | ALA |
| 18 | AR | 45 | SER |
| 19 | AS | 28 | LYS |
| 20 | AT | 11 | SER |
| 20 | AT | 74 | LYS |
| 22 | B0 | 5 | LYS |
| 22 | B0 | 14 | ARG |
| 22 | B0 | 44 | ARG |
| 23 | B1 | 10 | LYS |
| 23 | B1 | 11 | ARG |
| 23 | B1 | 14 | VAL |
| 23 | B1 | 26 | ARG |
| 23 | B1 | 33 | LYS |
| 23 | B1 | 48 | LYS |
| 23 | B1 | 65 | SER |
| 23 | B1 | 81 | LYS |
| 23 | B1 | 83 | GLU |
| 23 | B1 | 86 | SER |
| 23 | B1 | 94 | LEU |
| 24 | B2 | 16 | LEU |
| 24 | B2 | 32 | LEU |
| 24 | B2 | 35 | LEU |
| 24 | B2 | 41 | ILE |
| 24 | B2 | 52 | ASP |
| 26 | B4 | 6 | HIS |
| 26 | B4 | 7 | PRO |
| 26 | B4 | 10 | VAL |
| 26 | B4 | 11 | PRO |
| 26 | B4 | 23 | GLU |
| 26 | B4 | 25 | TYR |
| 26 | B4 | 27 | THR |
| 26 | B4 | 29 | PRO |
| 27 | B5 | 4 | HIS |
| 27 | B5 | 32 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | B5 | 33 | CYS |
| 27 | B5 | 47 | PRO |
| 27 | B5 | 49 | CYS |
| 28 | B6 | 17 | LYS |
| 28 | B6 | 20 | ASN |
| 28 | B6 | 31 | PRO |
| 28 | B6 | 33 | LYS |
| 28 | B6 | 49 | HIS |
| 30 | B8 | 30 | ARG |
| 30 | B8 | 35 | GLN |
| 30 | B8 | 36 | LYS |
| 30 | B8 | 37 | SER |
| 30 | B8 | 52 | LYS |
| 33 | BD | 26 | LYS |
| 33 | BD | 28 | GLU |
| 33 | BD | 33 | LEU |
| 33 | BD | 159 | ALA |
| 33 | BD | 225 | ALA |
| 33 | BD | 267 | SER |
| 34 | BE | 2 | LYS |
| 34 | BE | 4 | ILE |
| 34 | BE | 53 | PRO |
| 34 | BE | 54 | GLN |
| 34 | BE | 57 | LYS |
| 34 | BE | 77 | ILE |
| 34 | BE | 82 | ARG |
| 34 | BE | 88 | GLY |
| 34 | BE | 90 | THR |
| 34 | BE | 93 | VAL |
| 34 | BE | 118 | LYS |
| 34 | BE | 129 | HIS |
| 35 | BF | 2 | LYS |
| 35 | BF | 89 | VAL |
| 36 | BG | 14 | GLU |
| 36 | BG | 47 | LYS |
| 36 | BG | 82 | LEU |
| 36 | BG | 86 | MET |
| 36 | BG | 87 | PRO |
| 36 | BG | 90 | LEU |
| 36 | BG | 96 | ARG |
| 36 | BG | 153 | ARG |
| 37 | BH | 13 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | BH | 41 | MET |
| 37 | BH | 89 | ILE |
| 37 | BH | 90 | LYS |
| 37 | BH | 126 | PRO |
| 37 | BH | 138 | LYS |
| 37 | BH | 153 | LYS |
| 37 | BH | 154 | PRO |
| 37 | BH | 155 | SER |
| 37 | BH | 156 | ALA |
| 37 | BH | 157 | TYR |
| 37 | BH | 165 | ALA |
| 37 | BH | 170 | ARG |
| 38 | BI | 93 | THR |
| 38 | BI | 133 | HIS |
| 39 | BN | 58 | ASP |
| 39 | BN | 74 | ARG |
| 39 | BN | 78 | TYR |
| 39 | BN | 79 | PRO |
| 39 | BN | 96 | GLU |
| 39 | BN | 130 | HIS |
| 40 | BO | 48 | PRO |
| 41 | BP | 6 | LEU |
| 41 | BP | 11 | GLY |
| 41 | BP | 14 | LYS |
| 41 | BP | 15 | ARG |
| 41 | BP | 18 | ARG |
| 41 | BP | 34 | GLY |
| 41 | BP | 35 | HIS |
| 41 | BP | 47 | ASP |
| 41 | BP | 48 | PRO |
| 41 | BP | 52 | GLU |
| 41 | BP | 56 | SER |
| 41 | BP | 57 | THR |
| 41 | BP | 58 | THR |
| 41 | BP | 65 | ARG |
| 41 | BP | 106 | LEU |
| 41 | BP | 107 | LYS |
| 41 | BP | 141 | ALA |
| 41 | BP | 146 | VAL |
| 41 | BP | 147 | LEU |
| 42 | BQ | 8 | LYS |
| 42 | BQ | 21 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BQ | 25 | ASP |
| 42 | BQ | 30 | GLY |
| 42 | BQ | 79 | LEU |
| 42 | BQ | 134 | ARG |
| 43 | BR | 4 | LEU |
| 43 | BR | 5 | LYS |
| 43 | BR | 8 | ARG |
| 43 | BR | 88 | ARG |
| 43 | BR | 117 | VAL |
| 44 | BS | 17 | ARG |
| 44 | BS | 57 | LYS |
| 44 | BS | 59 | LYS |
| 44 | BS | 67 | ARG |
| 44 | BS | 89 | ARG |
| 44 | BS | 92 | TYR |
| 44 | BS | 102 | ALA |
| 45 | BT | 13 | ARG |
| 45 | BT | 18 | ASP |
| 45 | BT | 24 | PRO |
| 45 | BT | 26 | ASP |
| 45 | BT | 30 | VAL |
| 45 | BT | 35 | LYS |
| 45 | BT | 58 | ASN |
| 45 | BT | 80 | SER |
| 45 | BT | 94 | ALA |
| 45 | BT | 107 | ASP |
| 45 | BT | 129 | ARG |
| 46 | BU | 32 | PHE |
| 46 | BU | 90 | VAL |
| 47 | BV | 23 | GLU |
| 47 | BV | 44 | LYS |
| 47 | BV | 47 | VAL |
| 47 | BV | 51 | VAL |
| 47 | BV | 52 | VAL |
| 47 | BV | 69 | LYS |
| 47 | BV | 73 | SER |
| 47 | BV | 80 | GLN |
| 47 | BV | 86 | GLY |
| 47 | BV | 90 | PRO |
| 48 | BW | 11 | ARG |
| 48 | BW | 58 | ALA |
| 49 | BX | 6 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | BX | 25 | LYS |
| 49 | BX | 34 | ALA |
| 49 | BX | 35 | THR |
| 49 | BX | 36 | LYS |
| 49 | BX | 60 | ARG |
| 49 | BX | 77 | LYS |
| 49 | BX | 84 | ALA |
| 49 | BX | 86 | GLY |
| 49 | BX | 89 | ILE |
| 50 | BY | 3 | VAL |
| 50 | BY | 7 | VAL |
| 50 | BY | 17 | SER |
| 50 | BY | 30 | VAL |
| 50 | BY | 38 | ILE |
| 50 | BY | 42 | VAL |
| 50 | BY | 48 | ALA |
| 50 | BY | 55 | TYR |
| 50 | BY | 56 | PRO |
| 50 | BY | 62 | GLU |
| 50 | BY | 77 | PRO |
| 50 | BY | 78 | ALA |
| 50 | BY | 98 | VAL |
| 50 | BY | 99 | CYS |
| 51 | BZ | 8 | TYR |
| 51 | BZ | 56 | VAL |
| 51 | BZ | 65 | GLN |
| 51 | BZ | 101 | PRO |
| 51 | BZ | 111 | VAL |
| 51 | BZ | 152 | ALA |
| 51 | BZ | 168 | GLU |
| 2 | CB | 15 | VAL |
| 2 | CB | 154 | LEU |
| 2 | CB | 165 | VAL |
| 2 | CB | 194 | PRO |
| 2 | CB | 195 | ASP |
| 3 | CC | 47 | LEU |
| 3 | CC | 189 | ALA |
| 4 | CD | 3 | ARG |
| 4 | CD | 13 | ARG |
| 4 | CD | 14 | ARG |
| 4 | CD | 44 | GLY |
| 4 | CD | 129 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | CD | 163 | GLU |
| 5 | CE | 37 | ARG |
| 6 | CF | 15 | ASP |
| 6 | CF | 40 | VAL |
| 6 | CF | 81 | ILE |
| 7 | CG | 7 | ALA |
| 7 | CG | 33 | ASP |
| 8 | CH | 54 | ASP |
| 9 | CI | 124 | GLN |
| 9 | CI | 125 | TYR |
| 10 | CJ | 59 | SER |
| 12 | CL | 27 | LEU |
| 12 | CL | 47 | LYS |
| 12 | CL | 65 | GLU |
| 12 | CL | 91 | LYS |
| 12 | CL | 115 | LYS |
| 13 | CM | 12 | ASN |
| 13 | CM | 83 | ASP |
| 13 | CM | 106 | ASN |
| 17 | CQ | 34 | LYS |
| 18 | CR | 20 | ALA |
| 18 | CR | 45 | SER |
| 19 | CS | 28 | LYS |
| 20 | CT | 11 | SER |
| 20 | CT | 74 | LYS |
| 22 | D0 | 5 | LYS |
| 22 | D0 | 14 | ARG |
| 22 | D0 | 44 | ARG |
| 23 | D1 | 10 | LYS |
| 23 | D1 | 11 | ARG |
| 23 | D1 | 14 | VAL |
| 23 | D1 | 26 | ARG |
| 23 | D1 | 48 | LYS |
| 23 | D1 | 65 | SER |
| 23 | D1 | 81 | LYS |
| 23 | D1 | 83 | GLU |
| 23 | D1 | 86 | SER |
| 23 | D1 | 94 | LEU |
| 24 | D2 | 16 | LEU |
| 24 | D2 | 32 | LEU |
| 24 | D2 | 35 | LEU |
| 24 | D2 | 41 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | D2 | 52 | ASP |
| 26 | D4 | 6 | HIS |
| 26 | D4 | 7 | PRO |
| 26 | D4 | 10 | VAL |
| 26 | D4 | 11 | PRO |
| 26 | D4 | 23 | GLU |
| 26 | D4 | 25 | TYR |
| 26 | D4 | 27 | THR |
| 26 | D4 | 29 | PRO |
| 27 | D5 | 4 | HIS |
| 27 | D5 | 32 | PRO |
| 27 | D5 | 33 | CYS |
| 27 | D5 | 47 | PRO |
| 27 | D5 | 49 | CYS |
| 28 | D6 | 17 | LYS |
| 28 | D6 | 20 | ASN |
| 28 | D6 | 31 | PRO |
| 28 | D6 | 33 | LYS |
| 28 | D6 | 49 | HIS |
| 30 | D8 | 30 | ARG |
| 30 | D8 | 35 | GLN |
| 30 | D8 | 36 | LYS |
| 30 | D8 | 37 | SER |
| 30 | D8 | 52 | LYS |
| 33 | DD | 26 | LYS |
| 33 | DD | 28 | GLU |
| 33 | DD | 33 | LEU |
| 33 | DD | 159 | ALA |
| 33 | DD | 225 | ALA |
| 34 | DE | 2 | LYS |
| 34 | DE | 4 | ILE |
| 34 | DE | 54 | GLN |
| 34 | DE | 77 | ILE |
| 34 | DE | 82 | ARG |
| 34 | DE | 88 | GLY |
| 34 | DE | 90 | THR |
| 34 | DE | 93 | VAL |
| 34 | DE | 118 | LYS |
| 34 | DE | 129 | HIS |
| 35 | DF | 2 | LYS |
| 35 | DF | 89 | VAL |
| 36 | DG | 14 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | DG | 47 | LYS |
| 36 | DG | 82 | LEU |
| 36 | DG | 86 | MET |
| 36 | DG | 87 | PRO |
| 36 | DG | 90 | LEU |
| 36 | DG | 96 | ARG |
| 36 | DG | 153 | ARG |
| 37 | DH | 13 | LYS |
| 37 | DH | 41 | MET |
| 37 | DH | 89 | ILE |
| 37 | DH | 90 | LYS |
| 37 | DH | 126 | PRO |
| 37 | DH | 138 | LYS |
| 37 | DH | 153 | LYS |
| 37 | DH | 154 | PRO |
| 37 | DH | 155 | SER |
| 37 | DH | 157 | TYR |
| 37 | DH | 165 | ALA |
| 37 | DH | 170 | ARG |
| 38 | DI | 78 | THR |
| 38 | DI | 93 | THR |
| 38 | DI | 133 | HIS |
| 39 | DN | 58 | ASP |
| 39 | DN | 68 | GLU |
| 39 | DN | 74 | ARG |
| 39 | DN | 78 | TYR |
| 39 | DN | 79 | PRO |
| 39 | DN | 96 | GLU |
| 39 | DN | 130 | HIS |
| 40 | DO | 48 | PRO |
| 41 | DP | 6 | LEU |
| 41 | DP | 11 | GLY |
| 41 | DP | 14 | LYS |
| 41 | DP | 15 | ARG |
| 41 | DP | 17 | LYS |
| 41 | DP | 18 | ARG |
| 41 | DP | 34 | GLY |
| 41 | DP | 35 | HIS |
| 41 | DP | 36 | LYS |
| 41 | DP | 42 | SER |
| 41 | DP | 47 | ASP |
| 41 | DP | 52 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | DP | 56 | SER |
| 41 | DP | 57 | THR |
| 41 | DP | 58 | THR |
| 41 | DP | 65 | ARG |
| 41 | DP | 103 | ALA |
| 41 | DP | 106 | LEU |
| 41 | DP | 107 | LYS |
| 41 | DP | 141 | ALA |
| 41 | DP | 146 | VAL |
| 41 | DP | 147 | LEU |
| 42 | DQ | 8 | LYS |
| 42 | DQ | 21 | THR |
| 42 | DQ | 25 | ASP |
| 42 | DQ | 30 | GLY |
| 42 | DQ | 79 | LEU |
| 43 | DR | 4 | LEU |
| 43 | DR | 5 | LYS |
| 43 | DR | 8 | ARG |
| 43 | DR | 88 | ARG |
| 43 | DR | 117 | VAL |
| 44 | DS | 17 | ARG |
| 44 | DS | 57 | LYS |
| 44 | DS | 59 | LYS |
| 44 | DS | 67 | ARG |
| 44 | DS | 89 | ARG |
| 44 | DS | 90 | GLY |
| 44 | DS | 92 | TYR |
| 44 | DS | 102 | ALA |
| 45 | DT | 13 | ARG |
| 45 | DT | 18 | ASP |
| 45 | DT | 24 | PRO |
| 45 | DT | 26 | ASP |
| 45 | DT | 30 | VAL |
| 45 | DT | 35 | LYS |
| 45 | DT | 58 | ASN |
| 45 | DT | 80 | SER |
| 45 | DT | 94 | ALA |
| 45 | DT | 107 | ASP |
| 45 | DT | 129 | ARG |
| 46 | DU | 32 | PHE |
| 46 | DU | 90 | VAL |
| 47 | DV | 23 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | DV | 44 | LYS |
| 47 | DV | 47 | VAL |
| 47 | DV | 51 | VAL |
| 47 | DV | 73 | SER |
| 47 | DV | 80 | GLN |
| 47 | DV | 86 | GLY |
| 47 | DV | 90 | PRO |
| 48 | DW | 11 | ARG |
| 49 | DX | 6 | ASP |
| 49 | DX | 25 | LYS |
| 49 | DX | 34 | ALA |
| 49 | DX | 35 | THR |
| 49 | DX | 36 | LYS |
| 49 | DX | 60 | ARG |
| 49 | DX | 77 | LYS |
| 49 | DX | 84 | ALA |
| 49 | DX | 86 | GLY |
| 49 | DX | 89 | ILE |
| 50 | DY | 3 | VAL |
| 50 | DY | 7 | VAL |
| 50 | DY | 17 | SER |
| 50 | DY | 30 | VAL |
| 50 | DY | 38 | ILE |
| 50 | DY | 42 | VAL |
| 50 | DY | 48 | ALA |
| 50 | DY | 55 | TYR |
| 50 | DY | 56 | PRO |
| 50 | DY | 62 | GLU |
| 50 | DY | 77 | PRO |
| 50 | DY | 78 | ALA |
| 50 | DY | 98 | VAL |
| 50 | DY | 99 | CYS |
| 51 | DZ | 8 | TYR |
| 51 | DZ | 56 | VAL |
| 51 | DZ | 65 | GLN |
| 51 | DZ | 101 | PRO |
| 51 | DZ | 111 | VAL |
| 51 | DZ | 152 | ALA |
| 51 | DZ | 168 | GLU |
| 2 | AB | 18 | GLY |
| 2 | AB | 24 | TRP |
| 2 | AB | 52 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 97 | TRP |
| 2 | AB | 239 | VAL |
| 3 | AC | 12 | LEU |
| 3 | AC | 101 | LEU |
| 3 | AC | 145 | GLY |
| 3 | AC | 156 | ARG |
| 4 | AD | 10 | ARG |
| 4 | AD | 42 | GLN |
| 4 | AD | 47 | ARG |
| 4 | AD | 60 | GLU |
| 4 | AD | 110 | PHE |
| 5 | AE | 72 | GLN |
| 5 | AE | 146 | ALA |
| 7 | AG | 7 | ALA |
| 7 | AG | 131 | LYS |
| 9 | AI | 23 | ASN |
| 9 | AI | 100 | GLY |
| 9 | AI | 117 | HIS |
| 11 | AK | 48 | ILE |
| 12 | AL | 28 | LYS |
| 12 | AL | 64 | TYR |
| 12 | AL | 83 | VAL |
| 13 | AM | 100 | GLY |
| 14 | AN | 16 | PHE |
| 16 | AP | 11 | SER |
| 16 | AP | 28 | ARG |
| 17 | AQ | 49 | GLU |
| 17 | AQ | 61 | GLU |
| 19 | AS | 10 | PHE |
| 19 | AS | 29 | ARG |
| 19 | AS | 80 | TYR |
| 20 | AT | 95 | ALA |
| 20 | AT | 101 | GLY |
| 23 | B1 | 27 | GLU |
| 23 | B1 | 49 | VAL |
| 23 | B1 | 64 | ALA |
| 23 | B1 | 79 | GLY |
| 24 | B2 | 42 | GLY |
| 24 | B2 | 49 | LYS |
| 24 | B2 | 51 | ARG |
| 25 | B3 | 13 | ILE |
| 26 | B4 | 9 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | B4 | 16 | CYS |
| 26 | B4 | 20 | ASN |
| 27 | B5 | 48 | GLU |
| 27 | B5 | 52 | TYR |
| 27 | B5 | 57 | VAL |
| 28 | B6 | 19 | ARG |
| 28 | B6 | 23 | THR |
| 28 | B6 | 29 | ASN |
| 28 | B6 | 43 | CYS |
| 28 | B6 | 52 | VAL |
| 30 | B8 | 3 | LYS |
| 30 | B8 | 32 | LEU |
| 30 | B8 | 51 | ALA |
| 30 | B8 | 64 | TYR |
| 33 | BD | 3 | VAL |
| 33 | BD | 34 | VAL |
| 33 | BD | 156 | ALA |
| 33 | BD | 210 | GLY |
| 33 | BD | 239 | ARG |
| 33 | BD | 241 | PRO |
| 34 | BE | 17 | ASP |
| 34 | BE | 60 | ASN |
| 34 | BE | 71 | GLY |
| 34 | BE | 72 | VAL |
| 35 | BF | 14 | PRO |
| 35 | BF | 21 | ALA |
| 35 | BF | 66 | PRO |
| 35 | BF | 127 | GLU |
| 36 | BG | 30 | GLU |
| 37 | BH | 44 | VAL |
| 37 | BH | 47 | GLU |
| 37 | BH | 84 | SER |
| 37 | BH | 92 | ILE |
| 37 | BH | 93 | GLY |
| 37 | BH | 98 | LEU |
| 38 | BI | 13 | GLY |
| 38 | BI | 30 | LEU |
| 38 | BI | 42 | SER |
| 38 | BI | 78 | THR |
| 38 | BI | 120 | ILE |
| 38 | BI | 128 | LEU |
| 38 | BI | 145 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | BN | 57 | ALA |
| 39 | BN | 68 | GLU |
| 39 | BN | 95 | PRO |
| 40 | BO | 5 | GLN |
| 41 | BP | 17 | LYS |
| 41 | BP | 31 | ALA |
| 41 | BP | 36 | LYS |
| 41 | BP | 42 | SER |
| 41 | BP | 49 | ARG |
| 41 | BP | 66 | GLY |
| 41 | BP | 98 | GLU |
| 41 | BP | 103 | ALA |
| 41 | BP | 104 | GLY |
| 41 | BP | 108 | LYS |
| 42 | BQ | 19 | GLY |
| 42 | BQ | 83 | MET |
| 43 | BR | 107 | ASP |
| 44 | BS | 14 | VAL |
| 44 | BS | 45 | GLY |
| 44 | BS | 58 | LEU |
| 44 | BS | 85 | VAL |
| 44 | BS | 90 | GLY |
| 44 | BS | 94 | TYR |
| 44 | BS | 96 | GLY |
| 44 | BS | 100 | ALA |
| 45 | BT | 28 | VAL |
| 45 | BT | 83 | ILE |
| 46 | BU | 91 | ASP |
| 46 | BU | 92 | ARG |
| 47 | BV | 28 | GLU |
| 47 | BV | 41 | GLY |
| 47 | BV | 50 | PRO |
| 47 | BV | 53 | GLU |
| 47 | BV | 54 | GLY |
| 47 | BV | 55 | ALA |
| 47 | BV | 68 | LYS |
| 47 | BV | 70 | ILE |
| 47 | BV | 72 | VAL |
| 47 | BV | 91 | TYR |
| 48 | BW | 56 | ALA |
| 48 | BW | 63 | ASP |
| 48 | BW | 65 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | BX | 41 | ASN |
| 49 | BX | 59 | VAL |
| 49 | BX | 72 | LYS |
| 49 | BX | 74 | PRO |
| 50 | BY | 80 | GLY |
| 50 | BY | 81 | LYS |
| 50 | BY | 90 | LEU |
| 51 | BZ | 80 | ARG |
| 51 | BZ | 81 | ARG |
| 51 | BZ | 119 | GLU |
| 2 | CB | 18 | GLY |
| 2 | CB | 24 | TRP |
| 2 | CB | 52 | GLU |
| 2 | CB | 97 | TRP |
| 2 | CB | 239 | VAL |
| 3 | CC | 4 | LYS |
| 3 | CC | 12 | LEU |
| 3 | CC | 145 | GLY |
| 3 | CC | 156 | ARG |
| 4 | CD | 5 | ILE |
| 4 | CD | 42 | GLN |
| 4 | CD | 47 | ARG |
| 4 | CD | 60 | GLU |
| 4 | CD | 110 | PHE |
| 5 | CE | 72 | GLN |
| 5 | CE | 115 | VAL |
| 5 | CE | 146 | ALA |
| 7 | CG | 131 | LYS |
| 8 | CH | 2 | LEU |
| 9 | CI | 23 | ASN |
| 9 | CI | 100 | GLY |
| 9 | CI | 117 | HIS |
| 11 | CK | 48 | ILE |
| 12 | CL | 28 | LYS |
| 12 | CL | 64 | TYR |
| 12 | CL | 83 | VAL |
| 12 | CL | 106 | ASP |
| 13 | CM | 100 | GLY |
| 14 | CN | 16 | PHE |
| 17 | CQ | 49 | GLU |
| 17 | CQ | 61 | GLU |
| 19 | CS | 10 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | CS | 29 | ARG |
| 19 | CS | 80 | TYR |
| 20 | CT | 95 | ALA |
| 20 | CT | 101 | GLY |
| 23 | D1 | 27 | GLU |
| 23 | D1 | 33 | LYS |
| 23 | D1 | 49 | VAL |
| 23 | D1 | 64 | ALA |
| 23 | D1 | 79 | GLY |
| 24 | D2 | 42 | GLY |
| 24 | D2 | 49 | LYS |
| 25 | D3 | 13 | ILE |
| 26 | D4 | 9 | LEU |
| 26 | D4 | 16 | CYS |
| 26 | D4 | 20 | ASN |
| 26 | D4 | 31 | ILE |
| 27 | D5 | 37 | LYS |
| 27 | D5 | 48 | GLU |
| 27 | D5 | 52 | TYR |
| 27 | D5 | 57 | VAL |
| 28 | D6 | 19 | ARG |
| 28 | D6 | 23 | THR |
| 28 | D6 | 52 | VAL |
| 30 | D8 | 32 | LEU |
| 30 | D8 | 51 | ALA |
| 30 | D8 | 64 | TYR |
| 33 | DD | 3 | VAL |
| 33 | DD | 156 | ALA |
| 33 | DD | 241 | PRO |
| 33 | DD | 242 | ARG |
| 33 | DD | 267 | SER |
| 34 | DE | 17 | ASP |
| 34 | DE | 53 | PRO |
| 34 | DE | 57 | LYS |
| 34 | DE | 71 | GLY |
| 34 | DE | 72 | VAL |
| 34 | DE | 131 | ALA |
| 35 | DF | 7 | TYR |
| 35 | DF | 14 | PRO |
| 35 | DF | 21 | ALA |
| 35 | DF | 66 | PRO |
| 35 | DF | 127 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | DG | 30 | GLU |
| 36 | DG | 115 | ARG |
| 37 | DH | 44 | VAL |
| 37 | DH | 84 | SER |
| 37 | DH | 92 | ILE |
| 37 | DH | 93 | GLY |
| 37 | DH | 98 | LEU |
| 37 | DH | 156 | ALA |
| 38 | DI | 13 | GLY |
| 38 | DI | 30 | LEU |
| 38 | DI | 42 | SER |
| 38 | DI | 89 | TYR |
| 38 | DI | 120 | ILE |
| 38 | DI | 128 | LEU |
| 38 | DI | 145 | VAL |
| 39 | DN | 57 | ALA |
| 39 | DN | 95 | PRO |
| 40 | DO | 5 | GLN |
| 41 | DP | 31 | ALA |
| 41 | DP | 32 | THR |
| 41 | DP | 48 | PRO |
| 41 | DP | 49 | ARG |
| 41 | DP | 66 | GLY |
| 41 | DP | 98 | GLU |
| 41 | DP | 104 | GLY |
| 41 | DP | 108 | LYS |
| 42 | DQ | 19 | GLY |
| 42 | DQ | 83 | MET |
| 42 | DQ | 134 | ARG |
| 43 | DR | 107 | ASP |
| 43 | DR | 116 | LEU |
| 44 | DS | 14 | VAL |
| 44 | DS | 45 | GLY |
| 44 | DS | 58 | LEU |
| 44 | DS | 77 | ALA |
| 44 | DS | 85 | VAL |
| 44 | DS | 94 | TYR |
| 44 | DS | 96 | GLY |
| 44 | DS | 100 | ALA |
| 45 | DT | 28 | VAL |
| 45 | DT | 83 | ILE |
| 46 | DU | 89 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | DU | 91 | ASP |
| 46 | DU | 92 | ARG |
| 47 | DV | 28 | GLU |
| 47 | DV | 41 | GLY |
| 47 | DV | 50 | PRO |
| 47 | DV | 52 | VAL |
| 47 | DV | 53 | GLU |
| 47 | DV | 54 | GLY |
| 47 | DV | 55 | ALA |
| 47 | DV | 68 | LYS |
| 47 | DV | 69 | LYS |
| 47 | DV | 70 | ILE |
| 47 | DV | 72 | VAL |
| 47 | DV | 91 | TYR |
| 48 | DW | 56 | ALA |
| 48 | DW | 58 | ALA |
| 48 | DW | 63 | ASP |
| 49 | DX | 37 | THR |
| 49 | DX | 41 | ASN |
| 49 | DX | 59 | VAL |
| 49 | DX | 72 | LYS |
| 49 | DX | 81 | VAL |
| 50 | DY | 24 | VAL |
| 50 | DY | 80 | GLY |
| 50 | DY | 90 | LEU |
| 51 | DZ | 80 | ARG |
| 51 | DZ | 81 | ARG |
| 51 | DZ | 119 | GLU |
| 51 | DZ | 142 | SER |
| 2 | AB | 26 | PRO |
| 2 | AB | 106 | LYS |
| 2 | AB | 204 | ASN |
| 3 | AC | 4 | LYS |
| 4 | AD | 4 | TYR |
| 4 | AD | 5 | ILE |
| 4 | AD | 189 | PRO |
| 6 | AF | 39 | LYS |
| 6 | AF | 96 | PRO |
| 8 | AH | 63 | LEU |
| 9 | AI | 25 | LYS |
| 10 | AJ | 36 | GLY |
| 12 | AL | 18 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | AL | 23 | LYS |
| 12 | AL | 63 | GLY |
| 12 | AL | 106 | ASP |
| 13 | AM | 21 | TYR |
| 14 | AN | 52 | GLN |
| 16 | AP | 17 | TYR |
| 16 | AP | 76 | GLN |
| 17 | AQ | 3 | LYS |
| 17 | AQ | 4 | LYS |
| 19 | AS | 27 | GLU |
| 20 | AT | 49 | ALA |
| 20 | AT | 97 | ALA |
| 21 | AU | 25 | LYS |
| 24 | B2 | 40 | SER |
| 25 | B3 | 2 | PRO |
| 26 | B4 | 3 | GLU |
| 26 | B4 | 24 | THR |
| 26 | B4 | 30 | GLU |
| 26 | B4 | 31 | ILE |
| 27 | B5 | 37 | LYS |
| 28 | B6 | 18 | ARG |
| 28 | B6 | 28 | ARG |
| 30 | B8 | 31 | HIS |
| 33 | BD | 242 | ARG |
| 34 | BE | 58 | ARG |
| 34 | BE | 131 | ALA |
| 35 | BF | 7 | TYR |
| 35 | BF | 11 | VAL |
| 35 | BF | 25 | PRO |
| 35 | BF | 133 | ASN |
| 36 | BG | 21 | ARG |
| 36 | BG | 43 | LEU |
| 36 | BG | 115 | ARG |
| 36 | BG | 128 | ARG |
| 37 | BH | 117 | PRO |
| 37 | BH | 151 | ILE |
| 37 | BH | 159 | GLU |
| 38 | BI | 14 | ASP |
| 38 | BI | 89 | TYR |
| 38 | BI | 134 | PRO |
| 39 | BN | 127 | ASP |
| 39 | BN | 129 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | BP | 23 | PRO |
| 41 | BP | 32 | THR |
| 41 | BP | 40 | SER |
| 41 | BP | 89 | ALA |
| 41 | BP | 102 | ARG |
| 41 | BP | 110 | TYR |
| 42 | BQ | 11 | LYS |
| 42 | BQ | 15 | GLY |
| 42 | BQ | 89 | ASN |
| 42 | BQ | 136 | ALA |
| 43 | BR | 116 | LEU |
| 44 | BS | 15 | ARG |
| 44 | BS | 23 | ARG |
| 44 | BS | 77 | ALA |
| 45 | BT | 115 | ARG |
| 46 | BU | 89 | GLU |
| 46 | BU | 109 | LEU |
| 47 | BV | 3 | ALA |
| 48 | BW | 59 | VAL |
| 49 | BX | 24 | GLY |
| 49 | BX | 37 | THR |
| 49 | BX | 71 | GLY |
| 49 | BX | 73 | ARG |
| 49 | BX | 81 | VAL |
| 50 | BY | 24 | VAL |
| 50 | BY | 29 | GLU |
| 50 | BY | 39 | VAL |
| 50 | BY | 66 | PRO |
| 51 | BZ | 52 | SER |
| 51 | BZ | 142 | SER |
| 51 | BZ | 166 | SER |
| 2 | CB | 26 | PRO |
| 2 | CB | 106 | LYS |
| 3 | CC | 100 | ALA |
| 3 | CC | 101 | LEU |
| 4 | CD | 4 | TYR |
| 4 | CD | 7 | PRO |
| 4 | CD | 10 | ARG |
| 4 | CD | 189 | PRO |
| 6 | CF | 39 | LYS |
| 6 | CF | 96 | PRO |
| 8 | CH | 63 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | CI | 25 | LYS |
| 10 | CJ | 36 | GLY |
| 11 | CK | 100 | ALA |
| 12 | CL | 63 | GLY |
| 13 | CM | 21 | TYR |
| 14 | CN | 52 | GLN |
| 16 | CP | 17 | TYR |
| 16 | CP | 28 | ARG |
| 16 | CP | 76 | GLN |
| 17 | CQ | 3 | LYS |
| 17 | CQ | 4 | LYS |
| 19 | CS | 27 | GLU |
| 20 | CT | 97 | ALA |
| 21 | CU | 25 | LYS |
| 24 | D2 | 40 | SER |
| 24 | D2 | 51 | ARG |
| 25 | D3 | 2 | PRO |
| 26 | D4 | 3 | GLU |
| 26 | D4 | 24 | THR |
| 26 | D4 | 30 | GLU |
| 28 | D6 | 18 | ARG |
| 28 | D6 | 28 | ARG |
| 28 | D6 | 29 | ASN |
| 28 | D6 | 43 | CYS |
| 30 | D8 | 3 | LYS |
| 30 | D8 | 25 | MET |
| 30 | D8 | 31 | HIS |
| 30 | D8 | 38 | GLY |
| 33 | DD | 34 | VAL |
| 34 | DE | 60 | ASN |
| 34 | DE | 76 | ARG |
| 35 | DF | 11 | VAL |
| 35 | DF | 25 | PRO |
| 36 | DG | 21 | ARG |
| 36 | DG | 43 | LEU |
| 37 | DH | 47 | GLU |
| 37 | DH | 117 | PRO |
| 37 | DH | 159 | GLU |
| 38 | DI | 14 | ASP |
| 38 | DI | 134 | PRO |
| 39 | DN | 127 | ASP |
| 39 | DN | 129 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | DP | 23 | PRO |
| 41 | DP | 89 | ALA |
| 41 | DP | 102 | ARG |
| 41 | DP | 110 | TYR |
| 42 | DQ | 11 | LYS |
| 42 | DQ | 20 | ALA |
| 42 | DQ | 51 | ARG |
| 42 | DQ | 89 | ASN |
| 42 | DQ | 136 | ALA |
| 44 | DS | 15 | ARG |
| 45 | DT | 115 | ARG |
| 47 | DV | 3 | ALA |
| 47 | DV | 19 | LYS |
| 47 | DV | 71 | LEU |
| 47 | DV | 74 | LYS |
| 48 | DW | 65 | LEU |
| 49 | DX | 24 | GLY |
| 49 | DX | 71 | GLY |
| 49 | DX | 73 | ARG |
| 49 | DX | 74 | PRO |
| 49 | DX | 88 | LYS |
| 50 | DY | 29 | GLU |
| 50 | DY | 39 | VAL |
| 50 | DY | 66 | PRO |
| 50 | DY | 81 | LYS |
| 51 | DZ | 52 | SER |
| 51 | DZ | 64 | GLY |
| 51 | DZ | 166 | SER |
| 2 | AB | 130 | ARG |
| 2 | AB | 240 | GLN |
| 3 | AC | 100 | ALA |
| 4 | AD | 7 | PRO |
| 4 | AD | 24 | GLU |
| 5 | AE | 71 | LEU |
| 5 | AE | 129 | ILE |
| 5 | AE | 132 | ALA |
| 8 | AH | 68 | ARG |
| 10 | AJ | 23 | ILE |
| 11 | AK | 100 | ALA |
| 11 | AK | 106 | LYS |
| 12 | AL | 51 | ALA |
| 15 | AO | 73 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | AO | 88 | ARG |
| 16 | AP | 16 | HIS |
| 16 | AP | 39 | TYR |
| 19 | AS | 30 | LEU |
| 20 | AT | 84 | LEU |
| 23 | B1 | 28 | GLY |
| 28 | B6 | 44 | ARG |
| 30 | B8 | 38 | GLY |
| 34 | BE | 76 | ARG |
| 34 | BE | 89 | ASP |
| 35 | BF | 9 | ILE |
| 35 | BF | 10 | PRO |
| 35 | BF | 67 | GLN |
| 36 | BG | 81 | LYS |
| 37 | BH | 21 | PRO |
| 37 | BH | 81 | GLU |
| 38 | BI | 53 | ALA |
| 38 | BI | 85 | GLU |
| 39 | BN | 83 | LYS |
| 41 | BP | 109 | GLY |
| 42 | BQ | 51 | ARG |
| 44 | BS | 13 | ARG |
| 44 | BS | 24 | LEU |
| 44 | BS | 53 | SER |
| 44 | BS | 103 | GLU |
| 45 | BT | 41 | ARG |
| 45 | BT | 55 | ASN |
| 45 | BT | 59 | THR |
| 47 | BV | 15 | GLU |
| 47 | BV | 19 | LYS |
| 47 | BV | 71 | LEU |
| 47 | BV | 74 | LYS |
| 49 | BX | 4 | ALA |
| 49 | BX | 88 | LYS |
| 50 | BY | 21 | LYS |
| 50 | BY | 67 | LEU |
| 51 | BZ | 64 | GLY |
| 2 | CB | 84 | GLU |
| 2 | CB | 130 | ARG |
| 2 | CB | 240 | GLN |
| 3 | CC | 15 | THR |
| 10 | CJ | 23 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | CK | 106 | LYS |
| 12 | CL | 18 | VAL |
| 12 | CL | 23 | LYS |
| 12 | CL | 51 | ALA |
| 15 | CO | 88 | ARG |
| 16 | CP | 11 | SER |
| 16 | CP | 16 | HIS |
| 16 | CP | 39 | TYR |
| 16 | CP | 69 | THR |
| 19 | CS | 30 | LEU |
| 20 | CT | 49 | ALA |
| 23 | D1 | 28 | GLY |
| 23 | D1 | 82 | LEU |
| 33 | DD | 210 | GLY |
| 34 | DE | 58 | ARG |
| 34 | DE | 89 | ASP |
| 35 | DF | 9 | ILE |
| 35 | DF | 10 | PRO |
| 36 | DG | 81 | LYS |
| 36 | DG | 128 | ARG |
| 37 | DH | 21 | PRO |
| 37 | DH | 81 | GLU |
| 38 | DI | 85 | GLU |
| 41 | DP | 33 | ARG |
| 41 | DP | 40 | SER |
| 41 | DP | 109 | GLY |
| 43 | DR | 12 | ARG |
| 44 | DS | 23 | ARG |
| 44 | DS | 24 | LEU |
| 44 | DS | 53 | SER |
| 44 | DS | 103 | GLU |
| 46 | DU | 109 | LEU |
| 47 | DV | 15 | GLU |
| 48 | DW | 6 | ILE |
| 48 | DW | 57 | ASN |
| 49 | DX | 4 | ALA |
| 49 | DX | 19 | ALA |
| 49 | DX | 68 | ARG |
| 50 | DY | 21 | LYS |
| 50 | DY | 37 | VAL |
| 2 | AB | 229 | VAL |
| 3 | AC | 15 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 60 | ALA |
| 3 | AC | 61 | ALA |
| 4 | AD | 181 | MET |
| 5 | AE | 8 | GLU |
| 5 | AE | 77 | PRO |
| 8 | AH | 86 | ILE |
| 9 | AI | 97 | LYS |
| 12 | AL | 19 | ARG |
| 16 | AP | 69 | THR |
| 18 | AR | 87 | ARG |
| 20 | AT | 98 | PRO |
| 22 | B0 | 83 | PRO |
| 23 | B1 | 82 | LEU |
| 24 | B2 | 33 | MET |
| 34 | BE | 132 | HIS |
| 35 | BF | 24 | LEU |
| 36 | BG | 117 | PHE |
| 36 | BG | 129 | GLY |
| 36 | BG | 130 | ASN |
| 36 | BG | 140 | ILE |
| 37 | BH | 85 | LYS |
| 37 | BH | 139 | GLN |
| 39 | BN | 134 | ARG |
| 40 | BO | 29 | ASN |
| 41 | BP | 37 | GLY |
| 42 | BQ | 7 | MET |
| 42 | BQ | 20 | ALA |
| 43 | BR | 12 | ARG |
| 44 | BS | 54 | LEU |
| 46 | BU | 85 | LYS |
| 46 | BU | 102 | GLU |
| 47 | BV | 79 | VAL |
| 48 | BW | 6 | ILE |
| 48 | BW | 57 | ASN |
| 48 | BW | 93 | ALA |
| 50 | BY | 27 | VAL |
| 50 | BY | 37 | VAL |
| 50 | BY | 53 | PRO |
| 51 | BZ | 41 | LEU |
| 51 | BZ | 136 | PHE |
| 2 | CB | 204 | ASN |
| 2 | CB | 229 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CC | 60 | ALA |
| 3 | CC | 61 | ALA |
| 4 | CD | 17 | VAL |
| 4 | CD | 24 | GLU |
| 4 | CD | 181 | MET |
| 5 | CE | 77 | PRO |
| 5 | CE | 129 | ILE |
| 5 | CE | 132 | ALA |
| 5 | CE | 140 | ARG |
| 8 | CH | 68 | ARG |
| 8 | CH | 86 | ILE |
| 9 | CI | 97 | LYS |
| 11 | CK | 62 | GLN |
| 12 | CL | 19 | ARG |
| 15 | CO | 73 | GLU |
| 18 | CR | 78 | LEU |
| 18 | CR | 87 | ARG |
| 20 | CT | 98 | PRO |
| 24 | D2 | 33 | MET |
| 24 | D2 | 45 | SER |
| 24 | D2 | 48 | HIS |
| 34 | DE | 144 | ARG |
| 34 | DE | 201 | THR |
| 35 | DF | 24 | LEU |
| 36 | DG | 117 | PHE |
| 36 | DG | 130 | ASN |
| 36 | DG | 140 | ILE |
| 37 | DH | 151 | ILE |
| 39 | DN | 4 | TYR |
| 39 | DN | 83 | LYS |
| 44 | DS | 13 | ARG |
| 45 | DT | 41 | ARG |
| 47 | DV | 79 | VAL |
| 50 | DY | 53 | PRO |
| 50 | DY | 67 | LEU |
| 51 | DZ | 41 | LEU |
| 51 | DZ | 136 | PHE |
| 2 | AB | 191 | ASP |
| 4 | AD | 17 | VAL |
| 5 | AE | 133 | TYR |
| 9 | AI | 24 | GLY |
| 9 | AI | 123 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | AK | 62 | GLN |
| 16 | AP | 41 | PRO |
| 19 | AS | 5 | LEU |
| 30 | B8 | 25 | MET |
| 37 | BH | 158 | HIS |
| 39 | BN | 94 | HIS |
| 41 | BP | 38 | GLN |
| 41 | BP | 140 | ALA |
| 43 | BR | 106 | GLY |
| 44 | BS | 98 | VAL |
| 49 | BX | 68 | ARG |
| 49 | BX | 69 | TYR |
| 50 | BY | 40 | GLU |
| 5 | CE | 71 | LEU |
| 9 | CI | 24 | GLY |
| 9 | CI | 123 | PRO |
| 11 | CK | 105 | VAL |
| 15 | CO | 38 | ARG |
| 16 | CP | 41 | PRO |
| 18 | CR | 57 | GLY |
| 19 | CS | 5 | LEU |
| 22 | D0 | 83 | PRO |
| 28 | D6 | 44 | ARG |
| 33 | DD | 239 | ARG |
| 36 | DG | 22 | ARG |
| 37 | DH | 85 | LYS |
| 39 | DN | 94 | HIS |
| 41 | DP | 38 | GLN |
| 43 | DR | 42 | LYS |
| 45 | DT | 59 | THR |
| 46 | DU | 85 | LYS |
| 47 | DV | 64 | HIS |
| 50 | DY | 26 | LYS |
| 50 | DY | 27 | VAL |
| 51 | DZ | 6 | LYS |
| 5 | AE | 148 | VAL |
| 8 | AH | 51 | VAL |
| 16 | AP | 15 | PRO |
| 36 | BG | 68 | PRO |
| 38 | BI | 34 | GLY |
| 39 | BN | 80 | GLY |
| 41 | BP | 24 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BQ | 90 | VAL |
| 5 | CE | 128 | PRO |
| 8 | CH | 51 | VAL |
| 36 | DG | 129 | GLY |
| 38 | DI | 34 | GLY |
| 39 | DN | 80 | GLY |
| 39 | DN | 134 | ARG |
| 42 | DQ | 90 | VAL |
| 43 | DR | 106 | GLY |
| 3 | AC | 108 | ASN |
| 5 | AE | 128 | PRO |
| 10 | AJ | 91 | PRO |
| 11 | AK | 105 | VAL |
| 17 | AQ | 80 | GLY |
| 18 | AR | 57 | GLY |
| 39 | BN | 77 | GLY |
| 47 | BV | 22 | VAL |
| 50 | BY | 31 | LEU |
| 50 | BY | 96 | ILE |
| 3 | CC | 108 | ASN |
| 5 | CE | 148 | VAL |
| 8 | CH | 118 | VAL |
| 10 | CJ | 91 | PRO |
| 17 | CQ | 80 | GLY |
| 36 | DG | 68 | PRO |
| 50 | DY | 31 | LEU |
| 4 | AD | 56 | VAL |
| 8 | AH | 118 | VAL |
| 23 | B1 | 22 | GLY |
| 41 | BP | 144 | GLU |
| 4 | CD | 56 | VAL |
| 7 | CG | 14 | PRO |
| 16 | CP | 15 | PRO |
| 18 | CR | 22 | VAL |
| 34 | DE | 56 | PRO |
| 38 | DI | 111 | PRO |
| 41 | DP | 24 | GLY |
| 46 | DU | 102 | GLU |
| 47 | DV | 22 | VAL |
| 50 | DY | 18 | GLY |
| 51 | DZ | 47 | VAL |
| 3 | AC | 66 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 81 | GLY |
| 7 | AG | 14 | PRO |
| 15 | AO | 19 | PRO |
| 16 | AP | 66 | PRO |
| 38 | BI | 111 | PRO |
| 5 | CE | 49 | PRO |
| 16 | CP | 66 | PRO |
| 35 | DF | 84 | VAL |
| 41 | DP | 144 | GLU |
| 42 | DQ | 15 | GLY |
| 44 | DS | 98 | VAL |
| 48 | DW | 59 | VAL |
| 51 | DZ | 39 | VAL |
| 34 | BE | 61 | ARG |
| 3 | CC | 66 | VAL |
| 3 | CC | 81 | GLY |
| 25 | D3 | 59 | VAL |
| 33 | DD | 35 | LYS |
| 39 | DN | 77 | GLY |
| 38 | DI | 132 | PRO |
| 38 | BI | 132 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | AB | 202/220 (92%) | 178 (88%) | 24 (12%) | 5 | 22 |
| 2 | CB | 202/220 (92%) | 178 (88%) | 24 (12%) | 5 | 22 |
| 3 | AC | 160/188 (85%) | 153 (96%) | 7 (4%) | 28 | 65 |
| 3 | CC | 160/188 (85%) | 153 (96%) | 7 (4%) | 28 | 65 |
| 4 | AD | 180/181 (99%) | 150 (83%) | 30 (17%) | 2 | 11 |
| 4 | CD | 180/181 (99%) | 153 (85%) | 27 (15%) | 3 | 14 |
| 5 | AE | 115/122 (94%) | 97 (84%) | 18 (16%) | 2 | 13 |
| 5 | CE | 115/122 (94%) | 97 (84%) | 18 (16%) | 2 | 13 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 6 | AF | 90/90 (100%) | 80 (89%) | 10 (11%) | 6 | 25 |
| 6 | CF | 90/90 (100%) | 79 (88%) | 11 (12%) | 5 | 21 |
| 7 | AG | 126/127 (99%) | 123 (98%) | 3 (2%) | 49 | 79 |
| 7 | CG | 126/127 (99%) | 122 (97%) | 4 (3%) | 39 | 74 |
| 8 | AH | 119/119 (100%) | 110 (92%) | 9 (8%) | 13 | 43 |
| 8 | CH | 119/119 (100%) | 110 (92%) | 9 (8%) | 13 | 43 |
| 9 | AI | 98/99 (99%) | 88 (90%) | 10 (10%) | 7 | 28 |
| 9 | CI | 98/99 (99%) | 89 (91%) | 9 (9%) | 9 | 34 |
| 10 | AJ | 88/92 (96%) | 78 (89%) | 10 (11%) | 5 | 24 |
| 10 | CJ | 88/92 (96%) | 78 (89%) | 10 (11%) | 5 | 24 |
| 11 | AK | 90/99 (91%) | 84 (93%) | 6 (7%) | 16 | 49 |
| 11 | CK | 90/99 (91%) | 84 (93%) | 6 (7%) | 16 | 49 |
| 12 | AL | 104/111 (94%) | 93 (89%) | 11 (11%) | 6 | 26 |
| 12 | CL | 104/111 (94%) | 92 (88%) | 12 (12%) | 5 | 24 |
| 13 | AM | 93/101 (92%) | 87 (94%) | 6 (6%) | 17 | 50 |
| 13 | CM | 93/101 (92%) | 88 (95%) | 5 (5%) | 22 | 57 |
| 14 | AN | 49/50 (98%) | 46 (94%) | 3 (6%) | 18 | 53 |
| 14 | CN | 49/50 (98%) | 46 (94%) | 3 (6%) | 18 | 53 |
| 15 | AO | 79/80 (99%) | 71 (90%) | 8 (10%) | 7 | 29 |
| 15 | CO | 79/80 (99%) | 71 (90%) | 8 (10%) | 7 | 29 |
| 16 | AP | 72/74 (97%) | 57 (79%) | 15 (21%) | 1 | 5 |
| 16 | CP | 72/74 (97%) | 57 (79%) | 15 (21%) | 1 | 5 |
| 17 | AQ | 94/97 (97%) | 89 (95%) | 5 (5%) | 22 | 58 |
| 17 | CQ | 94/97 (97%) | 89 (95%) | 5 (5%) | 22 | 58 |
| 18 | AR | 61/77 (79%) | 56 (92%) | 5 (8%) | 11 | 39 |
| 18 | CR | 61/77 (79%) | 57 (93%) | 4 (7%) | 16 | 49 |
| 19 | AS | 69/80 (86%) | 62 (90%) | 7 (10%) | 7 | 29 |
| 19 | CS | 69/80 (86%) | 62 (90%) | 7 (10%) | 7 | 29 |
| 20 | AT | 76/82 (93%) | 65 (86%) | 11 (14%) | 3 | 15 |
| 20 | CT | 76/82 (93%) | 65 (86%) | 11 (14%) | 3 | 15 |
| 21 | AU | 19/22 (86%) | 19 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 21 | CU | 19/22 (86%) | 19 (100%) | 0 | 100 | 100 |
| 22 | B0 | 61/67 (91%) | 53 (87%) | 8 (13%) | 4 | 18 |
| 22 | D0 | 61/67 (91%) | 53 (87%) | 8 (13%) | 4 | 18 |
| 23 | B1 | 73/83 (88%) | 53 (73%) | 20 (27%) | 0 | 2 |
| 23 | D1 | 73/83 (88%) | 55 (75%) | 18 (25%) | 0 | 3 |
| 24 | B2 | 46/67 (69%) | 26 (56%) | 20 (44%) | 0 | 0 |
| 24 | D2 | 46/67 (69%) | 27 (59%) | 19 (41%) | 0 | 0 |
| 25 | B3 | 51/52 (98%) | 48 (94%) | 3 (6%) | 19 | 54 |
| 25 | D3 | 51/52 (98%) | 48 (94%) | 3 (6%) | 19 | 54 |
| 27 | B5 | 51/52 (98%) | 38 (74%) | 13 (26%) | 0 | 3 |
| 27 | D5 | 51/52 (98%) | 38 (74%) | 13 (26%) | 0 | 3 |
| 28 | B6 | 43/52 (83%) | 25 (58%) | 18 (42%) | 0 | 0 |
| 28 | D6 | 43/52 (83%) | 26 (60%) | 17 (40%) | 0 | 0 |
| 29 | B7 | 41/42 (98%) | 33 (80%) | 8 (20%) | 1 | 7 |
| 29 | D7 | 41/42 (98%) | 33 (80%) | 8 (20%) | 1 | 7 |
| 30 | B8 | 53/55 (96%) | 42 (79%) | 11 (21%) | 1 | 5 |
| 30 | D8 | 53/55 (96%) | 43 (81%) | 10 (19%) | 1 | 8 |
| 33 | BD | 213/218 (98%) | 168 (79%) | 45 (21%) | 1 | 5 |
| 33 | DD | 213/218 (98%) | 169 (79%) | 44 (21%) | 1 | 6 |
| 34 | BE | 165/166 (99%) | 125 (76%) | 40 (24%) | 0 | 3 |
| 34 | DE | 165/166 (99%) | 126 (76%) | 39 (24%) | 1 | 3 |
| 35 | BF | 165/166 (99%) | 127 (77%) | 38 (23%) | 1 | 4 |
| 35 | DF | 165/166 (99%) | 129 (78%) | 36 (22%) | 1 | 5 |
| 36 | BG | 155/156 (99%) | 136 (88%) | 19 (12%) | 4 | 21 |
| 36 | DG | 155/156 (99%) | 135 (87%) | 20 (13%) | 4 | 19 |
| 37 | BH | 132/148 (89%) | 107 (81%) | 25 (19%) | 1 | 8 |
| 37 | DH | 132/148 (89%) | 108 (82%) | 24 (18%) | 1 | 9 |
| 38 | BI | 122/124 (98%) | 105 (86%) | 17 (14%) | 3 | 16 |
| 38 | DI | 122/124 (98%) | 105 (86%) | 17 (14%) | 3 | 16 |
| 39 | BN | 117/119 (98%) | 78 (67%) | 39 (33%) | 0 | 1 |
| 39 | DN | 117/119 (98%) | 78 (67%) | 39 (33%) | 0 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-------------|----|
| 40 | BO | 100/100 (100%) | 85 (85%) | 15 (15%) | 3 | 14 |
| 40 | DO | 100/100 (100%) | 85 (85%) | 15 (15%) | 3 | 14 |
| 41 | BP | 112/116 (97%) | 73 (65%) | 39 (35%) | 0 | 1 |
| 41 | DP | 112/116 (97%) | 71 (63%) | 41 (37%) | 0 | 1 |
| 42 | BQ | 106/111 (96%) | 80 (76%) | 26 (24%) | 0 | 3 |
| 42 | DQ | 106/111 (96%) | 81 (76%) | 25 (24%) | 1 | 3 |
| 43 | BR | 100/101 (99%) | 72 (72%) | 28 (28%) | 0 | 2 |
| 43 | DR | 100/101 (99%) | 73 (73%) | 27 (27%) | 0 | 2 |
| 44 | BS | 77/88 (88%) | 52 (68%) | 25 (32%) | 0 | 1 |
| 44 | DS | 77/88 (88%) | 52 (68%) | 25 (32%) | 0 | 1 |
| 45 | BT | 116/127 (91%) | 86 (74%) | 30 (26%) | 0 | 2 |
| 45 | DT | 116/127 (91%) | 88 (76%) | 28 (24%) | 0 | 3 |
| 46 | BU | 92/94 (98%) | 76 (83%) | 16 (17%) | 2 | 10 |
| 46 | DU | 92/94 (98%) | 75 (82%) | 17 (18%) | 1 | 8 |
| 47 | BV | 82/82 (100%) | 53 (65%) | 29 (35%) | 0 | 1 |
| 47 | DV | 82/82 (100%) | 54 (66%) | 28 (34%) | 0 | 1 |
| 48 | BW | 91/92 (99%) | 76 (84%) | 15 (16%) | 2 | 11 |
| 48 | DW | 91/92 (99%) | 76 (84%) | 15 (16%) | 2 | 11 |
| 49 | BX | 74/78 (95%) | 55 (74%) | 19 (26%) | 0 | 3 |
| 49 | DX | 74/78 (95%) | 54 (73%) | 20 (27%) | 0 | 2 |
| 50 | BY | 84/91 (92%) | 58 (69%) | 26 (31%) | 0 | 1 |
| 50 | DY | 84/91 (92%) | 58 (69%) | 26 (31%) | 0 | 1 |
| 51 | BZ | 155/179 (87%) | 131 (84%) | 24 (16%) | 2 | 13 |
| 51 | DZ | 155/179 (87%) | 131 (84%) | 24 (16%) | 2 | 13 |
| All | All | 9322/9874 (94%) | 7707 (83%) | 1615 (17%) | 2 | 10 |

All (1615) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 10 | LEU |
| 2 | AB | 15 | VAL |
| 2 | AB | 17 | PHE |
| 2 | AB | 22 | LYS |
| 2 | AB | 24 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 36 | ARG |
| 2 | AB | 42 | ILE |
| 2 | AB | 69 | LEU |
| 2 | AB | 111 | ARG |
| 2 | AB | 130 | ARG |
| 2 | AB | 137 | ARG |
| 2 | AB | 145 | LEU |
| 2 | AB | 164 | VAL |
| 2 | AB | 165 | VAL |
| 2 | AB | 172 | ILE |
| 2 | AB | 178 | ARG |
| 2 | AB | 185 | ILE |
| 2 | AB | 187 | LEU |
| 2 | AB | 189 | ASP |
| 2 | AB | 193 | ASP |
| 2 | AB | 205 | ASP |
| 2 | AB | 206 | ASP |
| 2 | AB | 215 | LEU |
| 2 | AB | 221 | LEU |
| 3 | AC | 5 | ILE |
| 3 | AC | 12 | LEU |
| 3 | AC | 16 | ARG |
| 3 | AC | 27 | LYS |
| 3 | AC | 104 | GLN |
| 3 | AC | 127 | ARG |
| 3 | AC | 131 | ARG |
| 4 | AD | 3 | ARG |
| 4 | AD | 8 | VAL |
| 4 | AD | 9 | CYS |
| 4 | AD | 11 | LEU |
| 4 | AD | 12 | CYS |
| 4 | AD | 15 | GLU |
| 4 | AD | 19 | LEU |
| 4 | AD | 21 | LEU |
| 4 | AD | 24 | GLU |
| 4 | AD | 25 | ARG |
| 4 | AD | 45 | GLN |
| 4 | AD | 58 | LEU |
| 4 | AD | 64 | LEU |
| 4 | AD | 68 | TYR |
| 4 | AD | 94 | LEU |
| 4 | AD | 98 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AD | 110 | PHE |
| 4 | AD | 119 | GLN |
| 4 | AD | 122 | ARG |
| 4 | AD | 127 | THR |
| 4 | AD | 131 | ARG |
| 4 | AD | 132 | ARG |
| 4 | AD | 135 | LEU |
| 4 | AD | 138 | TYR |
| 4 | AD | 158 | ILE |
| 4 | AD | 170 | VAL |
| 4 | AD | 194 | LEU |
| 4 | AD | 196 | LEU |
| 4 | AD | 204 | ILE |
| 4 | AD | 209 | ARG |
| 5 | AE | 12 | LEU |
| 5 | AE | 20 | GLN |
| 5 | AE | 25 | ARG |
| 5 | AE | 31 | LEU |
| 5 | AE | 41 | VAL |
| 5 | AE | 55 | VAL |
| 5 | AE | 73 | ASN |
| 5 | AE | 76 | ILE |
| 5 | AE | 78 | HIS |
| 5 | AE | 79 | GLU |
| 5 | AE | 87 | SER |
| 5 | AE | 91 | LEU |
| 5 | AE | 98 | THR |
| 5 | AE | 101 | ILE |
| 5 | AE | 110 | LEU |
| 5 | AE | 115 | VAL |
| 5 | AE | 143 | ARG |
| 5 | AE | 147 | ASP |
| 6 | AF | 7 | ASN |
| 6 | AF | 18 | GLN |
| 6 | AF | 23 | LYS |
| 6 | AF | 45 | LEU |
| 6 | AF | 46 | ARG |
| 6 | AF | 55 | ASP |
| 6 | AF | 63 | TYR |
| 6 | AF | 65 | VAL |
| 6 | AF | 83 | ASP |
| 6 | AF | 98 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AG | 79 | ARG |
| 7 | AG | 136 | LYS |
| 7 | AG | 137 | LYS |
| 8 | AH | 1 | MET |
| 8 | AH | 10 | LEU |
| 8 | AH | 25 | ASP |
| 8 | AH | 41 | ARG |
| 8 | AH | 52 | ASP |
| 8 | AH | 95 | VAL |
| 8 | AH | 102 | ARG |
| 8 | AH | 114 | THR |
| 8 | AH | 127 | LEU |
| 9 | AI | 10 | ARG |
| 9 | AI | 95 | LYS |
| 9 | AI | 99 | LEU |
| 9 | AI | 102 | LEU |
| 9 | AI | 112 | LYS |
| 9 | AI | 113 | LYS |
| 9 | AI | 114 | TYR |
| 9 | AI | 121 | ARG |
| 9 | AI | 125 | TYR |
| 9 | AI | 128 | ARG |
| 10 | AJ | 12 | ASP |
| 10 | AJ | 22 | LYS |
| 10 | AJ | 45 | ARG |
| 10 | AJ | 47 | PHE |
| 10 | AJ | 50 | ILE |
| 10 | AJ | 57 | LYS |
| 10 | AJ | 62 | HIS |
| 10 | AJ | 74 | ILE |
| 10 | AJ | 80 | LYS |
| 10 | AJ | 96 | ILE |
| 11 | AK | 29 | ILE |
| 11 | AK | 47 | VAL |
| 11 | AK | 92 | GLU |
| 11 | AK | 107 | SER |
| 11 | AK | 125 | PHE |
| 11 | AK | 127 | LYS |
| 12 | AL | 20 | LYS |
| 12 | AL | 41 | ARG |
| 12 | AL | 42 | THR |
| 12 | AL | 52 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | AL | 53 | ARG |
| 12 | AL | 62 | SER |
| 12 | AL | 66 | VAL |
| 12 | AL | 67 | THR |
| 12 | AL | 89 | ARG |
| 12 | AL | 102 | ARG |
| 12 | AL | 116 | SER |
| 13 | AM | 48 | LEU |
| 13 | AM | 66 | LEU |
| 13 | AM | 70 | LEU |
| 13 | AM | 82 | MET |
| 13 | AM | 93 | ARG |
| 13 | AM | 108 | ARG |
| 14 | AN | 18 | VAL |
| 14 | AN | 42 | ILE |
| 14 | AN | 44 | LEU |
| 15 | AO | 3 | ILE |
| 15 | AO | 17 | ARG |
| 15 | AO | 24 | SER |
| 15 | AO | 31 | LEU |
| 15 | AO | 41 | GLU |
| 15 | AO | 65 | ARG |
| 15 | AO | 66 | LEU |
| 15 | AO | 82 | ILE |
| 16 | AP | 2 | VAL |
| 16 | AP | 8 | ARG |
| 16 | AP | 11 | SER |
| 16 | AP | 16 | HIS |
| 16 | AP | 20 | VAL |
| 16 | AP | 22 | THR |
| 16 | AP | 27 | LYS |
| 16 | AP | 28 | ARG |
| 16 | AP | 32 | TYR |
| 16 | AP | 39 | TYR |
| 16 | AP | 43 | LYS |
| 16 | AP | 48 | TRP |
| 16 | AP | 69 | THR |
| 16 | AP | 79 | VAL |
| 16 | AP | 82 | GLN |
| 17 | AQ | 52 | LYS |
| 17 | AQ | 57 | VAL |
| 17 | AQ | 60 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | AQ | 63 | ARG |
| 17 | AQ | 68 | ARG |
| 18 | AR | 32 | ARG |
| 18 | AR | 47 | THR |
| 18 | AR | 53 | ARG |
| 18 | AR | 70 | ILE |
| 18 | AR | 87 | ARG |
| 19 | AS | 5 | LEU |
| 19 | AS | 6 | LYS |
| 19 | AS | 7 | LYS |
| 19 | AS | 22 | LEU |
| 19 | AS | 27 | GLU |
| 19 | AS | 44 | MET |
| 19 | AS | 49 | ILE |
| 20 | AT | 9 | ASN |
| 20 | AT | 26 | ASN |
| 20 | AT | 27 | LYS |
| 20 | AT | 30 | LYS |
| 20 | AT | 41 | ILE |
| 20 | AT | 56 | MET |
| 20 | AT | 57 | ARG |
| 20 | AT | 62 | LEU |
| 20 | AT | 74 | LYS |
| 20 | AT | 75 | ASN |
| 20 | AT | 93 | GLU |
| 22 | B0 | 11 | ARG |
| 22 | B0 | 14 | ARG |
| 22 | B0 | 20 | ARG |
| 22 | B0 | 25 | ARG |
| 22 | B0 | 36 | ILE |
| 22 | B0 | 70 | GLN |
| 22 | B0 | 72 | ARG |
| 22 | B0 | 84 | LEU |
| 23 | B1 | 12 | PRO |
| 23 | B1 | 13 | ILE |
| 23 | B1 | 14 | VAL |
| 23 | B1 | 21 | ARG |
| 23 | B1 | 25 | LYS |
| 23 | B1 | 26 | ARG |
| 23 | B1 | 34 | THR |
| 23 | B1 | 37 | ILE |
| 23 | B1 | 41 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | B1 | 42 | GLN |
| 23 | B1 | 46 | LEU |
| 23 | B1 | 47 | GLN |
| 23 | B1 | 48 | LYS |
| 23 | B1 | 53 | VAL |
| 23 | B1 | 62 | VAL |
| 23 | B1 | 65 | SER |
| 23 | B1 | 67 | ILE |
| 23 | B1 | 86 | SER |
| 23 | B1 | 89 | GLU |
| 23 | B1 | 94 | LEU |
| 24 | B2 | 12 | GLU |
| 24 | B2 | 14 | ARG |
| 24 | B2 | 22 | GLU |
| 24 | B2 | 26 | ARG |
| 24 | B2 | 28 | LYS |
| 24 | B2 | 30 | ARG |
| 24 | B2 | 31 | GLU |
| 24 | B2 | 32 | LEU |
| 24 | B2 | 33 | MET |
| 24 | B2 | 35 | LEU |
| 24 | B2 | 36 | ARG |
| 24 | B2 | 44 | LEU |
| 24 | B2 | 45 | SER |
| 24 | B2 | 46 | GLN |
| 24 | B2 | 47 | ASN |
| 24 | B2 | 50 | ILE |
| 24 | B2 | 51 | ARG |
| 24 | B2 | 53 | LEU |
| 24 | B2 | 56 | GLN |
| 24 | B2 | 59 | ARG |
| 25 | B3 | 8 | LEU |
| 25 | B3 | 35 | ARG |
| 25 | B3 | 58 | VAL |
| 27 | B5 | 3 | LYS |
| 27 | B5 | 4 | HIS |
| 27 | B5 | 6 | VAL |
| 27 | B5 | 11 | THR |
| 27 | B5 | 16 | ARG |
| 27 | B5 | 26 | THR |
| 27 | B5 | 29 | THR |
| 27 | B5 | 40 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | B5 | 44 | THR |
| 27 | B5 | 49 | CYS |
| 27 | B5 | 55 | ARG |
| 27 | B5 | 56 | LYS |
| 27 | B5 | 58 | LEU |
| 28 | B6 | 9 | LEU |
| 28 | B6 | 10 | LEU |
| 28 | B6 | 14 | THR |
| 28 | B6 | 18 | ARG |
| 28 | B6 | 19 | ARG |
| 28 | B6 | 24 | GLU |
| 28 | B6 | 30 | THR |
| 28 | B6 | 35 | GLU |
| 28 | B6 | 37 | ARG |
| 28 | B6 | 41 | PRO |
| 28 | B6 | 42 | TRP |
| 28 | B6 | 43 | CYS |
| 28 | B6 | 44 | ARG |
| 28 | B6 | 46 | HIS |
| 28 | B6 | 47 | THR |
| 28 | B6 | 48 | VAL |
| 28 | B6 | 51 | GLU |
| 28 | B6 | 52 | VAL |
| 29 | B7 | 1 | MET |
| 29 | B7 | 8 | ASN |
| 29 | B7 | 9 | ARG |
| 29 | B7 | 10 | ARG |
| 29 | B7 | 24 | THR |
| 29 | B7 | 32 | LYS |
| 29 | B7 | 41 | ARG |
| 29 | B7 | 48 | LYS |
| 30 | B8 | 4 | MET |
| 30 | B8 | 6 | THR |
| 30 | B8 | 13 | ARG |
| 30 | B8 | 23 | VAL |
| 30 | B8 | 32 | LEU |
| 30 | B8 | 39 | LYS |
| 30 | B8 | 44 | LYS |
| 30 | B8 | 47 | LYS |
| 30 | B8 | 49 | VAL |
| 30 | B8 | 56 | GLU |
| 30 | B8 | 62 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | BD | 5 | LYS |
| 33 | BD | 13 | ARG |
| 33 | BD | 17 | THR |
| 33 | BD | 26 | LYS |
| 33 | BD | 31 | LYS |
| 33 | BD | 43 | ARG |
| 33 | BD | 44 | ASN |
| 33 | BD | 46 | GLN |
| 33 | BD | 61 | LEU |
| 33 | BD | 64 | ILE |
| 33 | BD | 65 | ILE |
| 33 | BD | 71 | ASP |
| 33 | BD | 73 | VAL |
| 33 | BD | 88 | ARG |
| 33 | BD | 89 | SER |
| 33 | BD | 94 | LEU |
| 33 | BD | 95 | LEU |
| 33 | BD | 98 | VAL |
| 33 | BD | 103 | ARG |
| 33 | BD | 105 | ILE |
| 33 | BD | 106 | ILE |
| 33 | BD | 111 | LEU |
| 33 | BD | 112 | GLN |
| 33 | BD | 116 | GLN |
| 33 | BD | 117 | VAL |
| 33 | BD | 127 | VAL |
| 33 | BD | 142 | VAL |
| 33 | BD | 161 | THR |
| 33 | BD | 166 | GLN |
| 33 | BD | 168 | ARG |
| 33 | BD | 173 | VAL |
| 33 | BD | 192 | THR |
| 33 | BD | 198 | ASN |
| 33 | BD | 211 | ARG |
| 33 | BD | 212 | SER |
| 33 | BD | 217 | ARG |
| 33 | BD | 221 | VAL |
| 33 | BD | 229 | VAL |
| 33 | BD | 242 | ARG |
| 33 | BD | 254 | THR |
| 33 | BD | 255 | LYS |
| 33 | BD | 257 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 33 | BD | 259 | THR |
| 33 | BD | 265 | PRO |
| 33 | BD | 271 | ILE |
| 34 | BE | 1 | MET |
| 34 | BE | 7 | VAL |
| 34 | BE | 12 | THR |
| 34 | BE | 21 | VAL |
| 34 | BE | 23 | VAL |
| 34 | BE | 24 | THR |
| 34 | BE | 33 | VAL |
| 34 | BE | 34 | VAL |
| 34 | BE | 47 | VAL |
| 34 | BE | 52 | LEU |
| 34 | BE | 60 | ASN |
| 34 | BE | 63 | LEU |
| 34 | BE | 66 | HIS |
| 34 | BE | 67 | PHE |
| 34 | BE | 69 | LYS |
| 34 | BE | 73 | GLU |
| 34 | BE | 75 | VAL |
| 34 | BE | 76 | ARG |
| 34 | BE | 77 | ILE |
| 34 | BE | 79 | ARG |
| 34 | BE | 82 | ARG |
| 34 | BE | 111 | ARG |
| 34 | BE | 116 | VAL |
| 34 | BE | 118 | LYS |
| 34 | BE | 119 | ARG |
| 34 | BE | 133 | LYS |
| 34 | BE | 134 | ILE |
| 34 | BE | 144 | ARG |
| 34 | BE | 152 | LYS |
| 34 | BE | 154 | LYS |
| 34 | BE | 160 | TYR |
| 34 | BE | 163 | GLU |
| 34 | BE | 169 | ASN |
| 34 | BE | 171 | GLU |
| 34 | BE | 175 | VAL |
| 34 | BE | 181 | LEU |
| 34 | BE | 197 | ILE |
| 34 | BE | 199 | ARG |
| 34 | BE | 202 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | BE | 203 | LYS |
| 35 | BF | 7 | TYR |
| 35 | BF | 20 | LEU |
| 35 | BF | 23 | ASP |
| 35 | BF | 28 | ILE |
| 35 | BF | 33 | LEU |
| 35 | BF | 38 | ARG |
| 35 | BF | 41 | LEU |
| 35 | BF | 46 | ARG |
| 35 | BF | 48 | THR |
| 35 | BF | 50 | SER |
| 35 | BF | 53 | THR |
| 35 | BF | 56 | GLU |
| 35 | BF | 57 | VAL |
| 35 | BF | 66 | PRO |
| 35 | BF | 74 | ARG |
| 35 | BF | 78 | ILE |
| 35 | BF | 82 | ILE |
| 35 | BF | 106 | ARG |
| 35 | BF | 112 | MET |
| 35 | BF | 116 | ASP |
| 35 | BF | 127 | GLU |
| 35 | BF | 137 | LYS |
| 35 | BF | 140 | LEU |
| 35 | BF | 160 | ASN |
| 35 | BF | 162 | LEU |
| 35 | BF | 164 | ARG |
| 35 | BF | 165 | ARG |
| 35 | BF | 168 | ARG |
| 35 | BF | 170 | LEU |
| 35 | BF | 175 | THR |
| 35 | BF | 183 | VAL |
| 35 | BF | 192 | LEU |
| 35 | BF | 194 | MET |
| 35 | BF | 197 | ASP |
| 35 | BF | 199 | TRP |
| 35 | BF | 201 | VAL |
| 35 | BF | 204 | ASN |
| 35 | BF | 206 | ILE |
| 36 | BG | 7 | LEU |
| 36 | BG | 16 | ARG |
| 36 | BG | 22 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | BG | 28 | VAL |
| 36 | BG | 34 | LEU |
| 36 | BG | 35 | GLU |
| 36 | BG | 39 | ILE |
| 36 | BG | 49 | ASP |
| 36 | BG | 58 | GLN |
| 36 | BG | 60 | LEU |
| 36 | BG | 63 | ILE |
| 36 | BG | 67 | LYS |
| 36 | BG | 80 | PHE |
| 36 | BG | 125 | PHE |
| 36 | BG | 143 | GLU |
| 36 | BG | 155 | MET |
| 36 | BG | 161 | THR |
| 36 | BG | 166 | ASP |
| 36 | BG | 174 | GLU |
| 37 | BH | 34 | GLU |
| 37 | BH | 41 | MET |
| 37 | BH | 46 | GLU |
| 37 | BH | 53 | GLU |
| 37 | BH | 70 | THR |
| 37 | BH | 71 | LEU |
| 37 | BH | 83 | TYR |
| 37 | BH | 95 | ARG |
| 37 | BH | 103 | LEU |
| 37 | BH | 105 | LEU |
| 37 | BH | 110 | SER |
| 37 | BH | 111 | HIS |
| 37 | BH | 122 | THR |
| 37 | BH | 134 | SER |
| 37 | BH | 136 | ILE |
| 37 | BH | 137 | ASP |
| 37 | BH | 141 | VAL |
| 37 | BH | 143 | GLN |
| 37 | BH | 149 | ARG |
| 37 | BH | 152 | ARG |
| 37 | BH | 153 | LYS |
| 37 | BH | 157 | TYR |
| 37 | BH | 159 | GLU |
| 37 | BH | 163 | TYR |
| 37 | BH | 170 | ARG |
| 38 | BI | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | BI | 12 | LEU |
| 38 | BI | 20 | ASP |
| 38 | BI | 22 | LYS |
| 38 | BI | 38 | LEU |
| 38 | BI | 40 | THR |
| 38 | BI | 51 | ILE |
| 38 | BI | 56 | LYS |
| 38 | BI | 58 | LEU |
| 38 | BI | 82 | ARG |
| 38 | BI | 88 | ILE |
| 38 | BI | 101 | LEU |
| 38 | BI | 109 | ILE |
| 38 | BI | 122 | GLU |
| 38 | BI | 129 | THR |
| 38 | BI | 142 | VAL |
| 38 | BI | 144 | VAL |
| 39 | BN | 2 | LYS |
| 39 | BN | 4 | TYR |
| 39 | BN | 5 | VAL |
| 39 | BN | 14 | VAL |
| 39 | BN | 16 | ILE |
| 39 | BN | 19 | GLU |
| 39 | BN | 23 | LEU |
| 39 | BN | 25 | ARG |
| 39 | BN | 28 | THR |
| 39 | BN | 33 | LEU |
| 39 | BN | 34 | LEU |
| 39 | BN | 37 | LYS |
| 39 | BN | 41 | ASP |
| 39 | BN | 45 | ASN |
| 39 | BN | 46 | VAL |
| 39 | BN | 48 | MET |
| 39 | BN | 55 | VAL |
| 39 | BN | 58 | ASP |
| 39 | BN | 60 | ILE |
| 39 | BN | 62 | VAL |
| 39 | BN | 63 | THR |
| 39 | BN | 65 | LYS |
| 39 | BN | 67 | LEU |
| 39 | BN | 69 | GLN |
| 39 | BN | 75 | TYR |
| 39 | BN | 78 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | BN | 82 | LEU |
| 39 | BN | 84 | LYS |
| 39 | BN | 85 | ILE |
| 39 | BN | 87 | LEU |
| 39 | BN | 98 | VAL |
| 39 | BN | 99 | LEU |
| 39 | BN | 112 | LEU |
| 39 | BN | 119 | ARG |
| 39 | BN | 120 | LEU |
| 39 | BN | 121 | LYS |
| 39 | BN | 130 | HIS |
| 39 | BN | 134 | ARG |
| 39 | BN | 138 | LEU |
| 40 | BO | 3 | GLN |
| 40 | BO | 8 | LEU |
| 40 | BO | 13 | ASN |
| 40 | BO | 22 | ILE |
| 40 | BO | 24 | VAL |
| 40 | BO | 28 | SER |
| 40 | BO | 47 | ILE |
| 40 | BO | 52 | VAL |
| 40 | BO | 63 | VAL |
| 40 | BO | 75 | SER |
| 40 | BO | 87 | ILE |
| 40 | BO | 88 | ASN |
| 40 | BO | 104 | ARG |
| 40 | BO | 108 | GLU |
| 40 | BO | 112 | MET |
| 41 | BP | 13 | ASN |
| 41 | BP | 16 | ARG |
| 41 | BP | 17 | LYS |
| 41 | BP | 18 | ARG |
| 41 | BP | 19 | VAL |
| 41 | BP | 21 | ARG |
| 41 | BP | 32 | THR |
| 41 | BP | 33 | ARG |
| 41 | BP | 39 | LYS |
| 41 | BP | 40 | SER |
| 41 | BP | 45 | LEU |
| 41 | BP | 47 | ASP |
| 41 | BP | 52 | GLU |
| 41 | BP | 55 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | BP | 57 | THR |
| 41 | BP | 59 | LEU |
| 41 | BP | 61 | ARG |
| 41 | BP | 62 | LEU |
| 41 | BP | 65 | ARG |
| 41 | BP | 67 | MET |
| 41 | BP | 70 | GLN |
| 41 | BP | 75 | ILE |
| 41 | BP | 77 | ARG |
| 41 | BP | 85 | LEU |
| 41 | BP | 100 | LEU |
| 41 | BP | 101 | VAL |
| 41 | BP | 102 | ARG |
| 41 | BP | 110 | TYR |
| 41 | BP | 111 | ARG |
| 41 | BP | 112 | LEU |
| 41 | BP | 114 | ILE |
| 41 | BP | 115 | LEU |
| 41 | BP | 123 | LEU |
| 41 | BP | 125 | VAL |
| 41 | BP | 135 | LEU |
| 41 | BP | 138 | LEU |
| 41 | BP | 144 | GLU |
| 41 | BP | 147 | LEU |
| 41 | BP | 148 | LEU |
| 42 | BQ | 6 | ARG |
| 42 | BQ | 9 | TYR |
| 42 | BQ | 13 | GLN |
| 42 | BQ | 18 | LYS |
| 42 | BQ | 22 | LYS |
| 42 | BQ | 27 | VAL |
| 42 | BQ | 29 | PHE |
| 42 | BQ | 35 | VAL |
| 42 | BQ | 45 | GLN |
| 42 | BQ | 52 | VAL |
| 42 | BQ | 54 | MET |
| 42 | BQ | 55 | VAL |
| 42 | BQ | 58 | PHE |
| 42 | BQ | 63 | LYS |
| 42 | BQ | 80 | GLU |
| 42 | BQ | 81 | VAL |
| 42 | BQ | 82 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BQ | 87 | LYS |
| 42 | BQ | 91 | GLU |
| 42 | BQ | 103 | MET |
| 42 | BQ | 109 | VAL |
| 42 | BQ | 115 | MET |
| 42 | BQ | 127 | ILE |
| 42 | BQ | 132 | VAL |
| 42 | BQ | 139 | GLU |
| 42 | BQ | 141 | GLN |
| 43 | BR | 2 | ARG |
| 43 | BR | 5 | LYS |
| 43 | BR | 6 | SER |
| 43 | BR | 8 | ARG |
| 43 | BR | 15 | SER |
| 43 | BR | 16 | HIS |
| 43 | BR | 18 | LEU |
| 43 | BR | 28 | LEU |
| 43 | BR | 29 | LEU |
| 43 | BR | 30 | THR |
| 43 | BR | 36 | THR |
| 43 | BR | 44 | LEU |
| 43 | BR | 45 | ARG |
| 43 | BR | 53 | HIS |
| 43 | BR | 60 | LEU |
| 43 | BR | 65 | LEU |
| 43 | BR | 67 | LEU |
| 43 | BR | 71 | GLN |
| 43 | BR | 74 | LYS |
| 43 | BR | 75 | LEU |
| 43 | BR | 79 | LEU |
| 43 | BR | 99 | LYS |
| 43 | BR | 100 | LEU |
| 43 | BR | 103 | ARG |
| 43 | BR | 104 | ARG |
| 43 | BR | 115 | GLU |
| 43 | BR | 117 | VAL |
| 43 | BR | 118 | GLU |
| 44 | BS | 11 | LYS |
| 44 | BS | 15 | ARG |
| 44 | BS | 17 | ARG |
| 44 | BS | 30 | ARG |
| 44 | BS | 33 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | BS | 36 | TYR |
| 44 | BS | 48 | LEU |
| 44 | BS | 50 | SER |
| 44 | BS | 54 | LEU |
| 44 | BS | 56 | LEU |
| 44 | BS | 58 | LEU |
| 44 | BS | 61 | ASN |
| 44 | BS | 69 | VAL |
| 44 | BS | 73 | LEU |
| 44 | BS | 80 | LEU |
| 44 | BS | 83 | LYS |
| 44 | BS | 84 | GLN |
| 44 | BS | 85 | VAL |
| 44 | BS | 89 | ARG |
| 44 | BS | 92 | TYR |
| 44 | BS | 93 | LYS |
| 44 | BS | 95 | HIS |
| 44 | BS | 97 | ARG |
| 44 | BS | 98 | VAL |
| 44 | BS | 106 | ARG |
| 45 | BT | 3 | ARG |
| 45 | BT | 11 | GLU |
| 45 | BT | 13 | ARG |
| 45 | BT | 15 | VAL |
| 45 | BT | 16 | ARG |
| 45 | BT | 17 | THR |
| 45 | BT | 18 | ASP |
| 45 | BT | 24 | PRO |
| 45 | BT | 29 | ARG |
| 45 | BT | 32 | TYR |
| 45 | BT | 33 | LYS |
| 45 | BT | 38 | ASN |
| 45 | BT | 41 | ARG |
| 45 | BT | 53 | ARG |
| 45 | BT | 58 | ASN |
| 45 | BT | 59 | THR |
| 45 | BT | 62 | THR |
| 45 | BT | 63 | VAL |
| 45 | BT | 64 | ARG |
| 45 | BT | 65 | LYS |
| 45 | BT | 77 | PRO |
| 45 | BT | 82 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | BT | 88 | ILE |
| 45 | BT | 96 | ARG |
| 45 | BT | 98 | LYS |
| 45 | BT | 99 | LEU |
| 45 | BT | 108 | ARG |
| 45 | BT | 112 | ARG |
| 45 | BT | 115 | ARG |
| 45 | BT | 128 | GLU |
| 46 | BU | 8 | VAL |
| 46 | BU | 34 | LYS |
| 46 | BU | 55 | ARG |
| 46 | BU | 56 | ASP |
| 46 | BU | 64 | ARG |
| 46 | BU | 70 | ARG |
| 46 | BU | 74 | LEU |
| 46 | BU | 77 | SER |
| 46 | BU | 83 | LEU |
| 46 | BU | 88 | ILE |
| 46 | BU | 89 | GLU |
| 46 | BU | 92 | ARG |
| 46 | BU | 93 | LYS |
| 46 | BU | 95 | LEU |
| 46 | BU | 97 | ASP |
| 46 | BU | 102 | GLU |
| 47 | BV | 2 | PHE |
| 47 | BV | 7 | THR |
| 47 | BV | 14 | VAL |
| 47 | BV | 15 | GLU |
| 47 | BV | 18 | LEU |
| 47 | BV | 19 | LYS |
| 47 | BV | 21 | ARG |
| 47 | BV | 22 | VAL |
| 47 | BV | 23 | GLU |
| 47 | BV | 28 | GLU |
| 47 | BV | 32 | THR |
| 47 | BV | 35 | LEU |
| 47 | BV | 37 | VAL |
| 47 | BV | 38 | LEU |
| 47 | BV | 40 | LEU |
| 47 | BV | 56 | SER |
| 47 | BV | 62 | LEU |
| 47 | BV | 66 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | BV | 71 | LEU |
| 47 | BV | 78 | LYS |
| 47 | BV | 80 | GLN |
| 47 | BV | 82 | ARG |
| 47 | BV | 83 | ARG |
| 47 | BV | 88 | ARG |
| 47 | BV | 89 | GLN |
| 47 | BV | 92 | THR |
| 47 | BV | 93 | GLU |
| 47 | BV | 98 | GLU |
| 47 | BV | 100 | ARG |
| 48 | BW | 4 | LYS |
| 48 | BW | 11 | ARG |
| 48 | BW | 17 | VAL |
| 48 | BW | 19 | LEU |
| 48 | BW | 20 | VAL |
| 48 | BW | 23 | LEU |
| 48 | BW | 33 | ARG |
| 48 | BW | 50 | VAL |
| 48 | BW | 51 | LEU |
| 48 | BW | 64 | MET |
| 48 | BW | 69 | LEU |
| 48 | BW | 82 | LEU |
| 48 | BW | 96 | ILE |
| 48 | BW | 106 | ILE |
| 48 | BW | 107 | LEU |
| 49 | BX | 3 | THR |
| 49 | BX | 12 | VAL |
| 49 | BX | 15 | GLU |
| 49 | BX | 25 | LYS |
| 49 | BX | 27 | THR |
| 49 | BX | 30 | VAL |
| 49 | BX | 33 | LYS |
| 49 | BX | 35 | THR |
| 49 | BX | 36 | LYS |
| 49 | BX | 38 | GLU |
| 49 | BX | 39 | ILE |
| 49 | BX | 45 | THR |
| 49 | BX | 49 | VAL |
| 49 | BX | 55 | ASN |
| 49 | BX | 60 | ARG |
| 49 | BX | 65 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | BX | 76 | ARG |
| 49 | BX | 78 | LYS |
| 49 | BX | 88 | LYS |
| 50 | BY | 2 | ARG |
| 50 | BY | 6 | HIS |
| 50 | BY | 7 | VAL |
| 50 | BY | 8 | LYS |
| 50 | BY | 13 | VAL |
| 50 | BY | 38 | ILE |
| 50 | BY | 42 | VAL |
| 50 | BY | 46 | LYS |
| 50 | BY | 47 | LYS |
| 50 | BY | 49 | VAL |
| 50 | BY | 55 | TYR |
| 50 | BY | 60 | PHE |
| 50 | BY | 62 | GLU |
| 50 | BY | 66 | PRO |
| 50 | BY | 70 | SER |
| 50 | BY | 71 | LYS |
| 50 | BY | 75 | ILE |
| 50 | BY | 76 | CYS |
| 50 | BY | 81 | LYS |
| 50 | BY | 86 | ARG |
| 50 | BY | 89 | PHE |
| 50 | BY | 90 | LEU |
| 50 | BY | 94 | LYS |
| 50 | BY | 96 | ILE |
| 50 | BY | 97 | ARG |
| 50 | BY | 99 | CYS |
| 51 | BZ | 6 | LYS |
| 51 | BZ | 19 | ARG |
| 51 | BZ | 27 | VAL |
| 51 | BZ | 42 | VAL |
| 51 | BZ | 53 | ILE |
| 51 | BZ | 72 | ARG |
| 51 | BZ | 73 | GLN |
| 51 | BZ | 79 | ARG |
| 51 | BZ | 81 | ARG |
| 51 | BZ | 86 | VAL |
| 51 | BZ | 87 | ASP |
| 51 | BZ | 93 | ASP |
| 51 | BZ | 97 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | BZ | 98 | MET |
| 51 | BZ | 117 | LEU |
| 51 | BZ | 121 | HIS |
| 51 | BZ | 124 | ILE |
| 51 | BZ | 128 | VAL |
| 51 | BZ | 140 | ASP |
| 51 | BZ | 150 | LEU |
| 51 | BZ | 151 | HIS |
| 51 | BZ | 153 | SER |
| 51 | BZ | 166 | SER |
| 51 | BZ | 171 | ILE |
| 2 | CB | 10 | LEU |
| 2 | CB | 15 | VAL |
| 2 | CB | 17 | PHE |
| 2 | CB | 22 | LYS |
| 2 | CB | 24 | TRP |
| 2 | CB | 36 | ARG |
| 2 | CB | 42 | ILE |
| 2 | CB | 69 | LEU |
| 2 | CB | 111 | ARG |
| 2 | CB | 130 | ARG |
| 2 | CB | 137 | ARG |
| 2 | CB | 145 | LEU |
| 2 | CB | 164 | VAL |
| 2 | CB | 165 | VAL |
| 2 | CB | 172 | ILE |
| 2 | CB | 178 | ARG |
| 2 | CB | 185 | ILE |
| 2 | CB | 187 | LEU |
| 2 | CB | 189 | ASP |
| 2 | CB | 193 | ASP |
| 2 | CB | 205 | ASP |
| 2 | CB | 206 | ASP |
| 2 | CB | 215 | LEU |
| 2 | CB | 221 | LEU |
| 3 | CC | 5 | ILE |
| 3 | CC | 12 | LEU |
| 3 | CC | 16 | ARG |
| 3 | CC | 27 | LYS |
| 3 | CC | 104 | GLN |
| 3 | CC | 127 | ARG |
| 3 | CC | 131 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | CD | 3 | ARG |
| 4 | CD | 8 | VAL |
| 4 | CD | 9 | CYS |
| 4 | CD | 11 | LEU |
| 4 | CD | 15 | GLU |
| 4 | CD | 19 | LEU |
| 4 | CD | 21 | LEU |
| 4 | CD | 24 | GLU |
| 4 | CD | 25 | ARG |
| 4 | CD | 45 | GLN |
| 4 | CD | 58 | LEU |
| 4 | CD | 64 | LEU |
| 4 | CD | 68 | TYR |
| 4 | CD | 94 | LEU |
| 4 | CD | 119 | GLN |
| 4 | CD | 122 | ARG |
| 4 | CD | 127 | THR |
| 4 | CD | 131 | ARG |
| 4 | CD | 132 | ARG |
| 4 | CD | 135 | LEU |
| 4 | CD | 138 | TYR |
| 4 | CD | 158 | ILE |
| 4 | CD | 170 | VAL |
| 4 | CD | 194 | LEU |
| 4 | CD | 196 | LEU |
| 4 | CD | 204 | ILE |
| 4 | CD | 209 | ARG |
| 5 | CE | 12 | LEU |
| 5 | CE | 20 | GLN |
| 5 | CE | 25 | ARG |
| 5 | CE | 31 | LEU |
| 5 | CE | 41 | VAL |
| 5 | CE | 55 | VAL |
| 5 | CE | 73 | ASN |
| 5 | CE | 76 | ILE |
| 5 | CE | 78 | HIS |
| 5 | CE | 79 | GLU |
| 5 | CE | 87 | SER |
| 5 | CE | 91 | LEU |
| 5 | CE | 98 | THR |
| 5 | CE | 101 | ILE |
| 5 | CE | 110 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CE | 115 | VAL |
| 5 | CE | 143 | ARG |
| 5 | CE | 147 | ASP |
| 6 | CF | 7 | ASN |
| 6 | CF | 18 | GLN |
| 6 | CF | 21 | LEU |
| 6 | CF | 23 | LYS |
| 6 | CF | 45 | LEU |
| 6 | CF | 46 | ARG |
| 6 | CF | 55 | ASP |
| 6 | CF | 63 | TYR |
| 6 | CF | 65 | VAL |
| 6 | CF | 83 | ASP |
| 6 | CF | 98 | LEU |
| 7 | CG | 79 | ARG |
| 7 | CG | 120 | ILE |
| 7 | CG | 136 | LYS |
| 7 | CG | 137 | LYS |
| 8 | CH | 1 | MET |
| 8 | CH | 10 | LEU |
| 8 | CH | 25 | ASP |
| 8 | CH | 41 | ARG |
| 8 | CH | 52 | ASP |
| 8 | CH | 95 | VAL |
| 8 | CH | 102 | ARG |
| 8 | CH | 114 | THR |
| 8 | CH | 127 | LEU |
| 9 | CI | 10 | ARG |
| 9 | CI | 95 | LYS |
| 9 | CI | 99 | LEU |
| 9 | CI | 102 | LEU |
| 9 | CI | 113 | LYS |
| 9 | CI | 114 | TYR |
| 9 | CI | 121 | ARG |
| 9 | CI | 125 | TYR |
| 9 | CI | 128 | ARG |
| 10 | CJ | 12 | ASP |
| 10 | CJ | 22 | LYS |
| 10 | CJ | 45 | ARG |
| 10 | CJ | 47 | PHE |
| 10 | CJ | 50 | ILE |
| 10 | CJ | 57 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | CJ | 62 | HIS |
| 10 | CJ | 74 | ILE |
| 10 | CJ | 80 | LYS |
| 10 | CJ | 96 | ILE |
| 11 | CK | 29 | ILE |
| 11 | CK | 47 | VAL |
| 11 | CK | 92 | GLU |
| 11 | CK | 107 | SER |
| 11 | CK | 125 | PHE |
| 11 | CK | 127 | LYS |
| 12 | CL | 20 | LYS |
| 12 | CL | 41 | ARG |
| 12 | CL | 42 | THR |
| 12 | CL | 52 | LEU |
| 12 | CL | 53 | ARG |
| 12 | CL | 62 | SER |
| 12 | CL | 66 | VAL |
| 12 | CL | 85 | ILE |
| 12 | CL | 89 | ARG |
| 12 | CL | 92 | ASP |
| 12 | CL | 102 | ARG |
| 12 | CL | 116 | SER |
| 13 | CM | 48 | LEU |
| 13 | CM | 66 | LEU |
| 13 | CM | 70 | LEU |
| 13 | CM | 93 | ARG |
| 13 | CM | 108 | ARG |
| 14 | CN | 18 | VAL |
| 14 | CN | 42 | ILE |
| 14 | CN | 44 | LEU |
| 15 | CO | 3 | ILE |
| 15 | CO | 17 | ARG |
| 15 | CO | 24 | SER |
| 15 | CO | 31 | LEU |
| 15 | CO | 41 | GLU |
| 15 | CO | 65 | ARG |
| 15 | CO | 66 | LEU |
| 15 | CO | 82 | ILE |
| 16 | CP | 2 | VAL |
| 16 | CP | 8 | ARG |
| 16 | CP | 11 | SER |
| 16 | CP | 16 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | CP | 20 | VAL |
| 16 | CP | 22 | THR |
| 16 | CP | 27 | LYS |
| 16 | CP | 28 | ARG |
| 16 | CP | 32 | TYR |
| 16 | CP | 39 | TYR |
| 16 | CP | 43 | LYS |
| 16 | CP | 48 | TRP |
| 16 | CP | 69 | THR |
| 16 | CP | 79 | VAL |
| 16 | CP | 82 | GLN |
| 17 | CQ | 52 | LYS |
| 17 | CQ | 57 | VAL |
| 17 | CQ | 60 | ILE |
| 17 | CQ | 63 | ARG |
| 17 | CQ | 68 | ARG |
| 18 | CR | 47 | THR |
| 18 | CR | 53 | ARG |
| 18 | CR | 70 | ILE |
| 18 | CR | 87 | ARG |
| 19 | CS | 5 | LEU |
| 19 | CS | 6 | LYS |
| 19 | CS | 7 | LYS |
| 19 | CS | 22 | LEU |
| 19 | CS | 27 | GLU |
| 19 | CS | 44 | MET |
| 19 | CS | 49 | ILE |
| 20 | CT | 9 | ASN |
| 20 | CT | 26 | ASN |
| 20 | CT | 27 | LYS |
| 20 | CT | 30 | LYS |
| 20 | CT | 41 | ILE |
| 20 | CT | 56 | MET |
| 20 | CT | 57 | ARG |
| 20 | CT | 62 | LEU |
| 20 | CT | 74 | LYS |
| 20 | CT | 75 | ASN |
| 20 | CT | 93 | GLU |
| 22 | D0 | 11 | ARG |
| 22 | D0 | 14 | ARG |
| 22 | D0 | 20 | ARG |
| 22 | D0 | 25 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | D0 | 36 | ILE |
| 22 | D0 | 70 | GLN |
| 22 | D0 | 72 | ARG |
| 22 | D0 | 84 | LEU |
| 23 | D1 | 12 | PRO |
| 23 | D1 | 13 | ILE |
| 23 | D1 | 14 | VAL |
| 23 | D1 | 21 | ARG |
| 23 | D1 | 25 | LYS |
| 23 | D1 | 26 | ARG |
| 23 | D1 | 34 | THR |
| 23 | D1 | 37 | ILE |
| 23 | D1 | 41 | ARG |
| 23 | D1 | 42 | GLN |
| 23 | D1 | 46 | LEU |
| 23 | D1 | 48 | LYS |
| 23 | D1 | 56 | GLN |
| 23 | D1 | 62 | VAL |
| 23 | D1 | 65 | SER |
| 23 | D1 | 67 | ILE |
| 23 | D1 | 89 | GLU |
| 23 | D1 | 94 | LEU |
| 24 | D2 | 12 | GLU |
| 24 | D2 | 14 | ARG |
| 24 | D2 | 22 | GLU |
| 24 | D2 | 26 | ARG |
| 24 | D2 | 30 | ARG |
| 24 | D2 | 31 | GLU |
| 24 | D2 | 32 | LEU |
| 24 | D2 | 33 | MET |
| 24 | D2 | 35 | LEU |
| 24 | D2 | 36 | ARG |
| 24 | D2 | 44 | LEU |
| 24 | D2 | 45 | SER |
| 24 | D2 | 46 | GLN |
| 24 | D2 | 47 | ASN |
| 24 | D2 | 50 | ILE |
| 24 | D2 | 51 | ARG |
| 24 | D2 | 53 | LEU |
| 24 | D2 | 56 | GLN |
| 24 | D2 | 59 | ARG |
| 25 | D3 | 8 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | D3 | 35 | ARG |
| 25 | D3 | 58 | VAL |
| 27 | D5 | 3 | LYS |
| 27 | D5 | 4 | HIS |
| 27 | D5 | 6 | VAL |
| 27 | D5 | 11 | THR |
| 27 | D5 | 16 | ARG |
| 27 | D5 | 26 | THR |
| 27 | D5 | 29 | THR |
| 27 | D5 | 40 | LYS |
| 27 | D5 | 44 | THR |
| 27 | D5 | 49 | CYS |
| 27 | D5 | 55 | ARG |
| 27 | D5 | 56 | LYS |
| 27 | D5 | 58 | LEU |
| 28 | D6 | 9 | LEU |
| 28 | D6 | 10 | LEU |
| 28 | D6 | 14 | THR |
| 28 | D6 | 18 | ARG |
| 28 | D6 | 19 | ARG |
| 28 | D6 | 24 | GLU |
| 28 | D6 | 30 | THR |
| 28 | D6 | 35 | GLU |
| 28 | D6 | 37 | ARG |
| 28 | D6 | 42 | TRP |
| 28 | D6 | 43 | CYS |
| 28 | D6 | 44 | ARG |
| 28 | D6 | 46 | HIS |
| 28 | D6 | 47 | THR |
| 28 | D6 | 48 | VAL |
| 28 | D6 | 51 | GLU |
| 28 | D6 | 52 | VAL |
| 29 | D7 | 1 | MET |
| 29 | D7 | 8 | ASN |
| 29 | D7 | 9 | ARG |
| 29 | D7 | 10 | ARG |
| 29 | D7 | 24 | THR |
| 29 | D7 | 32 | LYS |
| 29 | D7 | 41 | ARG |
| 29 | D7 | 48 | LYS |
| 30 | D8 | 4 | MET |
| 30 | D8 | 6 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 30 | D8 | 13 | ARG |
| 30 | D8 | 23 | VAL |
| 30 | D8 | 32 | LEU |
| 30 | D8 | 39 | LYS |
| 30 | D8 | 44 | LYS |
| 30 | D8 | 47 | LYS |
| 30 | D8 | 49 | VAL |
| 30 | D8 | 56 | GLU |
| 33 | DD | 5 | LYS |
| 33 | DD | 13 | ARG |
| 33 | DD | 17 | THR |
| 33 | DD | 26 | LYS |
| 33 | DD | 31 | LYS |
| 33 | DD | 43 | ARG |
| 33 | DD | 44 | ASN |
| 33 | DD | 46 | GLN |
| 33 | DD | 61 | LEU |
| 33 | DD | 64 | ILE |
| 33 | DD | 65 | ILE |
| 33 | DD | 71 | ASP |
| 33 | DD | 73 | VAL |
| 33 | DD | 88 | ARG |
| 33 | DD | 89 | SER |
| 33 | DD | 94 | LEU |
| 33 | DD | 95 | LEU |
| 33 | DD | 98 | VAL |
| 33 | DD | 103 | ARG |
| 33 | DD | 105 | ILE |
| 33 | DD | 106 | ILE |
| 33 | DD | 111 | LEU |
| 33 | DD | 112 | GLN |
| 33 | DD | 116 | GLN |
| 33 | DD | 117 | VAL |
| 33 | DD | 127 | VAL |
| 33 | DD | 142 | VAL |
| 33 | DD | 161 | THR |
| 33 | DD | 165 | ILE |
| 33 | DD | 166 | GLN |
| 33 | DD | 173 | VAL |
| 33 | DD | 192 | THR |
| 33 | DD | 198 | ASN |
| 33 | DD | 211 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | DD | 212 | SER |
| 33 | DD | 217 | ARG |
| 33 | DD | 221 | VAL |
| 33 | DD | 229 | VAL |
| 33 | DD | 242 | ARG |
| 33 | DD | 254 | THR |
| 33 | DD | 255 | LYS |
| 33 | DD | 257 | LEU |
| 33 | DD | 259 | THR |
| 33 | DD | 271 | ILE |
| 34 | DE | 1 | MET |
| 34 | DE | 7 | VAL |
| 34 | DE | 12 | THR |
| 34 | DE | 21 | VAL |
| 34 | DE | 23 | VAL |
| 34 | DE | 24 | THR |
| 34 | DE | 33 | VAL |
| 34 | DE | 47 | VAL |
| 34 | DE | 52 | LEU |
| 34 | DE | 60 | ASN |
| 34 | DE | 63 | LEU |
| 34 | DE | 66 | HIS |
| 34 | DE | 67 | PHE |
| 34 | DE | 69 | LYS |
| 34 | DE | 73 | GLU |
| 34 | DE | 75 | VAL |
| 34 | DE | 76 | ARG |
| 34 | DE | 77 | ILE |
| 34 | DE | 79 | ARG |
| 34 | DE | 82 | ARG |
| 34 | DE | 111 | ARG |
| 34 | DE | 116 | VAL |
| 34 | DE | 118 | LYS |
| 34 | DE | 119 | ARG |
| 34 | DE | 133 | LYS |
| 34 | DE | 134 | ILE |
| 34 | DE | 144 | ARG |
| 34 | DE | 152 | LYS |
| 34 | DE | 154 | LYS |
| 34 | DE | 160 | TYR |
| 34 | DE | 163 | GLU |
| 34 | DE | 169 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DE | 170 | LEU |
| 34 | DE | 171 | GLU |
| 34 | DE | 175 | VAL |
| 34 | DE | 181 | LEU |
| 34 | DE | 197 | ILE |
| 34 | DE | 202 | LYS |
| 34 | DE | 203 | LYS |
| 35 | DF | 7 | TYR |
| 35 | DF | 20 | LEU |
| 35 | DF | 23 | ASP |
| 35 | DF | 28 | ILE |
| 35 | DF | 33 | LEU |
| 35 | DF | 38 | ARG |
| 35 | DF | 41 | LEU |
| 35 | DF | 46 | ARG |
| 35 | DF | 48 | THR |
| 35 | DF | 50 | SER |
| 35 | DF | 53 | THR |
| 35 | DF | 56 | GLU |
| 35 | DF | 57 | VAL |
| 35 | DF | 74 | ARG |
| 35 | DF | 78 | ILE |
| 35 | DF | 106 | ARG |
| 35 | DF | 112 | MET |
| 35 | DF | 116 | ASP |
| 35 | DF | 127 | GLU |
| 35 | DF | 137 | LYS |
| 35 | DF | 140 | LEU |
| 35 | DF | 160 | ASN |
| 35 | DF | 162 | LEU |
| 35 | DF | 164 | ARG |
| 35 | DF | 165 | ARG |
| 35 | DF | 168 | ARG |
| 35 | DF | 170 | LEU |
| 35 | DF | 175 | THR |
| 35 | DF | 183 | VAL |
| 35 | DF | 192 | LEU |
| 35 | DF | 194 | MET |
| 35 | DF | 197 | ASP |
| 35 | DF | 199 | TRP |
| 35 | DF | 201 | VAL |
| 35 | DF | 204 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | DF | 206 | ILE |
| 36 | DG | 7 | LEU |
| 36 | DG | 16 | ARG |
| 36 | DG | 22 | ARG |
| 36 | DG | 28 | VAL |
| 36 | DG | 34 | LEU |
| 36 | DG | 35 | GLU |
| 36 | DG | 39 | ILE |
| 36 | DG | 45 | GLU |
| 36 | DG | 49 | ASP |
| 36 | DG | 58 | GLN |
| 36 | DG | 60 | LEU |
| 36 | DG | 63 | ILE |
| 36 | DG | 67 | LYS |
| 36 | DG | 80 | PHE |
| 36 | DG | 125 | PHE |
| 36 | DG | 143 | GLU |
| 36 | DG | 155 | MET |
| 36 | DG | 161 | THR |
| 36 | DG | 166 | ASP |
| 36 | DG | 174 | GLU |
| 37 | DH | 34 | GLU |
| 37 | DH | 41 | MET |
| 37 | DH | 46 | GLU |
| 37 | DH | 53 | GLU |
| 37 | DH | 71 | LEU |
| 37 | DH | 83 | TYR |
| 37 | DH | 95 | ARG |
| 37 | DH | 103 | LEU |
| 37 | DH | 105 | LEU |
| 37 | DH | 110 | SER |
| 37 | DH | 111 | HIS |
| 37 | DH | 122 | THR |
| 37 | DH | 134 | SER |
| 37 | DH | 136 | ILE |
| 37 | DH | 137 | ASP |
| 37 | DH | 141 | VAL |
| 37 | DH | 143 | GLN |
| 37 | DH | 149 | ARG |
| 37 | DH | 152 | ARG |
| 37 | DH | 153 | LYS |
| 37 | DH | 157 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | DH | 159 | GLU |
| 37 | DH | 163 | TYR |
| 37 | DH | 170 | ARG |
| 38 | DI | 1 | MET |
| 38 | DI | 12 | LEU |
| 38 | DI | 20 | ASP |
| 38 | DI | 22 | LYS |
| 38 | DI | 38 | LEU |
| 38 | DI | 40 | THR |
| 38 | DI | 51 | ILE |
| 38 | DI | 56 | LYS |
| 38 | DI | 58 | LEU |
| 38 | DI | 82 | ARG |
| 38 | DI | 88 | ILE |
| 38 | DI | 101 | LEU |
| 38 | DI | 109 | ILE |
| 38 | DI | 122 | GLU |
| 38 | DI | 129 | THR |
| 38 | DI | 142 | VAL |
| 38 | DI | 144 | VAL |
| 39 | DN | 2 | LYS |
| 39 | DN | 4 | TYR |
| 39 | DN | 5 | VAL |
| 39 | DN | 14 | VAL |
| 39 | DN | 16 | ILE |
| 39 | DN | 19 | GLU |
| 39 | DN | 23 | LEU |
| 39 | DN | 25 | ARG |
| 39 | DN | 28 | THR |
| 39 | DN | 33 | LEU |
| 39 | DN | 34 | LEU |
| 39 | DN | 37 | LYS |
| 39 | DN | 41 | ASP |
| 39 | DN | 45 | ASN |
| 39 | DN | 46 | VAL |
| 39 | DN | 48 | MET |
| 39 | DN | 55 | VAL |
| 39 | DN | 58 | ASP |
| 39 | DN | 60 | ILE |
| 39 | DN | 62 | VAL |
| 39 | DN | 63 | THR |
| 39 | DN | 65 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | DN | 67 | LEU |
| 39 | DN | 69 | GLN |
| 39 | DN | 75 | TYR |
| 39 | DN | 78 | TYR |
| 39 | DN | 82 | LEU |
| 39 | DN | 84 | LYS |
| 39 | DN | 85 | ILE |
| 39 | DN | 87 | LEU |
| 39 | DN | 98 | VAL |
| 39 | DN | 99 | LEU |
| 39 | DN | 112 | LEU |
| 39 | DN | 119 | ARG |
| 39 | DN | 120 | LEU |
| 39 | DN | 121 | LYS |
| 39 | DN | 130 | HIS |
| 39 | DN | 134 | ARG |
| 39 | DN | 138 | LEU |
| 40 | DO | 3 | GLN |
| 40 | DO | 8 | LEU |
| 40 | DO | 13 | ASN |
| 40 | DO | 22 | ILE |
| 40 | DO | 24 | VAL |
| 40 | DO | 28 | SER |
| 40 | DO | 47 | ILE |
| 40 | DO | 52 | VAL |
| 40 | DO | 63 | VAL |
| 40 | DO | 75 | SER |
| 40 | DO | 87 | ILE |
| 40 | DO | 88 | ASN |
| 40 | DO | 104 | ARG |
| 40 | DO | 108 | GLU |
| 40 | DO | 112 | MET |
| 41 | DP | 13 | ASN |
| 41 | DP | 15 | ARG |
| 41 | DP | 16 | ARG |
| 41 | DP | 17 | LYS |
| 41 | DP | 18 | ARG |
| 41 | DP | 19 | VAL |
| 41 | DP | 21 | ARG |
| 41 | DP | 32 | THR |
| 41 | DP | 33 | ARG |
| 41 | DP | 39 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | DP | 40 | SER |
| 41 | DP | 45 | LEU |
| 41 | DP | 47 | ASP |
| 41 | DP | 52 | GLU |
| 41 | DP | 55 | ARG |
| 41 | DP | 57 | THR |
| 41 | DP | 59 | LEU |
| 41 | DP | 61 | ARG |
| 41 | DP | 62 | LEU |
| 41 | DP | 65 | ARG |
| 41 | DP | 67 | MET |
| 41 | DP | 70 | GLN |
| 41 | DP | 75 | ILE |
| 41 | DP | 77 | ARG |
| 41 | DP | 85 | LEU |
| 41 | DP | 95 | VAL |
| 41 | DP | 100 | LEU |
| 41 | DP | 101 | VAL |
| 41 | DP | 102 | ARG |
| 41 | DP | 110 | TYR |
| 41 | DP | 111 | ARG |
| 41 | DP | 112 | LEU |
| 41 | DP | 114 | ILE |
| 41 | DP | 115 | LEU |
| 41 | DP | 123 | LEU |
| 41 | DP | 125 | VAL |
| 41 | DP | 135 | LEU |
| 41 | DP | 138 | LEU |
| 41 | DP | 144 | GLU |
| 41 | DP | 147 | LEU |
| 41 | DP | 148 | LEU |
| 42 | DQ | 6 | ARG |
| 42 | DQ | 9 | TYR |
| 42 | DQ | 13 | GLN |
| 42 | DQ | 18 | LYS |
| 42 | DQ | 22 | LYS |
| 42 | DQ | 27 | VAL |
| 42 | DQ | 29 | PHE |
| 42 | DQ | 35 | VAL |
| 42 | DQ | 45 | GLN |
| 42 | DQ | 52 | VAL |
| 42 | DQ | 54 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | DQ | 55 | VAL |
| 42 | DQ | 63 | LYS |
| 42 | DQ | 80 | GLU |
| 42 | DQ | 81 | VAL |
| 42 | DQ | 82 | ARG |
| 42 | DQ | 91 | GLU |
| 42 | DQ | 103 | MET |
| 42 | DQ | 106 | VAL |
| 42 | DQ | 109 | VAL |
| 42 | DQ | 115 | MET |
| 42 | DQ | 127 | ILE |
| 42 | DQ | 132 | VAL |
| 42 | DQ | 139 | GLU |
| 42 | DQ | 141 | GLN |
| 43 | DR | 2 | ARG |
| 43 | DR | 5 | LYS |
| 43 | DR | 6 | SER |
| 43 | DR | 8 | ARG |
| 43 | DR | 16 | HIS |
| 43 | DR | 18 | LEU |
| 43 | DR | 28 | LEU |
| 43 | DR | 29 | LEU |
| 43 | DR | 30 | THR |
| 43 | DR | 36 | THR |
| 43 | DR | 44 | LEU |
| 43 | DR | 45 | ARG |
| 43 | DR | 56 | LYS |
| 43 | DR | 60 | LEU |
| 43 | DR | 65 | LEU |
| 43 | DR | 67 | LEU |
| 43 | DR | 71 | GLN |
| 43 | DR | 74 | LYS |
| 43 | DR | 75 | LEU |
| 43 | DR | 79 | LEU |
| 43 | DR | 99 | LYS |
| 43 | DR | 100 | LEU |
| 43 | DR | 103 | ARG |
| 43 | DR | 104 | ARG |
| 43 | DR | 115 | GLU |
| 43 | DR | 117 | VAL |
| 43 | DR | 118 | GLU |
| 44 | DS | 11 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | DS | 15 | ARG |
| 44 | DS | 17 | ARG |
| 44 | DS | 30 | ARG |
| 44 | DS | 33 | LYS |
| 44 | DS | 36 | TYR |
| 44 | DS | 48 | LEU |
| 44 | DS | 50 | SER |
| 44 | DS | 54 | LEU |
| 44 | DS | 56 | LEU |
| 44 | DS | 58 | LEU |
| 44 | DS | 61 | ASN |
| 44 | DS | 69 | VAL |
| 44 | DS | 73 | LEU |
| 44 | DS | 80 | LEU |
| 44 | DS | 83 | LYS |
| 44 | DS | 84 | GLN |
| 44 | DS | 85 | VAL |
| 44 | DS | 89 | ARG |
| 44 | DS | 92 | TYR |
| 44 | DS | 93 | LYS |
| 44 | DS | 95 | HIS |
| 44 | DS | 97 | ARG |
| 44 | DS | 98 | VAL |
| 44 | DS | 106 | ARG |
| 45 | DT | 3 | ARG |
| 45 | DT | 13 | ARG |
| 45 | DT | 15 | VAL |
| 45 | DT | 16 | ARG |
| 45 | DT | 17 | THR |
| 45 | DT | 18 | ASP |
| 45 | DT | 24 | PRO |
| 45 | DT | 29 | ARG |
| 45 | DT | 32 | TYR |
| 45 | DT | 33 | LYS |
| 45 | DT | 38 | ASN |
| 45 | DT | 41 | ARG |
| 45 | DT | 53 | ARG |
| 45 | DT | 58 | ASN |
| 45 | DT | 59 | THR |
| 45 | DT | 62 | THR |
| 45 | DT | 63 | VAL |
| 45 | DT | 64 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | DT | 65 | LYS |
| 45 | DT | 82 | LEU |
| 45 | DT | 88 | ILE |
| 45 | DT | 96 | ARG |
| 45 | DT | 98 | LYS |
| 45 | DT | 99 | LEU |
| 45 | DT | 108 | ARG |
| 45 | DT | 112 | ARG |
| 45 | DT | 115 | ARG |
| 45 | DT | 128 | GLU |
| 46 | DU | 8 | VAL |
| 46 | DU | 27 | LEU |
| 46 | DU | 34 | LYS |
| 46 | DU | 55 | ARG |
| 46 | DU | 56 | ASP |
| 46 | DU | 64 | ARG |
| 46 | DU | 70 | ARG |
| 46 | DU | 74 | LEU |
| 46 | DU | 77 | SER |
| 46 | DU | 83 | LEU |
| 46 | DU | 88 | ILE |
| 46 | DU | 89 | GLU |
| 46 | DU | 90 | VAL |
| 46 | DU | 92 | ARG |
| 46 | DU | 93 | LYS |
| 46 | DU | 97 | ASP |
| 46 | DU | 102 | GLU |
| 47 | DV | 2 | PHE |
| 47 | DV | 14 | VAL |
| 47 | DV | 15 | GLU |
| 47 | DV | 18 | LEU |
| 47 | DV | 19 | LYS |
| 47 | DV | 21 | ARG |
| 47 | DV | 22 | VAL |
| 47 | DV | 23 | GLU |
| 47 | DV | 28 | GLU |
| 47 | DV | 32 | THR |
| 47 | DV | 35 | LEU |
| 47 | DV | 37 | VAL |
| 47 | DV | 38 | LEU |
| 47 | DV | 40 | LEU |
| 47 | DV | 56 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | DV | 62 | LEU |
| 47 | DV | 66 | ARG |
| 47 | DV | 71 | LEU |
| 47 | DV | 78 | LYS |
| 47 | DV | 80 | GLN |
| 47 | DV | 82 | ARG |
| 47 | DV | 83 | ARG |
| 47 | DV | 88 | ARG |
| 47 | DV | 89 | GLN |
| 47 | DV | 92 | THR |
| 47 | DV | 93 | GLU |
| 47 | DV | 98 | GLU |
| 47 | DV | 100 | ARG |
| 48 | DW | 4 | LYS |
| 48 | DW | 11 | ARG |
| 48 | DW | 17 | VAL |
| 48 | DW | 19 | LEU |
| 48 | DW | 20 | VAL |
| 48 | DW | 23 | LEU |
| 48 | DW | 33 | ARG |
| 48 | DW | 50 | VAL |
| 48 | DW | 51 | LEU |
| 48 | DW | 64 | MET |
| 48 | DW | 69 | LEU |
| 48 | DW | 82 | LEU |
| 48 | DW | 96 | ILE |
| 48 | DW | 106 | ILE |
| 48 | DW | 107 | LEU |
| 49 | DX | 3 | THR |
| 49 | DX | 12 | VAL |
| 49 | DX | 15 | GLU |
| 49 | DX | 21 | PHE |
| 49 | DX | 25 | LYS |
| 49 | DX | 27 | THR |
| 49 | DX | 30 | VAL |
| 49 | DX | 33 | LYS |
| 49 | DX | 35 | THR |
| 49 | DX | 36 | LYS |
| 49 | DX | 38 | GLU |
| 49 | DX | 39 | ILE |
| 49 | DX | 45 | THR |
| 49 | DX | 49 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | DX | 55 | ASN |
| 49 | DX | 60 | ARG |
| 49 | DX | 65 | ARG |
| 49 | DX | 76 | ARG |
| 49 | DX | 78 | LYS |
| 49 | DX | 88 | LYS |
| 50 | DY | 2 | ARG |
| 50 | DY | 6 | HIS |
| 50 | DY | 7 | VAL |
| 50 | DY | 8 | LYS |
| 50 | DY | 13 | VAL |
| 50 | DY | 38 | ILE |
| 50 | DY | 42 | VAL |
| 50 | DY | 46 | LYS |
| 50 | DY | 47 | LYS |
| 50 | DY | 49 | VAL |
| 50 | DY | 55 | TYR |
| 50 | DY | 60 | PHE |
| 50 | DY | 62 | GLU |
| 50 | DY | 66 | PRO |
| 50 | DY | 70 | SER |
| 50 | DY | 71 | LYS |
| 50 | DY | 75 | ILE |
| 50 | DY | 76 | CYS |
| 50 | DY | 81 | LYS |
| 50 | DY | 86 | ARG |
| 50 | DY | 89 | PHE |
| 50 | DY | 90 | LEU |
| 50 | DY | 94 | LYS |
| 50 | DY | 96 | ILE |
| 50 | DY | 97 | ARG |
| 50 | DY | 99 | CYS |
| 51 | DZ | 6 | LYS |
| 51 | DZ | 19 | ARG |
| 51 | DZ | 27 | VAL |
| 51 | DZ | 42 | VAL |
| 51 | DZ | 53 | ILE |
| 51 | DZ | 72 | ARG |
| 51 | DZ | 73 | GLN |
| 51 | DZ | 79 | ARG |
| 51 | DZ | 81 | ARG |
| 51 | DZ | 86 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | DZ | 87 | ASP |
| 51 | DZ | 93 | ASP |
| 51 | DZ | 97 | GLU |
| 51 | DZ | 98 | MET |
| 51 | DZ | 117 | LEU |
| 51 | DZ | 121 | HIS |
| 51 | DZ | 124 | ILE |
| 51 | DZ | 128 | VAL |
| 51 | DZ | 140 | ASP |
| 51 | DZ | 150 | LEU |
| 51 | DZ | 151 | HIS |
| 51 | DZ | 153 | SER |
| 51 | DZ | 166 | SER |
| 51 | DZ | 171 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (291) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 19 | HIS |
| 2 | AB | 40 | HIS |
| 2 | AB | 135 | GLN |
| 2 | AB | 146 | GLN |
| 2 | AB | 204 | ASN |
| 3 | AC | 3 | ASN |
| 3 | AC | 6 | HIS |
| 3 | AC | 28 | GLN |
| 3 | AC | 37 | GLN |
| 3 | AC | 69 | HIS |
| 3 | AC | 118 | GLN |
| 3 | AC | 170 | GLN |
| 4 | AD | 62 | GLN |
| 4 | AD | 77 | ASN |
| 4 | AD | 123 | HIS |
| 4 | AD | 129 | ASN |
| 5 | AE | 20 | GLN |
| 5 | AE | 78 | HIS |
| 6 | AF | 7 | ASN |
| 6 | AF | 18 | GLN |
| 6 | AF | 27 | GLN |
| 6 | AF | 64 | GLN |
| 6 | AF | 100 | ASN |
| 7 | AG | 13 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AG | 37 | ASN |
| 7 | AG | 84 | ASN |
| 7 | AG | 97 | GLN |
| 7 | AG | 106 | GLN |
| 8 | AH | 82 | HIS |
| 9 | AI | 117 | HIS |
| 9 | AI | 124 | GLN |
| 10 | AJ | 13 | HIS |
| 10 | AJ | 78 | ASN |
| 11 | AK | 117 | ASN |
| 12 | AL | 8 | ASN |
| 12 | AL | 49 | ASN |
| 12 | AL | 75 | HIS |
| 13 | AM | 77 | ASN |
| 15 | AO | 37 | ASN |
| 15 | AO | 46 | HIS |
| 16 | AP | 13 | HIS |
| 16 | AP | 76 | GLN |
| 16 | AP | 82 | GLN |
| 17 | AQ | 16 | GLN |
| 19 | AS | 53 | ASN |
| 20 | AT | 26 | ASN |
| 20 | AT | 75 | ASN |
| 22 | B0 | 29 | GLN |
| 23 | B1 | 19 | GLN |
| 23 | B1 | 66 | HIS |
| 24 | B2 | 38 | GLN |
| 24 | B2 | 46 | GLN |
| 24 | B2 | 47 | ASN |
| 24 | B2 | 56 | GLN |
| 25 | B3 | 19 | GLN |
| 25 | B3 | 46 | ASN |
| 25 | B3 | 52 | HIS |
| 27 | B5 | 4 | HIS |
| 27 | B5 | 43 | HIS |
| 28 | B6 | 20 | ASN |
| 28 | B6 | 26 | ASN |
| 28 | B6 | 32 | ASN |
| 29 | B7 | 8 | ASN |
| 29 | B7 | 36 | GLN |
| 30 | B8 | 35 | GLN |
| 33 | BD | 58 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | BD | 96 | HIS |
| 33 | BD | 126 | GLN |
| 33 | BD | 143 | HIS |
| 33 | BD | 164 | GLN |
| 33 | BD | 166 | GLN |
| 33 | BD | 186 | HIS |
| 33 | BD | 198 | ASN |
| 34 | BE | 48 | GLN |
| 34 | BE | 54 | GLN |
| 34 | BE | 55 | ASN |
| 34 | BE | 66 | HIS |
| 34 | BE | 85 | ASN |
| 34 | BE | 129 | HIS |
| 34 | BE | 132 | HIS |
| 34 | BE | 169 | ASN |
| 34 | BE | 192 | ASN |
| 35 | BF | 69 | HIS |
| 35 | BF | 75 | HIS |
| 35 | BF | 160 | ASN |
| 35 | BF | 169 | ASN |
| 36 | BG | 40 | ASN |
| 36 | BG | 58 | GLN |
| 36 | BG | 66 | GLN |
| 37 | BH | 65 | HIS |
| 37 | BH | 143 | GLN |
| 37 | BH | 147 | ASN |
| 37 | BH | 158 | HIS |
| 38 | BI | 43 | ASN |
| 38 | BI | 104 | GLN |
| 38 | BI | 105 | HIS |
| 38 | BI | 133 | HIS |
| 39 | BN | 45 | ASN |
| 39 | BN | 69 | GLN |
| 39 | BN | 130 | HIS |
| 40 | BO | 3 | GLN |
| 40 | BO | 13 | ASN |
| 40 | BO | 82 | ASN |
| 40 | BO | 89 | ASN |
| 41 | BP | 13 | ASN |
| 41 | BP | 81 | GLN |
| 41 | BP | 128 | HIS |
| 42 | BQ | 13 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BQ | 141 | GLN |
| 43 | BR | 13 | HIS |
| 43 | BR | 16 | HIS |
| 43 | BR | 23 | ASN |
| 43 | BR | 24 | GLN |
| 43 | BR | 53 | HIS |
| 43 | BR | 71 | GLN |
| 43 | BR | 91 | GLN |
| 44 | BS | 34 | HIS |
| 44 | BS | 61 | ASN |
| 44 | BS | 68 | GLN |
| 45 | BT | 38 | ASN |
| 45 | BT | 43 | GLN |
| 45 | BT | 58 | ASN |
| 45 | BT | 90 | GLN |
| 46 | BU | 49 | HIS |
| 46 | BU | 75 | ASN |
| 46 | BU | 94 | ASN |
| 47 | BV | 11 | GLN |
| 47 | BV | 64 | HIS |
| 47 | BV | 87 | HIS |
| 47 | BV | 89 | GLN |
| 48 | BW | 34 | ASN |
| 48 | BW | 57 | ASN |
| 48 | BW | 61 | ASN |
| 48 | BW | 62 | HIS |
| 48 | BW | 102 | HIS |
| 48 | BW | 111 | HIS |
| 49 | BX | 31 | HIS |
| 49 | BX | 41 | ASN |
| 49 | BX | 55 | ASN |
| 49 | BX | 87 | GLN |
| 51 | BZ | 30 | ASN |
| 51 | BZ | 54 | HIS |
| 51 | BZ | 55 | HIS |
| 51 | BZ | 151 | HIS |
| 2 | CB | 19 | HIS |
| 2 | CB | 40 | HIS |
| 2 | CB | 135 | GLN |
| 2 | CB | 146 | GLN |
| 2 | CB | 204 | ASN |
| 3 | CC | 3 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CC | 6 | HIS |
| 3 | CC | 28 | GLN |
| 3 | CC | 37 | GLN |
| 3 | CC | 69 | HIS |
| 3 | CC | 118 | GLN |
| 3 | CC | 170 | GLN |
| 4 | CD | 62 | GLN |
| 4 | CD | 77 | ASN |
| 4 | CD | 123 | HIS |
| 4 | CD | 129 | ASN |
| 5 | CE | 20 | GLN |
| 5 | CE | 72 | GLN |
| 5 | CE | 78 | HIS |
| 6 | CF | 7 | ASN |
| 6 | CF | 18 | GLN |
| 6 | CF | 27 | GLN |
| 6 | CF | 64 | GLN |
| 6 | CF | 100 | ASN |
| 7 | CG | 13 | GLN |
| 7 | CG | 37 | ASN |
| 7 | CG | 84 | ASN |
| 7 | CG | 97 | GLN |
| 7 | CG | 106 | GLN |
| 7 | CG | 153 | HIS |
| 8 | CH | 82 | HIS |
| 9 | CI | 117 | HIS |
| 9 | CI | 124 | GLN |
| 10 | CJ | 13 | HIS |
| 10 | CJ | 78 | ASN |
| 11 | CK | 38 | ASN |
| 11 | CK | 117 | ASN |
| 12 | CL | 8 | ASN |
| 12 | CL | 49 | ASN |
| 12 | CL | 75 | HIS |
| 13 | CM | 77 | ASN |
| 15 | CO | 37 | ASN |
| 15 | CO | 46 | HIS |
| 16 | CP | 13 | HIS |
| 16 | CP | 76 | GLN |
| 16 | CP | 82 | GLN |
| 17 | CQ | 16 | GLN |
| 19 | CS | 53 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | CT | 26 | ASN |
| 20 | CT | 75 | ASN |
| 22 | D0 | 29 | GLN |
| 23 | D1 | 19 | GLN |
| 23 | D1 | 66 | HIS |
| 24 | D2 | 38 | GLN |
| 24 | D2 | 46 | GLN |
| 24 | D2 | 47 | ASN |
| 24 | D2 | 56 | GLN |
| 25 | D3 | 19 | GLN |
| 25 | D3 | 46 | ASN |
| 25 | D3 | 52 | HIS |
| 27 | D5 | 4 | HIS |
| 27 | D5 | 43 | HIS |
| 28 | D6 | 20 | ASN |
| 28 | D6 | 26 | ASN |
| 28 | D6 | 32 | ASN |
| 29 | D7 | 8 | ASN |
| 29 | D7 | 36 | GLN |
| 30 | D8 | 35 | GLN |
| 33 | DD | 58 | HIS |
| 33 | DD | 96 | HIS |
| 33 | DD | 126 | GLN |
| 33 | DD | 143 | HIS |
| 33 | DD | 164 | GLN |
| 33 | DD | 166 | GLN |
| 33 | DD | 186 | HIS |
| 33 | DD | 198 | ASN |
| 34 | DE | 48 | GLN |
| 34 | DE | 54 | GLN |
| 34 | DE | 55 | ASN |
| 34 | DE | 60 | ASN |
| 34 | DE | 66 | HIS |
| 34 | DE | 85 | ASN |
| 34 | DE | 129 | HIS |
| 34 | DE | 132 | HIS |
| 34 | DE | 169 | ASN |
| 34 | DE | 192 | ASN |
| 35 | DF | 69 | HIS |
| 35 | DF | 75 | HIS |
| 35 | DF | 160 | ASN |
| 35 | DF | 169 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | DG | 40 | ASN |
| 36 | DG | 66 | GLN |
| 36 | DG | 108 | ASN |
| 37 | DH | 65 | HIS |
| 37 | DH | 147 | ASN |
| 37 | DH | 158 | HIS |
| 38 | DI | 43 | ASN |
| 38 | DI | 104 | GLN |
| 38 | DI | 133 | HIS |
| 39 | DN | 45 | ASN |
| 39 | DN | 69 | GLN |
| 39 | DN | 130 | HIS |
| 40 | DO | 3 | GLN |
| 40 | DO | 13 | ASN |
| 40 | DO | 82 | ASN |
| 40 | DO | 89 | ASN |
| 41 | DP | 13 | ASN |
| 41 | DP | 81 | GLN |
| 41 | DP | 128 | HIS |
| 42 | DQ | 12 | GLN |
| 42 | DQ | 13 | GLN |
| 42 | DQ | 141 | GLN |
| 43 | DR | 13 | HIS |
| 43 | DR | 16 | HIS |
| 43 | DR | 23 | ASN |
| 43 | DR | 24 | GLN |
| 43 | DR | 53 | HIS |
| 43 | DR | 71 | GLN |
| 43 | DR | 91 | GLN |
| 44 | DS | 34 | HIS |
| 44 | DS | 61 | ASN |
| 44 | DS | 68 | GLN |
| 45 | DT | 38 | ASN |
| 45 | DT | 43 | GLN |
| 45 | DT | 58 | ASN |
| 45 | DT | 90 | GLN |
| 46 | DU | 49 | HIS |
| 46 | DU | 75 | ASN |
| 46 | DU | 94 | ASN |
| 47 | DV | 11 | GLN |
| 47 | DV | 64 | HIS |
| 47 | DV | 87 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | DV | 89 | GLN |
| 48 | DW | 34 | ASN |
| 48 | DW | 57 | ASN |
| 48 | DW | 61 | ASN |
| 48 | DW | 62 | HIS |
| 48 | DW | 102 | HIS |
| 48 | DW | 111 | HIS |
| 49 | DX | 31 | HIS |
| 49 | DX | 41 | ASN |
| 49 | DX | 55 | ASN |
| 49 | DX | 87 | GLN |
| 51 | DZ | 30 | ASN |
| 51 | DZ | 54 | HIS |
| 51 | DZ | 55 | HIS |
| 51 | DZ | 151 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1503/1522 (98%) | 283 (18%) | 29 (1%) |
| 1 | CA | 1503/1522 (98%) | 280 (18%) | 29 (1%) |
| 31 | BA | 2723/2787 (97%) | 723 (26%) | 73 (2%) |
| 31 | DA | 2723/2787 (97%) | 726 (26%) | 70 (2%) |
| 32 | BB | 118/122 (96%) | 35 (29%) | 1 (0%) |
| 32 | DB | 118/122 (96%) | 34 (28%) | 1 (0%) |
| All | All | 8688/8862 (98%) | 2081 (23%) | 203 (2%) |

All (2081) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 9 | G |
| 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 | 61 | G |
| 1 | AA | 80 | G |
| 1 | AA | 81 | U |
| 1 | AA | 90 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 91 | C |
| 1 | AA | 97 | G |
| 1 | AA | 98 | G |
| 1 | AA | 101 | A |
| 1 | AA | 108 | G |
| 1 | AA | 115 | G |
| 1 | AA | 116 | A |
| 1 | AA | 119 | A |
| 1 | AA | 120 | A |
| 1 | AA | 121 | C |
| 1 | AA | 131 | C |
| 1 | AA | 138 | G |
| 1 | AA | 144 | G |
| 1 | AA | 147 | G |
| 1 | AA | 150 | C |
| 1 | AA | 152 | A |
| 1 | AA | 163 | C |
| 1 | AA | 168 | G |
| 1 | AA | 172 | A |
| 1 | AA | 173 | U |
| 1 | AA | 181 | G |
| 1 | AA | 182 | U |
| 1 | AA | 189(G) | G |
| 1 | AA | 189(H) | G |
| 1 | AA | 189(J) | G |
| 1 | AA | 195 | A |
| 1 | AA | 197 | A |
| 1 | AA | 199 | G |
| 1 | AA | 201 | C |
| 1 | AA | 202 | U |
| 1 | AA | 203 | U |
| 1 | AA | 216 | G |
| 1 | AA | 220 | G |
| 1 | AA | 243 | A |
| 1 | AA | 244 | U |
| 1 | AA | 247 | G |
| 1 | AA | 251 | G |
| 1 | AA | 266 | G |
| 1 | AA | 267 | C |
| 1 | AA | 280 | C |
| 1 | AA | 281 | G |
| 1 | AA | 289 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 296 | U |
| 1 | AA | 297 | G |
| 1 | AA | 298 | A |
| 1 | AA | 301 | G |
| 1 | AA | 306 | G |
| 1 | AA | 328 | C |
| 1 | AA | 329 | A |
| 1 | AA | 332 | G |
| 1 | AA | 343 | U |
| 1 | AA | 345 | C |
| 1 | AA | 351 | G |
| 1 | AA | 352 | C |
| 1 | AA | 353 | A |
| 1 | AA | 354 | G |
| 1 | AA | 357 | G |
| 1 | AA | 367 | U |
| 1 | AA | 372 | C |
| 1 | AA | 373 | A |
| 1 | AA | 384 | G |
| 1 | AA | 388 | G |
| 1 | AA | 390 | C |
| 1 | AA | 397 | A |
| 1 | AA | 398 | C |
| 1 | AA | 406 | G |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 414 | A |
| 1 | AA | 418 | C |
| 1 | AA | 419 | C |
| 1 | AA | 422 | C |
| 1 | AA | 424 | G |
| 1 | AA | 427 | U |
| 1 | AA | 429 | U |
| 1 | AA | 430 | A |
| 1 | AA | 435 | C |
| 1 | AA | 437 | U |
| 1 | AA | 439 | A |
| 1 | AA | 442 | C |
| 1 | AA | 448 | A |
| 1 | AA | 452 | A |
| 1 | AA | 461 | A |
| 1 | AA | 472 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 484 | G |
| 1 | AA | 485 | G |
| 1 | AA | 487 | A |
| 1 | AA | 496 | A |
| 1 | AA | 498 | U |
| 1 | AA | 499 | A |
| 1 | AA | 505 | G |
| 1 | AA | 508 | C |
| 1 | AA | 509 | A |
| 1 | AA | 510 | A |
| 1 | AA | 511 | C |
| 1 | AA | 513 | C |
| 1 | AA | 518 | C |
| 1 | AA | 527 | G |
| 1 | AA | 531 | U |
| 1 | AA | 532 | A |
| 1 | AA | 533 | A |
| 1 | AA | 534 | U |
| 1 | AA | 547 | A |
| 1 | AA | 559 | A |
| 1 | AA | 561 | U |
| 1 | AA | 562 | C |
| 1 | AA | 563 | A |
| 1 | AA | 572 | A |
| 1 | AA | 573 | A |
| 1 | AA | 575 | G |
| 1 | AA | 576 | G |
| 1 | AA | 588 | G |
| 1 | AA | 596 | C |
| 1 | AA | 616 | G |
| 1 | AA | 623 | C |
| 1 | AA | 630 | G |
| 1 | AA | 632 | A |
| 1 | AA | 653 | A |
| 1 | AA | 665 | A |
| 1 | AA | 671 | G |
| 1 | AA | 674 | G |
| 1 | AA | 687 | A |
| 1 | AA | 688 | G |
| 1 | AA | 693 | G |
| 1 | AA | 724 | G |
| 1 | AA | 725 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 731 | G |
| 1 | AA | 748 | C |
| 1 | AA | 749 | C |
| 1 | AA | 753 | A |
| 1 | AA | 754 | C |
| 1 | AA | 755 | G |
| 1 | AA | 760 | G |
| 1 | AA | 765 | G |
| 1 | AA | 766 | A |
| 1 | AA | 777 | A |
| 1 | AA | 782 | A |
| 1 | AA | 786 | G |
| 1 | AA | 792 | A |
| 1 | AA | 793 | U |
| 1 | AA | 794 | A |
| 1 | AA | 817 | C |
| 1 | AA | 818 | G |
| 1 | AA | 827 | U |
| 1 | AA | 828 | A |
| 1 | AA | 833 | U |
| 1 | AA | 836 | G |
| 1 | AA | 839 | U |
| 1 | AA | 840 | C |
| 1 | AA | 841 | U |
| 1 | AA | 848 | C |
| 1 | AA | 859 | A |
| 1 | AA | 864 | A |
| 1 | AA | 869 | G |
| 1 | AA | 870 | U |
| 1 | AA | 872 | A |
| 1 | AA | 902 | G |
| 1 | AA | 914 | A |
| 1 | AA | 916 | G |
| 1 | AA | 927 | G |
| 1 | AA | 934 | C |
| 1 | AA | 935 | A |
| 1 | AA | 960 | U |
| 1 | AA | 961 | U |
| 1 | AA | 968 | A |
| 1 | AA | 969 | A |
| 1 | AA | 971 | G |
| 1 | AA | 972 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 974 | A |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 978 | A |
| 1 | AA | 980 | C |
| 1 | AA | 991 | U |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 1005 | A |
| 1 | AA | 1026 | G |
| 1 | AA | 1050 | G |
| 1 | AA | 1053 | G |
| 1 | AA | 1054 | C |
| 1 | AA | 1064 | G |
| 1 | AA | 1065 | U |
| 1 | AA | 1066 | C |
| 1 | AA | 1067 | A |
| 1 | AA | 1068 | G |
| 1 | AA | 1081 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1101 | A |
| 1 | AA | 1103 | C |
| 1 | AA | 1113 | C |
| 1 | AA | 1117 | G |
| 1 | AA | 1118 | C |
| 1 | AA | 1124 | G |
| 1 | AA | 1125 | U |
| 1 | AA | 1126 | U |
| 1 | AA | 1127 | G |
| 1 | AA | 1129 | C |
| 1 | AA | 1136 | U |
| 1 | AA | 1137 | C |
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1146 | A |
| 1 | AA | 1152 | A |
| 1 | AA | 1159 | U |
| 1 | AA | 1160 | G |
| 1 | AA | 1196 | U |
| 1 | AA | 1197 | G |
| 1 | AA | 1202 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1204 | A |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1225 | A |
| 1 | AA | 1227 | A |
| 1 | AA | 1238 | A |
| 1 | AA | 1249 | C |
| 1 | AA | 1255 | G |
| 1 | AA | 1256 | A |
| 1 | AA | 1257 | U |
| 1 | AA | 1280 | A |
| 1 | AA | 1281 | U |
| 1 | AA | 1282 | C |
| 1 | AA | 1286 | A |
| 1 | AA | 1287 | A |
| 1 | AA | 1294 | G |
| 1 | AA | 1299 | A |
| 1 | AA | 1300 | G |
| 1 | AA | 1301 | U |
| 1 | AA | 1302 | U |
| 1 | AA | 1305 | G |
| 1 | AA | 1310 | G |
| 1 | AA | 1312 | G |
| 1 | AA | 1317 | C |
| 1 | AA | 1320 | C |
| 1 | AA | 1322 | C |
| 1 | AA | 1323 | G |
| 1 | AA | 1331 | G |
| 1 | AA | 1332 | A |
| 1 | AA | 1334 | G |
| 1 | AA | 1335 | C |
| 1 | AA | 1338 | G |
| 1 | AA | 1347 | G |
| 1 | AA | 1363 | C |
| 1 | AA | 1364 | U |
| 1 | AA | 1370 | G |
| 1 | AA | 1388 | C |
| 1 | AA | 1397 | C |
| 1 | AA | 1416 | G |
| 1 | AA | 1419 | G |
| 1 | AA | 1442 | G |
| 1 | AA | 1442(A) | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1442(B) | A |
| 1 | AA | 1443 | G |
| 1 | AA | 1447 | A |
| 1 | AA | 1452 | C |
| 1 | AA | 1456 | G |
| 1 | AA | 1457 | G |
| 1 | AA | 1492 | A |
| 1 | AA | 1493 | A |
| 1 | AA | 1494 | G |
| 1 | AA | 1497 | G |
| 1 | AA | 1499 | A |
| 1 | AA | 1502 | A |
| 1 | AA | 1504 | G |
| 1 | AA | 1505 | G |
| 1 | AA | 1506 | U |
| 1 | AA | 1507 | A |
| 1 | AA | 1517 | G |
| 1 | AA | 1520 | G |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 31 | BA | 10 | G |
| 31 | BA | 12 | U |
| 31 | BA | 15 | G |
| 31 | BA | 34 | C |
| 31 | BA | 35 | G |
| 31 | BA | 36 | G |
| 31 | BA | 45 | C |
| 31 | BA | 49 | A |
| 31 | BA | 50 | U |
| 31 | BA | 51 | G |
| 31 | BA | 55 | G |
| 31 | BA | 61 | G |
| 31 | BA | 64 | A |
| 31 | BA | 71 | A |
| 31 | BA | 72 | U |
| 31 | BA | 74 | A |
| 31 | BA | 75 | G |
| 31 | BA | 84 | A |
| 31 | BA | 90 | U |
| 31 | BA | 92 | A |
| 31 | BA | 94 | C |
| 31 | BA | 95 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 31 | BA | 100 | G |
| 31 | BA | 102 | G |
| 31 | BA | 103 | A |
| 31 | BA | 105 | C |
| 31 | BA | 117 | G |
| 31 | BA | 118 | A |
| 31 | BA | 119 | A |
| 31 | BA | 120 | U |
| 31 | BA | 125 | G |
| 31 | BA | 129 | C |
| 31 | BA | 131 | G |
| 31 | BA | 137 | C |
| 31 | BA | 139(A) | G |
| 31 | BA | 142 | A |
| 31 | BA | 142(A) | C |
| 31 | BA | 146 | G |
| 31 | BA | 154(A) | C |
| 31 | BA | 157 | U |
| 31 | BA | 158 | U |
| 31 | BA | 171 | G |
| 31 | BA | 173 | G |
| 31 | BA | 174 | C |
| 31 | BA | 175 | G |
| 31 | BA | 182 | A |
| 31 | BA | 188 | G |
| 31 | BA | 196 | A |
| 31 | BA | 197 | A |
| 31 | BA | 199 | A |
| 31 | BA | 204 | A |
| 31 | BA | 205 | G |
| 31 | BA | 214 | G |
| 31 | BA | 215 | G |
| 31 | BA | 216 | A |
| 31 | BA | 221 | A |
| 31 | BA | 222 | A |
| 31 | BA | 225 | A |
| 31 | BA | 228 | A |
| 31 | BA | 229 | A |
| 31 | BA | 233 | A |
| 31 | BA | 248 | G |
| 31 | BA | 250 | G |
| 31 | BA | 252 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 31 | BA | 266 | G |
| 31 | BA | 271(J) | C |
| 31 | BA | 271(K) | U |
| 31 | BA | 271(L) | U |
| 31 | BA | 271(M) | G |
| 31 | BA | 271(N) | U |
| 31 | BA | 271(O) | C |
| 31 | BA | 271(P) | C |
| 31 | BA | 271(R) | G |
| 31 | BA | 271(U) | G |
| 31 | BA | 272 | G |
| 31 | BA | 272(B) | G |
| 31 | BA | 272(H) | C |
| 31 | BA | 272(I) | U |
| 31 | BA | 272(J) | C |
| 31 | BA | 274 | G |
| 31 | BA | 275 | G |
| 31 | BA | 279 | C |
| 31 | BA | 281 | G |
| 31 | BA | 286 | C |
| 31 | BA | 287 | C |
| 31 | BA | 298 | G |
| 31 | BA | 299 | A |
| 31 | BA | 310 | A |
| 31 | BA | 311 | A |
| 31 | BA | 324 | A |
| 31 | BA | 329 | G |
| 31 | BA | 330 | A |
| 31 | BA | 332 | A |
| 31 | BA | 346 | A |
| 31 | BA | 347 | A |
| 31 | BA | 350 | U |
| 31 | BA | 352 | G |
| 31 | BA | 353 | G |
| 31 | BA | 362 | U |
| 31 | BA | 363(B) | G |
| 31 | BA | 363(C) | G |
| 31 | BA | 363(D) | G |
| 31 | BA | 363(E) | U |
| 31 | BA | 363(F) | A |
| 31 | BA | 370 | G |
| 31 | BA | 372 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | BA | 386 | G |
| 31 | BA | 389 | G |
| 31 | BA | 405 | U |
| 31 | BA | 406 | G |
| 31 | BA | 407 | G |
| 31 | BA | 411 | G |
| 31 | BA | 412 | A |
| 31 | BA | 418 | G |
| 31 | BA | 428 | A |
| 31 | BA | 444 | C |
| 31 | BA | 448 | U |
| 31 | BA | 454 | A |
| 31 | BA | 456 | C |
| 31 | BA | 457 | A |
| 31 | BA | 462 | C |
| 31 | BA | 463 | G |
| 31 | BA | 466 | A |
| 31 | BA | 469 | G |
| 31 | BA | 470 | A |
| 31 | BA | 472 | A |
| 31 | BA | 473 | G |
| 31 | BA | 474 | G |
| 31 | BA | 475 | U |
| 31 | BA | 479 | A |
| 31 | BA | 481 | G |
| 31 | BA | 494 | G |
| 31 | BA | 505 | A |
| 31 | BA | 508 | G |
| 31 | BA | 509 | C |
| 31 | BA | 511 | U |
| 31 | BA | 512 | G |
| 31 | BA | 528 | A |
| 31 | BA | 530 | G |
| 31 | BA | 531 | C |
| 31 | BA | 532 | A |
| 31 | BA | 533 | G |
| 31 | BA | 542 | C |
| 31 | BA | 543 | C |
| 31 | BA | 547 | A |
| 31 | BA | 548 | A |
| 31 | BA | 549 | G |
| 31 | BA | 563 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 31 | BA | 571 | A |
| 31 | BA | 573 | G |
| 31 | BA | 575 | A |
| 31 | BA | 586 | A |
| 31 | BA | 587 | C |
| 31 | BA | 588 | U |
| 31 | BA | 602 | G |
| 31 | BA | 603 | A |
| 31 | BA | 604 | G |
| 31 | BA | 607 | U |
| 31 | BA | 610 | G |
| 31 | BA | 614(B) | G |
| 31 | BA | 615 | G |
| 31 | BA | 618 | C |
| 31 | BA | 619 | G |
| 31 | BA | 622 | G |
| 31 | BA | 627 | A |
| 31 | BA | 637 | A |
| 31 | BA | 643 | A |
| 31 | BA | 644 | A |
| 31 | BA | 645 | C |
| 31 | BA | 646 | A |
| 31 | BA | 647 | G |
| 31 | BA | 650 | C |
| 31 | BA | 651 | G |
| 31 | BA | 652 | C |
| 31 | BA | 656 | G |
| 31 | BA | 657 | U |
| 31 | BA | 667 | U |
| 31 | BA | 669 | G |
| 31 | BA | 670 | A |
| 31 | BA | 671 | C |
| 31 | BA | 686 | G |
| 31 | BA | 701 | G |
| 31 | BA | 708 | C |
| 31 | BA | 721 | C |
| 31 | BA | 722 | A |
| 31 | BA | 730 | C |
| 31 | BA | 745 | G |
| 31 | BA | 746 | A |
| 31 | BA | 747 | U |
| 31 | BA | 752 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | BA | 753 | C |
| 31 | BA | 762 | U |
| 31 | BA | 765 | G |
| 31 | BA | 768 | G |
| 31 | BA | 775 | G |
| 31 | BA | 776 | G |
| 31 | BA | 782 | A |
| 31 | BA | 784 | A |
| 31 | BA | 785 | G |
| 31 | BA | 787 | U |
| 31 | BA | 789 | A |
| 31 | BA | 790 | C |
| 31 | BA | 791 | C |
| 31 | BA | 792 | G |
| 31 | BA | 805 | G |
| 31 | BA | 808 | G |
| 31 | BA | 812 | C |
| 31 | BA | 819 | A |
| 31 | BA | 824 | A |
| 31 | BA | 826 | U |
| 31 | BA | 827 | U |
| 31 | BA | 830 | G |
| 31 | BA | 831 | G |
| 31 | BA | 832 | G |
| 31 | BA | 856 | C |
| 31 | BA | 859 | G |
| 31 | BA | 861 | A |
| 31 | BA | 865 | C |
| 31 | BA | 866 | A |
| 31 | BA | 872 | A |
| 31 | BA | 878 | A |
| 31 | BA | 883 | G |
| 31 | BA | 884 | C |
| 31 | BA | 892 | G |
| 31 | BA | 894 | C |
| 31 | BA | 896 | A |
| 31 | BA | 897 | C |
| 31 | BA | 898 | C |
| 31 | BA | 899 | A |
| 31 | BA | 900 | A |
| 31 | BA | 901 | A |
| 31 | BA | 910 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 31 | BA | 917 | A |
| 31 | BA | 918 | A |
| 31 | BA | 919 | G |
| 31 | BA | 923 | C |
| 31 | BA | 926 | A |
| 31 | BA | 932 | G |
| 31 | BA | 934 | G |
| 31 | BA | 938 | G |
| 31 | BA | 941 | A |
| 31 | BA | 945 | A |
| 31 | BA | 946 | G |
| 31 | BA | 958 | U |
| 31 | BA | 959 | A |
| 31 | BA | 961 | C |
| 31 | BA | 974 | G |
| 31 | BA | 975 | C |
| 31 | BA | 975(A) | G |
| 31 | BA | 983 | A |
| 31 | BA | 990 | A |
| 31 | BA | 991 | C |
| 31 | BA | 996 | A |
| 31 | BA | 997 | G |
| 31 | BA | 1005 | C |
| 31 | BA | 1010 | A |
| 31 | BA | 1011 | G |
| 31 | BA | 1012 | U |
| 31 | BA | 1013 | C |
| 31 | BA | 1016 | G |
| 31 | BA | 1020 | A |
| 31 | BA | 1022 | G |
| 31 | BA | 1023 | U |
| 31 | BA | 1025 | G |
| 31 | BA | 1026 | U |
| 31 | BA | 1033 | U |
| 31 | BA | 1038 | C |
| 31 | BA | 1039 | G |
| 31 | BA | 1041 | C |
| 31 | BA | 1042 | G |
| 31 | BA | 1043 | C |
| 31 | BA | 1044 | G |
| 31 | BA | 1045 | A |
| 31 | BA | 1047 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | BA | 1048 | A |
| 31 | BA | 1049 | C |
| 31 | BA | 1051 | G |
| 31 | BA | 1052 | C |
| 31 | BA | 1053 | C |
| 31 | BA | 1106 | A |
| 31 | BA | 1107 | G |
| 31 | BA | 1110 | G |
| 31 | BA | 1112 | G |
| 31 | BA | 1113 | U |
| 31 | BA | 1114 | G |
| 31 | BA | 1115 | G |
| 31 | BA | 1117 | G |
| 31 | BA | 1126 | A |
| 31 | BA | 1129 | A |
| 31 | BA | 1130 | U |
| 31 | BA | 1135 | C |
| 31 | BA | 1136 | G |
| 31 | BA | 1139 | G |
| 31 | BA | 1142 | U |
| 31 | BA | 1155 | A |
| 31 | BA | 1156 | A |
| 31 | BA | 1159 | U |
| 31 | BA | 1169 | G |
| 31 | BA | 1171 | G |
| 31 | BA | 1173 | G |
| 31 | BA | 1174 | A |
| 31 | BA | 1175 | U |
| 31 | BA | 1176 | G |
| 31 | BA | 1177 | A |
| 31 | BA | 1178 | C |
| 31 | BA | 1179 | C |
| 31 | BA | 1180 | C |
| 31 | BA | 1183 | G |
| 31 | BA | 1195 | G |
| 31 | BA | 1210 | A |
| 31 | BA | 1211 | U |
| 31 | BA | 1213 | A |
| 31 | BA | 1220 | A |
| 31 | BA | 1221 | C |
| 31 | BA | 1240 | U |
| 31 | BA | 1251 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | BA | 1252 | G |
| 31 | BA | 1253 | A |
| 31 | BA | 1255 | U |
| 31 | BA | 1256 | G |
| 31 | BA | 1265 | A |
| 31 | BA | 1271 | G |
| 31 | BA | 1272 | A |
| 31 | BA | 1273 | U |
| 31 | BA | 1284 | A |
| 31 | BA | 1287 | A |
| 31 | BA | 1298 | C |
| 31 | BA | 1300 | U |
| 31 | BA | 1301 | A |
| 31 | BA | 1309 | G |
| 31 | BA | 1311 | G |
| 31 | BA | 1313 | U |
| 31 | BA | 1314 | C |
| 31 | BA | 1321 | A |
| 31 | BA | 1341 | U |
| 31 | BA | 1345 | C |
| 31 | BA | 1349 | A |
| 31 | BA | 1359 | A |
| 31 | BA | 1360 | A |
| 31 | BA | 1364 | G |
| 31 | BA | 1365 | A |
| 31 | BA | 1368 | G |
| 31 | BA | 1378 | A |
| 31 | BA | 1379 | A |
| 31 | BA | 1380 | G |
| 31 | BA | 1384 | A |
| 31 | BA | 1385 | G |
| 31 | BA | 1386 | C |
| 31 | BA | 1388 | G |
| 31 | BA | 1395 | A |
| 31 | BA | 1397 | U |
| 31 | BA | 1398 | C |
| 31 | BA | 1406 | U |
| 31 | BA | 1407 | C |
| 31 | BA | 1416 | G |
| 31 | BA | 1417 | C |
| 31 | BA | 1419 | A |
| 31 | BA | 1420 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | BA | 1421 | G |
| 31 | BA | 1428 | C |
| 31 | BA | 1436 | G |
| 31 | BA | 1437 | C |
| 31 | BA | 1445 | A |
| 31 | BA | 1448 | G |
| 31 | BA | 1449 | A |
| 31 | BA | 1450 | G |
| 31 | BA | 1455 | G |
| 31 | BA | 1458 | C |
| 31 | BA | 1459 | G |
| 31 | BA | 1460 | A |
| 31 | BA | 1461 | G |
| 31 | BA | 1462 | C |
| 31 | BA | 1466 | G |
| 31 | BA | 1467 | C |
| 31 | BA | 1471 | A |
| 31 | BA | 1472 | A |
| 31 | BA | 1474 | C |
| 31 | BA | 1475 | G |
| 31 | BA | 1476 | C |
| 31 | BA | 1477 | A |
| 31 | BA | 1479 | G |
| 31 | BA | 1481 | U |
| 31 | BA | 1482 | G |
| 31 | BA | 1485 | G |
| 31 | BA | 1488 | G |
| 31 | BA | 1490 | A |
| 31 | BA | 1491 | G |
| 31 | BA | 1493 | C |
| 31 | BA | 1494 | A |
| 31 | BA | 1495 | A |
| 31 | BA | 1497 | U |
| 31 | BA | 1498 | C |
| 31 | BA | 1501 | C |
| 31 | BA | 1502 | C |
| 31 | BA | 1503 | U |
| 31 | BA | 1505 | C |
| 31 | BA | 1508 | A |
| 31 | BA | 1509 | C |
| 31 | BA | 1509(A) | A |
| 31 | BA | 1511 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 31 | BA | 1512 | U |
| 31 | BA | 1513 | C |
| 31 | BA | 1515 | G |
| 31 | BA | 1520 | G |
| 31 | BA | 1526 | G |
| 31 | BA | 1528 | A |
| 31 | BA | 1528(A) | A |
| 31 | BA | 1529 | G |
| 31 | BA | 1530 | C |
| 31 | BA | 1531 | C |
| 31 | BA | 1532 | C |
| 31 | BA | 1533 | G |
| 31 | BA | 1543 | C |
| 31 | BA | 1545 | A |
| 31 | BA | 1546 | C |
| 31 | BA | 1558 | A |
| 31 | BA | 1559 | G |
| 31 | BA | 1566 | A |
| 31 | BA | 1569 | A |
| 31 | BA | 1578 | U |
| 31 | BA | 1580 | A |
| 31 | BA | 1581 | G |
| 31 | BA | 1584 | C |
| 31 | BA | 1586 | A |
| 31 | BA | 1588 | C |
| 31 | BA | 1591 | G |
| 31 | BA | 1593 | G |
| 31 | BA | 1594 | G |
| 31 | BA | 1597 | A |
| 31 | BA | 1598 | C |
| 31 | BA | 1603 | A |
| 31 | BA | 1608 | A |
| 31 | BA | 1609 | A |
| 31 | BA | 1610 | A |
| 31 | BA | 1617 | C |
| 31 | BA | 1618 | A |
| 31 | BA | 1625 | C |
| 31 | BA | 1635 | G |
| 31 | BA | 1640 | C |
| 31 | BA | 1648 | C |
| 31 | BA | 1652 | A |
| 31 | BA | 1653 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | BA | 1654 | A |
| 31 | BA | 1655 | A |
| 31 | BA | 1674 | G |
| 31 | BA | 1694 | C |
| 31 | BA | 1695 | G |
| 31 | BA | 1696 | G |
| 31 | BA | 1697 | G |
| 31 | BA | 1698 | A |
| 31 | BA | 1700 | A |
| 31 | BA | 1701 | A |
| 31 | BA | 1703 | G |
| 31 | BA | 1721 | G |
| 31 | BA | 1722 | A |
| 31 | BA | 1739 | U |
| 31 | BA | 1741 | A |
| 31 | BA | 1742 | G |
| 31 | BA | 1744 | C |
| 31 | BA | 1746 | G |
| 31 | BA | 1749 | A |
| 31 | BA | 1756 | G |
| 31 | BA | 1763 | G |
| 31 | BA | 1764 | G |
| 31 | BA | 1773 | A |
| 31 | BA | 1780 | A |
| 31 | BA | 1781 | C |
| 31 | BA | 1782 | C |
| 31 | BA | 1791 | A |
| 31 | BA | 1799 | G |
| 31 | BA | 1800 | C |
| 31 | BA | 1801 | G |
| 31 | BA | 1813 | G |
| 31 | BA | 1816 | G |
| 31 | BA | 1820 | U |
| 31 | BA | 1822 | G |
| 31 | BA | 1827 | C |
| 31 | BA | 1828 | G |
| 31 | BA | 1829 | A |
| 31 | BA | 1835 | G |
| 31 | BA | 1838 | C |
| 31 | BA | 1840 | G |
| 31 | BA | 1847 | A |
| 31 | BA | 1858 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | BA | 1865 | G |
| 31 | BA | 1866 | C |
| 31 | BA | 1877 | A |
| 31 | BA | 1878 | G |
| 31 | BA | 1882 | C |
| 31 | BA | 1885 | A |
| 31 | BA | 1889 | A |
| 31 | BA | 1900 | A |
| 31 | BA | 1902 | C |
| 31 | BA | 1903 | G |
| 31 | BA | 1906 | G |
| 31 | BA | 1913 | A |
| 31 | BA | 1914 | C |
| 31 | BA | 1929 | G |
| 31 | BA | 1930 | G |
| 31 | BA | 1934 | C |
| 31 | BA | 1935 | G |
| 31 | BA | 1936 | A |
| 31 | BA | 1938 | A |
| 31 | BA | 1948 | G |
| 31 | BA | 1955 | U |
| 31 | BA | 1962 | C |
| 31 | BA | 1963 | U |
| 31 | BA | 1964 | G |
| 31 | BA | 1967 | C |
| 31 | BA | 1969 | A |
| 31 | BA | 1970 | A |
| 31 | BA | 1971 | A |
| 31 | BA | 1972 | A |
| 31 | BA | 1982 | C |
| 31 | BA | 1992 | G |
| 31 | BA | 1993 | U |
| 31 | BA | 1997 | G |
| 31 | BA | 2018 | G |
| 31 | BA | 2020 | A |
| 31 | BA | 2021 | C |
| 31 | BA | 2023 | G |
| 31 | BA | 2030 | A |
| 31 | BA | 2031 | A |
| 31 | BA | 2033 | A |
| 31 | BA | 2036 | C |
| 31 | BA | 2039 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | BA | 2043 | C |
| 31 | BA | 2055 | C |
| 31 | BA | 2056 | G |
| 31 | BA | 2060 | A |
| 31 | BA | 2061 | G |
| 31 | BA | 2062 | A |
| 31 | BA | 2069 | G |
| 31 | BA | 2071 | A |
| 31 | BA | 2095 | C |
| 31 | BA | 2099 | U |
| 31 | BA | 2100 | G |
| 31 | BA | 2103 | C |
| 31 | BA | 2104 | G |
| 31 | BA | 2187 | G |
| 31 | BA | 2190 | G |
| 31 | BA | 2191 | G |
| 31 | BA | 2192 | G |
| 31 | BA | 2193 | G |
| 31 | BA | 2197 | U |
| 31 | BA | 2198 | A |
| 31 | BA | 2199 | A |
| 31 | BA | 2200 | C |
| 31 | BA | 2201 | C |
| 31 | BA | 2203 | U |
| 31 | BA | 2206 | G |
| 31 | BA | 2207 | G |
| 31 | BA | 2208 | A |
| 31 | BA | 2218 | U |
| 31 | BA | 2219 | G |
| 31 | BA | 2225 | A |
| 31 | BA | 2226 | C |
| 31 | BA | 2238 | G |
| 31 | BA | 2263 | C |
| 31 | BA | 2268 | A |
| 31 | BA | 2272 | U |
| 31 | BA | 2273 | A |
| 31 | BA | 2275 | C |
| 31 | BA | 2280 | G |
| 31 | BA | 2283 | C |
| 31 | BA | 2287 | A |
| 31 | BA | 2288 | A |
| 31 | BA | 2289 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | BA | 2298 | A |
| 31 | BA | 2303 | G |
| 31 | BA | 2305 | A |
| 31 | BA | 2307 | G |
| 31 | BA | 2308 | G |
| 31 | BA | 2309 | A |
| 31 | BA | 2311 | A |
| 31 | BA | 2316 | C |
| 31 | BA | 2318 | G |
| 31 | BA | 2319 | G |
| 31 | BA | 2320 | A |
| 31 | BA | 2321 | G |
| 31 | BA | 2324 | C |
| 31 | BA | 2325 | G |
| 31 | BA | 2327 | A |
| 31 | BA | 2334 | G |
| 31 | BA | 2336 | A |
| 31 | BA | 2340 | G |
| 31 | BA | 2342 | C |
| 31 | BA | 2346 | A |
| 31 | BA | 2347 | C |
| 31 | BA | 2350 | C |
| 31 | BA | 2360 | A |
| 31 | BA | 2361 | A |
| 31 | BA | 2372 | G |
| 31 | BA | 2377 | A |
| 31 | BA | 2383 | G |
| 31 | BA | 2385 | C |
| 31 | BA | 2387 | U |
| 31 | BA | 2388 | A |
| 31 | BA | 2402 | C |
| 31 | BA | 2403 | C |
| 31 | BA | 2404 | C |
| 31 | BA | 2405 | G |
| 31 | BA | 2406 | U |
| 31 | BA | 2410 | G |
| 31 | BA | 2422 | A |
| 31 | BA | 2423 | U |
| 31 | BA | 2425 | A |
| 31 | BA | 2427 | C |
| 31 | BA | 2429 | G |
| 31 | BA | 2430 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | BA | 2431 | U |
| 31 | BA | 2435 | A |
| 31 | BA | 2439 | A |
| 31 | BA | 2440 | C |
| 31 | BA | 2441 | C |
| 31 | BA | 2448 | A |
| 31 | BA | 2449 | U |
| 31 | BA | 2464 | C |
| 31 | BA | 2465 | C |
| 31 | BA | 2468 | G |
| 31 | BA | 2469 | A |
| 31 | BA | 2470 | G |
| 31 | BA | 2471 | C |
| 31 | BA | 2476 | A |
| 31 | BA | 2477 | C |
| 31 | BA | 2478 | A |
| 31 | BA | 2487 | G |
| 31 | BA | 2489 | G |
| 31 | BA | 2492 | U |
| 31 | BA | 2502 | G |
| 31 | BA | 2505 | G |
| 31 | BA | 2506 | U |
| 31 | BA | 2507 | C |
| 31 | BA | 2518 | A |
| 31 | BA | 2520 | C |
| 31 | BA | 2524 | G |
| 31 | BA | 2525 | G |
| 31 | BA | 2529 | G |
| 31 | BA | 2535 | G |
| 31 | BA | 2543 | G |
| 31 | BA | 2554 | U |
| 31 | BA | 2564 | A |
| 31 | BA | 2566 | A |
| 31 | BA | 2567 | G |
| 31 | BA | 2569 | G |
| 31 | BA | 2582 | G |
| 31 | BA | 2585 | U |
| 31 | BA | 2586 | C |
| 31 | BA | 2601 | C |
| 31 | BA | 2602 | A |
| 31 | BA | 2603 | G |
| 31 | BA | 2604 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 31 | BA | 2609 | U |
| 31 | BA | 2611 | U |
| 31 | BA | 2612 | C |
| 31 | BA | 2613 | U |
| 31 | BA | 2615 | U |
| 31 | BA | 2630 | G |
| 31 | BA | 2637 | U |
| 31 | BA | 2638 | G |
| 31 | BA | 2654 | A |
| 31 | BA | 2655 | G |
| 31 | BA | 2656 | U |
| 31 | BA | 2657 | A |
| 31 | BA | 2658 | C |
| 31 | BA | 2659 | G |
| 31 | BA | 2660 | A |
| 31 | BA | 2661 | G |
| 31 | BA | 2662 | A |
| 31 | BA | 2663 | G |
| 31 | BA | 2673 | G |
| 31 | BA | 2682 | U |
| 31 | BA | 2688 | U |
| 31 | BA | 2690 | C |
| 31 | BA | 2702 | U |
| 31 | BA | 2703 | C |
| 31 | BA | 2707 | G |
| 31 | BA | 2712 | U |
| 31 | BA | 2712(A) | A |
| 31 | BA | 2713 | A |
| 31 | BA | 2714 | G |
| 31 | BA | 2726 | U |
| 31 | BA | 2731 | G |
| 31 | BA | 2733 | A |
| 31 | BA | 2752 | C |
| 31 | BA | 2753 | A |
| 31 | BA | 2754 | U |
| 31 | BA | 2755 | C |
| 31 | BA | 2757 | A |
| 31 | BA | 2758 | A |
| 31 | BA | 2762 | G |
| 31 | BA | 2764 | A |
| 31 | BA | 2765 | A |
| 31 | BA | 2766 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 31 | BA | 2778 | A |
| 31 | BA | 2779 | U |
| 31 | BA | 2781 | A |
| 31 | BA | 2789 | C |
| 31 | BA | 2790 | A |
| 31 | BA | 2791 | C |
| 31 | BA | 2794 | C |
| 31 | BA | 2795 | G |
| 31 | BA | 2801(A) | A |
| 31 | BA | 2802 | G |
| 31 | BA | 2803 | C |
| 31 | BA | 2807 | G |
| 31 | BA | 2808 | U |
| 31 | BA | 2818 | G |
| 31 | BA | 2820 | A |
| 31 | BA | 2821 | A |
| 31 | BA | 2833 | G |
| 31 | BA | 2835 | A |
| 31 | BA | 2836 | U |
| 31 | BA | 2844 | G |
| 31 | BA | 2847 | U |
| 31 | BA | 2849 | U |
| 31 | BA | 2860 | A |
| 31 | BA | 2872 | G |
| 31 | BA | 2880 | C |
| 31 | BA | 2892 | A |
| 31 | BA | 2894 | G |
| 31 | BA | 2895 | U |
| 31 | BA | 2897 | U |
| 32 | BB | 8 | U |
| 32 | BB | 9 | G |
| 32 | BB | 12 | C |
| 32 | BB | 15 | A |
| 32 | BB | 20 | C |
| 32 | BB | 22 | U |
| 32 | BB | 27 | C |
| 32 | BB | 33 | G |
| 32 | BB | 40 | U |
| 32 | BB | 41 | U |
| 32 | BB | 42 | C |
| 32 | BB | 43 | C |
| 32 | BB | 44 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BB | 45 | A |
| 32 | BB | 46 | A |
| 32 | BB | 47 | C |
| 32 | BB | 52 | A |
| 32 | BB | 53 | A |
| 32 | BB | 56 | G |
| 32 | BB | 63 | G |
| 32 | BB | 64 | C |
| 32 | BB | 73 | A |
| 32 | BB | 74 | U |
| 32 | BB | 75 | G |
| 32 | BB | 81 | G |
| 32 | BB | 85 | G |
| 32 | BB | 87 | G |
| 32 | BB | 88 | C |
| 32 | BB | 89 | G |
| 32 | BB | 90 | A |
| 32 | BB | 91 | C |
| 32 | BB | 102 | A |
| 32 | BB | 106 | G |
| 32 | BB | 110 | G |
| 32 | BB | 118 | G |
| 1 | CA | 9 | G |
| 1 | CA | 32 | A |
| 1 | CA | 39 | G |
| 1 | CA | 48 | C |
| 1 | CA | 50 | A |
| 1 | CA | 51 | A |
| 1 | CA | 61 | G |
| 1 | CA | 80 | G |
| 1 | CA | 81 | U |
| 1 | CA | 90 | U |
| 1 | CA | 91 | C |
| 1 | CA | 97 | G |
| 1 | CA | 98 | G |
| 1 | CA | 101 | A |
| 1 | CA | 108 | G |
| 1 | CA | 115 | G |
| 1 | CA | 116 | A |
| 1 | CA | 119 | A |
| 1 | CA | 120 | A |
| 1 | CA | 121 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 131 | C |
| 1 | CA | 138 | G |
| 1 | CA | 144 | G |
| 1 | CA | 147 | G |
| 1 | CA | 150 | C |
| 1 | CA | 163 | C |
| 1 | CA | 168 | G |
| 1 | CA | 172 | A |
| 1 | CA | 173 | U |
| 1 | CA | 181 | G |
| 1 | CA | 182 | U |
| 1 | CA | 189(G) | G |
| 1 | CA | 189(H) | G |
| 1 | CA | 189(J) | G |
| 1 | CA | 195 | A |
| 1 | CA | 197 | A |
| 1 | CA | 199 | G |
| 1 | CA | 201 | C |
| 1 | CA | 202 | U |
| 1 | CA | 203 | U |
| 1 | CA | 216 | G |
| 1 | CA | 220 | G |
| 1 | CA | 243 | A |
| 1 | CA | 244 | U |
| 1 | CA | 247 | G |
| 1 | CA | 251 | G |
| 1 | CA | 266 | G |
| 1 | CA | 267 | C |
| 1 | CA | 280 | C |
| 1 | CA | 281 | G |
| 1 | CA | 289 | G |
| 1 | CA | 296 | U |
| 1 | CA | 297 | G |
| 1 | CA | 298 | A |
| 1 | CA | 301 | G |
| 1 | CA | 328 | C |
| 1 | CA | 329 | A |
| 1 | CA | 332 | G |
| 1 | CA | 343 | U |
| 1 | CA | 345 | C |
| 1 | CA | 351 | G |
| 1 | CA | 352 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 353 | A |
| 1 | CA | 354 | G |
| 1 | CA | 357 | G |
| 1 | CA | 367 | U |
| 1 | CA | 372 | C |
| 1 | CA | 373 | A |
| 1 | CA | 384 | G |
| 1 | CA | 388 | G |
| 1 | CA | 390 | C |
| 1 | CA | 397 | A |
| 1 | CA | 398 | C |
| 1 | CA | 406 | G |
| 1 | CA | 412 | A |
| 1 | CA | 413 | G |
| 1 | CA | 414 | A |
| 1 | CA | 418 | C |
| 1 | CA | 419 | C |
| 1 | CA | 422 | C |
| 1 | CA | 424 | G |
| 1 | CA | 427 | U |
| 1 | CA | 429 | U |
| 1 | CA | 430 | A |
| 1 | CA | 435 | C |
| 1 | CA | 437 | U |
| 1 | CA | 439 | A |
| 1 | CA | 442 | C |
| 1 | CA | 448 | A |
| 1 | CA | 452 | A |
| 1 | CA | 461 | A |
| 1 | CA | 472 | A |
| 1 | CA | 484 | G |
| 1 | CA | 485 | G |
| 1 | CA | 487 | A |
| 1 | CA | 496 | A |
| 1 | CA | 498 | U |
| 1 | CA | 499 | A |
| 1 | CA | 505 | G |
| 1 | CA | 508 | C |
| 1 | CA | 509 | A |
| 1 | CA | 510 | A |
| 1 | CA | 511 | C |
| 1 | CA | 513 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 518 | C |
| 1 | CA | 527 | G |
| 1 | CA | 531 | U |
| 1 | CA | 532 | A |
| 1 | CA | 533 | A |
| 1 | CA | 534 | U |
| 1 | CA | 547 | A |
| 1 | CA | 559 | A |
| 1 | CA | 561 | U |
| 1 | CA | 562 | C |
| 1 | CA | 563 | A |
| 1 | CA | 572 | A |
| 1 | CA | 573 | A |
| 1 | CA | 575 | G |
| 1 | CA | 576 | G |
| 1 | CA | 588 | G |
| 1 | CA | 596 | C |
| 1 | CA | 616 | G |
| 1 | CA | 623 | C |
| 1 | CA | 630 | G |
| 1 | CA | 632 | A |
| 1 | CA | 653 | A |
| 1 | CA | 665 | A |
| 1 | CA | 671 | G |
| 1 | CA | 674 | G |
| 1 | CA | 687 | A |
| 1 | CA | 688 | G |
| 1 | CA | 693 | G |
| 1 | CA | 724 | G |
| 1 | CA | 725 | G |
| 1 | CA | 731 | G |
| 1 | CA | 748 | C |
| 1 | CA | 749 | C |
| 1 | CA | 753 | A |
| 1 | CA | 754 | C |
| 1 | CA | 755 | G |
| 1 | CA | 760 | G |
| 1 | CA | 765 | G |
| 1 | CA | 766 | A |
| 1 | CA | 777 | A |
| 1 | CA | 782 | A |
| 1 | CA | 786 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 792 | A |
| 1 | CA | 793 | U |
| 1 | CA | 794 | A |
| 1 | CA | 815 | A |
| 1 | CA | 817 | C |
| 1 | CA | 818 | G |
| 1 | CA | 827 | U |
| 1 | CA | 828 | A |
| 1 | CA | 833 | U |
| 1 | CA | 836 | G |
| 1 | CA | 839 | U |
| 1 | CA | 840 | C |
| 1 | CA | 841 | U |
| 1 | CA | 848 | C |
| 1 | CA | 859 | A |
| 1 | CA | 864 | A |
| 1 | CA | 870 | U |
| 1 | CA | 872 | A |
| 1 | CA | 902 | G |
| 1 | CA | 914 | A |
| 1 | CA | 916 | G |
| 1 | CA | 927 | G |
| 1 | CA | 934 | C |
| 1 | CA | 935 | A |
| 1 | CA | 960 | U |
| 1 | CA | 961 | U |
| 1 | CA | 968 | A |
| 1 | CA | 969 | A |
| 1 | CA | 971 | G |
| 1 | CA | 972 | C |
| 1 | CA | 974 | A |
| 1 | CA | 975 | A |
| 1 | CA | 976 | G |
| 1 | CA | 977 | A |
| 1 | CA | 978 | A |
| 1 | CA | 980 | C |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |
| 1 | CA | 993 | G |
| 1 | CA | 1005 | A |
| 1 | CA | 1026 | G |
| 1 | CA | 1050 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1053 | G |
| 1 | CA | 1054 | C |
| 1 | CA | 1064 | G |
| 1 | CA | 1065 | U |
| 1 | CA | 1066 | C |
| 1 | CA | 1067 | A |
| 1 | CA | 1068 | G |
| 1 | CA | 1081 | G |
| 1 | CA | 1095 | U |
| 1 | CA | 1101 | A |
| 1 | CA | 1103 | C |
| 1 | CA | 1113 | C |
| 1 | CA | 1117 | G |
| 1 | CA | 1118 | C |
| 1 | CA | 1124 | G |
| 1 | CA | 1125 | U |
| 1 | CA | 1126 | U |
| 1 | CA | 1127 | G |
| 1 | CA | 1129 | C |
| 1 | CA | 1136 | U |
| 1 | CA | 1137 | C |
| 1 | CA | 1138 | G |
| 1 | CA | 1139 | G |
| 1 | CA | 1146 | A |
| 1 | CA | 1152 | A |
| 1 | CA | 1159 | U |
| 1 | CA | 1160 | G |
| 1 | CA | 1196 | U |
| 1 | CA | 1197 | G |
| 1 | CA | 1202 | G |
| 1 | CA | 1204 | A |
| 1 | CA | 1212 | U |
| 1 | CA | 1213 | A |
| 1 | CA | 1214 | C |
| 1 | CA | 1225 | A |
| 1 | CA | 1227 | A |
| 1 | CA | 1238 | A |
| 1 | CA | 1249 | C |
| 1 | CA | 1255 | G |
| 1 | CA | 1256 | A |
| 1 | CA | 1257 | U |
| 1 | CA | 1280 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 1281 | U |
| 1 | CA | 1282 | C |
| 1 | CA | 1286 | A |
| 1 | CA | 1287 | A |
| 1 | CA | 1294 | G |
| 1 | CA | 1299 | A |
| 1 | CA | 1300 | G |
| 1 | CA | 1301 | U |
| 1 | CA | 1302 | U |
| 1 | CA | 1305 | G |
| 1 | CA | 1310 | G |
| 1 | CA | 1312 | G |
| 1 | CA | 1317 | C |
| 1 | CA | 1320 | C |
| 1 | CA | 1322 | C |
| 1 | CA | 1323 | G |
| 1 | CA | 1331 | G |
| 1 | CA | 1332 | A |
| 1 | CA | 1335 | C |
| 1 | CA | 1338 | G |
| 1 | CA | 1347 | G |
| 1 | CA | 1363 | C |
| 1 | CA | 1364 | U |
| 1 | CA | 1370 | G |
| 1 | CA | 1388 | C |
| 1 | CA | 1397 | C |
| 1 | CA | 1416 | G |
| 1 | CA | 1419 | G |
| 1 | CA | 1442 | G |
| 1 | CA | 1442(A) | G |
| 1 | CA | 1442(B) | A |
| 1 | CA | 1443 | G |
| 1 | CA | 1447 | A |
| 1 | CA | 1452 | C |
| 1 | CA | 1456 | G |
| 1 | CA | 1457 | G |
| 1 | CA | 1492 | A |
| 1 | CA | 1493 | A |
| 1 | CA | 1494 | G |
| 1 | CA | 1497 | G |
| 1 | CA | 1499 | A |
| 1 | CA | 1502 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1504 | G |
| 1 | CA | 1505 | G |
| 1 | CA | 1506 | U |
| 1 | CA | 1507 | A |
| 1 | CA | 1517 | G |
| 1 | CA | 1520 | G |
| 1 | CA | 1529 | G |
| 1 | CA | 1530 | G |
| 31 | DA | 10 | G |
| 31 | DA | 12 | U |
| 31 | DA | 15 | G |
| 31 | DA | 34 | C |
| 31 | DA | 35 | G |
| 31 | DA | 36 | G |
| 31 | DA | 45 | C |
| 31 | DA | 49 | A |
| 31 | DA | 50 | U |
| 31 | DA | 51 | G |
| 31 | DA | 55 | G |
| 31 | DA | 61 | G |
| 31 | DA | 64 | A |
| 31 | DA | 69 | C |
| 31 | DA | 70 | G |
| 31 | DA | 71 | A |
| 31 | DA | 72 | U |
| 31 | DA | 74 | A |
| 31 | DA | 75 | G |
| 31 | DA | 84 | A |
| 31 | DA | 90 | U |
| 31 | DA | 92 | A |
| 31 | DA | 94 | C |
| 31 | DA | 95 | G |
| 31 | DA | 100 | G |
| 31 | DA | 102 | G |
| 31 | DA | 103 | A |
| 31 | DA | 117 | G |
| 31 | DA | 118 | A |
| 31 | DA | 119 | A |
| 31 | DA | 120 | U |
| 31 | DA | 125 | G |
| 31 | DA | 129 | C |
| 31 | DA | 131 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 31 | DA | 137 | C |
| 31 | DA | 139(A) | G |
| 31 | DA | 142 | A |
| 31 | DA | 142(A) | C |
| 31 | DA | 146 | G |
| 31 | DA | 147 | U |
| 31 | DA | 154(A) | C |
| 31 | DA | 157 | U |
| 31 | DA | 158 | U |
| 31 | DA | 171 | G |
| 31 | DA | 173 | G |
| 31 | DA | 174 | C |
| 31 | DA | 175 | G |
| 31 | DA | 182 | A |
| 31 | DA | 188 | G |
| 31 | DA | 196 | A |
| 31 | DA | 197 | A |
| 31 | DA | 199 | A |
| 31 | DA | 204 | A |
| 31 | DA | 205 | G |
| 31 | DA | 214 | G |
| 31 | DA | 215 | G |
| 31 | DA | 216 | A |
| 31 | DA | 221 | A |
| 31 | DA | 222 | A |
| 31 | DA | 225 | A |
| 31 | DA | 228 | A |
| 31 | DA | 229 | A |
| 31 | DA | 233 | A |
| 31 | DA | 248 | G |
| 31 | DA | 250 | G |
| 31 | DA | 252 | G |
| 31 | DA | 266 | G |
| 31 | DA | 271(J) | C |
| 31 | DA | 271(K) | U |
| 31 | DA | 271(L) | U |
| 31 | DA | 271(M) | G |
| 31 | DA | 271(N) | U |
| 31 | DA | 271(O) | C |
| 31 | DA | 271(P) | C |
| 31 | DA | 271(R) | G |
| 31 | DA | 271(U) | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | DA | 272 | G |
| 31 | DA | 272(B) | G |
| 31 | DA | 272(H) | C |
| 31 | DA | 272(I) | U |
| 31 | DA | 272(J) | C |
| 31 | DA | 274 | G |
| 31 | DA | 275 | G |
| 31 | DA | 279 | C |
| 31 | DA | 281 | G |
| 31 | DA | 286 | C |
| 31 | DA | 287 | C |
| 31 | DA | 298 | G |
| 31 | DA | 299 | A |
| 31 | DA | 310 | A |
| 31 | DA | 311 | A |
| 31 | DA | 324 | A |
| 31 | DA | 329 | G |
| 31 | DA | 330 | A |
| 31 | DA | 332 | A |
| 31 | DA | 346 | A |
| 31 | DA | 347 | A |
| 31 | DA | 352 | G |
| 31 | DA | 353 | G |
| 31 | DA | 362 | U |
| 31 | DA | 363(B) | G |
| 31 | DA | 363(C) | G |
| 31 | DA | 363(D) | G |
| 31 | DA | 363(E) | U |
| 31 | DA | 363(F) | A |
| 31 | DA | 370 | G |
| 31 | DA | 372 | G |
| 31 | DA | 386 | G |
| 31 | DA | 389 | G |
| 31 | DA | 405 | U |
| 31 | DA | 406 | G |
| 31 | DA | 407 | G |
| 31 | DA | 411 | G |
| 31 | DA | 412 | A |
| 31 | DA | 416 | C |
| 31 | DA | 418 | G |
| 31 | DA | 428 | A |
| 31 | DA | 444 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | DA | 448 | U |
| 31 | DA | 454 | A |
| 31 | DA | 456 | C |
| 31 | DA | 457 | A |
| 31 | DA | 466 | A |
| 31 | DA | 469 | G |
| 31 | DA | 470 | A |
| 31 | DA | 472 | A |
| 31 | DA | 473 | G |
| 31 | DA | 474 | G |
| 31 | DA | 475 | U |
| 31 | DA | 479 | A |
| 31 | DA | 481 | G |
| 31 | DA | 494 | G |
| 31 | DA | 496 | G |
| 31 | DA | 505 | A |
| 31 | DA | 508 | G |
| 31 | DA | 509 | C |
| 31 | DA | 511 | U |
| 31 | DA | 512 | G |
| 31 | DA | 528 | A |
| 31 | DA | 530 | G |
| 31 | DA | 531 | C |
| 31 | DA | 532 | A |
| 31 | DA | 533 | G |
| 31 | DA | 542 | C |
| 31 | DA | 543 | C |
| 31 | DA | 547 | A |
| 31 | DA | 548 | A |
| 31 | DA | 549 | G |
| 31 | DA | 563 | G |
| 31 | DA | 571 | A |
| 31 | DA | 573 | G |
| 31 | DA | 575 | A |
| 31 | DA | 586 | A |
| 31 | DA | 587 | C |
| 31 | DA | 588 | U |
| 31 | DA | 602 | G |
| 31 | DA | 603 | A |
| 31 | DA | 604 | G |
| 31 | DA | 607 | U |
| 31 | DA | 610 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | DA | 614(B) | G |
| 31 | DA | 615 | G |
| 31 | DA | 618 | C |
| 31 | DA | 619 | G |
| 31 | DA | 622 | G |
| 31 | DA | 627 | A |
| 31 | DA | 637 | A |
| 31 | DA | 643 | A |
| 31 | DA | 644 | A |
| 31 | DA | 645 | C |
| 31 | DA | 646 | A |
| 31 | DA | 647 | G |
| 31 | DA | 650 | C |
| 31 | DA | 651 | G |
| 31 | DA | 652 | C |
| 31 | DA | 656 | G |
| 31 | DA | 657 | U |
| 31 | DA | 667 | U |
| 31 | DA | 669 | G |
| 31 | DA | 670 | A |
| 31 | DA | 671 | C |
| 31 | DA | 686 | G |
| 31 | DA | 701 | G |
| 31 | DA | 708 | C |
| 31 | DA | 721 | C |
| 31 | DA | 722 | A |
| 31 | DA | 730 | C |
| 31 | DA | 745 | G |
| 31 | DA | 752 | A |
| 31 | DA | 753 | C |
| 31 | DA | 762 | U |
| 31 | DA | 765 | G |
| 31 | DA | 768 | G |
| 31 | DA | 775 | G |
| 31 | DA | 776 | G |
| 31 | DA | 782 | A |
| 31 | DA | 784 | A |
| 31 | DA | 785 | G |
| 31 | DA | 787 | U |
| 31 | DA | 789 | A |
| 31 | DA | 790 | C |
| 31 | DA | 791 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 31 | DA | 792 | G |
| 31 | DA | 805 | G |
| 31 | DA | 812 | C |
| 31 | DA | 819 | A |
| 31 | DA | 824 | A |
| 31 | DA | 826 | U |
| 31 | DA | 827 | U |
| 31 | DA | 830 | G |
| 31 | DA | 831 | G |
| 31 | DA | 856 | C |
| 31 | DA | 859 | G |
| 31 | DA | 861 | A |
| 31 | DA | 865 | C |
| 31 | DA | 866 | A |
| 31 | DA | 872 | A |
| 31 | DA | 878 | A |
| 31 | DA | 883 | G |
| 31 | DA | 884 | C |
| 31 | DA | 892 | G |
| 31 | DA | 894 | C |
| 31 | DA | 896 | A |
| 31 | DA | 897 | C |
| 31 | DA | 898 | C |
| 31 | DA | 899 | A |
| 31 | DA | 901 | A |
| 31 | DA | 910 | A |
| 31 | DA | 917 | A |
| 31 | DA | 918 | A |
| 31 | DA | 919 | G |
| 31 | DA | 923 | C |
| 31 | DA | 926 | A |
| 31 | DA | 932 | G |
| 31 | DA | 938 | G |
| 31 | DA | 941 | A |
| 31 | DA | 945 | A |
| 31 | DA | 946 | G |
| 31 | DA | 958 | U |
| 31 | DA | 959 | A |
| 31 | DA | 961 | C |
| 31 | DA | 974 | G |
| 31 | DA | 975 | C |
| 31 | DA | 975(A) | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | DA | 983 | A |
| 31 | DA | 990 | A |
| 31 | DA | 991 | C |
| 31 | DA | 996 | A |
| 31 | DA | 997 | G |
| 31 | DA | 1005 | C |
| 31 | DA | 1010 | A |
| 31 | DA | 1011 | G |
| 31 | DA | 1012 | U |
| 31 | DA | 1013 | C |
| 31 | DA | 1016 | G |
| 31 | DA | 1020 | A |
| 31 | DA | 1022 | G |
| 31 | DA | 1023 | U |
| 31 | DA | 1025 | G |
| 31 | DA | 1026 | U |
| 31 | DA | 1033 | U |
| 31 | DA | 1038 | C |
| 31 | DA | 1039 | G |
| 31 | DA | 1041 | C |
| 31 | DA | 1042 | G |
| 31 | DA | 1043 | C |
| 31 | DA | 1044 | G |
| 31 | DA | 1045 | A |
| 31 | DA | 1047 | G |
| 31 | DA | 1048 | A |
| 31 | DA | 1049 | C |
| 31 | DA | 1051 | G |
| 31 | DA | 1052 | C |
| 31 | DA | 1053 | C |
| 31 | DA | 1106 | A |
| 31 | DA | 1107 | G |
| 31 | DA | 1110 | G |
| 31 | DA | 1112 | G |
| 31 | DA | 1113 | U |
| 31 | DA | 1114 | G |
| 31 | DA | 1115 | G |
| 31 | DA | 1117 | G |
| 31 | DA | 1126 | A |
| 31 | DA | 1129 | A |
| 31 | DA | 1130 | U |
| 31 | DA | 1135 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | DA | 1136 | G |
| 31 | DA | 1139 | G |
| 31 | DA | 1142 | U |
| 31 | DA | 1155 | A |
| 31 | DA | 1156 | A |
| 31 | DA | 1159 | U |
| 31 | DA | 1169 | G |
| 31 | DA | 1171 | G |
| 31 | DA | 1173 | G |
| 31 | DA | 1174 | A |
| 31 | DA | 1175 | U |
| 31 | DA | 1176 | G |
| 31 | DA | 1177 | A |
| 31 | DA | 1178 | C |
| 31 | DA | 1179 | C |
| 31 | DA | 1180 | C |
| 31 | DA | 1183 | G |
| 31 | DA | 1195 | G |
| 31 | DA | 1210 | A |
| 31 | DA | 1211 | U |
| 31 | DA | 1213 | A |
| 31 | DA | 1220 | A |
| 31 | DA | 1221 | C |
| 31 | DA | 1230 | C |
| 31 | DA | 1240 | U |
| 31 | DA | 1242 | A |
| 31 | DA | 1251 | C |
| 31 | DA | 1252 | G |
| 31 | DA | 1253 | A |
| 31 | DA | 1255 | U |
| 31 | DA | 1256 | G |
| 31 | DA | 1265 | A |
| 31 | DA | 1271 | G |
| 31 | DA | 1272 | A |
| 31 | DA | 1273 | U |
| 31 | DA | 1284 | A |
| 31 | DA | 1287 | A |
| 31 | DA | 1298 | C |
| 31 | DA | 1300 | U |
| 31 | DA | 1301 | A |
| 31 | DA | 1309 | G |
| 31 | DA | 1311 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | DA | 1313 | U |
| 31 | DA | 1314 | C |
| 31 | DA | 1321 | A |
| 31 | DA | 1329 | U |
| 31 | DA | 1332 | G |
| 31 | DA | 1341 | U |
| 31 | DA | 1345 | C |
| 31 | DA | 1349 | A |
| 31 | DA | 1359 | A |
| 31 | DA | 1360 | A |
| 31 | DA | 1364 | G |
| 31 | DA | 1365 | A |
| 31 | DA | 1368 | G |
| 31 | DA | 1378 | A |
| 31 | DA | 1379 | A |
| 31 | DA | 1380 | G |
| 31 | DA | 1384 | A |
| 31 | DA | 1385 | G |
| 31 | DA | 1386 | C |
| 31 | DA | 1388 | G |
| 31 | DA | 1395 | A |
| 31 | DA | 1397 | U |
| 31 | DA | 1398 | C |
| 31 | DA | 1406 | U |
| 31 | DA | 1407 | C |
| 31 | DA | 1416 | G |
| 31 | DA | 1417 | C |
| 31 | DA | 1419 | A |
| 31 | DA | 1420 | U |
| 31 | DA | 1421 | G |
| 31 | DA | 1427 | A |
| 31 | DA | 1428 | C |
| 31 | DA | 1436 | G |
| 31 | DA | 1437 | C |
| 31 | DA | 1445 | A |
| 31 | DA | 1448 | G |
| 31 | DA | 1449 | A |
| 31 | DA | 1450 | G |
| 31 | DA | 1455 | G |
| 31 | DA | 1458 | C |
| 31 | DA | 1459 | G |
| 31 | DA | 1460 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 31 | DA | 1461 | G |
| 31 | DA | 1462 | C |
| 31 | DA | 1466 | G |
| 31 | DA | 1467 | C |
| 31 | DA | 1471 | A |
| 31 | DA | 1472 | A |
| 31 | DA | 1474 | C |
| 31 | DA | 1475 | G |
| 31 | DA | 1476 | C |
| 31 | DA | 1477 | A |
| 31 | DA | 1479 | G |
| 31 | DA | 1480 | G |
| 31 | DA | 1481 | U |
| 31 | DA | 1482 | G |
| 31 | DA | 1485 | G |
| 31 | DA | 1487 | G |
| 31 | DA | 1488 | G |
| 31 | DA | 1490 | A |
| 31 | DA | 1491 | G |
| 31 | DA | 1493 | C |
| 31 | DA | 1494 | A |
| 31 | DA | 1495 | A |
| 31 | DA | 1497 | U |
| 31 | DA | 1498 | C |
| 31 | DA | 1501 | C |
| 31 | DA | 1502 | C |
| 31 | DA | 1503 | U |
| 31 | DA | 1505 | C |
| 31 | DA | 1508 | A |
| 31 | DA | 1509 | C |
| 31 | DA | 1509(A) | A |
| 31 | DA | 1511 | C |
| 31 | DA | 1512 | U |
| 31 | DA | 1513 | C |
| 31 | DA | 1515 | G |
| 31 | DA | 1520 | G |
| 31 | DA | 1526 | G |
| 31 | DA | 1528 | A |
| 31 | DA | 1528(A) | A |
| 31 | DA | 1529 | G |
| 31 | DA | 1530 | C |
| 31 | DA | 1531 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | DA | 1532 | C |
| 31 | DA | 1533 | G |
| 31 | DA | 1543 | C |
| 31 | DA | 1545 | A |
| 31 | DA | 1546 | C |
| 31 | DA | 1558 | A |
| 31 | DA | 1559 | G |
| 31 | DA | 1566 | A |
| 31 | DA | 1569 | A |
| 31 | DA | 1578 | U |
| 31 | DA | 1579 | A |
| 31 | DA | 1580 | A |
| 31 | DA | 1581 | G |
| 31 | DA | 1584 | C |
| 31 | DA | 1586 | A |
| 31 | DA | 1588 | C |
| 31 | DA | 1591 | G |
| 31 | DA | 1593 | G |
| 31 | DA | 1594 | G |
| 31 | DA | 1597 | A |
| 31 | DA | 1598 | C |
| 31 | DA | 1603 | A |
| 31 | DA | 1608 | A |
| 31 | DA | 1609 | A |
| 31 | DA | 1617 | C |
| 31 | DA | 1618 | A |
| 31 | DA | 1625 | C |
| 31 | DA | 1635 | G |
| 31 | DA | 1640 | C |
| 31 | DA | 1648 | C |
| 31 | DA | 1652 | A |
| 31 | DA | 1653 | G |
| 31 | DA | 1654 | A |
| 31 | DA | 1655 | A |
| 31 | DA | 1674 | G |
| 31 | DA | 1678 | G |
| 31 | DA | 1694 | C |
| 31 | DA | 1695 | G |
| 31 | DA | 1696 | G |
| 31 | DA | 1697 | G |
| 31 | DA | 1698 | A |
| 31 | DA | 1700 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | DA | 1701 | A |
| 31 | DA | 1703 | G |
| 31 | DA | 1721 | G |
| 31 | DA | 1722 | A |
| 31 | DA | 1739 | U |
| 31 | DA | 1741 | A |
| 31 | DA | 1742 | G |
| 31 | DA | 1744 | C |
| 31 | DA | 1746 | G |
| 31 | DA | 1749 | A |
| 31 | DA | 1756 | G |
| 31 | DA | 1763 | G |
| 31 | DA | 1764 | G |
| 31 | DA | 1773 | A |
| 31 | DA | 1780 | A |
| 31 | DA | 1781 | C |
| 31 | DA | 1782 | C |
| 31 | DA | 1791 | A |
| 31 | DA | 1799 | G |
| 31 | DA | 1800 | C |
| 31 | DA | 1801 | G |
| 31 | DA | 1813 | G |
| 31 | DA | 1816 | G |
| 31 | DA | 1820 | U |
| 31 | DA | 1822 | G |
| 31 | DA | 1827 | C |
| 31 | DA | 1828 | G |
| 31 | DA | 1829 | A |
| 31 | DA | 1835 | G |
| 31 | DA | 1838 | C |
| 31 | DA | 1840 | G |
| 31 | DA | 1847 | A |
| 31 | DA | 1858 | G |
| 31 | DA | 1865 | G |
| 31 | DA | 1866 | C |
| 31 | DA | 1877 | A |
| 31 | DA | 1878 | G |
| 31 | DA | 1882 | C |
| 31 | DA | 1885 | A |
| 31 | DA | 1889 | A |
| 31 | DA | 1900 | A |
| 31 | DA | 1902 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | DA | 1903 | G |
| 31 | DA | 1906 | G |
| 31 | DA | 1913 | A |
| 31 | DA | 1914 | C |
| 31 | DA | 1915 | U |
| 31 | DA | 1929 | G |
| 31 | DA | 1930 | G |
| 31 | DA | 1934 | C |
| 31 | DA | 1935 | G |
| 31 | DA | 1936 | A |
| 31 | DA | 1938 | A |
| 31 | DA | 1948 | G |
| 31 | DA | 1955 | U |
| 31 | DA | 1962 | C |
| 31 | DA | 1963 | U |
| 31 | DA | 1964 | G |
| 31 | DA | 1967 | C |
| 31 | DA | 1969 | A |
| 31 | DA | 1970 | A |
| 31 | DA | 1971 | A |
| 31 | DA | 1972 | A |
| 31 | DA | 1982 | C |
| 31 | DA | 1992 | G |
| 31 | DA | 1993 | U |
| 31 | DA | 1997 | G |
| 31 | DA | 2018 | G |
| 31 | DA | 2020 | A |
| 31 | DA | 2021 | C |
| 31 | DA | 2023 | G |
| 31 | DA | 2030 | A |
| 31 | DA | 2031 | A |
| 31 | DA | 2033 | A |
| 31 | DA | 2036 | C |
| 31 | DA | 2039 | C |
| 31 | DA | 2043 | C |
| 31 | DA | 2055 | C |
| 31 | DA | 2056 | G |
| 31 | DA | 2058 | A |
| 31 | DA | 2060 | A |
| 31 | DA | 2061 | G |
| 31 | DA | 2062 | A |
| 31 | DA | 2069 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | DA | 2071 | A |
| 31 | DA | 2095 | C |
| 31 | DA | 2100 | G |
| 31 | DA | 2103 | C |
| 31 | DA | 2104 | G |
| 31 | DA | 2187 | G |
| 31 | DA | 2190 | G |
| 31 | DA | 2191 | G |
| 31 | DA | 2192 | G |
| 31 | DA | 2193 | G |
| 31 | DA | 2198 | A |
| 31 | DA | 2199 | A |
| 31 | DA | 2200 | C |
| 31 | DA | 2203 | U |
| 31 | DA | 2206 | G |
| 31 | DA | 2207 | G |
| 31 | DA | 2208 | A |
| 31 | DA | 2218 | U |
| 31 | DA | 2219 | G |
| 31 | DA | 2225 | A |
| 31 | DA | 2226 | C |
| 31 | DA | 2238 | G |
| 31 | DA | 2263 | C |
| 31 | DA | 2268 | A |
| 31 | DA | 2272 | U |
| 31 | DA | 2273 | A |
| 31 | DA | 2275 | C |
| 31 | DA | 2278 | A |
| 31 | DA | 2280 | G |
| 31 | DA | 2283 | C |
| 31 | DA | 2287 | A |
| 31 | DA | 2288 | A |
| 31 | DA | 2289 | G |
| 31 | DA | 2298 | A |
| 31 | DA | 2303 | G |
| 31 | DA | 2305 | A |
| 31 | DA | 2307 | G |
| 31 | DA | 2308 | G |
| 31 | DA | 2309 | A |
| 31 | DA | 2311 | A |
| 31 | DA | 2316 | C |
| 31 | DA | 2318 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | DA | 2319 | G |
| 31 | DA | 2320 | A |
| 31 | DA | 2321 | G |
| 31 | DA | 2324 | C |
| 31 | DA | 2325 | G |
| 31 | DA | 2327 | A |
| 31 | DA | 2334 | G |
| 31 | DA | 2336 | A |
| 31 | DA | 2340 | G |
| 31 | DA | 2342 | C |
| 31 | DA | 2347 | C |
| 31 | DA | 2350 | C |
| 31 | DA | 2360 | A |
| 31 | DA | 2361 | A |
| 31 | DA | 2372 | G |
| 31 | DA | 2383 | G |
| 31 | DA | 2385 | C |
| 31 | DA | 2387 | U |
| 31 | DA | 2388 | A |
| 31 | DA | 2393 | A |
| 31 | DA | 2402 | C |
| 31 | DA | 2403 | C |
| 31 | DA | 2404 | C |
| 31 | DA | 2405 | G |
| 31 | DA | 2406 | U |
| 31 | DA | 2410 | G |
| 31 | DA | 2422 | A |
| 31 | DA | 2423 | U |
| 31 | DA | 2425 | A |
| 31 | DA | 2427 | C |
| 31 | DA | 2429 | G |
| 31 | DA | 2430 | A |
| 31 | DA | 2431 | U |
| 31 | DA | 2435 | A |
| 31 | DA | 2439 | A |
| 31 | DA | 2440 | C |
| 31 | DA | 2441 | C |
| 31 | DA | 2448 | A |
| 31 | DA | 2449 | U |
| 31 | DA | 2464 | C |
| 31 | DA | 2465 | C |
| 31 | DA | 2468 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | DA | 2469 | A |
| 31 | DA | 2470 | G |
| 31 | DA | 2471 | C |
| 31 | DA | 2475 | C |
| 31 | DA | 2476 | A |
| 31 | DA | 2477 | C |
| 31 | DA | 2478 | A |
| 31 | DA | 2487 | G |
| 31 | DA | 2489 | G |
| 31 | DA | 2492 | U |
| 31 | DA | 2497 | A |
| 31 | DA | 2502 | G |
| 31 | DA | 2505 | G |
| 31 | DA | 2506 | U |
| 31 | DA | 2507 | C |
| 31 | DA | 2510 | C |
| 31 | DA | 2518 | A |
| 31 | DA | 2520 | C |
| 31 | DA | 2524 | G |
| 31 | DA | 2525 | G |
| 31 | DA | 2529 | G |
| 31 | DA | 2535 | G |
| 31 | DA | 2543 | G |
| 31 | DA | 2554 | U |
| 31 | DA | 2564 | A |
| 31 | DA | 2566 | A |
| 31 | DA | 2567 | G |
| 31 | DA | 2569 | G |
| 31 | DA | 2582 | G |
| 31 | DA | 2585 | U |
| 31 | DA | 2586 | C |
| 31 | DA | 2601 | C |
| 31 | DA | 2602 | A |
| 31 | DA | 2603 | G |
| 31 | DA | 2604 | U |
| 31 | DA | 2608 | G |
| 31 | DA | 2609 | U |
| 31 | DA | 2610 | C |
| 31 | DA | 2611 | U |
| 31 | DA | 2612 | C |
| 31 | DA | 2613 | U |
| 31 | DA | 2615 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 31 | DA | 2630 | G |
| 31 | DA | 2637 | U |
| 31 | DA | 2638 | G |
| 31 | DA | 2654 | A |
| 31 | DA | 2655 | G |
| 31 | DA | 2656 | U |
| 31 | DA | 2657 | A |
| 31 | DA | 2658 | C |
| 31 | DA | 2659 | G |
| 31 | DA | 2660 | A |
| 31 | DA | 2661 | G |
| 31 | DA | 2662 | A |
| 31 | DA | 2663 | G |
| 31 | DA | 2673 | G |
| 31 | DA | 2682 | U |
| 31 | DA | 2690 | C |
| 31 | DA | 2701 | C |
| 31 | DA | 2702 | U |
| 31 | DA | 2703 | C |
| 31 | DA | 2707 | G |
| 31 | DA | 2712 | U |
| 31 | DA | 2712(A) | A |
| 31 | DA | 2713 | A |
| 31 | DA | 2714 | G |
| 31 | DA | 2726 | U |
| 31 | DA | 2731 | G |
| 31 | DA | 2733 | A |
| 31 | DA | 2752 | C |
| 31 | DA | 2753 | A |
| 31 | DA | 2754 | U |
| 31 | DA | 2757 | A |
| 31 | DA | 2758 | A |
| 31 | DA | 2762 | G |
| 31 | DA | 2764 | A |
| 31 | DA | 2765 | A |
| 31 | DA | 2766 | G |
| 31 | DA | 2778 | A |
| 31 | DA | 2779 | U |
| 31 | DA | 2781 | A |
| 31 | DA | 2789 | C |
| 31 | DA | 2790 | A |
| 31 | DA | 2791 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 31 | DA | 2794 | C |
| 31 | DA | 2795 | G |
| 31 | DA | 2801(A) | A |
| 31 | DA | 2802 | G |
| 31 | DA | 2803 | C |
| 31 | DA | 2807 | G |
| 31 | DA | 2808 | U |
| 31 | DA | 2818 | G |
| 31 | DA | 2820 | A |
| 31 | DA | 2821 | A |
| 31 | DA | 2833 | G |
| 31 | DA | 2835 | A |
| 31 | DA | 2849 | U |
| 31 | DA | 2860 | A |
| 31 | DA | 2872 | G |
| 31 | DA | 2880 | C |
| 31 | DA | 2892 | A |
| 31 | DA | 2894 | G |
| 31 | DA | 2895 | U |
| 31 | DA | 2897 | U |
| 32 | DB | 8 | U |
| 32 | DB | 9 | G |
| 32 | DB | 12 | C |
| 32 | DB | 15 | A |
| 32 | DB | 20 | C |
| 32 | DB | 22 | U |
| 32 | DB | 27 | C |
| 32 | DB | 33 | G |
| 32 | DB | 40 | U |
| 32 | DB | 41 | U |
| 32 | DB | 42 | C |
| 32 | DB | 43 | C |
| 32 | DB | 44 | G |
| 32 | DB | 45 | A |
| 32 | DB | 46 | A |
| 32 | DB | 47 | C |
| 32 | DB | 52 | A |
| 32 | DB | 53 | A |
| 32 | DB | 56 | G |
| 32 | DB | 63 | G |
| 32 | DB | 64 | C |
| 32 | DB | 73 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DB | 74 | U |
| 32 | DB | 75 | G |
| 32 | DB | 85 | G |
| 32 | DB | 87 | G |
| 32 | DB | 88 | C |
| 32 | DB | 89 | G |
| 32 | DB | 90 | A |
| 32 | DB | 91 | C |
| 32 | DB | 102 | A |
| 32 | DB | 106 | G |
| 32 | DB | 110 | G |
| 32 | DB | 118 | G |

All (203) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 60 | A |
| 1 | AA | 79 | G |
| 1 | AA | 115 | G |
| 1 | AA | 119 | A |
| 1 | AA | 243 | A |
| 1 | AA | 250 | A |
| 1 | AA | 266 | G |
| 1 | AA | 328 | C |
| 1 | AA | 353 | A |
| 1 | AA | 366 | C |
| 1 | AA | 428 | G |
| 1 | AA | 429 | U |
| 1 | AA | 484 | G |
| 1 | AA | 509 | A |
| 1 | AA | 533 | A |
| 1 | AA | 560 | U |
| 1 | AA | 687 | A |
| 1 | AA | 748 | C |
| 1 | AA | 913 | A |
| 1 | AA | 991 | U |
| 1 | AA | 992 | U |
| 1 | AA | 1049 | U |
| 1 | AA | 1064 | G |
| 1 | AA | 1065 | U |
| 1 | AA | 1067 | A |
| 1 | AA | 1201 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 1285 | A |
| 1 | AA | 1498 | U |
| 1 | AA | 1504 | G |
| 31 | BA | 34 | C |
| 31 | BA | 49 | A |
| 31 | BA | 50 | U |
| 31 | BA | 71 | A |
| 31 | BA | 128 | C |
| 31 | BA | 249 | C |
| 31 | BA | 272 | G |
| 31 | BA | 331 | A |
| 31 | BA | 352 | G |
| 31 | BA | 363(E) | U |
| 31 | BA | 472 | A |
| 31 | BA | 474 | G |
| 31 | BA | 542 | C |
| 31 | BA | 587 | C |
| 31 | BA | 603 | A |
| 31 | BA | 651 | G |
| 31 | BA | 669 | G |
| 31 | BA | 671 | C |
| 31 | BA | 685 | A |
| 31 | BA | 746 | A |
| 31 | BA | 752 | A |
| 31 | BA | 764 | A |
| 31 | BA | 774 | A |
| 31 | BA | 790 | C |
| 31 | BA | 827 | U |
| 31 | BA | 958 | U |
| 31 | BA | 974 | G |
| 31 | BA | 1022 | G |
| 31 | BA | 1112 | G |
| 31 | BA | 1176 | G |
| 31 | BA | 1210 | A |
| 31 | BA | 1250 | G |
| 31 | BA | 1300 | U |
| 31 | BA | 1378 | A |
| 31 | BA | 1379 | A |
| 31 | BA | 1397 | U |
| 31 | BA | 1419 | A |
| 31 | BA | 1427 | A |
| 31 | BA | 1459 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | BA | 1494 | A |
| 31 | BA | 1508 | A |
| 31 | BA | 1544 | A |
| 31 | BA | 1558 | A |
| 31 | BA | 1608 | A |
| 31 | BA | 1617 | C |
| 31 | BA | 1652 | A |
| 31 | BA | 1653 | G |
| 31 | BA | 1694 | C |
| 31 | BA | 1697 | G |
| 31 | BA | 1740 | G |
| 31 | BA | 1819 | A |
| 31 | BA | 1934 | C |
| 31 | BA | 1962 | C |
| 31 | BA | 1970 | A |
| 31 | BA | 1992 | G |
| 31 | BA | 2225 | A |
| 31 | BA | 2405 | G |
| 31 | BA | 2406 | U |
| 31 | BA | 2422 | A |
| 31 | BA | 2439 | A |
| 31 | BA | 2542 | A |
| 31 | BA | 2610 | C |
| 31 | BA | 2660 | A |
| 31 | BA | 2661 | G |
| 31 | BA | 2662 | A |
| 31 | BA | 2689 | U |
| 31 | BA | 2712 | U |
| 31 | BA | 2726 | U |
| 31 | BA | 2756 | U |
| 31 | BA | 2796 | U |
| 31 | BA | 2849 | U |
| 31 | BA | 2859 | G |
| 31 | BA | 2873 | A |
| 32 | BB | 109 | C |
| 1 | CA | 60 | A |
| 1 | CA | 79 | G |
| 1 | CA | 115 | G |
| 1 | CA | 119 | A |
| 1 | CA | 243 | A |
| 1 | CA | 250 | A |
| 1 | CA | 266 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 328 | C |
| 1 | CA | 353 | A |
| 1 | CA | 366 | C |
| 1 | CA | 428 | G |
| 1 | CA | 429 | U |
| 1 | CA | 484 | G |
| 1 | CA | 509 | A |
| 1 | CA | 533 | A |
| 1 | CA | 560 | U |
| 1 | CA | 687 | A |
| 1 | CA | 748 | C |
| 1 | CA | 913 | A |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |
| 1 | CA | 1049 | U |
| 1 | CA | 1064 | G |
| 1 | CA | 1065 | U |
| 1 | CA | 1067 | A |
| 1 | CA | 1201 | A |
| 1 | CA | 1285 | A |
| 1 | CA | 1498 | U |
| 1 | CA | 1504 | G |
| 31 | DA | 34 | C |
| 31 | DA | 49 | A |
| 31 | DA | 50 | U |
| 31 | DA | 71 | A |
| 31 | DA | 128 | C |
| 31 | DA | 249 | C |
| 31 | DA | 272 | G |
| 31 | DA | 331 | A |
| 31 | DA | 352 | G |
| 31 | DA | 363(E) | U |
| 31 | DA | 472 | A |
| 31 | DA | 474 | G |
| 31 | DA | 542 | C |
| 31 | DA | 587 | C |
| 31 | DA | 603 | A |
| 31 | DA | 651 | G |
| 31 | DA | 669 | G |
| 31 | DA | 671 | C |
| 31 | DA | 685 | A |
| 31 | DA | 746 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | DA | 752 | A |
| 31 | DA | 764 | A |
| 31 | DA | 774 | A |
| 31 | DA | 790 | C |
| 31 | DA | 827 | U |
| 31 | DA | 958 | U |
| 31 | DA | 1022 | G |
| 31 | DA | 1112 | G |
| 31 | DA | 1176 | G |
| 31 | DA | 1210 | A |
| 31 | DA | 1250 | G |
| 31 | DA | 1300 | U |
| 31 | DA | 1378 | A |
| 31 | DA | 1379 | A |
| 31 | DA | 1397 | U |
| 31 | DA | 1419 | A |
| 31 | DA | 1427 | A |
| 31 | DA | 1459 | G |
| 31 | DA | 1494 | A |
| 31 | DA | 1504 | C |
| 31 | DA | 1508 | A |
| 31 | DA | 1544 | A |
| 31 | DA | 1558 | A |
| 31 | DA | 1608 | A |
| 31 | DA | 1617 | C |
| 31 | DA | 1652 | A |
| 31 | DA | 1653 | G |
| 31 | DA | 1694 | C |
| 31 | DA | 1697 | G |
| 31 | DA | 1740 | G |
| 31 | DA | 1819 | A |
| 31 | DA | 1934 | C |
| 31 | DA | 1962 | C |
| 31 | DA | 1970 | A |
| 31 | DA | 1992 | G |
| 31 | DA | 2225 | A |
| 31 | DA | 2405 | G |
| 31 | DA | 2422 | A |
| 31 | DA | 2439 | A |
| 31 | DA | 2542 | A |
| 31 | DA | 2610 | C |
| 31 | DA | 2660 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 31 | DA | 2661 | G |
| 31 | DA | 2662 | A |
| 31 | DA | 2689 | U |
| 31 | DA | 2726 | U |
| 31 | DA | 2756 | U |
| 31 | DA | 2796 | U |
| 31 | DA | 2859 | G |
| 31 | DA | 2873 | A |
| 32 | DB | 109 | C |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 838 ligands modelled in this entry, 836 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 | $\# Z > 2$ |
| 55 | ERY | DA | 3330 | - | 53,53,53 | 1.23 | 5 (9%) | 82,82,82 | 0.98 | 5 (6%) |
| 55 | ERY | BA | 3364 | - | 53,53,53 | 1.23 | 5 (9%) | 82,82,82 | 0.98 | 5 (6%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|--------------|---------|
| 55 | ERY | DA | 3330 | - | - | 4/72/107/107 | 0/3/3/3 |
| 55 | ERY | BA | 3364 | - | - | 4/72/107/107 | 0/3/3/3 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 55 | BA | 3364 | ERY | C6-C5 | 3.26 | 1.61 | 1.55 |
| 55 | DA | 3330 | ERY | C6-C5 | 3.24 | 1.61 | 1.55 |
| 55 | BA | 3364 | ERY | C7-C6 | 2.47 | 1.58 | 1.54 |
| 55 | DA | 3330 | ERY | C7-C6 | 2.44 | 1.58 | 1.54 |
| 55 | DA | 3330 | ERY | O2-C13 | 2.18 | 1.50 | 1.46 |
| 55 | BA | 3364 | ERY | O2-C13 | 2.17 | 1.50 | 1.46 |
| 55 | DA | 3330 | ERY | C2-C3 | 2.14 | 1.60 | 1.55 |
| 55 | BA | 3364 | ERY | C2-C3 | 2.14 | 1.60 | 1.55 |
| 55 | BA | 3364 | ERY | O4-C18 | 2.03 | 1.49 | 1.44 |
| 55 | DA | 3330 | ERY | O4-C18 | 2.02 | 1.49 | 1.44 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55 | DA | 3330 | ERY | C3-C2-C1 | -2.61 | 104.69 | 110.01 |
| 55 | BA | 3364 | ERY | C3-C2-C1 | -2.60 | 104.70 | 110.01 |
| 55 | DA | 3330 | ERY | C25-C24-C23 | -2.44 | 106.45 | 109.97 |
| 55 | BA | 3364 | ERY | C25-C24-C23 | -2.43 | 106.46 | 109.97 |
| 55 | DA | 3330 | ERY | C6-C5-C4 | -2.16 | 111.00 | 114.05 |
| 55 | BA | 3364 | ERY | C6-C5-C4 | -2.14 | 111.03 | 114.05 |
| 55 | BA | 3364 | ERY | O5-C16-C17 | 2.12 | 106.95 | 103.81 |
| 55 | DA | 3330 | ERY | O5-C16-C17 | 2.12 | 106.95 | 103.81 |
| 55 | DA | 3330 | ERY | O13-C12-C35 | -2.02 | 103.62 | 107.78 |
| 55 | BA | 3364 | ERY | O13-C12-C35 | -2.01 | 103.64 | 107.78 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 55 | DA | 3330 | ERY | O9-C22-O7-C5 |
| 55 | BA | 3364 | ERY | O9-C22-O7-C5 |
| 55 | DA | 3330 | ERY | O7-C5-C6-C7 |
| 55 | BA | 3364 | ERY | O7-C5-C6-C7 |
| 55 | BA | 3364 | ERY | C23-C22-O7-C5 |
| 55 | DA | 3330 | ERY | C23-C22-O7-C5 |
| 55 | DA | 3330 | ERY | C25-C24-N1-C29 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 55 | BA | 3364 | ERY | C25-C24-N1-C29 |

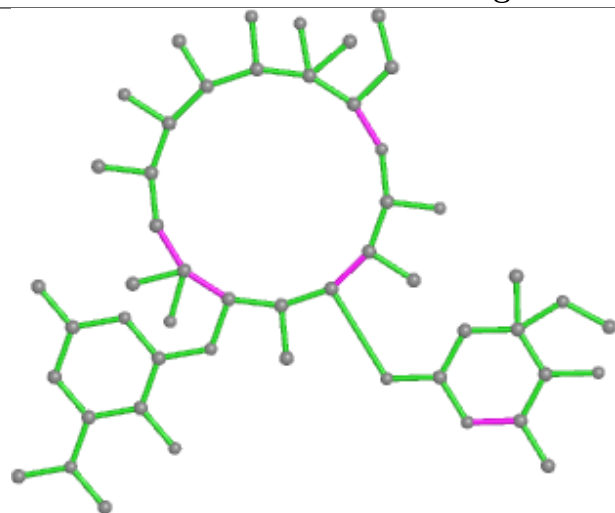
There are no ring outliers.

2 monomers are involved in 3 short contacts:

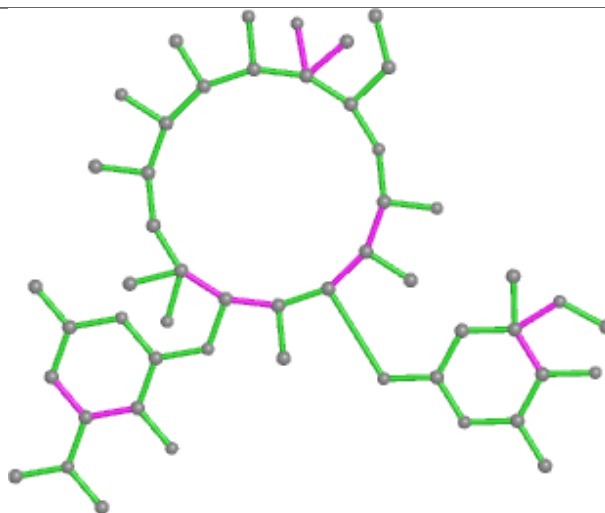
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 55 | DA | 3330 | ERY | 2 | 0 |
| 55 | BA | 3364 | ERY | 1 | 0 |

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

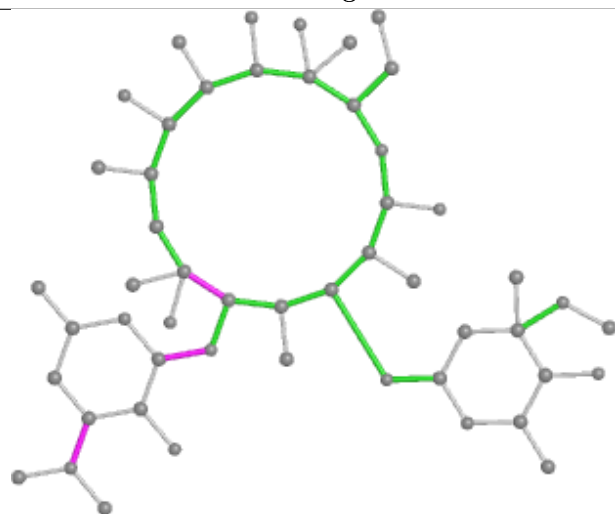
Ligand ERY DA 3330



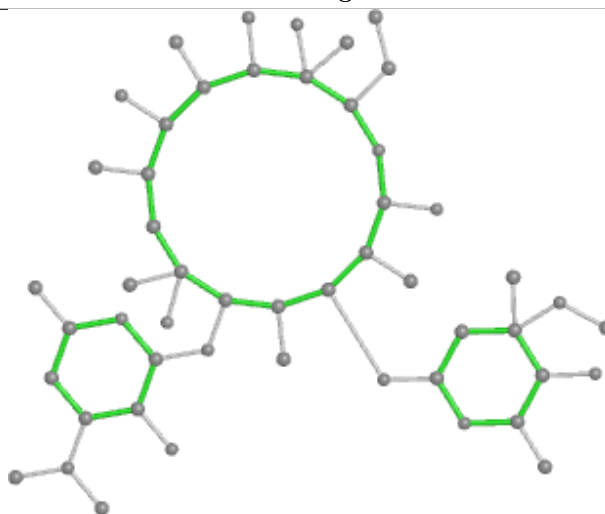
Bond lengths



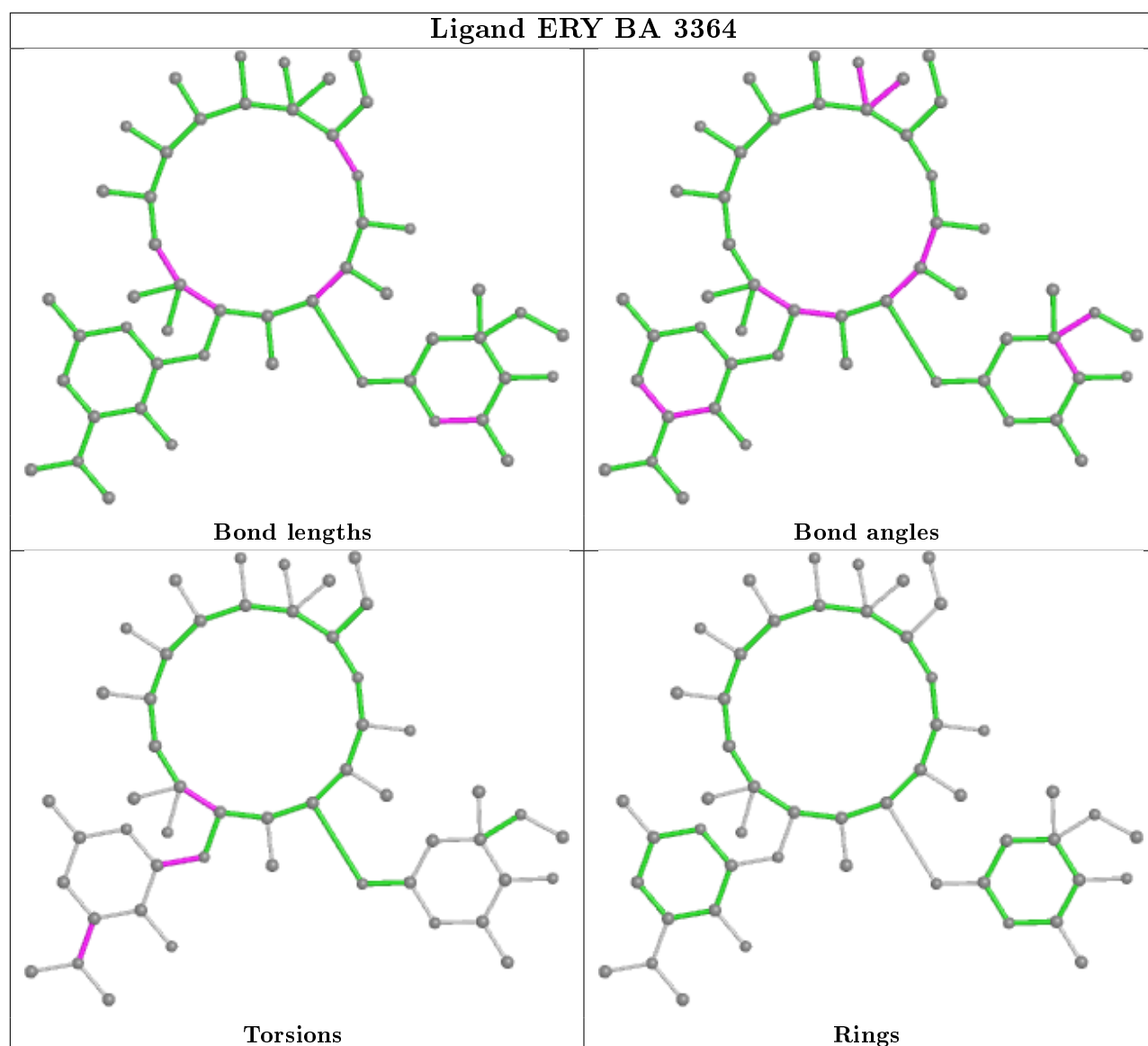
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 13 | CM | 3 |
| 13 | AM | 3 |
| 36 | DG | 1 |
| 36 | BG | 1 |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 9 | AI | 1 |
| 9 | CI | 1 |
| 28 | D6 | 1 |
| 28 | B6 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | CM | 69:GLU | C | 70:LEU | N | 5.58 |
| 1 | AM | 69:GLU | C | 70:LEU | N | 5.57 |
| 1 | DG | 112:PRO | C | 113:ARG | N | 4.82 |
| 1 | BG | 112:PRO | C | 113:ARG | N | 4.80 |
| 1 | CM | 97:PRO | C | 98:VAL | N | 4.38 |
| 1 | AM | 97:PRO | C | 98:VAL | N | 4.37 |
| 1 | B6 | 46:HIS | C | 47:THR | N | 3.94 |
| 1 | D6 | 46:HIS | C | 47:THR | N | 3.92 |
| 1 | CM | 112:GLY | C | 113:PRO | N | 3.74 |
| 1 | AM | 112:GLY | C | 113:PRO | N | 3.73 |
| 1 | AI | 53:VAL | C | 54:ASP | N | 3.24 |
| 1 | CI | 53:VAL | C | 54:ASP | N | 3.23 |

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1504/1522 (98%) | 1.15 | 305 (20%) 1 0 | 46, 116, 201, 202 | 0 |
| 1 | CA | 1504/1522 (98%) | 1.11 | 300 (19%) 1 0 | 50, 115, 201, 203 | 0 |
| 2 | AB | 235/256 (91%) | 1.22 | 64 (27%) 0 0 | 99, 157, 195, 200 | 0 |
| 2 | CB | 235/256 (91%) | 1.57 | 77 (32%) 0 0 | 99, 162, 195, 201 | 0 |
| 3 | AC | 207/239 (86%) | 1.17 | 47 (22%) 0 0 | 108, 163, 190, 198 | 0 |
| 3 | CC | 207/239 (86%) | 1.86 | 75 (36%) 0 0 | 110, 168, 192, 198 | 0 |
| 4 | AD | 208/209 (99%) | 0.55 | 21 (10%) 7 2 | 65, 126, 175, 189 | 0 |
| 4 | CD | 208/209 (99%) | 0.48 | 17 (8%) 11 3 | 66, 124, 173, 191 | 0 |
| 5 | AE | 151/160 (94%) | 0.37 | 15 (9%) 7 2 | 65, 111, 162, 199 | 0 |
| 5 | CE | 151/160 (94%) | 0.81 | 21 (13%) 2 1 | 72, 115, 172, 198 | 0 |
| 6 | AF | 101/101 (100%) | 0.35 | 5 (4%) 28 10 | 82, 123, 173, 192 | 0 |
| 6 | CF | 101/101 (100%) | 0.56 | 16 (15%) 2 1 | 84, 130, 177, 196 | 0 |
| 7 | AG | 155/156 (99%) | 1.83 | 65 (41%) 0 0 | 126, 177, 196, 201 | 0 |
| 7 | CG | 155/156 (99%) | 2.26 | 73 (47%) 0 0 | 122, 177, 196, 200 | 0 |
| 8 | AH | 138/138 (100%) | 0.10 | 4 (2%) 51 23 | 78, 113, 157, 171 | 0 |
| 8 | CH | 138/138 (100%) | 0.14 | 2 (1%) 75 49 | 79, 115, 162, 171 | 0 |
| 9 | AI | 127/128 (99%) | 2.65 | 71 (55%) 0 0 | 132, 189, 200, 201 | 0 |
| 9 | CI | 127/128 (99%) | 2.90 | 74 (58%) 0 0 | 131, 190, 200, 202 | 0 |
| 10 | AJ | 99/105 (94%) | 3.50 | 69 (69%) 0 0 | 119, 178, 199, 200 | 0 |
| 10 | CJ | 99/105 (94%) | 3.97 | 76 (76%) 0 0 | 116, 182, 200, 201 | 0 |
| 11 | AK | 119/129 (92%) | 0.74 | 23 (19%) 1 0 | 63, 113, 163, 199 | 0 |
| 11 | CK | 119/129 (92%) | 0.94 | 21 (17%) 1 0 | 64, 116, 165, 199 | 0 |
| 12 | AL | 125/135 (92%) | 0.66 | 15 (12%) 4 1 | 59, 98, 164, 201 | 0 |
| 12 | CL | 125/135 (92%) | 0.71 | 16 (12%) 3 1 | 58, 99, 167, 201 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å²) | | Q<0.9 | |
|-----|-------|---------------|--------|----------|----------|-----|--------------------|---|
| 13 | AM | 115/126 (91%) | 3.05 | 64 (55%) | 0 | 0 | 157, 191, 200, 201 | 0 |
| 13 | CM | 115/126 (91%) | 2.33 | 56 (48%) | 0 | 0 | 152, 189, 199, 201 | 0 |
| 14 | AN | 60/61 (98%) | 1.99 | 22 (36%) | 0 | 0 | 112, 172, 197, 199 | 0 |
| 14 | CN | 60/61 (98%) | 1.74 | 16 (26%) | 0 | 0 | 112, 171, 197, 199 | 0 |
| 15 | AO | 88/89 (98%) | 0.30 | 6 (6%) | 17 | 5 | 70, 105, 160, 169 | 0 |
| 15 | CO | 88/89 (98%) | 0.37 | 5 (5%) | 23 | 8 | 71, 107, 162, 171 | 0 |
| 16 | AP | 84/88 (95%) | 1.23 | 24 (28%) | 0 | 0 | 82, 109, 170, 187 | 0 |
| 16 | CP | 84/88 (95%) | 1.10 | 23 (27%) | 0 | 0 | 80, 107, 165, 183 | 0 |
| 17 | AQ | 100/105 (95%) | 0.51 | 9 (9%) | 9 | 3 | 71, 104, 154, 185 | 0 |
| 17 | CQ | 100/105 (95%) | 0.28 | 7 (7%) | 16 | 5 | 74, 103, 154, 190 | 0 |
| 18 | AR | 70/88 (79%) | 0.92 | 7 (10%) | 7 | 2 | 80, 116, 173, 182 | 0 |
| 18 | CR | 70/88 (79%) | 1.36 | 20 (28%) | 0 | 0 | 83, 124, 175, 185 | 0 |
| 19 | AS | 79/93 (84%) | 3.31 | 58 (73%) | 0 | 0 | 127, 192, 200, 200 | 0 |
| 19 | CS | 79/93 (84%) | 3.42 | 53 (67%) | 0 | 0 | 131, 190, 200, 201 | 0 |
| 20 | AT | 99/106 (93%) | 0.58 | 10 (10%) | 7 | 2 | 75, 115, 162, 186 | 0 |
| 20 | CT | 99/106 (93%) | 0.48 | 10 (10%) | 7 | 2 | 74, 115, 160, 189 | 0 |
| 21 | AU | 25/27 (92%) | 5.05 | 21 (84%) | 0 | 0 | 144, 182, 197, 199 | 0 |
| 21 | CU | 25/27 (92%) | 3.57 | 17 (68%) | 0 | 0 | 139, 173, 194, 197 | 0 |
| 22 | B0 | 85/85 (100%) | 0.56 | 9 (10%) | 6 | 2 | 39, 60, 177, 193 | 0 |
| 22 | D0 | 85/85 (100%) | 0.69 | 8 (9%) | 8 | 3 | 44, 65, 177, 193 | 0 |
| 23 | B1 | 89/98 (90%) | 0.19 | 2 (2%) | 62 | 33 | 39, 64, 143, 170 | 0 |
| 23 | D1 | 89/98 (90%) | 0.16 | 5 (5%) | 24 | 8 | 41, 66, 144, 183 | 0 |
| 24 | B2 | 51/72 (70%) | 0.72 | 3 (5%) | 22 | 7 | 47, 85, 185, 196 | 0 |
| 24 | D2 | 51/72 (70%) | 0.45 | 4 (7%) | 13 | 4 | 53, 92, 191, 198 | 0 |
| 25 | B3 | 60/60 (100%) | 0.08 | 2 (3%) | 46 | 20 | 36, 59, 135, 186 | 0 |
| 25 | D3 | 60/60 (100%) | 0.30 | 4 (6%) | 17 | 5 | 42, 66, 141, 182 | 0 |
| 26 | B4 | 32/71 (45%) | -0.22 | 0 | 100 | 100 | 133, 155, 186, 193 | 0 |
| 26 | D4 | 32/71 (45%) | 0.46 | 5 (15%) | 2 | 1 | 143, 169, 187, 197 | 0 |
| 27 | B5 | 58/60 (96%) | 0.46 | 5 (8%) | 10 | 3 | 20, 47, 177, 199 | 0 |
| 27 | D5 | 58/60 (96%) | 0.17 | 7 (12%) | 4 | 1 | 23, 50, 176, 199 | 0 |
| 28 | B6 | 45/54 (83%) | 1.07 | 8 (17%) | 1 | 0 | 41, 74, 129, 184 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 28 | D6 | 45/54 (83%) | 0.91 | 11 (24%) 0 0 | 44, 77, 143, 178 | 0 |
| 29 | B7 | 49/49 (100%) | 0.11 | 4 (8%) 11 3 | 26, 33, 119, 175 | 0 |
| 29 | D7 | 49/49 (100%) | 0.17 | 3 (6%) 21 7 | 26, 35, 126, 174 | 0 |
| 30 | B8 | 64/65 (98%) | 0.42 | 4 (6%) 20 6 | 33, 54, 148, 179 | 0 |
| 30 | D8 | 64/65 (98%) | 0.09 | 2 (3%) 49 21 | 36, 58, 148, 180 | 0 |
| 31 | BA | 2725/2787 (97%) | 0.30 | 90 (3%) 46 20 | 25, 47, 144, 203 | 0 |
| 31 | DA | 2725/2787 (97%) | 0.20 | 141 (5%) 27 10 | 25, 52, 155, 202 | 0 |
| 32 | BB | 119/122 (97%) | 0.59 | 5 (4%) 36 14 | 44, 92, 137, 191 | 0 |
| 32 | DB | 119/122 (97%) | 1.08 | 31 (26%) 0 0 | 51, 101, 165, 190 | 0 |
| 33 | BD | 272/276 (98%) | -0.15 | 4 (1%) 73 46 | 25, 49, 105, 183 | 0 |
| 33 | DD | 272/276 (98%) | -0.24 | 3 (1%) 80 56 | 23, 53, 109, 172 | 0 |
| 34 | BE | 205/206 (99%) | 0.06 | 7 (3%) 45 19 | 26, 54, 140, 193 | 0 |
| 34 | DE | 205/206 (99%) | -0.02 | 5 (2%) 59 30 | 30, 58, 146, 193 | 0 |
| 35 | BF | 208/210 (99%) | 0.37 | 15 (7%) 15 4 | 21, 65, 175, 198 | 0 |
| 35 | DF | 208/210 (99%) | 0.27 | 17 (8%) 11 3 | 27, 68, 175, 199 | 0 |
| 36 | BG | 181/182 (99%) | 1.04 | 36 (19%) 1 0 | 95, 145, 191, 201 | 0 |
| 36 | DG | 181/182 (99%) | 2.41 | 91 (50%) 0 0 | 104, 162, 195, 202 | 0 |
| 37 | BH | 160/180 (88%) | 0.50 | 12 (7%) 14 4 | 62, 103, 161, 193 | 0 |
| 37 | DH | 160/180 (88%) | 1.25 | 46 (28%) 0 0 | 68, 117, 171, 193 | 0 |
| 38 | BI | 146/148 (98%) | 0.52 | 17 (11%) 4 1 | 56, 144, 191, 200 | 0 |
| 38 | DI | 146/148 (98%) | 2.88 | 65 (44%) 0 0 | 52, 164, 194, 201 | 0 |
| 39 | BN | 139/140 (99%) | 0.13 | 6 (4%) 35 13 | 35, 63, 136, 190 | 0 |
| 39 | DN | 139/140 (99%) | -0.16 | 3 (2%) 62 33 | 41, 69, 144, 191 | 0 |
| 40 | BO | 122/122 (100%) | -0.18 | 0 100 100 | 34, 57, 109, 141 | 0 |
| 40 | DO | 122/122 (100%) | -0.43 | 0 100 100 | 37, 59, 116, 146 | 0 |
| 41 | BP | 146/150 (97%) | 0.56 | 12 (8%) 11 3 | 23, 83, 151, 201 | 0 |
| 41 | DP | 146/150 (97%) | 0.52 | 19 (13%) 3 1 | 25, 88, 155, 201 | 0 |
| 42 | BQ | 136/141 (96%) | 0.54 | 9 (6%) 18 5 | 38, 68, 149, 195 | 0 |
| 42 | DQ | 136/141 (96%) | 0.41 | 13 (9%) 8 2 | 43, 74, 146, 195 | 0 |
| 43 | BR | 117/118 (99%) | -0.18 | 1 (0%) 84 63 | 29, 45, 120, 144 | 0 |
| 43 | DR | 117/118 (99%) | -0.30 | 1 (0%) 84 63 | 31, 51, 125, 143 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | BS | 99/112 (88%) | 0.47 | 6 (6%) 21 7 | 49, 98, 144, 184 | 0 |
| 44 | DS | 99/112 (88%) | 0.91 | 21 (21%) 0 0 | 59, 105, 160, 188 | 0 |
| 45 | BT | 132/146 (90%) | 0.29 | 7 (5%) 26 10 | 43, 76, 154, 194 | 0 |
| 45 | DT | 132/146 (90%) | 0.27 | 14 (10%) 6 2 | 47, 79, 162, 197 | 0 |
| 46 | BU | 117/118 (99%) | 0.14 | 3 (2%) 56 27 | 29, 51, 121, 190 | 0 |
| 46 | DU | 117/118 (99%) | 0.27 | 16 (13%) 3 1 | 35, 58, 130, 192 | 0 |
| 47 | BV | 101/101 (100%) | 0.85 | 10 (9%) 7 2 | 32, 98, 188, 199 | 0 |
| 47 | DV | 101/101 (100%) | 0.75 | 12 (11%) 4 1 | 39, 105, 189, 199 | 0 |
| 48 | BW | 113/113 (100%) | -0.28 | 0 100 100 | 27, 39, 106, 171 | 0 |
| 48 | DW | 113/113 (100%) | -0.44 | 1 (0%) 84 63 | 28, 43, 109, 180 | 0 |
| 49 | BX | 93/96 (96%) | 0.25 | 3 (3%) 47 20 | 37, 63, 144, 187 | 0 |
| 49 | DX | 93/96 (96%) | 0.05 | 1 (1%) 80 56 | 40, 66, 144, 186 | 0 |
| 50 | BY | 101/110 (91%) | 0.94 | 13 (12%) 3 1 | 44, 92, 194, 201 | 0 |
| 50 | DY | 101/110 (91%) | 0.70 | 18 (17%) 1 0 | 53, 99, 192, 201 | 0 |
| 51 | BZ | 177/206 (85%) | 0.16 | 4 (2%) 60 31 | 58, 103, 152, 180 | 0 |
| 51 | DZ | 177/206 (85%) | 0.69 | 25 (14%) 2 1 | 63, 110, 156, 188 | 0 |
| All | All | 20062/20918 (95%) | 0.70 | 2789 (13%) 2 1 | 20, 90, 194, 203 | 0 |

All (2789) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 88 | A | 18.5 |
| 1 | AA | 89 | C | 17.8 |
| 35 | BF | 208 | GLY | 17.7 |
| 42 | BQ | 140 | ALA | 17.0 |
| 34 | DE | 205 | ALA | 17.0 |
| 1 | CA | 1149 | C | 16.7 |
| 31 | DA | 2802 | G | 15.6 |
| 42 | DQ | 140 | ALA | 14.8 |
| 2 | CB | 7 | VAL | 14.3 |
| 10 | CJ | 67 | THR | 14.2 |
| 38 | DI | 143 | SER | 14.1 |
| 38 | DI | 91 | SER | 14.1 |
| 13 | AM | 25 | ILE | 14.1 |
| 3 | CC | 159 | GLY | 14.0 |
| 31 | DA | 652 | C | 14.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 42 | DQ | 141 | GLN | 14.0 |
| 42 | BQ | 141 | GLN | 13.9 |
| 38 | DI | 100 | ALA | 13.9 |
| 10 | CJ | 17 | ASP | 13.8 |
| 1 | CA | 84 | U | 13.6 |
| 13 | AM | 24 | GLY | 13.5 |
| 38 | DI | 119 | PRO | 13.5 |
| 21 | AU | 5 | ASP | 13.2 |
| 19 | CS | 79 | THR | 12.9 |
| 10 | CJ | 10 | GLY | 12.7 |
| 31 | BA | 897 | C | 12.3 |
| 1 | AA | 90 | U | 12.2 |
| 38 | DI | 109 | ILE | 11.7 |
| 35 | BF | 207 | GLY | 11.6 |
| 25 | D3 | 60 | GLU | 11.5 |
| 1 | CA | 345 | C | 11.5 |
| 50 | BY | 51 | VAL | 11.4 |
| 3 | CC | 160 | ALA | 11.4 |
| 35 | DF | 12 | LEU | 11.3 |
| 38 | DI | 120 | ILE | 11.3 |
| 10 | AJ | 39 | PRO | 11.0 |
| 12 | CL | 129 | ALA | 10.9 |
| 10 | CJ | 16 | LEU | 10.8 |
| 36 | BG | 87 | PRO | 10.8 |
| 9 | CI | 124 | GLN | 10.8 |
| 35 | BF | 12 | LEU | 10.8 |
| 10 | AJ | 38 | ILE | 10.7 |
| 38 | DI | 81 | VAL | 10.7 |
| 7 | CG | 5 | ARG | 10.7 |
| 36 | BG | 88 | ILE | 10.7 |
| 38 | DI | 121 | LYS | 10.7 |
| 31 | DA | 897 | C | 10.5 |
| 31 | BA | 2104 | G | 10.5 |
| 1 | CA | 1027 | C | 10.4 |
| 1 | CA | 1026 | G | 10.4 |
| 3 | CC | 208 | ILE | 10.4 |
| 38 | DI | 68 | LEU | 10.4 |
| 13 | AM | 3 | ARG | 10.3 |
| 2 | AB | 7 | VAL | 10.3 |
| 31 | DA | 2104 | G | 10.3 |
| 35 | DF | 208 | GLY | 10.3 |
| 10 | CJ | 27 | ALA | 10.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 9 | AI | 81 | ILE | 10.0 |
| 9 | CI | 127 | LYS | 10.0 |
| 13 | AM | 7 | VAL | 10.0 |
| 45 | DT | 39 | ARG | 10.0 |
| 38 | DI | 74 | ASN | 10.0 |
| 22 | B0 | 85 | ALA | 10.0 |
| 27 | B5 | 59 | GLU | 9.9 |
| 42 | DQ | 24 | GLY | 9.9 |
| 38 | BI | 90 | GLY | 9.9 |
| 38 | DI | 86 | THR | 9.8 |
| 1 | CA | 83 | U | 9.8 |
| 11 | CK | 12 | ARG | 9.8 |
| 51 | DZ | 113 | ALA | 9.8 |
| 19 | CS | 80 | TYR | 9.8 |
| 9 | CI | 126 | SER | 9.8 |
| 38 | DI | 89 | TYR | 9.7 |
| 38 | DI | 111 | PRO | 9.7 |
| 35 | DF | 207 | GLY | 9.7 |
| 21 | CU | 5 | ASP | 9.5 |
| 1 | CA | 1001 | A | 9.5 |
| 9 | AI | 2 | GLU | 9.5 |
| 1 | AA | 1001(A) | G | 9.4 |
| 12 | AL | 129 | ALA | 9.4 |
| 1 | AA | 91 | C | 9.4 |
| 9 | AI | 85 | LEU | 9.4 |
| 27 | D5 | 58 | LEU | 9.4 |
| 1 | CA | 1024 | G | 9.3 |
| 14 | CN | 60 | SER | 9.3 |
| 1 | AA | 1260 | C | 9.3 |
| 31 | BA | 652 | C | 9.3 |
| 1 | CA | 1141 | C | 9.3 |
| 50 | DY | 52 | SER | 9.3 |
| 1 | CA | 344 | A | 9.2 |
| 19 | CS | 25 | LYS | 9.2 |
| 14 | CN | 61 | TRP | 9.2 |
| 31 | DA | 2803 | C | 9.2 |
| 22 | B0 | 6 | GLY | 9.2 |
| 31 | BA | 2101 | G | 9.1 |
| 21 | AU | 4 | GLY | 9.1 |
| 1 | CA | 82 | U | 9.1 |
| 1 | AA | 84 | U | 9.1 |
| 38 | DI | 118 | LYS | 9.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 7 | CG | 80 | VAL | 9.1 |
| 10 | AJ | 35 | SER | 9.1 |
| 19 | AS | 56 | GLN | 9.0 |
| 10 | AJ | 5 | ARG | 9.0 |
| 38 | DI | 61 | ARG | 9.0 |
| 1 | AA | 1002 | G | 9.0 |
| 14 | AN | 60 | SER | 9.0 |
| 1 | CA | 1033 | G | 8.8 |
| 47 | DV | 28 | GLU | 8.8 |
| 35 | BF | 24 | LEU | 8.8 |
| 3 | AC | 195 | VAL | 8.7 |
| 7 | CG | 4 | ARG | 8.7 |
| 3 | CC | 155 | GLY | 8.7 |
| 7 | AG | 4 | ARG | 8.7 |
| 34 | DE | 204 | ALA | 8.7 |
| 1 | CA | 1025 | U | 8.7 |
| 11 | CK | 89 | ALA | 8.6 |
| 36 | DG | 108 | ASN | 8.6 |
| 13 | AM | 6 | GLY | 8.6 |
| 42 | BQ | 24 | GLY | 8.6 |
| 10 | CJ | 70 | ARG | 8.6 |
| 3 | AC | 193 | TYR | 8.6 |
| 1 | CA | 1034 | G | 8.5 |
| 45 | BT | 39 | ARG | 8.5 |
| 13 | AM | 4 | ILE | 8.5 |
| 1 | AA | 1139 | G | 8.5 |
| 9 | AI | 96 | LEU | 8.5 |
| 36 | DG | 157 | ILE | 8.5 |
| 10 | CJ | 19 | SER | 8.5 |
| 1 | CA | 1001(A) | G | 8.5 |
| 19 | CS | 71 | LEU | 8.5 |
| 21 | CU | 8 | THR | 8.5 |
| 11 | CK | 11 | LYS | 8.4 |
| 3 | AC | 155 | GLY | 8.4 |
| 31 | BA | 2802 | G | 8.4 |
| 1 | CA | 88 | A | 8.4 |
| 14 | AN | 14 | PRO | 8.4 |
| 3 | CC | 158 | GLY | 8.4 |
| 13 | AM | 8 | GLU | 8.3 |
| 1 | CA | 1140 | C | 8.3 |
| 12 | AL | 128 | ALA | 8.3 |
| 38 | DI | 88 | ILE | 8.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | AI | 126 | SER | 8.2 |
| 19 | CS | 27 | GLU | 8.2 |
| 10 | CJ | 99 | LYS | 8.2 |
| 9 | CI | 18 | PHE | 8.2 |
| 2 | CB | 231 | GLU | 8.2 |
| 1 | AA | 1036 | G | 8.2 |
| 10 | CJ | 20 | ALA | 8.2 |
| 14 | CN | 2 | ALA | 8.2 |
| 2 | CB | 14 | GLY | 8.1 |
| 50 | BY | 59 | GLY | 8.1 |
| 36 | DG | 182 | LYS | 8.1 |
| 9 | CI | 17 | VAL | 8.1 |
| 1 | CA | 1150 | U | 8.1 |
| 9 | AI | 3 | GLN | 8.1 |
| 1 | AA | 79 | G | 8.1 |
| 7 | CG | 82 | GLY | 8.1 |
| 9 | CI | 128 | ARG | 8.1 |
| 10 | CJ | 18 | ALA | 8.1 |
| 18 | AR | 88 | LYS | 8.1 |
| 1 | CA | 1028 | C | 8.1 |
| 13 | AM | 64 | TRP | 8.1 |
| 21 | AU | 2 | GLY | 8.0 |
| 2 | CB | 232 | PRO | 8.0 |
| 24 | D2 | 35 | LEU | 8.0 |
| 31 | DA | 1052 | C | 8.0 |
| 10 | AJ | 37 | PRO | 7.9 |
| 19 | AS | 38 | SER | 7.9 |
| 22 | D0 | 3 | HIS | 7.9 |
| 19 | CS | 68 | GLY | 7.9 |
| 7 | AG | 5 | ARG | 7.9 |
| 10 | CJ | 100 | THR | 7.9 |
| 27 | B5 | 60 | VAL | 7.9 |
| 7 | AG | 3 | ARG | 7.9 |
| 19 | AS | 53 | ASN | 7.8 |
| 21 | AU | 21 | TYR | 7.8 |
| 38 | DI | 97 | ILE | 7.8 |
| 10 | CJ | 68 | HIS | 7.8 |
| 9 | CI | 92 | TYR | 7.7 |
| 9 | CI | 85 | LEU | 7.7 |
| 19 | CS | 26 | GLY | 7.7 |
| 1 | AA | 1001 | A | 7.6 |
| 1 | CA | 1023 | G | 7.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | CM | 42 | ALA | 7.6 |
| 13 | CM | 8 | GLU | 7.6 |
| 10 | AJ | 94 | VAL | 7.5 |
| 50 | DY | 51 | VAL | 7.5 |
| 1 | AA | 1030(B) | C | 7.5 |
| 19 | AS | 57 | HIS | 7.5 |
| 10 | AJ | 86 | MET | 7.5 |
| 19 | CS | 76 | PRO | 7.5 |
| 35 | BF | 133 | ASN | 7.5 |
| 10 | CJ | 91 | PRO | 7.5 |
| 13 | CM | 7 | VAL | 7.5 |
| 9 | AI | 89 | ASN | 7.5 |
| 10 | CJ | 69 | ASN | 7.5 |
| 46 | DU | 118 | GLY | 7.4 |
| 13 | CM | 84 | ILE | 7.4 |
| 31 | BA | 2796 | U | 7.4 |
| 19 | AS | 5 | LEU | 7.4 |
| 38 | DI | 65 | ALA | 7.4 |
| 2 | CB | 15 | VAL | 7.4 |
| 35 | DF | 11 | VAL | 7.4 |
| 31 | DA | 2106 | G | 7.4 |
| 36 | DG | 155 | MET | 7.4 |
| 7 | CG | 41 | ARG | 7.4 |
| 36 | DG | 142 | PRO | 7.3 |
| 1 | AA | 78 | G | 7.3 |
| 3 | AC | 159 | GLY | 7.3 |
| 2 | CB | 19 | HIS | 7.3 |
| 9 | CI | 63 | ILE | 7.3 |
| 38 | DI | 146 | ALA | 7.3 |
| 11 | CK | 13 | GLN | 7.2 |
| 21 | AU | 12 | LYS | 7.2 |
| 16 | CP | 48 | TRP | 7.2 |
| 36 | DG | 29 | TRP | 7.2 |
| 9 | CI | 3 | GLN | 7.2 |
| 36 | DG | 176 | LEU | 7.2 |
| 1 | AA | 1030(C) | G | 7.2 |
| 19 | CS | 69 | HIS | 7.2 |
| 2 | AB | 234 | PRO | 7.2 |
| 9 | AI | 128 | ARG | 7.2 |
| 19 | AS | 33 | THR | 7.1 |
| 2 | CB | 209 | ARG | 7.1 |
| 1 | AA | 1267 | C | 7.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 45 | BT | 2 | ASN | 7.1 |
| 11 | CK | 90 | GLY | 7.1 |
| 21 | AU | 17 | THR | 7.1 |
| 1 | CA | 961 | U | 7.1 |
| 47 | BV | 46 | VAL | 7.1 |
| 9 | CI | 7 | THR | 7.1 |
| 10 | AJ | 85 | LEU | 7.0 |
| 31 | BA | 2795 | G | 7.0 |
| 1 | AA | 1138 | G | 7.0 |
| 22 | D0 | 85 | ALA | 7.0 |
| 1 | CA | 1240 | U | 7.0 |
| 7 | AG | 17 | VAL | 7.0 |
| 9 | AI | 8 | GLY | 7.0 |
| 1 | AA | 80 | G | 6.9 |
| 1 | AA | 1182 | G | 6.9 |
| 50 | DY | 59 | GLY | 6.9 |
| 1 | AA | 1286 | A | 6.9 |
| 19 | CS | 49 | ILE | 6.9 |
| 22 | D0 | 4 | LYS | 6.9 |
| 7 | CG | 2 | ALA | 6.9 |
| 36 | DG | 35 | GLU | 6.9 |
| 12 | CL | 127 | GLU | 6.9 |
| 7 | CG | 81 | GLY | 6.9 |
| 32 | BB | 88 | C | 6.9 |
| 1 | CA | 89 | C | 6.9 |
| 1 | AA | 1235 | U | 6.9 |
| 31 | DA | 1531 | C | 6.9 |
| 13 | CM | 116 | THR | 6.9 |
| 10 | CJ | 34 | VAL | 6.8 |
| 14 | AN | 18 | VAL | 6.8 |
| 10 | AJ | 70 | ARG | 6.8 |
| 14 | CN | 8 | GLU | 6.8 |
| 13 | AM | 66 | LEU | 6.8 |
| 32 | DB | 58 | A | 6.8 |
| 4 | CD | 42 | GLN | 6.8 |
| 31 | BA | 1174 | A | 6.8 |
| 31 | DA | 2801(A) | A | 6.8 |
| 1 | CA | 1030(A) | G | 6.8 |
| 31 | DA | 2105 | C | 6.8 |
| 35 | DF | 1 | MET | 6.8 |
| 38 | DI | 123 | LEU | 6.8 |
| 19 | AS | 69 | HIS | 6.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | AM | 69 | GLU | 6.8 |
| 9 | CI | 89 | ASN | 6.8 |
| 38 | DI | 90 | GLY | 6.8 |
| 31 | BA | 2189 | U | 6.7 |
| 1 | AA | 985 | C | 6.7 |
| 1 | AA | 984 | C | 6.7 |
| 22 | D0 | 1 | MET | 6.7 |
| 21 | CU | 26 | LYS | 6.7 |
| 1 | AA | 999 | C | 6.7 |
| 36 | DG | 88 | ILE | 6.7 |
| 7 | AG | 18 | TYR | 6.7 |
| 7 | AG | 103 | TRP | 6.7 |
| 3 | CC | 207 | VAL | 6.7 |
| 10 | AJ | 10 | GLY | 6.6 |
| 50 | BY | 52 | SER | 6.6 |
| 36 | DG | 41 | GLN | 6.6 |
| 2 | CB | 11 | LEU | 6.6 |
| 31 | BA | 2103 | C | 6.6 |
| 36 | DG | 136 | ARG | 6.6 |
| 13 | CM | 5 | ALA | 6.6 |
| 13 | AM | 9 | ILE | 6.6 |
| 31 | BA | 275 | G | 6.6 |
| 1 | CA | 1032 | G | 6.6 |
| 9 | CI | 84 | ALA | 6.6 |
| 36 | DG | 135 | LEU | 6.6 |
| 1 | AA | 1128 | C | 6.6 |
| 9 | CI | 21 | PRO | 6.6 |
| 31 | BA | 1509 | C | 6.6 |
| 1 | CA | 1139 | G | 6.5 |
| 36 | DG | 107 | LEU | 6.5 |
| 3 | AC | 192 | THR | 6.5 |
| 1 | AA | 1026 | G | 6.5 |
| 21 | CU | 11 | GLY | 6.5 |
| 36 | DG | 134 | GLY | 6.5 |
| 38 | DI | 87 | LYS | 6.5 |
| 1 | AA | 1020 | U | 6.5 |
| 1 | CA | 1029 | C | 6.4 |
| 10 | AJ | 25 | GLU | 6.4 |
| 21 | AU | 8 | THR | 6.4 |
| 21 | AU | 7 | ARG | 6.4 |
| 10 | AJ | 17 | ASP | 6.4 |
| 1 | CA | 1030(B) | C | 6.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 31 | DA | 2793 | G | 6.4 |
| 7 | CG | 42 | ILE | 6.4 |
| 46 | BU | 118 | GLY | 6.4 |
| 1 | AA | 1024 | G | 6.4 |
| 36 | DG | 172 | LEU | 6.4 |
| 19 | CS | 52 | TYR | 6.4 |
| 3 | CC | 108 | ASN | 6.3 |
| 35 | DF | 25 | PRO | 6.3 |
| 31 | BA | 1531 | C | 6.3 |
| 10 | CJ | 59 | SER | 6.3 |
| 13 | CM | 107 | ALA | 6.3 |
| 14 | AN | 16 | PHE | 6.3 |
| 19 | AS | 74 | PHE | 6.3 |
| 3 | CC | 156 | ARG | 6.3 |
| 1 | AA | 1129 | C | 6.3 |
| 16 | AP | 11 | SER | 6.3 |
| 21 | AU | 3 | LYS | 6.3 |
| 31 | BA | 2105 | C | 6.3 |
| 9 | AI | 84 | ALA | 6.3 |
| 25 | B3 | 60 | GLU | 6.3 |
| 38 | DI | 69 | LYS | 6.3 |
| 1 | AA | 1131 | G | 6.2 |
| 1 | AA | 1222 | G | 6.2 |
| 1 | AA | 1127 | G | 6.2 |
| 31 | BA | 363(F) | A | 6.2 |
| 44 | DS | 56 | LEU | 6.2 |
| 10 | AJ | 4 | ILE | 6.2 |
| 19 | AS | 40 | ILE | 6.2 |
| 44 | DS | 31 | SER | 6.2 |
| 1 | CA | 1129 | C | 6.2 |
| 1 | AA | 1025 | U | 6.2 |
| 19 | CS | 5 | LEU | 6.2 |
| 9 | CI | 90 | PRO | 6.2 |
| 21 | AU | 18 | TYR | 6.2 |
| 38 | DI | 125 | GLU | 6.2 |
| 1 | CA | 1235 | U | 6.2 |
| 1 | CA | 1286 | A | 6.2 |
| 1 | AA | 933 | G | 6.2 |
| 1 | CA | 1260 | C | 6.2 |
| 38 | DI | 122 | GLU | 6.2 |
| 1 | AA | 1034 | G | 6.2 |
| 50 | DY | 50 | ARG | 6.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | CA | 1030 | C | 6.2 |
| 27 | D5 | 59 | GLU | 6.1 |
| 13 | AM | 96 | LEU | 6.1 |
| 21 | CU | 2 | GLY | 6.1 |
| 9 | CI | 5 | TYR | 6.1 |
| 34 | BE | 205 | ALA | 6.1 |
| 2 | CB | 233 | SER | 6.1 |
| 13 | AM | 63 | THR | 6.1 |
| 10 | AJ | 71 | LEU | 6.1 |
| 1 | CA | 1005 | A | 6.1 |
| 1 | CA | 1442(A) | G | 6.1 |
| 13 | AM | 62 | ASN | 6.1 |
| 38 | DI | 73 | GLU | 6.1 |
| 1 | CA | 1261 | A | 6.1 |
| 13 | AM | 59 | TYR | 6.1 |
| 3 | CC | 191 | THR | 6.1 |
| 23 | B1 | 96 | LYS | 6.1 |
| 37 | DH | 44 | VAL | 6.1 |
| 1 | CA | 1220 | G | 6.0 |
| 7 | CG | 113 | GLU | 6.0 |
| 31 | DA | 879 | G | 6.0 |
| 2 | CB | 10 | LEU | 6.0 |
| 47 | DV | 68 | LYS | 6.0 |
| 38 | DI | 66 | GLU | 6.0 |
| 13 | CM | 50 | GLU | 6.0 |
| 38 | DI | 76 | THR | 6.0 |
| 2 | AB | 213 | LEU | 6.0 |
| 1 | AA | 93 | G | 6.0 |
| 1 | CA | 1007 | C | 6.0 |
| 1 | AA | 1003 | G | 6.0 |
| 2 | CB | 236 | TYR | 6.0 |
| 38 | DI | 144 | VAL | 6.0 |
| 35 | DF | 24 | LEU | 6.0 |
| 13 | AM | 2 | ALA | 6.0 |
| 31 | DA | 1174 | A | 5.9 |
| 31 | DA | 2792 | G | 6.0 |
| 1 | AA | 1092 | A | 5.9 |
| 13 | CM | 51 | ALA | 5.9 |
| 19 | AS | 39 | THR | 5.9 |
| 9 | CI | 62 | TYR | 5.9 |
| 47 | DV | 45 | THR | 5.9 |
| 1 | CA | 1131 | G | 5.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | AB | 134 | GLU | 5.9 |
| 10 | CJ | 101 | VAL | 5.9 |
| 36 | BG | 50 | ALA | 5.9 |
| 2 | AB | 212 | GLN | 5.9 |
| 10 | CJ | 85 | LEU | 5.9 |
| 38 | DI | 70 | GLU | 5.8 |
| 12 | AL | 61 | THR | 5.8 |
| 10 | AJ | 27 | ALA | 5.8 |
| 1 | CA | 1338 | G | 5.8 |
| 7 | CG | 33 | ASP | 5.8 |
| 10 | CJ | 22 | LYS | 5.8 |
| 13 | AM | 29 | ARG | 5.8 |
| 10 | AJ | 36 | GLY | 5.8 |
| 36 | DG | 133 | LEU | 5.8 |
| 9 | AI | 82 | ALA | 5.8 |
| 10 | AJ | 16 | LEU | 5.8 |
| 1 | AA | 1029 | C | 5.8 |
| 31 | BA | 2801 | A | 5.8 |
| 31 | DA | 280 | C | 5.8 |
| 47 | BV | 68 | LYS | 5.8 |
| 1 | CA | 1030(C) | G | 5.8 |
| 42 | BQ | 91 | GLU | 5.8 |
| 1 | AA | 92 | C | 5.8 |
| 1 | AA | 1028 | C | 5.8 |
| 2 | AB | 11 | LEU | 5.8 |
| 2 | CB | 37 | ASN | 5.8 |
| 31 | DA | 1913 | A | 5.8 |
| 1 | CA | 1223 | C | 5.7 |
| 32 | DB | 59 | A | 5.7 |
| 31 | DA | 271(L) | U | 5.7 |
| 31 | DA | 883 | G | 5.7 |
| 38 | DI | 117 | GLU | 5.7 |
| 20 | AT | 104 | LEU | 5.7 |
| 21 | AU | 26 | LYS | 5.7 |
| 9 | AI | 87 | GLN | 5.7 |
| 2 | AB | 228 | GLY | 5.7 |
| 36 | DG | 33 | ARG | 5.7 |
| 37 | BH | 42 | ARG | 5.7 |
| 1 | AA | 1031 | G | 5.7 |
| 1 | AA | 1035 | A | 5.7 |
| 2 | AB | 133 | LYS | 5.7 |
| 4 | AD | 42 | GLN | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 38 | DI | 64 | GLU | 5.7 |
| 3 | CC | 65 | ALA | 5.7 |
| 31 | DA | 1509 | C | 5.7 |
| 1 | CA | 80 | G | 5.7 |
| 10 | CJ | 26 | ALA | 5.6 |
| 36 | BG | 73 | ALA | 5.6 |
| 31 | DA | 271(K) | U | 5.6 |
| 7 | AG | 112 | PRO | 5.6 |
| 9 | AI | 125 | TYR | 5.6 |
| 37 | DH | 30 | LYS | 5.6 |
| 3 | AC | 160 | ALA | 5.6 |
| 39 | BN | 1 | MET | 5.6 |
| 35 | BF | 11 | VAL | 5.6 |
| 28 | B6 | 34 | LEU | 5.6 |
| 1 | AA | 959 | A | 5.6 |
| 19 | AS | 59 | PRO | 5.6 |
| 3 | CC | 23 | TYR | 5.6 |
| 10 | CJ | 66 | ARG | 5.6 |
| 37 | DH | 158 | HIS | 5.6 |
| 10 | AJ | 40 | LEU | 5.5 |
| 31 | DA | 2796 | U | 5.5 |
| 38 | DI | 115 | ALA | 5.5 |
| 9 | AI | 47 | LEU | 5.5 |
| 3 | CC | 157 | ILE | 5.5 |
| 13 | AM | 26 | GLY | 5.5 |
| 38 | DI | 72 | LEU | 5.5 |
| 38 | DI | 58 | LEU | 5.5 |
| 1 | CA | 1278 | U | 5.5 |
| 10 | AJ | 72 | VAL | 5.5 |
| 36 | DG | 63 | ILE | 5.5 |
| 1 | AA | 345 | C | 5.5 |
| 50 | BY | 49 | VAL | 5.4 |
| 3 | CC | 194 | GLY | 5.4 |
| 18 | AR | 31 | LEU | 5.4 |
| 1 | CA | 1006 | C | 5.4 |
| 31 | DA | 2795 | G | 5.4 |
| 10 | AJ | 73 | ASP | 5.4 |
| 13 | AM | 116 | THR | 5.4 |
| 1 | AA | 1174 | G | 5.4 |
| 42 | DQ | 139 | GLU | 5.4 |
| 1 | AA | 344 | A | 5.4 |
| 1 | AA | 1223 | C | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 28 | B6 | 42 | TRP | 5.4 |
| 1 | CA | 1022 | G | 5.4 |
| 19 | AS | 49 | ILE | 5.4 |
| 1 | AA | 1236 | A | 5.4 |
| 19 | CS | 75 | ALA | 5.4 |
| 25 | B3 | 1 | MET | 5.4 |
| 9 | AI | 92 | TYR | 5.4 |
| 10 | AJ | 23 | ILE | 5.4 |
| 2 | CB | 237 | ALA | 5.4 |
| 32 | BB | 89 | G | 5.4 |
| 13 | AM | 98 | VAL | 5.3 |
| 20 | CT | 103 | GLY | 5.3 |
| 19 | CS | 81 | ARG | 5.3 |
| 1 | AA | 1000 | U | 5.3 |
| 34 | DE | 69 | LYS | 5.3 |
| 2 | CB | 208 | ILE | 5.3 |
| 9 | AI | 99 | LEU | 5.3 |
| 2 | CB | 234 | PRO | 5.3 |
| 7 | CG | 39 | ALA | 5.3 |
| 36 | DG | 65 | GLY | 5.3 |
| 8 | AH | 116 | LYS | 5.3 |
| 1 | AA | 1033 | G | 5.3 |
| 19 | CS | 82 | GLY | 5.3 |
| 10 | AJ | 91 | PRO | 5.3 |
| 36 | DG | 2 | PRO | 5.3 |
| 1 | CA | 970 | C | 5.3 |
| 1 | AA | 958 | A | 5.3 |
| 2 | CB | 80 | ILE | 5.3 |
| 11 | AK | 11 | LYS | 5.3 |
| 36 | DG | 8 | LYS | 5.3 |
| 32 | DB | 5 | C | 5.3 |
| 10 | AJ | 100 | THR | 5.3 |
| 1 | CA | 944 | G | 5.3 |
| 1 | CA | 1021 | G | 5.3 |
| 1 | AA | 1326 | C | 5.2 |
| 21 | AU | 11 | GLY | 5.2 |
| 31 | BA | 1914 | C | 5.2 |
| 2 | CB | 240 | GLN | 5.2 |
| 15 | AO | 88 | ARG | 5.2 |
| 1 | CA | 1148 | U | 5.2 |
| 31 | BA | 2799 | C | 5.2 |
| 19 | CS | 4 | SER | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | AC | 156 | ARG | 5.2 |
| 2 | CB | 210 | SER | 5.2 |
| 7 | CG | 32 | ARG | 5.2 |
| 13 | CM | 2 | ALA | 5.2 |
| 1 | CA | 1295 | G | 5.2 |
| 45 | DT | 2 | ASN | 5.2 |
| 36 | DG | 39 | ILE | 5.2 |
| 25 | D3 | 1 | MET | 5.2 |
| 19 | CS | 77 | THR | 5.2 |
| 19 | AS | 58 | VAL | 5.2 |
| 7 | CG | 99 | LEU | 5.2 |
| 9 | CI | 96 | LEU | 5.2 |
| 28 | D6 | 42 | TRP | 5.2 |
| 10 | CJ | 15 | THR | 5.2 |
| 38 | DI | 132 | PRO | 5.1 |
| 9 | CI | 87 | GLN | 5.1 |
| 1 | AA | 957 | U | 5.1 |
| 1 | AA | 1149 | C | 5.1 |
| 3 | CC | 183 | ASP | 5.1 |
| 10 | CJ | 98 | ILE | 5.1 |
| 33 | BD | 26 | LYS | 5.1 |
| 37 | DH | 97 | ARG | 5.1 |
| 1 | CA | 1042 | G | 5.1 |
| 9 | CI | 125 | TYR | 5.1 |
| 9 | AI | 90 | PRO | 5.1 |
| 47 | BV | 28 | GLU | 5.1 |
| 38 | DI | 124 | GLY | 5.1 |
| 37 | DH | 25 | LYS | 5.1 |
| 7 | CG | 123 | GLU | 5.1 |
| 1 | AA | 1148 | U | 5.1 |
| 19 | AS | 71 | LEU | 5.1 |
| 19 | CS | 48 | THR | 5.1 |
| 10 | CJ | 5 | ARG | 5.1 |
| 2 | CB | 115 | LEU | 5.1 |
| 19 | AS | 60 | VAL | 5.1 |
| 10 | CJ | 87 | THR | 5.1 |
| 3 | CC | 87 | LEU | 5.1 |
| 1 | AA | 1261 | A | 5.1 |
| 1 | AA | 1266 | G | 5.1 |
| 7 | CG | 40 | ALA | 5.1 |
| 7 | CG | 79 | ARG | 5.1 |
| 10 | CJ | 3 | LYS | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 10 | CJ | 8 | LEU | 5.0 |
| 10 | CJ | 23 | ILE | 5.0 |
| 9 | CI | 54 | ASP | 5.0 |
| 1 | AA | 1327 | C | 5.0 |
| 10 | AJ | 26 | ALA | 5.0 |
| 1 | CA | 1036 | G | 5.0 |
| 37 | DH | 32 | GLU | 5.0 |
| 2 | CB | 13 | ALA | 5.0 |
| 51 | BZ | 113 | ALA | 5.0 |
| 31 | DA | 1053 | C | 5.0 |
| 10 | CJ | 73 | ASP | 5.0 |
| 2 | CB | 41 | ILE | 5.0 |
| 13 | AM | 32 | GLU | 5.0 |
| 37 | BH | 44 | VAL | 5.0 |
| 10 | CJ | 74 | ILE | 5.0 |
| 1 | AA | 1257 | U | 5.0 |
| 7 | AG | 42 | ILE | 5.0 |
| 12 | AL | 127 | GLU | 5.0 |
| 13 | CM | 39 | ILE | 5.0 |
| 1 | CA | 1068 | G | 5.0 |
| 13 | AM | 87 | TYR | 5.0 |
| 31 | DA | 880 | G | 5.0 |
| 31 | DA | 2103 | C | 5.0 |
| 18 | CR | 19 | LYS | 5.0 |
| 1 | AA | 1032 | G | 5.0 |
| 19 | CS | 57 | HIS | 5.0 |
| 10 | AJ | 89 | ASP | 5.0 |
| 22 | D0 | 2 | ALA | 5.0 |
| 9 | CI | 93 | ARG | 5.0 |
| 1 | CA | 1092 | A | 5.0 |
| 10 | AJ | 8 | LEU | 4.9 |
| 31 | DA | 1532 | C | 4.9 |
| 3 | CC | 192 | THR | 4.9 |
| 42 | DQ | 91 | GLU | 4.9 |
| 7 | CG | 27 | ILE | 4.9 |
| 7 | AG | 6 | ARG | 4.9 |
| 1 | AA | 77 | G | 4.9 |
| 3 | CC | 58 | GLU | 4.9 |
| 13 | AM | 23 | TYR | 4.9 |
| 19 | CS | 10 | PHE | 4.9 |
| 1 | CA | 1031 | G | 4.9 |
| 36 | BG | 139 | LEU | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 9 | AI | 51 | ARG | 4.9 |
| 1 | AA | 1274 | G | 4.9 |
| 38 | DI | 126 | TYR | 4.9 |
| 5 | CE | 31 | LEU | 4.9 |
| 9 | CI | 111 | ARG | 4.9 |
| 14 | AN | 61 | TRP | 4.9 |
| 36 | DG | 34 | LEU | 4.9 |
| 1 | AA | 1030(D) | A | 4.9 |
| 36 | DG | 159 | VAL | 4.9 |
| 14 | AN | 19 | ARG | 4.9 |
| 1 | AA | 1224 | G | 4.9 |
| 2 | AB | 232 | PRO | 4.9 |
| 10 | CJ | 33 | GLN | 4.9 |
| 14 | AN | 17 | LYS | 4.9 |
| 22 | B0 | 7 | LEU | 4.9 |
| 3 | AC | 65 | ALA | 4.9 |
| 10 | AJ | 69 | ASN | 4.9 |
| 1 | CA | 90 | U | 4.9 |
| 1 | CA | 1156 | G | 4.8 |
| 13 | AM | 91 | ARG | 4.8 |
| 31 | BA | 1913 | A | 4.8 |
| 51 | DZ | 164 | ALA | 4.8 |
| 13 | AM | 36 | LYS | 4.8 |
| 13 | AM | 58 | GLU | 4.8 |
| 1 | CA | 1224 | G | 4.8 |
| 9 | AI | 88 | TYR | 4.8 |
| 9 | CI | 123 | PRO | 4.8 |
| 31 | BA | 2102 | U | 4.8 |
| 31 | DA | 275 | G | 4.8 |
| 1 | AA | 949 | A | 4.8 |
| 50 | DY | 86 | ARG | 4.8 |
| 7 | AG | 26 | PHE | 4.8 |
| 7 | CG | 34 | GLY | 4.8 |
| 18 | CR | 46 | GLU | 4.8 |
| 38 | DI | 57 | ARG | 4.8 |
| 1 | AA | 1137 | C | 4.8 |
| 19 | AS | 29 | ARG | 4.8 |
| 32 | BB | 87 | G | 4.8 |
| 1 | AA | 1023 | G | 4.8 |
| 13 | CM | 63 | THR | 4.8 |
| 12 | CL | 128 | ALA | 4.8 |
| 25 | D3 | 2 | PRO | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 9 | CI | 65 | VAL | 4.8 |
| 1 | CA | 1183 | A | 4.8 |
| 9 | AI | 15 | ALA | 4.8 |
| 31 | DA | 279 | C | 4.8 |
| 41 | BP | 150 | ALA | 4.8 |
| 17 | AQ | 27 | PHE | 4.7 |
| 1 | CA | 1030(D) | A | 4.7 |
| 5 | CE | 33 | VAL | 4.7 |
| 9 | CI | 53 | VAL | 4.7 |
| 47 | DV | 46 | VAL | 4.7 |
| 31 | BA | 1053 | C | 4.7 |
| 1 | AA | 1312 | G | 4.7 |
| 9 | AI | 77 | ILE | 4.7 |
| 10 | AJ | 98 | ILE | 4.7 |
| 19 | CS | 53 | ASN | 4.7 |
| 36 | BG | 2 | PRO | 4.7 |
| 1 | CA | 1035 | A | 4.7 |
| 35 | DF | 13 | SER | 4.7 |
| 10 | CJ | 45 | ARG | 4.7 |
| 36 | DG | 173 | LEU | 4.7 |
| 22 | B0 | 1 | MET | 4.7 |
| 36 | BG | 182 | LYS | 4.7 |
| 31 | DA | 884 | C | 4.7 |
| 31 | DA | 2804 | C | 4.7 |
| 32 | DB | 3 | C | 4.7 |
| 1 | AA | 947 | G | 4.7 |
| 10 | AJ | 24 | VAL | 4.7 |
| 22 | D0 | 9 | SER | 4.7 |
| 36 | DG | 138 | GLN | 4.7 |
| 1 | AA | 70 | G | 4.7 |
| 36 | DG | 131 | TYR | 4.7 |
| 1 | AA | 1206 | G | 4.7 |
| 3 | CC | 206 | GLU | 4.7 |
| 31 | DA | 1533 | G | 4.7 |
| 31 | DA | 1048 | A | 4.7 |
| 36 | DG | 100 | TRP | 4.7 |
| 41 | DP | 116 | GLY | 4.7 |
| 9 | AI | 46 | ALA | 4.6 |
| 7 | CG | 6 | ARG | 4.6 |
| 35 | DF | 10 | PRO | 4.6 |
| 1 | CA | 1128 | C | 4.6 |
| 1 | AA | 983 | A | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | CA | 1182 | G | 4.6 |
| 7 | CG | 119 | ARG | 4.6 |
| 11 | CK | 42 | TRP | 4.6 |
| 3 | AC | 207 | VAL | 4.6 |
| 3 | CC | 76 | VAL | 4.6 |
| 7 | CG | 16 | LEU | 4.6 |
| 36 | DG | 171 | ALA | 4.6 |
| 36 | DG | 132 | ASN | 4.6 |
| 9 | AI | 9 | ARG | 4.6 |
| 35 | BF | 25 | PRO | 4.6 |
| 13 | AM | 60 | VAL | 4.6 |
| 45 | DT | 36 | GLU | 4.6 |
| 6 | CF | 101 | ALA | 4.6 |
| 13 | CM | 26 | GLY | 4.6 |
| 37 | DH | 59 | ARG | 4.6 |
| 1 | CA | 540 | G | 4.6 |
| 38 | DI | 101 | LEU | 4.6 |
| 31 | BA | 2106 | G | 4.6 |
| 31 | DA | 1114 | G | 4.6 |
| 37 | DH | 34 | GLU | 4.6 |
| 14 | AN | 15 | LYS | 4.6 |
| 13 | CM | 64 | TRP | 4.6 |
| 3 | CC | 39 | ILE | 4.5 |
| 1 | AA | 1243 | C | 4.5 |
| 19 | AS | 25 | LYS | 4.5 |
| 47 | BV | 47 | VAL | 4.5 |
| 31 | DA | 878 | A | 4.5 |
| 3 | AC | 107 | GLN | 4.5 |
| 21 | AU | 6 | ARG | 4.5 |
| 13 | AM | 102 | ARG | 4.5 |
| 20 | AT | 69 | GLY | 4.5 |
| 3 | AC | 196 | LEU | 4.5 |
| 12 | CL | 28 | LYS | 4.5 |
| 31 | DA | 1106 | A | 4.5 |
| 38 | DI | 112 | LYS | 4.5 |
| 7 | CG | 154 | TYR | 4.5 |
| 50 | BY | 28 | LYS | 4.5 |
| 1 | AA | 1353 | G | 4.5 |
| 1 | CA | 1004 | A | 4.5 |
| 7 | AG | 31 | MET | 4.5 |
| 51 | BZ | 112 | ARG | 4.5 |
| 1 | AA | 1130 | A | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 1037 | C | 4.5 |
| 7 | CG | 104 | LEU | 4.5 |
| 3 | CC | 195 | VAL | 4.5 |
| 20 | CT | 9 | ASN | 4.5 |
| 37 | DH | 111 | HIS | 4.5 |
| 1 | AA | 979 | C | 4.5 |
| 1 | AA | 1006 | C | 4.5 |
| 10 | CJ | 86 | MET | 4.4 |
| 7 | AG | 30 | ILE | 4.4 |
| 9 | AI | 100 | GLY | 4.4 |
| 38 | DI | 84 | GLY | 4.4 |
| 1 | CA | 1138 | G | 4.4 |
| 1 | CA | 1142 | G | 4.4 |
| 31 | DA | 2833 | G | 4.4 |
| 21 | CU | 7 | ARG | 4.4 |
| 2 | AB | 230 | VAL | 4.4 |
| 2 | CB | 81 | VAL | 4.4 |
| 10 | CJ | 72 | VAL | 4.4 |
| 1 | AA | 1046 | A | 4.4 |
| 7 | CG | 31 | MET | 4.4 |
| 31 | BA | 878 | A | 4.4 |
| 7 | CG | 114 | ARG | 4.4 |
| 1 | CA | 1041 | A | 4.4 |
| 4 | AD | 3 | ARG | 4.4 |
| 1 | AA | 1018 | C | 4.4 |
| 1 | CA | 1389 | C | 4.4 |
| 10 | AJ | 99 | LYS | 4.4 |
| 14 | AN | 8 | GLU | 4.4 |
| 19 | AS | 27 | GLU | 4.4 |
| 13 | CM | 4 | ILE | 4.4 |
| 21 | AU | 22 | ARG | 4.4 |
| 5 | CE | 11 | ILE | 4.4 |
| 1 | AA | 950 | U | 4.4 |
| 24 | D2 | 43 | GLN | 4.4 |
| 46 | DU | 77 | SER | 4.4 |
| 1 | AA | 1093 | A | 4.4 |
| 20 | CT | 104 | LEU | 4.4 |
| 21 | CU | 25 | LYS | 4.4 |
| 1 | AA | 71 | C | 4.4 |
| 9 | CI | 20 | ARG | 4.4 |
| 17 | CQ | 101 | ARG | 4.4 |
| 2 | AB | 231 | GLU | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | AM | 72 | ALA | 4.4 |
| 21 | CU | 10 | ARG | 4.3 |
| 2 | CB | 133 | LYS | 4.3 |
| 10 | CJ | 13 | HIS | 4.3 |
| 42 | DQ | 90 | VAL | 4.3 |
| 20 | AT | 106 | ALA | 4.3 |
| 2 | AB | 19 | HIS | 4.3 |
| 44 | DS | 34 | HIS | 4.3 |
| 1 | CA | 1214 | C | 4.3 |
| 18 | CR | 34 | TYR | 4.3 |
| 35 | BF | 13 | SER | 4.3 |
| 9 | CI | 97 | LYS | 4.3 |
| 44 | DS | 55 | ALA | 4.3 |
| 1 | AA | 1231 | G | 4.3 |
| 27 | D5 | 60 | VAL | 4.3 |
| 50 | DY | 28 | LYS | 4.3 |
| 7 | CG | 103 | TRP | 4.3 |
| 2 | CB | 214 | ILE | 4.3 |
| 36 | DG | 160 | VAL | 4.3 |
| 21 | CU | 21 | TYR | 4.3 |
| 36 | BG | 86 | MET | 4.3 |
| 41 | DP | 118 | GLY | 4.3 |
| 10 | AJ | 41 | PRO | 4.3 |
| 19 | AS | 36 | ARG | 4.3 |
| 34 | BE | 204 | ALA | 4.3 |
| 1 | AA | 1234 | C | 4.3 |
| 31 | BA | 352 | G | 4.3 |
| 9 | CI | 88 | TYR | 4.3 |
| 31 | BA | 1532 | C | 4.3 |
| 31 | DA | 1909 | C | 4.3 |
| 7 | AG | 32 | ARG | 4.3 |
| 3 | CC | 200 | ALA | 4.3 |
| 1 | AA | 1005 | A | 4.3 |
| 35 | BF | 14 | PRO | 4.3 |
| 7 | AG | 99 | LEU | 4.3 |
| 21 | AU | 14 | TRP | 4.3 |
| 1 | AA | 1141 | C | 4.3 |
| 31 | BA | 2188 | C | 4.3 |
| 7 | CG | 26 | PHE | 4.3 |
| 31 | DA | 1051 | G | 4.3 |
| 7 | CG | 37 | ASN | 4.3 |
| 1 | AA | 1125 | U | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | AA | 1146 | A | 4.3 |
| 7 | CG | 130 | GLY | 4.3 |
| 31 | BA | 1052 | C | 4.3 |
| 17 | AQ | 78 | GLU | 4.3 |
| 1 | AA | 1175 | G | 4.3 |
| 1 | AA | 1159 | U | 4.2 |
| 10 | AJ | 77 | PRO | 4.2 |
| 10 | CJ | 71 | LEU | 4.2 |
| 1 | CA | 929 | G | 4.2 |
| 1 | CA | 953 | G | 4.2 |
| 2 | AB | 28 | PHE | 4.2 |
| 3 | AC | 102 | ASN | 4.2 |
| 9 | AI | 86 | VAL | 4.2 |
| 9 | AI | 101 | PHE | 4.2 |
| 10 | AJ | 20 | ALA | 4.2 |
| 13 | CM | 62 | ASN | 4.2 |
| 1 | CA | 1130 | A | 4.2 |
| 7 | AG | 76 | ARG | 4.2 |
| 44 | DS | 54 | LEU | 4.2 |
| 1 | CA | 428 | G | 4.2 |
| 1 | CA | 1086 | U | 4.2 |
| 31 | DA | 271(M) | G | 4.2 |
| 2 | CB | 163 | PHE | 4.2 |
| 1 | CA | 1243 | C | 4.2 |
| 24 | B2 | 35 | LEU | 4.2 |
| 47 | BV | 45 | THR | 4.2 |
| 1 | CA | 1293 | G | 4.2 |
| 31 | BA | 879 | G | 4.2 |
| 10 | CJ | 14 | LYS | 4.2 |
| 31 | DA | 2402 | C | 4.2 |
| 31 | BA | 892 | G | 4.2 |
| 32 | DB | 4 | C | 4.2 |
| 13 | AM | 33 | ALA | 4.2 |
| 10 | CJ | 89 | ASP | 4.2 |
| 36 | DG | 7 | LEU | 4.2 |
| 3 | AC | 64 | VAL | 4.2 |
| 10 | AJ | 74 | ILE | 4.2 |
| 46 | DU | 88 | ILE | 4.2 |
| 31 | DA | 1113 | U | 4.2 |
| 36 | DG | 168 | GLU | 4.2 |
| 10 | CJ | 92 | THR | 4.2 |
| 31 | DA | 2101 | G | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | BB | 90 | A | 4.2 |
| 7 | CG | 36 | LYS | 4.2 |
| 14 | CN | 35 | ARG | 4.2 |
| 36 | DG | 165 | THR | 4.2 |
| 1 | AA | 1447 | A | 4.2 |
| 1 | AA | 1313 | U | 4.2 |
| 12 | AL | 71 | PRO | 4.2 |
| 13 | AM | 65 | LYS | 4.2 |
| 2 | CB | 17 | PHE | 4.2 |
| 36 | DG | 80 | PHE | 4.2 |
| 32 | DB | 27 | C | 4.1 |
| 7 | AG | 134 | ALA | 4.1 |
| 13 | CM | 60 | VAL | 4.1 |
| 2 | CB | 128 | GLU | 4.1 |
| 37 | BH | 158 | HIS | 4.1 |
| 1 | CA | 1049 | U | 4.1 |
| 1 | CA | 1257 | U | 4.1 |
| 1 | AA | 1147 | C | 4.1 |
| 2 | AB | 137 | ARG | 4.1 |
| 2 | CB | 36 | ARG | 4.1 |
| 1 | CA | 1392 | G | 4.1 |
| 7 | AG | 7 | ALA | 4.1 |
| 19 | AS | 37 | ARG | 4.1 |
| 10 | CJ | 6 | ILE | 4.1 |
| 38 | DI | 108 | THR | 4.1 |
| 36 | BG | 146 | TYR | 4.1 |
| 36 | DG | 77 | ILE | 4.1 |
| 1 | CA | 984 | C | 4.1 |
| 7 | CG | 3 | ARG | 4.1 |
| 31 | DA | 2102 | U | 4.1 |
| 41 | DP | 121 | LYS | 4.1 |
| 21 | CU | 3 | LYS | 4.1 |
| 1 | CA | 1002 | G | 4.1 |
| 2 | AB | 148 | TYR | 4.1 |
| 7 | AG | 33 | ASP | 4.1 |
| 36 | DG | 32 | PRO | 4.1 |
| 7 | CG | 116 | ALA | 4.1 |
| 50 | DY | 48 | ALA | 4.1 |
| 1 | CA | 427 | U | 4.1 |
| 37 | DH | 60 | ARG | 4.1 |
| 38 | BI | 61 | ARG | 4.1 |
| 3 | CC | 60 | ALA | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CB | 18 | GLY | 4.1 |
| 42 | DQ | 23 | GLY | 4.1 |
| 10 | AJ | 19 | SER | 4.1 |
| 13 | AM | 67 | GLU | 4.1 |
| 14 | AN | 2 | ALA | 4.1 |
| 51 | DZ | 97 | GLU | 4.1 |
| 14 | AN | 7 | ILE | 4.1 |
| 16 | AP | 35 | LYS | 4.0 |
| 38 | DI | 131 | LYS | 4.0 |
| 2 | CB | 212 | GLN | 4.0 |
| 3 | AC | 2 | GLY | 4.0 |
| 13 | CM | 56 | LEU | 4.0 |
| 1 | AA | 1140 | C | 4.0 |
| 1 | CA | 1294 | G | 4.0 |
| 3 | CC | 44 | GLU | 4.0 |
| 13 | AM | 56 | LEU | 4.0 |
| 1 | AA | 1119 | C | 4.0 |
| 32 | DB | 117 | G | 4.0 |
| 19 | AS | 30 | LEU | 4.0 |
| 37 | DH | 58 | GLU | 4.0 |
| 7 | CG | 48 | LYS | 4.0 |
| 1 | CA | 1287 | A | 4.0 |
| 1 | AA | 993 | G | 4.0 |
| 31 | DA | 281 | G | 4.0 |
| 31 | DA | 882 | G | 4.0 |
| 9 | AI | 12 | GLU | 4.0 |
| 13 | AM | 85 | GLY | 4.0 |
| 19 | AS | 4 | SER | 4.0 |
| 36 | DG | 38 | VAL | 4.0 |
| 2 | CB | 21 | ARG | 4.0 |
| 9 | AI | 64 | THR | 4.0 |
| 34 | BE | 17 | ASP | 4.0 |
| 38 | DI | 85 | GLU | 4.0 |
| 2 | AB | 36 | ARG | 4.0 |
| 13 | CM | 15 | VAL | 4.0 |
| 3 | CC | 104 | GLN | 4.0 |
| 1 | AA | 1370 | G | 4.0 |
| 9 | CI | 70 | LYS | 4.0 |
| 19 | AS | 28 | LYS | 4.0 |
| 19 | AS | 51 | VAL | 4.0 |
| 1 | CA | 1096 | C | 4.0 |
| 32 | DB | 88 | C | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | AM | 22 | ILE | 4.0 |
| 4 | AD | 201 | GLN | 4.0 |
| 7 | AG | 37 | ASN | 4.0 |
| 31 | DA | 2310 | A | 4.0 |
| 1 | AA | 1233 | G | 4.0 |
| 1 | CA | 1186 | G | 4.0 |
| 1 | AA | 418 | C | 4.0 |
| 3 | CC | 91 | LEU | 4.0 |
| 1 | CA | 1172 | C | 4.0 |
| 1 | CA | 1395 | C | 4.0 |
| 6 | CF | 7 | ASN | 4.0 |
| 7 | AG | 91 | VAL | 4.0 |
| 13 | AM | 84 | ILE | 4.0 |
| 13 | CM | 43 | THR | 4.0 |
| 31 | BA | 1508 | A | 4.0 |
| 38 | DI | 129 | THR | 4.0 |
| 16 | CP | 39 | TYR | 3.9 |
| 2 | AB | 14 | GLY | 3.9 |
| 1 | AA | 998 | G | 3.9 |
| 19 | AS | 22 | LEU | 3.9 |
| 1 | CA | 1262 | C | 3.9 |
| 21 | AU | 23 | PRO | 3.9 |
| 16 | AP | 18 | ARG | 3.9 |
| 19 | CS | 24 | ALA | 3.9 |
| 1 | AA | 1132 | C | 3.9 |
| 1 | CA | 79 | G | 3.9 |
| 14 | AN | 33 | VAL | 3.9 |
| 3 | CC | 205 | GLY | 3.9 |
| 42 | BQ | 23 | GLY | 3.9 |
| 2 | AB | 214 | ILE | 3.9 |
| 3 | AC | 3 | ASN | 3.9 |
| 6 | CF | 67 | MET | 3.9 |
| 16 | AP | 19 | ILE | 3.9 |
| 13 | CM | 69 | GLU | 3.9 |
| 16 | CP | 40 | ASP | 3.9 |
| 19 | AS | 21 | GLU | 3.9 |
| 36 | DG | 163 | ALA | 3.9 |
| 7 | AG | 71 | PRO | 3.9 |
| 1 | CA | 1312 | G | 3.9 |
| 42 | DQ | 21 | THR | 3.9 |
| 37 | DH | 159 | GLU | 3.9 |
| 1 | CA | 1390 | U | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 3 | CC | 102 | ASN | 3.9 |
| 18 | CR | 88 | LYS | 3.9 |
| 14 | AN | 13 | THR | 3.9 |
| 36 | DG | 137 | GLU | 3.9 |
| 45 | DT | 92 | GLY | 3.9 |
| 1 | CA | 1160 | G | 3.9 |
| 3 | CC | 77 | ILE | 3.9 |
| 2 | CB | 207 | ALA | 3.9 |
| 3 | CC | 189 | ALA | 3.9 |
| 2 | CB | 230 | VAL | 3.9 |
| 9 | AI | 16 | ARG | 3.9 |
| 36 | BG | 72 | ARG | 3.9 |
| 10 | AJ | 62 | HIS | 3.9 |
| 22 | B0 | 5 | LYS | 3.9 |
| 32 | DB | 118 | G | 3.9 |
| 1 | AA | 1212 | U | 3.8 |
| 37 | DH | 94 | TYR | 3.8 |
| 2 | CB | 216 | SER | 3.8 |
| 13 | CM | 102 | ARG | 3.8 |
| 31 | BA | 2801(A) | A | 3.8 |
| 31 | DA | 899 | A | 3.8 |
| 19 | AS | 26 | GLY | 3.8 |
| 1 | AA | 223 | U | 3.8 |
| 1 | AA | 1030(A) | G | 3.8 |
| 1 | AA | 1124 | G | 3.8 |
| 1 | AA | 1220 | G | 3.8 |
| 38 | DI | 60 | GLU | 3.8 |
| 1 | AA | 994 | A | 3.8 |
| 1 | AA | 955 | U | 3.8 |
| 39 | BN | 129 | PRO | 3.8 |
| 1 | AA | 1241 | G | 3.8 |
| 1 | CA | 1174 | G | 3.8 |
| 5 | CE | 43 | LEU | 3.8 |
| 14 | AN | 59 | ALA | 3.8 |
| 47 | BV | 55 | ALA | 3.8 |
| 13 | CM | 16 | ASP | 3.8 |
| 13 | CM | 55 | ARG | 3.8 |
| 36 | DG | 16 | ARG | 3.8 |
| 37 | DH | 36 | PRO | 3.8 |
| 1 | AA | 951 | G | 3.8 |
| 1 | CA | 1207 | G | 3.8 |
| 2 | AB | 217 | ARG | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 16 | AP | 14 | ASN | 3.8 |
| 11 | CK | 109 | VAL | 3.8 |
| 36 | BG | 43 | LEU | 3.8 |
| 1 | AA | 1041 | A | 3.8 |
| 7 | AG | 2 | ALA | 3.8 |
| 9 | CI | 61 | ALA | 3.8 |
| 19 | CS | 78 | ARG | 3.8 |
| 31 | DA | 2794 | C | 3.8 |
| 13 | CM | 106 | ASN | 3.8 |
| 46 | DU | 75 | ASN | 3.8 |
| 2 | AB | 101 | MET | 3.8 |
| 3 | AC | 87 | LEU | 3.8 |
| 36 | DG | 158 | ALA | 3.8 |
| 1 | AA | 195 | A | 3.8 |
| 10 | CJ | 96 | ILE | 3.8 |
| 1 | CA | 841 | U | 3.8 |
| 2 | AB | 31 | TYR | 3.8 |
| 19 | CS | 55 | LYS | 3.8 |
| 38 | DI | 145 | VAL | 3.8 |
| 2 | CB | 99 | GLY | 3.8 |
| 29 | D7 | 48 | LYS | 3.8 |
| 38 | BI | 73 | GLU | 3.8 |
| 1 | CA | 346 | G | 3.8 |
| 31 | DA | 1044 | G | 3.8 |
| 17 | AQ | 73 | VAL | 3.8 |
| 11 | AK | 42 | TRP | 3.8 |
| 35 | DF | 133 | ASN | 3.8 |
| 31 | DA | 2799 | C | 3.8 |
| 10 | CJ | 65 | LEU | 3.8 |
| 13 | CM | 9 | ILE | 3.8 |
| 1 | AA | 427 | U | 3.8 |
| 10 | AJ | 101 | VAL | 3.8 |
| 7 | AG | 52 | GLU | 3.8 |
| 7 | AG | 113 | GLU | 3.8 |
| 21 | CU | 14 | TRP | 3.8 |
| 31 | BA | 882 | G | 3.8 |
| 46 | DU | 80 | ILE | 3.8 |
| 19 | CS | 67 | VAL | 3.8 |
| 19 | CS | 8 | GLY | 3.7 |
| 21 | AU | 19 | GLY | 3.7 |
| 46 | DU | 91 | ASP | 3.7 |
| 2 | AB | 10 | LEU | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 630 | G | 3.7 |
| 1 | AA | 1380 | U | 3.7 |
| 36 | BG | 49 | ASP | 3.7 |
| 38 | DI | 96 | ASP | 3.7 |
| 19 | CS | 9 | VAL | 3.7 |
| 1 | CA | 983 | A | 3.7 |
| 1 | AA | 932 | C | 3.7 |
| 1 | AA | 980 | C | 3.7 |
| 22 | D0 | 5 | LYS | 3.7 |
| 9 | CI | 2 | GLU | 3.7 |
| 44 | DS | 52 | SER | 3.7 |
| 1 | CA | 1050 | G | 3.7 |
| 1 | CA | 1097 | C | 3.7 |
| 1 | CA | 1266 | G | 3.7 |
| 1 | CA | 1136 | U | 3.7 |
| 31 | DA | 1108 | U | 3.7 |
| 9 | CI | 115 | GLY | 3.7 |
| 3 | CC | 43 | LEU | 3.7 |
| 13 | AM | 47 | ASP | 3.7 |
| 1 | CA | 1447 | A | 3.7 |
| 19 | AS | 19 | VAL | 3.7 |
| 31 | DA | 1112 | G | 3.7 |
| 11 | AK | 12 | ARG | 3.7 |
| 36 | DG | 25 | TYR | 3.7 |
| 35 | BF | 23 | ASP | 3.7 |
| 1 | AA | 956 | U | 3.7 |
| 31 | DA | 229 | A | 3.7 |
| 32 | DB | 90 | A | 3.7 |
| 16 | CP | 73 | LEU | 3.7 |
| 29 | D7 | 49 | ARG | 3.7 |
| 36 | BG | 152 | LEU | 3.7 |
| 1 | AA | 1271 | G | 3.7 |
| 1 | AA | 1272 | G | 3.7 |
| 2 | AB | 42 | ILE | 3.7 |
| 9 | AI | 110 | GLU | 3.7 |
| 9 | CI | 60 | ASP | 3.7 |
| 49 | BX | 91 | ALA | 3.7 |
| 50 | BY | 48 | ALA | 3.7 |
| 42 | BQ | 139 | GLU | 3.7 |
| 18 | AR | 40 | LEU | 3.7 |
| 9 | AI | 41 | VAL | 3.7 |
| 4 | CD | 152 | SER | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 9 | CI | 64 | THR | 3.7 |
| 31 | DA | 2660 | A | 3.7 |
| 50 | BY | 102 | CYS | 3.7 |
| 39 | DN | 1 | MET | 3.7 |
| 36 | DG | 169 | ALA | 3.7 |
| 31 | DA | 11 | G | 3.7 |
| 18 | CR | 48 | GLY | 3.7 |
| 1 | CA | 1248 | A | 3.7 |
| 10 | CJ | 97 | GLU | 3.7 |
| 19 | CS | 30 | LEU | 3.6 |
| 3 | CC | 53 | ALA | 3.6 |
| 1 | AA | 1287 | A | 3.6 |
| 1 | CA | 1326 | C | 3.6 |
| 7 | AG | 44 | TYR | 3.6 |
| 51 | DZ | 143 | GLY | 3.6 |
| 7 | AG | 12 | LEU | 3.6 |
| 19 | AS | 77 | THR | 3.6 |
| 1 | AA | 220 | G | 3.6 |
| 1 | CA | 1370 | G | 3.6 |
| 20 | AT | 105 | SER | 3.6 |
| 7 | AG | 80 | VAL | 3.6 |
| 3 | CC | 72 | LYS | 3.6 |
| 17 | CQ | 14 | LYS | 3.6 |
| 33 | DD | 26 | LYS | 3.6 |
| 1 | AA | 1044 | A | 3.6 |
| 27 | B5 | 58 | LEU | 3.6 |
| 3 | CC | 59 | ARG | 3.6 |
| 7 | CG | 117 | ALA | 3.6 |
| 9 | AI | 83 | ARG | 3.6 |
| 31 | DA | 362 | U | 3.6 |
| 1 | AA | 1120 | G | 3.6 |
| 36 | DG | 72 | ARG | 3.6 |
| 50 | DY | 92 | ASN | 3.6 |
| 1 | CA | 1164 | G | 3.6 |
| 1 | CA | 1173 | G | 3.6 |
| 2 | CB | 39 | ILE | 3.6 |
| 1 | CA | 1492 | A | 3.6 |
| 13 | AM | 10 | PRO | 3.6 |
| 18 | CR | 85 | LEU | 3.6 |
| 37 | DH | 42 | ARG | 3.6 |
| 44 | BS | 54 | LEU | 3.6 |
| 19 | AS | 55 | LYS | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | CC | 100 | ALA | 3.6 |
| 37 | DH | 24 | VAL | 3.6 |
| 1 | AA | 369 | C | 3.6 |
| 9 | AI | 19 | LEU | 3.6 |
| 16 | CP | 49 | LEU | 3.6 |
| 31 | DA | 1910 | G | 3.6 |
| 45 | DT | 40 | THR | 3.6 |
| 1 | CA | 1393 | U | 3.6 |
| 10 | AJ | 64 | GLU | 3.6 |
| 46 | DU | 89 | GLU | 3.6 |
| 9 | AI | 111 | ARG | 3.6 |
| 19 | AS | 78 | ARG | 3.6 |
| 9 | CI | 19 | LEU | 3.6 |
| 36 | DG | 27 | ASN | 3.6 |
| 19 | AS | 12 | ASP | 3.6 |
| 1 | AA | 961 | U | 3.6 |
| 1 | CA | 1353 | G | 3.6 |
| 2 | CB | 16 | HIS | 3.6 |
| 10 | CJ | 4 | ILE | 3.6 |
| 13 | AM | 97 | PRO | 3.6 |
| 22 | D0 | 6 | GLY | 3.6 |
| 3 | AC | 82 | GLU | 3.6 |
| 12 | AL | 113 | ARG | 3.6 |
| 1 | AA | 1116 | C | 3.6 |
| 27 | B5 | 2 | ALA | 3.6 |
| 18 | CR | 87 | ARG | 3.6 |
| 7 | AG | 47 | CYS | 3.6 |
| 41 | DP | 85 | LEU | 3.6 |
| 1 | CA | 952 | U | 3.6 |
| 1 | CA | 994 | A | 3.6 |
| 19 | CS | 40 | ILE | 3.6 |
| 31 | DA | 1466 | G | 3.6 |
| 37 | DH | 19 | VAL | 3.6 |
| 9 | CI | 27 | THR | 3.6 |
| 10 | CJ | 30 | SER | 3.6 |
| 19 | AS | 15 | LEU | 3.6 |
| 22 | B0 | 9 | SER | 3.6 |
| 2 | CB | 33 | TYR | 3.6 |
| 3 | AC | 127 | ARG | 3.5 |
| 16 | AP | 81 | ARG | 3.5 |
| 1 | AA | 1342 | C | 3.5 |
| 1 | CA | 1236 | A | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | AB | 39 | ILE | 3.5 |
| 37 | DH | 52 | VAL | 3.5 |
| 1 | AA | 1021 | G | 3.5 |
| 3 | CC | 64 | VAL | 3.5 |
| 3 | CC | 82 | GLU | 3.5 |
| 31 | DA | 2189 | U | 3.5 |
| 1 | CA | 1202 | G | 3.5 |
| 7 | CG | 17 | VAL | 3.5 |
| 36 | DG | 19 | LEU | 3.5 |
| 13 | CM | 12 | ASN | 3.5 |
| 38 | BI | 83 | ALA | 3.5 |
| 9 | CI | 91 | ASP | 3.5 |
| 32 | DB | 28 | C | 3.5 |
| 10 | AJ | 95 | GLU | 3.5 |
| 1 | CA | 1020 | U | 3.5 |
| 7 | AG | 81 | GLY | 3.5 |
| 31 | DA | 2805 | G | 3.5 |
| 36 | DG | 156 | ASP | 3.5 |
| 19 | CS | 36 | ARG | 3.5 |
| 36 | DG | 162 | THR | 3.5 |
| 32 | DB | 57 | A | 3.5 |
| 9 | AI | 62 | TYR | 3.5 |
| 45 | BT | 36 | GLU | 3.5 |
| 1 | AA | 1265 | G | 3.5 |
| 2 | AB | 190 | THR | 3.5 |
| 10 | AJ | 6 | ILE | 3.5 |
| 13 | CM | 49 | THR | 3.5 |
| 42 | BQ | 21 | THR | 3.5 |
| 10 | AJ | 21 | GLN | 3.5 |
| 29 | B7 | 47 | ARG | 3.5 |
| 14 | CN | 25 | VAL | 3.5 |
| 13 | AM | 103 | THR | 3.5 |
| 4 | CD | 7 | PRO | 3.5 |
| 13 | CM | 10 | PRO | 3.5 |
| 31 | DA | 1034 | G | 3.5 |
| 1 | AA | 946 | A | 3.5 |
| 15 | AO | 81 | LEU | 3.5 |
| 36 | BG | 34 | LEU | 3.5 |
| 20 | AT | 103 | GLY | 3.5 |
| 1 | AA | 953 | G | 3.5 |
| 1 | AA | 1173 | G | 3.5 |
| 31 | BA | 1048 | A | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 10 | AJ | 33 | GLN | 3.5 |
| 37 | BH | 156 | ALA | 3.5 |
| 4 | CD | 29 | PRO | 3.5 |
| 16 | AP | 59 | TRP | 3.5 |
| 4 | CD | 3 | ARG | 3.5 |
| 32 | DB | 26 | A | 3.5 |
| 19 | AS | 35 | SER | 3.5 |
| 7 | CG | 30 | ILE | 3.5 |
| 10 | AJ | 28 | ARG | 3.5 |
| 13 | AM | 71 | ARG | 3.5 |
| 7 | AG | 133 | GLY | 3.5 |
| 29 | B7 | 48 | LYS | 3.5 |
| 44 | DS | 57 | LYS | 3.5 |
| 1 | AA | 970 | C | 3.4 |
| 16 | CP | 47 | ASP | 3.4 |
| 1 | AA | 81 | U | 3.4 |
| 1 | CA | 1003 | G | 3.4 |
| 1 | CA | 1175 | G | 3.4 |
| 1 | CA | 1232 | U | 3.4 |
| 31 | BA | 271(K) | U | 3.4 |
| 50 | DY | 55 | TYR | 3.4 |
| 19 | CS | 70 | LYS | 3.4 |
| 9 | CI | 22 | GLY | 3.4 |
| 34 | DE | 54 | GLN | 3.4 |
| 31 | BA | 271(L) | U | 3.4 |
| 50 | DY | 61 | ILE | 3.4 |
| 1 | AA | 1275 | A | 3.4 |
| 1 | CA | 1094 | G | 3.4 |
| 31 | DA | 2100 | G | 3.4 |
| 10 | AJ | 83 | GLU | 3.4 |
| 4 | AD | 45 | GLN | 3.4 |
| 7 | AG | 36 | LYS | 3.4 |
| 13 | AM | 74 | VAL | 3.4 |
| 16 | CP | 17 | TYR | 3.4 |
| 36 | DG | 103 | LEU | 3.4 |
| 1 | AA | 1027 | C | 3.4 |
| 1 | CA | 160 | A | 3.4 |
| 7 | CG | 83 | ALA | 3.4 |
| 44 | DS | 33 | LYS | 3.4 |
| 1 | AA | 1300 | G | 3.4 |
| 3 | CC | 47 | LEU | 3.4 |
| 31 | BA | 883 | G | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CB | 211 | ILE | 3.4 |
| 10 | CJ | 28 | ARG | 3.4 |
| 36 | DG | 96 | ARG | 3.4 |
| 5 | CE | 21 | ALA | 3.4 |
| 1 | AA | 1019 | C | 3.4 |
| 1 | CA | 924 | C | 3.4 |
| 28 | B6 | 17 | LYS | 3.4 |
| 1 | AA | 927 | G | 3.4 |
| 1 | AA | 1368 | G | 3.4 |
| 1 | CA | 1222 | G | 3.4 |
| 9 | AI | 107 | ARG | 3.4 |
| 45 | DT | 132 | LYS | 3.4 |
| 1 | CA | 1137 | C | 3.4 |
| 13 | CM | 52 | GLU | 3.4 |
| 5 | AE | 130 | ASN | 3.4 |
| 20 | AT | 9 | ASN | 3.4 |
| 1 | AA | 969 | A | 3.4 |
| 1 | AA | 1318 | A | 3.4 |
| 3 | AC | 101 | LEU | 3.4 |
| 7 | CG | 35 | LYS | 3.4 |
| 14 | AN | 23 | ARG | 3.4 |
| 19 | CS | 56 | GLN | 3.4 |
| 37 | DH | 101 | ARG | 3.4 |
| 1 | AA | 97 | G | 3.4 |
| 1 | CA | 1305 | G | 3.4 |
| 2 | CB | 101 | MET | 3.4 |
| 9 | CI | 98 | PRO | 3.4 |
| 25 | D3 | 39 | ASP | 3.4 |
| 31 | BA | 884 | C | 3.4 |
| 4 | CD | 32 | ALA | 3.4 |
| 7 | CG | 108 | ALA | 3.4 |
| 13 | AM | 30 | ALA | 3.4 |
| 19 | AS | 41 | VAL | 3.4 |
| 3 | AC | 194 | GLY | 3.4 |
| 3 | CC | 90 | GLU | 3.4 |
| 47 | DV | 53 | GLU | 3.4 |
| 1 | CA | 950 | U | 3.4 |
| 27 | D5 | 2 | ALA | 3.4 |
| 31 | BA | 2402 | C | 3.4 |
| 1 | AA | 1157 | A | 3.4 |
| 9 | AI | 78 | LYS | 3.4 |
| 41 | BP | 139 | LYS | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | AB | 118 | LEU | 3.4 |
| 11 | AK | 19 | ALA | 3.4 |
| 19 | AS | 75 | ALA | 3.4 |
| 18 | AR | 29 | PHE | 3.4 |
| 36 | BG | 80 | PHE | 3.4 |
| 7 | CG | 68 | ASN | 3.4 |
| 10 | AJ | 78 | ASN | 3.4 |
| 9 | CI | 102 | LEU | 3.3 |
| 38 | DI | 128 | LEU | 3.3 |
| 1 | AA | 935 | A | 3.3 |
| 1 | AA | 1213 | A | 3.3 |
| 31 | DA | 900 | A | 3.3 |
| 9 | CI | 36 | TYR | 3.3 |
| 12 | AL | 28 | LYS | 3.3 |
| 41 | BP | 144 | GLU | 3.3 |
| 1 | AA | 1354 | C | 3.3 |
| 1 | CA | 1098 | C | 3.3 |
| 1 | CA | 1296 | C | 3.3 |
| 1 | AA | 976 | G | 3.3 |
| 19 | CS | 74 | PHE | 3.3 |
| 41 | DP | 150 | ALA | 3.3 |
| 3 | CC | 190 | ARG | 3.3 |
| 4 | AD | 36 | ARG | 3.3 |
| 28 | D6 | 20 | ASN | 3.3 |
| 2 | CB | 215 | LEU | 3.3 |
| 7 | AG | 77 | SER | 3.3 |
| 51 | DZ | 96 | VAL | 3.3 |
| 2 | AB | 13 | ALA | 3.3 |
| 16 | AP | 17 | TYR | 3.3 |
| 1 | AA | 1295 | G | 3.3 |
| 22 | B0 | 3 | HIS | 3.3 |
| 3 | AC | 189 | ALA | 3.3 |
| 3 | CC | 21 | ARG | 3.3 |
| 9 | AI | 93 | ARG | 3.3 |
| 1 | AA | 1115 | C | 3.3 |
| 5 | CE | 42 | GLY | 3.3 |
| 10 | AJ | 34 | VAL | 3.3 |
| 1 | CA | 698 | G | 3.3 |
| 12 | CL | 111 | LYS | 3.3 |
| 21 | CU | 9 | ARG | 3.3 |
| 1 | AA | 1248 | A | 3.3 |
| 10 | CJ | 38 | ILE | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | DH | 156 | ALA | 3.3 |
| 19 | CS | 45 | VAL | 3.3 |
| 1 | AA | 83 | U | 3.3 |
| 1 | AA | 1126 | U | 3.3 |
| 1 | CA | 81 | U | 3.3 |
| 3 | AC | 69 | HIS | 3.3 |
| 2 | AB | 187 | LEU | 3.3 |
| 7 | AG | 53 | LYS | 3.3 |
| 7 | CG | 118 | VAL | 3.3 |
| 19 | AS | 45 | VAL | 3.3 |
| 1 | AA | 417 | C | 3.3 |
| 31 | BA | 2477 | C | 3.3 |
| 13 | CM | 72 | ALA | 3.3 |
| 3 | AC | 184 | TYR | 3.3 |
| 1 | CA | 959 | A | 3.3 |
| 31 | DA | 1046 | A | 3.3 |
| 31 | DA | 1107 | G | 3.3 |
| 31 | DA | 1465 | G | 3.3 |
| 10 | CJ | 32 | ALA | 3.3 |
| 19 | AS | 61 | TYR | 3.3 |
| 20 | CT | 101 | GLY | 3.3 |
| 2 | CB | 76 | GLN | 3.3 |
| 19 | CS | 60 | VAL | 3.3 |
| 8 | AH | 55 | GLY | 3.3 |
| 9 | AI | 80 | GLY | 3.3 |
| 31 | DA | 2311 | A | 3.3 |
| 1 | CA | 1221 | G | 3.3 |
| 2 | AB | 233 | SER | 3.3 |
| 9 | AI | 7 | THR | 3.3 |
| 24 | D2 | 38 | GLN | 3.3 |
| 13 | CM | 13 | LYS | 3.3 |
| 36 | DG | 167 | GLU | 3.3 |
| 2 | CB | 213 | LEU | 3.3 |
| 7 | AG | 101 | LEU | 3.3 |
| 10 | CJ | 90 | LEU | 3.3 |
| 31 | BA | 2310 | A | 3.3 |
| 7 | AG | 35 | LYS | 3.3 |
| 31 | DA | 7 | G | 3.3 |
| 41 | BP | 107 | LYS | 3.3 |
| 18 | CR | 82 | THR | 3.3 |
| 16 | AP | 39 | TYR | 3.3 |
| 44 | DS | 36 | TYR | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 50 | BY | 88 | LYS | 3.3 |
| 1 | CA | 1212 | U | 3.2 |
| 1 | CA | 1219 | U | 3.2 |
| 31 | DA | 895 | U | 3.2 |
| 1 | CA | 1218 | C | 3.2 |
| 3 | CC | 111 | LEU | 3.2 |
| 9 | CI | 86 | VAL | 3.2 |
| 9 | CI | 95 | LYS | 3.2 |
| 44 | DS | 49 | VAL | 3.2 |
| 4 | CD | 69 | GLY | 3.2 |
| 6 | CF | 8 | ILE | 3.2 |
| 36 | DG | 152 | LEU | 3.2 |
| 1 | CA | 1249 | C | 3.2 |
| 6 | AF | 90 | VAL | 3.2 |
| 29 | B7 | 49 | ARG | 3.2 |
| 5 | CE | 78 | HIS | 3.2 |
| 9 | CI | 41 | VAL | 3.2 |
| 36 | BG | 137 | GLU | 3.2 |
| 5 | AE | 154 | GLY | 3.2 |
| 12 | AL | 52 | LEU | 3.2 |
| 14 | CN | 59 | ALA | 3.2 |
| 13 | AM | 49 | THR | 3.2 |
| 1 | AA | 965 | A | 3.2 |
| 28 | D6 | 39 | TYR | 3.2 |
| 1 | AA | 971 | G | 3.2 |
| 38 | BI | 70 | GLU | 3.2 |
| 1 | AA | 1229 | A | 3.2 |
| 1 | CA | 1093 | A | 3.2 |
| 1 | CA | 1229 | A | 3.2 |
| 49 | DX | 26 | TYR | 3.2 |
| 1 | CA | 1163 | C | 3.2 |
| 31 | BA | 2794 | C | 3.2 |
| 39 | BN | 68 | GLU | 3.2 |
| 16 | AP | 75 | ARG | 3.2 |
| 23 | D1 | 26 | ARG | 3.2 |
| 1 | AA | 96 | U | 3.2 |
| 1 | AA | 1160 | G | 3.2 |
| 1 | AA | 1240 | U | 3.2 |
| 1 | CA | 570 | G | 3.2 |
| 1 | CA | 1143 | G | 3.2 |
| 2 | AB | 16 | HIS | 3.2 |
| 1 | CA | 1146 | A | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | CA | 1349 | A | 3.2 |
| 9 | CI | 109 | VAL | 3.2 |
| 45 | BT | 132 | LYS | 3.2 |
| 1 | AA | 1045 | C | 3.2 |
| 31 | BA | 1530 | C | 3.2 |
| 21 | CU | 4 | GLY | 3.2 |
| 16 | AP | 29 | ASP | 3.2 |
| 37 | DH | 29 | PRO | 3.2 |
| 1 | AA | 1305 | G | 3.2 |
| 1 | CA | 928 | G | 3.2 |
| 7 | AG | 79 | ARG | 3.2 |
| 10 | CJ | 43 | ARG | 3.2 |
| 31 | DA | 2207 | G | 3.2 |
| 19 | CS | 39 | THR | 3.2 |
| 36 | BG | 145 | THR | 3.2 |
| 13 | AM | 61 | GLU | 3.2 |
| 21 | AU | 24 | ARG | 3.2 |
| 38 | DI | 127 | VAL | 3.2 |
| 31 | BA | 1108 | U | 3.2 |
| 1 | CA | 951 | G | 3.2 |
| 7 | CG | 29 | LYS | 3.2 |
| 19 | AS | 62 | ILE | 3.2 |
| 2 | AB | 96 | ARG | 3.2 |
| 2 | AB | 237 | ALA | 3.2 |
| 13 | CM | 75 | ALA | 3.2 |
| 37 | DH | 57 | ASP | 3.2 |
| 1 | CA | 194 | C | 3.2 |
| 1 | CA | 1045 | C | 3.2 |
| 1 | CA | 1244 | C | 3.2 |
| 2 | AB | 12 | GLU | 3.2 |
| 31 | DA | 271(J) | C | 3.2 |
| 31 | DA | 2791 | C | 3.2 |
| 3 | AC | 63 | ASN | 3.2 |
| 5 | CE | 6 | PHE | 3.2 |
| 11 | AK | 26 | ASN | 3.2 |
| 9 | AI | 17 | VAL | 3.2 |
| 1 | CA | 927 | G | 3.2 |
| 1 | CA | 958 | A | 3.2 |
| 1 | CA | 963 | G | 3.2 |
| 1 | CA | 1230 | C | 3.1 |
| 10 | CJ | 77 | PRO | 3.1 |
| 19 | AS | 32 | LYS | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 50 | DY | 87 | LYS | 3.1 |
| 3 | CC | 85 | ARG | 3.1 |
| 3 | AC | 180 | ALA | 3.1 |
| 6 | CF | 65 | VAL | 3.1 |
| 47 | DV | 5 | VAL | 3.1 |
| 51 | DZ | 70 | LEU | 3.1 |
| 1 | AA | 218 | C | 3.1 |
| 1 | CA | 1087 | G | 3.1 |
| 28 | D6 | 44 | ARG | 3.1 |
| 32 | DB | 60 | C | 3.1 |
| 38 | BI | 89 | TYR | 3.1 |
| 3 | CC | 101 | LEU | 3.1 |
| 3 | CC | 164 | ARG | 3.1 |
| 11 | AK | 98 | LEU | 3.1 |
| 17 | CQ | 25 | ARG | 3.1 |
| 16 | AP | 9 | PHE | 3.1 |
| 36 | DG | 180 | PHE | 3.1 |
| 1 | AA | 1221 | G | 3.1 |
| 1 | CA | 1302 | U | 3.1 |
| 37 | BH | 116 | GLU | 3.1 |
| 2 | CB | 148 | TYR | 3.1 |
| 10 | CJ | 84 | GLN | 3.1 |
| 31 | DA | 1914 | C | 3.1 |
| 32 | DB | 31 | C | 3.1 |
| 7 | CG | 78 | ARG | 3.1 |
| 9 | AI | 56 | LEU | 3.1 |
| 19 | CS | 63 | THR | 3.1 |
| 37 | DH | 108 | GLY | 3.1 |
| 36 | DG | 109 | VAL | 3.1 |
| 1 | AA | 992 | U | 3.1 |
| 1 | CA | 532 | A | 3.1 |
| 10 | CJ | 21 | GLN | 3.1 |
| 10 | AJ | 76 | ASN | 3.1 |
| 10 | CJ | 75 | ILE | 3.1 |
| 31 | BA | 2308 | G | 3.1 |
| 31 | BA | 2833 | G | 3.1 |
| 34 | DE | 17 | ASP | 3.1 |
| 36 | DG | 23 | PHE | 3.1 |
| 3 | CC | 204 | LEU | 3.1 |
| 1 | CA | 1066 | C | 3.1 |
| 9 | CI | 71 | SER | 3.1 |
| 1 | AA | 1283 | G | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CB | 31 | TYR | 3.1 |
| 1 | AA | 1091 | U | 3.1 |
| 1 | AA | 1232 | U | 3.1 |
| 10 | AJ | 30 | SER | 3.1 |
| 47 | DV | 47 | VAL | 3.1 |
| 1 | AA | 964 | A | 3.1 |
| 37 | DH | 106 | THR | 3.1 |
| 7 | CG | 38 | LEU | 3.1 |
| 9 | AI | 94 | ALA | 3.1 |
| 35 | BF | 128 | ALA | 3.1 |
| 9 | CI | 4 | TYR | 3.1 |
| 1 | AA | 1047 | G | 3.1 |
| 5 | CE | 45 | PHE | 3.1 |
| 31 | BA | 2100 | G | 3.1 |
| 11 | AK | 30 | VAL | 3.1 |
| 36 | DG | 86 | MET | 3.1 |
| 42 | BQ | 135 | ASP | 3.1 |
| 7 | AG | 16 | LEU | 3.1 |
| 11 | AK | 21 | ILE | 3.1 |
| 1 | AA | 944 | G | 3.1 |
| 20 | CT | 99 | LEU | 3.1 |
| 2 | AB | 144 | ARG | 3.1 |
| 1 | CA | 539 | A | 3.1 |
| 9 | AI | 95 | LYS | 3.1 |
| 50 | DY | 49 | VAL | 3.1 |
| 7 | CG | 25 | ALA | 3.1 |
| 12 | CL | 51 | ALA | 3.1 |
| 19 | CS | 59 | PRO | 3.1 |
| 21 | CU | 6 | ARG | 3.1 |
| 1 | AA | 841 | U | 3.1 |
| 1 | AA | 1056 | U | 3.1 |
| 31 | DA | 2893 | G | 3.1 |
| 36 | BG | 35 | GLU | 3.1 |
| 17 | AQ | 80 | GLY | 3.0 |
| 19 | AS | 18 | LYS | 3.0 |
| 13 | AM | 35 | GLU | 3.0 |
| 1 | AA | 1043 | C | 3.0 |
| 3 | CC | 81 | GLY | 3.0 |
| 10 | CJ | 54 | PHE | 3.0 |
| 37 | DH | 27 | LYS | 3.0 |
| 42 | DQ | 89 | ASN | 3.0 |
| 1 | CA | 957 | U | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 3 | AC | 15 | THR | 3.0 |
| 4 | CD | 10 | ARG | 3.0 |
| 7 | CG | 115 | ARG | 3.0 |
| 36 | DG | 75 | LYS | 3.0 |
| 1 | CA | 1265 | G | 3.0 |
| 9 | AI | 21 | PRO | 3.0 |
| 31 | DA | 352 | G | 3.0 |
| 7 | AG | 51 | GLN | 3.0 |
| 10 | CJ | 40 | LEU | 3.0 |
| 3 | AC | 39 | ILE | 3.0 |
| 37 | BH | 45 | VAL | 3.0 |
| 1 | AA | 1013 | G | 3.0 |
| 1 | CA | 922 | G | 3.0 |
| 1 | CA | 933 | G | 3.0 |
| 3 | AC | 91 | LEU | 3.0 |
| 1 | AA | 1252 | A | 3.0 |
| 1 | CA | 1115 | C | 3.0 |
| 31 | DA | 1032 | A | 3.0 |
| 9 | CI | 15 | ALA | 3.0 |
| 2 | AB | 140 | HIS | 3.0 |
| 7 | CG | 49 | ILE | 3.0 |
| 9 | CI | 26 | VAL | 3.0 |
| 13 | CM | 83 | ASP | 3.0 |
| 30 | B8 | 34 | TRP | 3.0 |
| 36 | DG | 26 | GLN | 3.0 |
| 10 | CJ | 76 | ASN | 3.0 |
| 7 | CG | 62 | PHE | 3.0 |
| 31 | DA | 2477 | C | 3.0 |
| 1 | CA | 1151 | A | 3.0 |
| 1 | CA | 1256 | A | 3.0 |
| 6 | CF | 91 | VAL | 3.0 |
| 10 | CJ | 55 | LYS | 3.0 |
| 41 | DP | 123 | LEU | 3.0 |
| 9 | AI | 5 | TYR | 3.0 |
| 9 | CI | 12 | GLU | 3.0 |
| 11 | AK | 94 | ALA | 3.0 |
| 31 | BA | 11 | G | 3.0 |
| 31 | DA | 271(I) | G | 3.0 |
| 31 | DA | 1527 | G | 3.0 |
| 37 | DH | 112 | PRO | 3.0 |
| 13 | CM | 24 | GLY | 3.0 |
| 11 | CK | 32 | ILE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 11 | CK | 31 | THR | 3.0 |
| 31 | DA | 1908 | C | 3.0 |
| 1 | AA | 1329 | A | 3.0 |
| 7 | AG | 156 | TRP | 3.0 |
| 4 | CD | 6 | GLY | 3.0 |
| 13 | CM | 67 | GLU | 3.0 |
| 19 | AS | 54 | GLY | 3.0 |
| 19 | AS | 79 | THR | 3.0 |
| 9 | AI | 123 | PRO | 3.0 |
| 1 | CA | 1369 | C | 3.0 |
| 10 | AJ | 32 | ALA | 3.0 |
| 11 | CK | 94 | ALA | 3.0 |
| 31 | DA | 1043 | C | 3.0 |
| 3 | AC | 66 | VAL | 3.0 |
| 7 | AG | 141 | VAL | 3.0 |
| 12 | CL | 112 | ASP | 3.0 |
| 19 | CS | 41 | VAL | 3.0 |
| 32 | DB | 105 | A | 3.0 |
| 36 | BG | 108 | ASN | 3.0 |
| 36 | DG | 94 | LEU | 3.0 |
| 31 | BA | 2186 | G | 3.0 |
| 19 | AS | 8 | GLY | 3.0 |
| 2 | AB | 41 | ILE | 3.0 |
| 13 | CM | 76 | ALA | 3.0 |
| 19 | CS | 50 | ALA | 3.0 |
| 1 | CA | 962 | C | 3.0 |
| 3 | CC | 162 | GLN | 3.0 |
| 1 | CA | 1283 | G | 2.9 |
| 13 | CM | 100 | GLY | 2.9 |
| 9 | CI | 16 | ARG | 2.9 |
| 31 | DA | 272(B) | G | 2.9 |
| 31 | DA | 1115 | G | 2.9 |
| 7 | CG | 91 | VAL | 2.9 |
| 17 | AQ | 53 | LEU | 2.9 |
| 36 | BG | 74 | LYS | 2.9 |
| 36 | BG | 75 | LYS | 2.9 |
| 49 | BX | 26 | TYR | 2.9 |
| 1 | AA | 1158 | C | 2.9 |
| 31 | DA | 1152 | C | 2.9 |
| 37 | DH | 109 | PHE | 2.9 |
| 3 | CC | 88 | ARG | 2.9 |
| 10 | CJ | 41 | PRO | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | AK | 28 | THR | 2.9 |
| 14 | AN | 28 | GLY | 2.9 |
| 14 | CN | 11 | LYS | 2.9 |
| 38 | DI | 62 | LYS | 2.9 |
| 1 | CA | 1121 | U | 2.9 |
| 31 | DA | 312 | G | 2.9 |
| 7 | AG | 8 | GLU | 2.9 |
| 35 | BF | 1 | MET | 2.9 |
| 50 | BY | 50 | ARG | 2.9 |
| 2 | AB | 75 | LYS | 2.9 |
| 3 | CC | 124 | ILE | 2.9 |
| 21 | AU | 13 | ILE | 2.9 |
| 31 | DA | 876 | C | 2.9 |
| 1 | CA | 1319 | A | 2.9 |
| 3 | CC | 22 | TRP | 2.9 |
| 7 | CG | 22 | LEU | 2.9 |
| 13 | CM | 87 | TYR | 2.9 |
| 22 | B0 | 2 | ALA | 2.9 |
| 16 | AP | 48 | TRP | 2.9 |
| 31 | DA | 2892 | A | 2.9 |
| 13 | AM | 57 | ARG | 2.9 |
| 1 | CA | 1127 | G | 2.9 |
| 1 | CA | 1144 | G | 2.9 |
| 7 | AG | 92 | SER | 2.9 |
| 9 | CI | 74 | ILE | 2.9 |
| 16 | AP | 7 | ALA | 2.9 |
| 19 | AS | 47 | HIS | 2.9 |
| 19 | CS | 31 | ILE | 2.9 |
| 19 | CS | 62 | ILE | 2.9 |
| 39 | DN | 129 | PRO | 2.9 |
| 31 | DA | 1049 | C | 2.9 |
| 2 | CB | 220 | ASP | 2.9 |
| 7 | AG | 29 | LYS | 2.9 |
| 38 | BI | 127 | VAL | 2.9 |
| 9 | AI | 114 | TYR | 2.9 |
| 1 | CA | 144 | G | 2.9 |
| 45 | DT | 93 | ARG | 2.9 |
| 7 | AG | 73 | MET | 2.9 |
| 3 | CC | 196 | LEU | 2.9 |
| 36 | DG | 28 | VAL | 2.9 |
| 38 | BI | 128 | LEU | 2.9 |
| 3 | CC | 184 | TYR | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 36 | DG | 104 | GLU | 2.9 |
| 1 | CA | 1008 | C | 2.9 |
| 1 | CA | 1217 | C | 2.9 |
| 9 | AI | 57 | GLY | 2.9 |
| 32 | DB | 56 | G | 2.9 |
| 37 | DH | 48 | GLY | 2.9 |
| 1 | AA | 1390 | U | 2.9 |
| 1 | CA | 1275 | A | 2.9 |
| 14 | AN | 20 | ALA | 2.9 |
| 39 | BN | 18 | ALA | 2.9 |
| 2 | AB | 38 | GLY | 2.9 |
| 50 | DY | 58 | GLY | 2.9 |
| 13 | CM | 17 | VAL | 2.9 |
| 1 | AA | 1363 | C | 2.9 |
| 31 | DA | 1467 | C | 2.9 |
| 1 | CA | 993 | G | 2.9 |
| 37 | DH | 83 | TYR | 2.9 |
| 31 | DA | 363(F) | A | 2.9 |
| 38 | BI | 131 | LYS | 2.9 |
| 44 | DS | 80 | LEU | 2.9 |
| 3 | CC | 71 | ALA | 2.9 |
| 27 | D5 | 53 | ALA | 2.9 |
| 12 | AL | 114 | LYS | 2.9 |
| 1 | CA | 1268 | A | 2.9 |
| 11 | CK | 108 | ILE | 2.9 |
| 7 | AG | 100 | ALA | 2.9 |
| 10 | CJ | 11 | PHE | 2.9 |
| 13 | AM | 51 | ALA | 2.9 |
| 41 | DP | 92 | GLU | 2.9 |
| 3 | AC | 181 | ASN | 2.9 |
| 10 | AJ | 15 | THR | 2.9 |
| 1 | AA | 426 | G | 2.9 |
| 1 | AA | 1207 | G | 2.9 |
| 2 | CB | 92 | TYR | 2.9 |
| 31 | DA | 1494 | A | 2.9 |
| 10 | CJ | 12 | ASP | 2.9 |
| 35 | DF | 2 | LYS | 2.9 |
| 50 | DY | 56 | PRO | 2.9 |
| 2 | CB | 235 | SER | 2.8 |
| 3 | AC | 144 | SER | 2.8 |
| 3 | AC | 128 | PHE | 2.8 |
| 7 | CG | 84 | ASN | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CB | 96 | ARG | 2.8 |
| 18 | CR | 47 | THR | 2.8 |
| 31 | BA | 1547 | C | 2.8 |
| 1 | AA | 532 | A | 2.8 |
| 1 | AA | 1280 | A | 2.8 |
| 1 | CA | 541 | G | 2.8 |
| 1 | AA | 1317 | C | 2.8 |
| 1 | AA | 1389 | C | 2.8 |
| 1 | CA | 960 | U | 2.8 |
| 1 | CA | 1200 | C | 2.8 |
| 1 | AA | 1289 | A | 2.8 |
| 1 | CA | 1503 | A | 2.8 |
| 2 | CB | 70 | PHE | 2.8 |
| 13 | CM | 57 | ARG | 2.8 |
| 18 | CR | 80 | PRO | 2.8 |
| 2 | CB | 241 | GLU | 2.8 |
| 31 | BA | 1107 | G | 2.8 |
| 39 | DN | 68 | GLU | 2.8 |
| 36 | DG | 64 | THR | 2.8 |
| 1 | AA | 1008 | C | 2.8 |
| 1 | AA | 1230 | C | 2.8 |
| 14 | CN | 29 | ARG | 2.8 |
| 11 | CK | 117 | ASN | 2.8 |
| 13 | AM | 115 | LYS | 2.8 |
| 18 | AR | 82 | THR | 2.8 |
| 13 | CM | 54 | VAL | 2.8 |
| 31 | DA | 1915 | U | 2.8 |
| 47 | DV | 96 | ILE | 2.8 |
| 36 | DG | 87 | PRO | 2.8 |
| 2 | CB | 143 | GLU | 2.8 |
| 37 | DH | 61 | HIS | 2.8 |
| 3 | AC | 179 | ARG | 2.8 |
| 15 | CO | 88 | ARG | 2.8 |
| 12 | CL | 32 | PHE | 2.8 |
| 46 | DU | 90 | VAL | 2.8 |
| 1 | AA | 354 | G | 2.8 |
| 1 | AA | 1311 | G | 2.8 |
| 16 | CP | 41 | PRO | 2.8 |
| 31 | DA | 2811 | G | 2.8 |
| 32 | DB | 1 | U | 2.8 |
| 3 | CC | 107 | GLN | 2.8 |
| 31 | DA | 898 | C | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | DG | 76 | SER | 2.8 |
| 11 | AK | 83 | ILE | 2.8 |
| 46 | DU | 79 | PHE | 2.8 |
| 51 | DZ | 146 | ILE | 2.8 |
| 1 | AA | 1360 | A | 2.8 |
| 2 | CB | 116 | GLU | 2.8 |
| 13 | AM | 107 | ALA | 2.8 |
| 19 | CS | 29 | ARG | 2.8 |
| 24 | B2 | 48 | HIS | 2.8 |
| 35 | DF | 128 | ALA | 2.8 |
| 38 | DI | 94 | ALA | 2.8 |
| 1 | AA | 428 | G | 2.8 |
| 1 | AA | 1310 | G | 2.8 |
| 1 | AA | 1347 | G | 2.8 |
| 10 | AJ | 46 | ARG | 2.8 |
| 10 | AJ | 81 | THR | 2.8 |
| 41 | DP | 119 | GLU | 2.8 |
| 1 | AA | 1503 | A | 2.8 |
| 1 | CA | 1285 | A | 2.8 |
| 1 | CA | 956 | U | 2.8 |
| 16 | CP | 6 | LEU | 2.8 |
| 38 | BI | 65 | ALA | 2.8 |
| 3 | CC | 74 | GLY | 2.8 |
| 7 | AG | 50 | ILE | 2.8 |
| 41 | DP | 91 | PHE | 2.8 |
| 1 | AA | 194 | C | 2.8 |
| 1 | CA | 945 | G | 2.8 |
| 1 | CA | 1117 | G | 2.8 |
| 2 | CB | 132 | LYS | 2.8 |
| 4 | AD | 152 | SER | 2.8 |
| 11 | CK | 129 | SER | 2.8 |
| 13 | AM | 40 | ASN | 2.8 |
| 46 | DU | 78 | THR | 2.8 |
| 37 | DH | 33 | LEU | 2.8 |
| 9 | AI | 30 | GLY | 2.8 |
| 1 | CA | 943 | U | 2.8 |
| 6 | AF | 94 | GLN | 2.8 |
| 6 | CF | 89 | MET | 2.8 |
| 19 | AS | 43 | GLU | 2.8 |
| 37 | BH | 41 | MET | 2.8 |
| 9 | CI | 29 | ASN | 2.8 |
| 3 | CC | 95 | THR | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 1011 | G | 2.8 |
| 32 | DB | 116 | G | 2.8 |
| 31 | BA | 362 | U | 2.8 |
| 1 | CA | 195 | A | 2.8 |
| 1 | CA | 1019 | C | 2.8 |
| 1 | CA | 1043 | C | 2.8 |
| 10 | AJ | 11 | PHE | 2.8 |
| 13 | CM | 53 | VAL | 2.8 |
| 1 | AA | 1446 | U | 2.7 |
| 51 | DZ | 98 | MET | 2.7 |
| 2 | CB | 154 | LEU | 2.7 |
| 9 | AI | 127 | LYS | 2.7 |
| 2 | AB | 136 | VAL | 2.7 |
| 28 | B6 | 20 | ASN | 2.7 |
| 36 | DG | 178 | PHE | 2.7 |
| 41 | DP | 84 | ASN | 2.7 |
| 3 | CC | 165 | THR | 2.7 |
| 9 | CI | 81 | ILE | 2.7 |
| 13 | CM | 41 | PRO | 2.7 |
| 36 | BG | 144 | ILE | 2.7 |
| 41 | DP | 144 | GLU | 2.7 |
| 1 | AA | 1218 | C | 2.7 |
| 1 | AA | 1362 | C | 2.7 |
| 31 | DA | 1505 | C | 2.7 |
| 2 | CB | 153 | ARG | 2.7 |
| 44 | BS | 11 | LYS | 2.7 |
| 1 | AA | 945 | G | 2.7 |
| 1 | AA | 954 | G | 2.7 |
| 1 | CA | 925 | G | 2.7 |
| 3 | CC | 177 | THR | 2.7 |
| 31 | BA | 896 | A | 2.7 |
| 6 | CF | 61 | LEU | 2.7 |
| 2 | AB | 227 | GLY | 2.7 |
| 14 | AN | 30 | ALA | 2.7 |
| 17 | CQ | 73 | VAL | 2.7 |
| 51 | DZ | 130 | PRO | 2.7 |
| 1 | AA | 540 | G | 2.7 |
| 1 | AA | 1017 | G | 2.7 |
| 3 | AC | 183 | ASP | 2.7 |
| 6 | CF | 39 | LYS | 2.7 |
| 9 | AI | 76 | ALA | 2.7 |
| 35 | BF | 21 | ALA | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 45 | BT | 92 | GLY | 2.7 |
| 1 | AA | 76 | C | 2.7 |
| 1 | AA | 1114 | C | 2.7 |
| 38 | BI | 74 | ASN | 2.7 |
| 10 | CJ | 31 | GLY | 2.7 |
| 31 | DA | 896 | A | 2.7 |
| 31 | DA | 2308 | G | 2.7 |
| 2 | AB | 32 | ILE | 2.7 |
| 18 | CR | 50 | ILE | 2.7 |
| 1 | CA | 1267 | C | 2.7 |
| 19 | CS | 38 | SER | 2.7 |
| 28 | D6 | 41 | PRO | 2.7 |
| 4 | CD | 41 | GLY | 2.7 |
| 9 | CI | 105 | ASP | 2.7 |
| 37 | DH | 123 | PHE | 2.7 |
| 2 | CB | 137 | ARG | 2.7 |
| 10 | AJ | 80 | LYS | 2.7 |
| 14 | CN | 4 | LYS | 2.7 |
| 9 | AI | 124 | GLN | 2.7 |
| 37 | DH | 16 | SER | 2.7 |
| 1 | AA | 1150 | U | 2.7 |
| 1 | AA | 1264 | C | 2.7 |
| 12 | AL | 74 | GLY | 2.7 |
| 16 | CP | 43 | LYS | 2.7 |
| 19 | CS | 72 | GLY | 2.7 |
| 31 | BA | 271(J) | C | 2.7 |
| 6 | CF | 90 | VAL | 2.7 |
| 2 | AB | 201 | ILE | 2.7 |
| 7 | CG | 44 | TYR | 2.7 |
| 11 | AK | 61 | ALA | 2.7 |
| 16 | CP | 19 | ILE | 2.7 |
| 31 | DA | 901 | A | 2.7 |
| 2 | AB | 229 | VAL | 2.7 |
| 2 | CB | 38 | GLY | 2.7 |
| 9 | AI | 20 | ARG | 2.7 |
| 15 | CO | 23 | GLY | 2.7 |
| 31 | DA | 361 | G | 2.7 |
| 5 | AE | 155 | GLU | 2.7 |
| 7 | CG | 134 | ALA | 2.7 |
| 13 | CM | 35 | GLU | 2.7 |
| 23 | D1 | 27 | GLU | 2.7 |
| 35 | DF | 199 | TRP | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | DG | 90 | LEU | 2.7 |
| 3 | CC | 2 | GLY | 2.7 |
| 10 | CJ | 94 | VAL | 2.7 |
| 33 | BD | 236 | GLY | 2.7 |
| 2 | AB | 236 | TYR | 2.7 |
| 5 | AE | 89 | ILE | 2.7 |
| 9 | AI | 122 | ALA | 2.7 |
| 13 | CM | 66 | LEU | 2.7 |
| 31 | DA | 1530 | C | 2.7 |
| 32 | DB | 23 | G | 2.7 |
| 32 | DB | 62 | C | 2.7 |
| 14 | AN | 29 | ARG | 2.7 |
| 16 | CP | 72 | ARG | 2.7 |
| 37 | DH | 43 | VAL | 2.7 |
| 37 | DH | 110 | SER | 2.7 |
| 1 | CA | 141 | A | 2.7 |
| 1 | CA | 1040 | U | 2.7 |
| 1 | CA | 1252 | A | 2.7 |
| 9 | AI | 23 | ASN | 2.7 |
| 9 | AI | 50 | LEU | 2.7 |
| 14 | CN | 19 | ARG | 2.7 |
| 32 | DB | 24 | G | 2.7 |
| 37 | DH | 107 | VAL | 2.7 |
| 4 | CD | 43 | HIS | 2.7 |
| 36 | DG | 73 | ALA | 2.7 |
| 2 | AB | 98 | LEU | 2.6 |
| 36 | DG | 62 | LEU | 2.6 |
| 1 | AA | 982 | U | 2.6 |
| 1 | CA | 974 | A | 2.6 |
| 1 | CA | 1159 | U | 2.6 |
| 51 | DZ | 170 | THR | 2.6 |
| 3 | CC | 78 | GLY | 2.6 |
| 5 | CE | 109 | ILE | 2.6 |
| 11 | CK | 39 | PRO | 2.6 |
| 2 | CB | 109 | SER | 2.6 |
| 19 | CS | 34 | TRP | 2.6 |
| 11 | CK | 27 | ASN | 2.6 |
| 24 | D2 | 37 | PHE | 2.6 |
| 15 | AO | 23 | GLY | 2.6 |
| 4 | AD | 200 | GLU | 2.6 |
| 7 | CG | 112 | PRO | 2.6 |
| 9 | CI | 9 | ARG | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 9 | CI | 107 | ARG | 2.6 |
| 10 | CJ | 9 | ARG | 2.6 |
| 10 | CJ | 37 | PRO | 2.6 |
| 1 | CA | 1277 | C | 2.6 |
| 9 | AI | 18 | PHE | 2.6 |
| 11 | AK | 43 | SER | 2.6 |
| 7 | CG | 28 | ASN | 2.6 |
| 18 | CR | 22 | VAL | 2.6 |
| 36 | DG | 36 | LYS | 2.6 |
| 5 | CE | 75 | THR | 2.6 |
| 38 | BI | 132 | PRO | 2.6 |
| 16 | AP | 80 | PHE | 2.6 |
| 36 | DG | 141 | PHE | 2.6 |
| 1 | CA | 1234 | C | 2.6 |
| 35 | BF | 134 | GLY | 2.6 |
| 36 | DG | 92 | VAL | 2.6 |
| 42 | DQ | 92 | GLY | 2.6 |
| 10 | AJ | 65 | LEU | 2.6 |
| 19 | AS | 48 | THR | 2.6 |
| 36 | DG | 43 | LEU | 2.6 |
| 1 | CA | 1017 | G | 2.6 |
| 26 | D4 | 18 | CYS | 2.6 |
| 31 | BA | 1533 | G | 2.6 |
| 31 | BA | 2793 | G | 2.6 |
| 36 | DG | 17 | PRO | 2.6 |
| 3 | AC | 158 | GLY | 2.6 |
| 7 | AG | 74 | GLU | 2.6 |
| 8 | CH | 30 | ARG | 2.6 |
| 16 | CP | 51 | VAL | 2.6 |
| 19 | AS | 68 | GLY | 2.6 |
| 31 | BA | 1916 | A | 2.6 |
| 37 | DH | 35 | VAL | 2.6 |
| 45 | DT | 34 | VAL | 2.6 |
| 1 | AA | 188 | C | 2.6 |
| 1 | AA | 1030 | C | 2.6 |
| 28 | B6 | 39 | TYR | 2.6 |
| 1 | CA | 991 | U | 2.6 |
| 2 | AB | 17 | PHE | 2.6 |
| 31 | DA | 271(N) | U | 2.6 |
| 1 | CA | 1185 | G | 2.6 |
| 7 | CG | 132 | GLY | 2.6 |
| 31 | BA | 1173 | G | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | DA | 875 | G | 2.6 |
| 7 | AG | 78 | ARG | 2.6 |
| 10 | AJ | 67 | THR | 2.6 |
| 14 | CN | 12 | ARG | 2.6 |
| 1 | CA | 1085 | U | 2.6 |
| 37 | BH | 47 | GLU | 2.6 |
| 1 | CA | 93 | G | 2.6 |
| 10 | CJ | 48 | THR | 2.6 |
| 13 | AM | 52 | GLU | 2.6 |
| 7 | CG | 137 | LYS | 2.6 |
| 13 | AM | 48 | LEU | 2.6 |
| 7 | AG | 96 | GLN | 2.6 |
| 36 | BG | 136 | ARG | 2.6 |
| 1 | CA | 348 | G | 2.6 |
| 4 | CD | 21 | LEU | 2.6 |
| 9 | CI | 50 | LEU | 2.6 |
| 31 | BA | 898 | C | 2.6 |
| 43 | DR | 33 | ARG | 2.6 |
| 47 | BV | 96 | ILE | 2.6 |
| 2 | CB | 112 | VAL | 2.6 |
| 44 | DS | 81 | GLY | 2.6 |
| 10 | CJ | 29 | ARG | 2.6 |
| 2 | AB | 211 | ILE | 2.6 |
| 1 | AA | 162 | A | 2.6 |
| 1 | AA | 1186 | G | 2.6 |
| 1 | AA | 1316 | G | 2.6 |
| 1 | CA | 15 | G | 2.6 |
| 1 | CA | 731 | G | 2.6 |
| 31 | DA | 1922 | G | 2.6 |
| 1 | AA | 624 | C | 2.6 |
| 1 | CA | 992 | U | 2.6 |
| 13 | CM | 59 | TYR | 2.6 |
| 9 | CI | 83 | ARG | 2.6 |
| 29 | D7 | 47 | ARG | 2.6 |
| 17 | AQ | 98 | LEU | 2.6 |
| 41 | DP | 122 | PRO | 2.6 |
| 11 | AK | 31 | THR | 2.6 |
| 18 | CR | 56 | THR | 2.6 |
| 16 | AP | 12 | LYS | 2.5 |
| 19 | AS | 70 | LYS | 2.5 |
| 41 | BP | 119 | GLU | 2.5 |
| 46 | DU | 76 | TYR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | CA | 16 | A | 2.5 |
| 1 | CA | 417 | C | 2.5 |
| 31 | DA | 1033 | U | 2.5 |
| 11 | AK | 129 | SER | 2.5 |
| 2 | CB | 51 | LEU | 2.5 |
| 38 | DI | 137 | PRO | 2.5 |
| 18 | CR | 49 | LYS | 2.5 |
| 2 | CB | 12 | GLU | 2.5 |
| 3 | AC | 100 | ALA | 2.5 |
| 44 | DS | 37 | ALA | 2.5 |
| 1 | AA | 472 | A | 2.5 |
| 1 | CA | 979 | C | 2.5 |
| 1 | CA | 1180 | A | 2.5 |
| 32 | DB | 29 | A | 2.5 |
| 1 | CA | 1206 | G | 2.5 |
| 7 | AG | 120 | ILE | 2.5 |
| 41 | BP | 121 | LYS | 2.5 |
| 31 | DA | 892 | G | 2.5 |
| 31 | DA | 1154 | G | 2.5 |
| 28 | D6 | 40 | CYS | 2.5 |
| 45 | DT | 123 | GLN | 2.5 |
| 50 | DY | 98 | VAL | 2.5 |
| 21 | CU | 12 | LYS | 2.5 |
| 37 | DH | 105 | LEU | 2.5 |
| 41 | DP | 88 | LEU | 2.5 |
| 44 | DS | 50 | SER | 2.5 |
| 1 | AA | 1183 | A | 2.5 |
| 36 | DG | 112 | PRO | 2.5 |
| 1 | CA | 1132 | C | 2.5 |
| 6 | CF | 4 | TYR | 2.5 |
| 7 | CG | 139 | GLU | 2.5 |
| 10 | CJ | 83 | GLU | 2.5 |
| 31 | DA | 272(J) | C | 2.5 |
| 16 | AP | 38 | TYR | 2.5 |
| 18 | CR | 83 | GLU | 2.5 |
| 42 | DQ | 80 | GLU | 2.5 |
| 7 | AG | 23 | VAL | 2.5 |
| 28 | B6 | 23 | THR | 2.5 |
| 31 | DA | 1525 | G | 2.5 |
| 51 | DZ | 88 | PHE | 2.5 |
| 1 | CA | 982 | U | 2.5 |
| 19 | CS | 51 | VAL | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 39 | BN | 131 | GLN | 2.5 |
| 1 | AA | 390 | C | 2.5 |
| 1 | AA | 488 | C | 2.5 |
| 28 | D6 | 13 | CYS | 2.5 |
| 1 | CA | 1184 | G | 2.5 |
| 36 | BG | 39 | ILE | 2.5 |
| 2 | AB | 33 | TYR | 2.5 |
| 7 | AG | 136 | LYS | 2.5 |
| 10 | AJ | 68 | HIS | 2.5 |
| 12 | CL | 99 | HIS | 2.5 |
| 31 | BA | 157 | U | 2.5 |
| 42 | BQ | 90 | VAL | 2.5 |
| 3 | CC | 181 | ASN | 2.5 |
| 45 | DT | 38 | ASN | 2.5 |
| 7 | AG | 27 | ILE | 2.5 |
| 31 | DA | 2801 | A | 2.5 |
| 10 | AJ | 7 | LYS | 2.5 |
| 1 | AA | 1181 | G | 2.5 |
| 1 | CA | 987 | G | 2.5 |
| 3 | AC | 154 | SER | 2.5 |
| 3 | CC | 193 | TYR | 2.5 |
| 9 | AI | 22 | GLY | 2.5 |
| 10 | AJ | 79 | ARG | 2.5 |
| 31 | BA | 881 | G | 2.5 |
| 44 | DS | 30 | ARG | 2.5 |
| 46 | DU | 109 | LEU | 2.5 |
| 10 | AJ | 87 | THR | 2.5 |
| 16 | CP | 9 | PHE | 2.5 |
| 1 | AA | 948 | C | 2.5 |
| 1 | AA | 1270 | C | 2.5 |
| 32 | DB | 6 | C | 2.5 |
| 9 | CI | 114 | TYR | 2.5 |
| 33 | BD | 268 | ARG | 2.5 |
| 44 | DS | 51 | ALA | 2.5 |
| 1 | AA | 1351 | U | 2.5 |
| 1 | CA | 426 | G | 2.5 |
| 31 | DA | 2302 | G | 2.5 |
| 47 | DV | 24 | LYS | 2.5 |
| 38 | BI | 67 | ARG | 2.5 |
| 1 | AA | 1161 | C | 2.5 |
| 1 | AA | 1332 | A | 2.5 |
| 2 | AB | 202 | PRO | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | BA | 279 | C | 2.5 |
| 31 | BA | 900 | A | 2.5 |
| 9 | CI | 78 | LYS | 2.5 |
| 23 | D1 | 78 | LYS | 2.5 |
| 3 | AC | 182 | ILE | 2.5 |
| 5 | AE | 109 | ILE | 2.5 |
| 36 | DG | 161 | THR | 2.5 |
| 37 | DH | 95 | ARG | 2.5 |
| 1 | CA | 1124 | G | 2.5 |
| 1 | CA | 1216 | G | 2.5 |
| 31 | DA | 1042 | G | 2.5 |
| 44 | DS | 72 | ALA | 2.5 |
| 34 | BE | 69 | LYS | 2.5 |
| 1 | CA | 418 | C | 2.5 |
| 1 | CA | 1162 | C | 2.5 |
| 1 | CA | 1322 | C | 2.5 |
| 31 | BA | 1546 | C | 2.5 |
| 3 | AC | 58 | GLU | 2.5 |
| 31 | BA | 2660 | A | 2.5 |
| 31 | DA | 1876 | A | 2.5 |
| 31 | DA | 2629 | A | 2.5 |
| 19 | CS | 44 | MET | 2.5 |
| 37 | DH | 46 | GLU | 2.5 |
| 2 | AB | 215 | LEU | 2.5 |
| 3 | CC | 103 | VAL | 2.5 |
| 4 | CD | 155 | LEU | 2.5 |
| 26 | D4 | 10 | VAL | 2.5 |
| 30 | B8 | 32 | LEU | 2.5 |
| 36 | BG | 89 | GLY | 2.5 |
| 37 | BH | 83 | TYR | 2.5 |
| 1 | AA | 1171 | G | 2.5 |
| 2 | AB | 80 | ILE | 2.5 |
| 7 | AG | 140 | ASP | 2.5 |
| 7 | CG | 64 | GLN | 2.5 |
| 2 | CB | 40 | HIS | 2.5 |
| 13 | AM | 99 | ARG | 2.5 |
| 31 | BA | 1176 | G | 2.5 |
| 31 | DA | 274 | G | 2.5 |
| 1 | CA | 218 | C | 2.4 |
| 1 | CA | 980 | C | 2.4 |
| 1 | CA | 1158 | C | 2.4 |
| 1 | CA | 1327 | C | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 1 | CA | 1354 | C | 2.4 |
| 31 | DA | 1547 | C | 2.4 |
| 11 | AK | 82 | VAL | 2.4 |
| 11 | CK | 80 | VAL | 2.4 |
| 13 | CM | 40 | ASN | 2.4 |
| 33 | DD | 236 | GLY | 2.4 |
| 43 | BR | 11 | ASN | 2.4 |
| 51 | DZ | 132 | ASN | 2.4 |
| 13 | AM | 104 | ARG | 2.4 |
| 16 | CP | 42 | ARG | 2.4 |
| 16 | CP | 76 | GLN | 2.4 |
| 38 | BI | 135 | GLU | 2.4 |
| 1 | CA | 292 | G | 2.4 |
| 1 | CA | 1271 | G | 2.4 |
| 4 | AD | 8 | VAL | 2.4 |
| 9 | AI | 109 | VAL | 2.4 |
| 11 | CK | 98 | LEU | 2.4 |
| 31 | BA | 271(M) | G | 2.4 |
| 38 | DI | 107 | VAL | 2.4 |
| 50 | BY | 27 | VAL | 2.4 |
| 31 | BA | 2803 | C | 2.4 |
| 2 | CB | 105 | PHE | 2.4 |
| 1 | CA | 1091 | U | 2.4 |
| 20 | CT | 8 | ARG | 2.4 |
| 3 | CC | 109 | PRO | 2.4 |
| 36 | BG | 66 | GLN | 2.4 |
| 5 | CE | 19 | MET | 2.4 |
| 13 | AM | 13 | LYS | 2.4 |
| 19 | AS | 50 | ALA | 2.4 |
| 45 | DT | 115 | ARG | 2.4 |
| 1 | AA | 1314 | C | 2.4 |
| 1 | AA | 1335 | C | 2.4 |
| 1 | CA | 1108 | G | 2.4 |
| 1 | CA | 1231 | G | 2.4 |
| 19 | AS | 63 | THR | 2.4 |
| 1 | AA | 1363(A) | A | 2.4 |
| 16 | CP | 15 | PRO | 2.4 |
| 2 | CB | 83 | MET | 2.4 |
| 6 | AF | 99 | ALA | 2.4 |
| 7 | CG | 85 | TYR | 2.4 |
| 46 | BU | 117 | GLN | 2.4 |
| 1 | AA | 1328 | C | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 1369 | C | 2.4 |
| 1 | CA | 1263 | C | 2.4 |
| 6 | AF | 48 | LEU | 2.4 |
| 27 | D5 | 55 | ARG | 2.4 |
| 37 | DH | 41 | MET | 2.4 |
| 1 | CA | 1347 | G | 2.4 |
| 31 | BA | 1912 | A | 2.4 |
| 38 | BI | 120 | ILE | 2.4 |
| 38 | DI | 79 | ILE | 2.4 |
| 3 | AC | 106 | VAL | 2.4 |
| 19 | CS | 33 | THR | 2.4 |
| 36 | DG | 93 | THR | 2.4 |
| 4 | AD | 6 | GLY | 2.4 |
| 36 | DG | 179 | PRO | 2.4 |
| 1 | AA | 952 | U | 2.4 |
| 1 | CA | 931 | C | 2.4 |
| 31 | BA | 12 | U | 2.4 |
| 45 | BT | 32 | TYR | 2.4 |
| 51 | DZ | 179 | ASP | 2.4 |
| 31 | DA | 330 | A | 2.4 |
| 31 | DA | 1528 | A | 2.4 |
| 3 | CC | 57 | ILE | 2.4 |
| 11 | AK | 29 | ILE | 2.4 |
| 31 | DA | 1526 | G | 2.4 |
| 3 | CC | 179 | ARG | 2.4 |
| 24 | B2 | 43 | GLN | 2.4 |
| 7 | CG | 105 | VAL | 2.4 |
| 7 | CG | 153 | HIS | 2.4 |
| 9 | CI | 13 | ALA | 2.4 |
| 16 | CP | 29 | ASP | 2.4 |
| 1 | CA | 1147 | C | 2.4 |
| 3 | AC | 126 | ARG | 2.4 |
| 19 | AS | 11 | VAL | 2.4 |
| 1 | AA | 1331 | G | 2.4 |
| 1 | CA | 347 | G | 2.4 |
| 1 | CA | 988 | G | 2.4 |
| 11 | AK | 27 | ASN | 2.4 |
| 36 | BG | 51 | ARG | 2.4 |
| 37 | BH | 101 | ARG | 2.4 |
| 1 | AA | 1330 | U | 2.4 |
| 1 | CA | 1391 | U | 2.4 |
| 1 | AA | 1051 | C | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | DA | 2183 | C | 2.4 |
| 44 | DS | 48 | LEU | 2.4 |
| 4 | AD | 23 | GLY | 2.4 |
| 50 | DY | 91 | GLU | 2.4 |
| 1 | AA | 98 | G | 2.4 |
| 1 | AA | 1190 | G | 2.4 |
| 1 | CA | 1047 | G | 2.4 |
| 31 | DA | 919 | G | 2.4 |
| 32 | DB | 87 | G | 2.4 |
| 37 | BH | 65 | HIS | 2.4 |
| 1 | CA | 1321 | C | 2.4 |
| 10 | CJ | 42 | THR | 2.4 |
| 20 | CT | 106 | ALA | 2.4 |
| 31 | DA | 1508 | A | 2.4 |
| 20 | AT | 72 | LEU | 2.4 |
| 6 | CF | 40 | VAL | 2.4 |
| 17 | AQ | 77 | VAL | 2.4 |
| 1 | AA | 1276 | G | 2.4 |
| 1 | CA | 920 | U | 2.4 |
| 1 | CA | 1401 | G | 2.4 |
| 5 | CE | 20 | GLN | 2.4 |
| 10 | AJ | 59 | SER | 2.4 |
| 30 | B8 | 37 | SER | 2.4 |
| 31 | BA | 1915 | U | 2.4 |
| 31 | DA | 1921 | G | 2.4 |
| 4 | AD | 184 | LYS | 2.4 |
| 47 | DV | 6 | LYS | 2.4 |
| 50 | BY | 91 | GLU | 2.4 |
| 32 | DB | 2 | C | 2.4 |
| 35 | DF | 7 | TYR | 2.4 |
| 5 | AE | 85 | GLY | 2.3 |
| 36 | DG | 44 | GLY | 2.3 |
| 1 | CA | 723 | U | 2.3 |
| 19 | CS | 21 | GLU | 2.3 |
| 19 | CS | 28 | LYS | 2.3 |
| 2 | AB | 121 | LEU | 2.3 |
| 2 | AB | 222 | ILE | 2.3 |
| 11 | AK | 60 | ALA | 2.3 |
| 27 | B5 | 53 | ALA | 2.3 |
| 1 | AA | 219 | C | 2.3 |
| 4 | CD | 35 | ARG | 2.3 |
| 7 | AG | 84 | ASN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | AC | 197 | GLY | 2.3 |
| 10 | AJ | 93 | GLY | 2.3 |
| 11 | AK | 17 | GLY | 2.3 |
| 34 | BE | 59 | VAL | 2.3 |
| 2 | AB | 95 | GLN | 2.3 |
| 11 | AK | 81 | ASP | 2.3 |
| 14 | CN | 58 | LYS | 2.3 |
| 31 | DA | 311 | A | 2.3 |
| 31 | DA | 1111 | A | 2.3 |
| 31 | DA | 1916 | A | 2.3 |
| 4 | CD | 131 | ARG | 2.3 |
| 10 | CJ | 88 | LEU | 2.3 |
| 18 | AR | 79 | LEU | 2.3 |
| 35 | DF | 14 | PRO | 2.3 |
| 20 | AT | 87 | LYS | 2.3 |
| 31 | BA | 1051 | G | 2.3 |
| 32 | DB | 89 | G | 2.3 |
| 51 | DZ | 114 | GLY | 2.3 |
| 1 | AA | 1352 | C | 2.3 |
| 7 | AG | 123 | GLU | 2.3 |
| 1 | AA | 986 | A | 2.3 |
| 1 | AA | 1319 | A | 2.3 |
| 1 | CA | 923 | A | 2.3 |
| 4 | AD | 4 | TYR | 2.3 |
| 1 | AA | 1136 | U | 2.3 |
| 1 | AA | 1393 | U | 2.3 |
| 7 | AG | 58 | PRO | 2.3 |
| 3 | CC | 80 | GLY | 2.3 |
| 36 | DG | 125 | PHE | 2.3 |
| 7 | CG | 96 | GLN | 2.3 |
| 41 | DP | 94 | GLU | 2.3 |
| 9 | CI | 51 | ARG | 2.3 |
| 3 | CC | 201 | TYR | 2.3 |
| 5 | AE | 17 | ALA | 2.3 |
| 31 | BA | 1112 | G | 2.3 |
| 44 | DS | 32 | LEU | 2.3 |
| 51 | DZ | 90 | VAL | 2.3 |
| 1 | AA | 1123 | A | 2.3 |
| 1 | CA | 697 | U | 2.3 |
| 5 | AE | 35 | GLY | 2.3 |
| 41 | BP | 104 | GLY | 2.3 |
| 10 | CJ | 61 | GLU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 16 | CP | 13 | HIS | 2.3 |
| 41 | DP | 149 | GLU | 2.3 |
| 7 | CG | 97 | GLN | 2.3 |
| 46 | BU | 75 | ASN | 2.3 |
| 51 | DZ | 87 | ASP | 2.3 |
| 1 | AA | 201 | C | 2.3 |
| 1 | CA | 419 | C | 2.3 |
| 31 | DA | 1166 | C | 2.3 |
| 1 | AA | 64 | G | 2.3 |
| 31 | BA | 919 | G | 2.3 |
| 36 | BG | 112 | PRO | 2.3 |
| 10 | AJ | 29 | ARG | 2.3 |
| 10 | AJ | 66 | ARG | 2.3 |
| 19 | CS | 43 | GLU | 2.3 |
| 21 | CU | 22 | ARG | 2.3 |
| 1 | AA | 171 | A | 2.3 |
| 1 | CA | 1502 | A | 2.3 |
| 3 | CC | 3 | ASN | 2.3 |
| 7 | AG | 106 | GLN | 2.3 |
| 13 | AM | 19 | LEU | 2.3 |
| 15 | AO | 22 | THR | 2.3 |
| 11 | AK | 84 | VAL | 2.3 |
| 13 | CM | 85 | GLY | 2.3 |
| 7 | AG | 72 | ARG | 2.3 |
| 1 | AA | 1208 | C | 2.3 |
| 1 | CA | 366 | C | 2.3 |
| 1 | CA | 990 | C | 2.3 |
| 2 | AB | 210 | SER | 2.3 |
| 13 | AM | 114 | ARG | 2.3 |
| 51 | DZ | 4 | ARG | 2.3 |
| 13 | AM | 46 | LYS | 2.3 |
| 31 | DA | 334 | C | 2.3 |
| 50 | DY | 88 | LYS | 2.3 |
| 1 | AA | 191 | G | 2.3 |
| 1 | AA | 1308 | U | 2.3 |
| 1 | AA | 151 | A | 2.3 |
| 2 | AB | 165 | VAL | 2.3 |
| 2 | CB | 34 | ALA | 2.3 |
| 6 | CF | 35 | ALA | 2.3 |
| 12 | AL | 64 | TYR | 2.3 |
| 28 | B6 | 21 | TYR | 2.3 |
| 11 | CK | 82 | VAL | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | CF | 3 | ARG | 2.3 |
| 4 | AD | 179 | GLU | 2.3 |
| 36 | BG | 105 | LYS | 2.3 |
| 44 | DS | 103 | GLU | 2.3 |
| 1 | AA | 470 | C | 2.3 |
| 2 | AB | 76 | GLN | 2.3 |
| 6 | AF | 98 | LEU | 2.3 |
| 2 | CB | 97 | TRP | 2.3 |
| 7 | CG | 120 | ILE | 2.3 |
| 7 | AG | 69 | VAL | 2.3 |
| 16 | AP | 58 | TYR | 2.3 |
| 33 | BD | 34 | VAL | 2.3 |
| 46 | DU | 113 | ALA | 2.3 |
| 38 | DI | 93 | THR | 2.3 |
| 1 | AA | 1009 | G | 2.3 |
| 1 | CA | 410 | G | 2.3 |
| 1 | CA | 538 | G | 2.3 |
| 1 | CA | 964 | A | 2.3 |
| 1 | CA | 1233 | G | 2.3 |
| 10 | CJ | 64 | GLU | 2.3 |
| 17 | CQ | 100 | LYS | 2.3 |
| 5 | AE | 19 | MET | 2.3 |
| 9 | CI | 99 | LEU | 2.3 |
| 26 | D4 | 31 | ILE | 2.3 |
| 38 | DI | 133 | HIS | 2.3 |
| 9 | CI | 94 | ALA | 2.3 |
| 50 | BY | 2 | ARG | 2.3 |
| 12 | CL | 74 | GLY | 2.3 |
| 17 | AQ | 14 | LYS | 2.3 |
| 31 | BA | 1467 | C | 2.3 |
| 1 | CA | 976 | G | 2.3 |
| 5 | AE | 129 | ILE | 2.3 |
| 10 | AJ | 45 | ARG | 2.3 |
| 10 | AJ | 96 | ILE | 2.3 |
| 2 | AB | 188 | ALA | 2.3 |
| 5 | CE | 34 | VAL | 2.3 |
| 9 | AI | 33 | PHE | 2.3 |
| 33 | DD | 154 | LYS | 2.3 |
| 16 | AP | 10 | GLY | 2.3 |
| 23 | D1 | 79 | GLY | 2.3 |
| 1 | AA | 1040 | U | 2.3 |
| 1 | AA | 1121 | U | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 1395 | C | 2.3 |
| 1 | CA | 921 | U | 2.3 |
| 5 | CE | 120 | THR | 2.3 |
| 31 | DA | 816 | C | 2.3 |
| 31 | DA | 877 | U | 2.3 |
| 31 | DA | 2666 | C | 2.3 |
| 32 | DB | 114 | C | 2.3 |
| 7 | CG | 71 | PRO | 2.3 |
| 13 | AM | 100 | GLY | 2.2 |
| 5 | AE | 43 | LEU | 2.2 |
| 18 | CR | 31 | LEU | 2.2 |
| 31 | BA | 1578 | U | 2.2 |
| 36 | DG | 118 | ARG | 2.2 |
| 44 | BS | 89 | ARG | 2.2 |
| 1 | AA | 419 | C | 2.2 |
| 1 | AA | 1259 | C | 2.2 |
| 2 | AB | 207 | ALA | 2.2 |
| 2 | CB | 150 | SER | 2.2 |
| 9 | CI | 80 | GLY | 2.2 |
| 36 | BG | 46 | ALA | 2.2 |
| 1 | AA | 1055 | A | 2.2 |
| 1 | CA | 969 | A | 2.2 |
| 38 | DI | 82 | ARG | 2.2 |
| 39 | BN | 134 | ARG | 2.2 |
| 3 | AC | 67 | THR | 2.2 |
| 31 | BA | 1709 | U | 2.2 |
| 1 | AA | 1378 | C | 2.2 |
| 9 | AI | 6 | GLY | 2.2 |
| 9 | CI | 6 | GLY | 2.2 |
| 20 | CT | 102 | GLY | 2.2 |
| 46 | DU | 117 | GLN | 2.2 |
| 7 | CG | 101 | LEU | 2.2 |
| 36 | BG | 94 | LEU | 2.2 |
| 1 | CA | 1374 | A | 2.2 |
| 31 | BA | 1046 | A | 2.2 |
| 31 | BA | 1494 | A | 2.2 |
| 36 | BG | 71 | THR | 2.2 |
| 51 | DZ | 69 | THR | 2.2 |
| 1 | AA | 1057 | G | 2.2 |
| 10 | AJ | 43 | ARG | 2.2 |
| 13 | CM | 38 | GLY | 2.2 |
| 15 | AO | 89 | GLY | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 19 | AS | 52 | TYR | 2.2 |
| 19 | AS | 80 | TYR | 2.2 |
| 31 | DA | 354 | G | 2.2 |
| 37 | DH | 18 | GLU | 2.2 |
| 41 | DP | 110 | TYR | 2.2 |
| 44 | BS | 36 | TYR | 2.2 |
| 2 | CB | 187 | LEU | 2.2 |
| 4 | AD | 208 | SER | 2.2 |
| 4 | AD | 70 | ILE | 2.2 |
| 5 | CE | 90 | VAL | 2.2 |
| 13 | CM | 25 | ILE | 2.2 |
| 36 | BG | 63 | ILE | 2.2 |
| 5 | CE | 130 | ASN | 2.2 |
| 20 | CT | 64 | ASP | 2.2 |
| 1 | CA | 1170 | A | 2.2 |
| 1 | CA | 1213 | A | 2.2 |
| 3 | CC | 117 | ALA | 2.2 |
| 15 | CO | 6 | GLU | 2.2 |
| 19 | AS | 72 | GLY | 2.2 |
| 28 | D6 | 23 | THR | 2.2 |
| 50 | DY | 54 | LYS | 2.2 |
| 1 | AA | 541 | G | 2.2 |
| 1 | CA | 1442 | G | 2.2 |
| 4 | AD | 175 | SER | 2.2 |
| 31 | BA | 1525 | G | 2.2 |
| 1 | CA | 930 | C | 2.2 |
| 2 | AB | 15 | VAL | 2.2 |
| 20 | CT | 88 | VAL | 2.2 |
| 7 | CG | 18 | TYR | 2.2 |
| 16 | AP | 70 | ALA | 2.2 |
| 37 | BH | 139 | GLN | 2.2 |
| 1 | CA | 609 | A | 2.2 |
| 1 | CA | 949 | A | 2.2 |
| 31 | DA | 2809 | A | 2.2 |
| 36 | DG | 3 | LEU | 2.2 |
| 51 | BZ | 144 | LEU | 2.2 |
| 2 | CB | 53 | ARG | 2.2 |
| 2 | CB | 217 | ARG | 2.2 |
| 3 | CC | 79 | ARG | 2.2 |
| 8 | AH | 30 | ARG | 2.2 |
| 12 | CL | 33 | ARG | 2.2 |
| 12 | CL | 113 | ARG | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | CM | 65 | LYS | 2.2 |
| 15 | AO | 82 | ILE | 2.2 |
| 51 | DZ | 112 | ARG | 2.2 |
| 13 | CM | 32 | GLU | 2.2 |
| 1 | CA | 1190 | G | 2.2 |
| 31 | BA | 281 | G | 2.2 |
| 31 | DA | 317 | G | 2.2 |
| 41 | BP | 120 | ALA | 2.2 |
| 9 | CI | 23 | ASN | 2.2 |
| 7 | AG | 137 | LYS | 2.2 |
| 17 | AQ | 99 | SER | 2.2 |
| 31 | DA | 2810 | A | 2.2 |
| 1 | AA | 699 | C | 2.2 |
| 1 | CA | 1069 | C | 2.2 |
| 2 | CB | 44 | LEU | 2.2 |
| 32 | DB | 30 | C | 2.2 |
| 38 | DI | 104 | GLN | 2.2 |
| 46 | DU | 74 | LEU | 2.2 |
| 1 | AA | 1022 | G | 2.2 |
| 16 | CP | 80 | PHE | 2.2 |
| 31 | BA | 2184 | G | 2.2 |
| 34 | BE | 76 | ARG | 2.2 |
| 1 | AA | 82 | U | 2.2 |
| 1 | AA | 921 | U | 2.2 |
| 36 | BG | 59 | GLU | 2.2 |
| 41 | BP | 118 | GLY | 2.2 |
| 1 | AA | 1350 | A | 2.2 |
| 7 | CG | 76 | ARG | 2.2 |
| 9 | AI | 104 | ARG | 2.2 |
| 38 | BI | 35 | LEU | 2.2 |
| 10 | AJ | 3 | LYS | 2.2 |
| 12 | CL | 114 | LYS | 2.2 |
| 18 | CR | 29 | PHE | 2.2 |
| 7 | CG | 156 | TRP | 2.2 |
| 1 | AA | 113 | G | 2.2 |
| 1 | AA | 631 | G | 2.2 |
| 1 | CA | 1276 | G | 2.2 |
| 1 | AA | 960 | U | 2.2 |
| 1 | CA | 1095 | U | 2.2 |
| 5 | CE | 9 | LYS | 2.2 |
| 12 | AL | 54 | LYS | 2.2 |
| 45 | DT | 118 | ARG | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | CA | 1191 | A | 2.2 |
| 16 | AP | 41 | PRO | 2.2 |
| 36 | DG | 122 | PRO | 2.2 |
| 7 | AG | 139 | GLU | 2.2 |
| 12 | CL | 43 | VAL | 2.2 |
| 2 | CB | 113 | HIS | 2.2 |
| 1 | CA | 1126 | U | 2.2 |
| 1 | CA | 1355 | G | 2.2 |
| 51 | DZ | 89 | PHE | 2.2 |
| 9 | AI | 32 | ASP | 2.2 |
| 12 | AL | 43 | VAL | 2.2 |
| 1 | AA | 1333 | A | 2.2 |
| 11 | AK | 91 | ARG | 2.2 |
| 31 | DA | 1847 | A | 2.2 |
| 41 | DP | 135 | LEU | 2.1 |
| 1 | AA | 1038 | C | 2.1 |
| 1 | AA | 1263 | C | 2.1 |
| 11 | CK | 100 | ALA | 2.1 |
| 32 | BB | 5 | C | 2.1 |
| 35 | DF | 115 | ALA | 2.1 |
| 13 | CM | 68 | GLY | 2.1 |
| 51 | DZ | 156 | LYS | 2.1 |
| 1 | AA | 1306 | A | 2.1 |
| 9 | CI | 117 | HIS | 2.1 |
| 16 | AP | 16 | HIS | 2.1 |
| 51 | DZ | 34 | ASN | 2.1 |
| 5 | AE | 132 | ALA | 2.1 |
| 16 | CP | 7 | ALA | 2.1 |
| 4 | CD | 115 | ARG | 2.1 |
| 9 | AI | 74 | ILE | 2.1 |
| 21 | AU | 15 | ARG | 2.1 |
| 41 | DP | 117 | GLU | 2.1 |
| 1 | CA | 1083 | U | 2.1 |
| 1 | CA | 1205 | U | 2.1 |
| 3 | CC | 188 | LEU | 2.1 |
| 9 | AI | 13 | ALA | 2.1 |
| 11 | CK | 28 | THR | 2.1 |
| 14 | CN | 13 | THR | 2.1 |
| 36 | DG | 11 | TYR | 2.1 |
| 1 | AA | 1294 | G | 2.1 |
| 1 | CA | 66 | G | 2.1 |
| 9 | AI | 37 | PHE | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | DG | 145 | THR | 2.1 |
| 2 | CB | 32 | ILE | 2.1 |
| 9 | CI | 14 | VAL | 2.1 |
| 14 | CN | 42 | ILE | 2.1 |
| 2 | CB | 202 | PRO | 2.1 |
| 26 | D4 | 11 | PRO | 2.1 |
| 30 | D8 | 37 | SER | 2.1 |
| 1 | CA | 1051 | C | 2.1 |
| 2 | AB | 37 | ASN | 2.1 |
| 10 | CJ | 46 | ARG | 2.1 |
| 2 | CB | 35 | GLU | 2.1 |
| 19 | AS | 17 | GLU | 2.1 |
| 21 | CU | 13 | ILE | 2.1 |
| 47 | BV | 60 | GLU | 2.1 |
| 1 | AA | 353 | A | 2.1 |
| 1 | CA | 814 | A | 2.1 |
| 1 | CA | 1009 | G | 2.1 |
| 15 | CO | 20 | GLY | 2.1 |
| 19 | AS | 44 | MET | 2.1 |
| 37 | DH | 93 | GLY | 2.1 |
| 16 | AP | 40 | ASP | 2.1 |
| 1 | AA | 1103 | C | 2.1 |
| 1 | CA | 470 | C | 2.1 |
| 3 | AC | 105 | GLU | 2.1 |
| 45 | BT | 40 | THR | 2.1 |
| 3 | AC | 104 | GLN | 2.1 |
| 5 | AE | 77 | PRO | 2.1 |
| 26 | D4 | 7 | PRO | 2.1 |
| 1 | AA | 1004 | A | 2.1 |
| 4 | AD | 38 | TYR | 2.1 |
| 31 | BA | 1445 | A | 2.1 |
| 1 | AA | 204 | U | 2.1 |
| 1 | CA | 786 | G | 2.1 |
| 1 | CA | 1258 | G | 2.1 |
| 1 | CA | 1368 | G | 2.1 |
| 19 | CS | 47 | HIS | 2.1 |
| 31 | BA | 508 | G | 2.1 |
| 31 | DA | 1878 | G | 2.1 |
| 31 | DA | 2894 | G | 2.1 |
| 1 | CA | 1378 | C | 2.1 |
| 9 | AI | 108 | VAL | 2.1 |
| 31 | BA | 1049 | C | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | DH | 99 | VAL | 2.1 |
| 2 | AB | 111 | ARG | 2.1 |
| 10 | AJ | 90 | LEU | 2.1 |
| 14 | AN | 12 | ARG | 2.1 |
| 4 | CD | 4 | TYR | 2.1 |
| 7 | CG | 43 | PHE | 2.1 |
| 41 | BP | 122 | PRO | 2.1 |
| 13 | AM | 53 | VAL | 2.1 |
| 27 | D5 | 57 | VAL | 2.1 |
| 1 | CA | 223 | U | 2.1 |
| 31 | DA | 2897 | U | 2.1 |
| 1 | AA | 928 | G | 2.1 |
| 1 | CA | 199 | G | 2.1 |
| 1 | CA | 1171 | G | 2.1 |
| 12 | CL | 29 | GLY | 2.1 |
| 32 | DB | 51 | G | 2.1 |
| 36 | DG | 170 | ARG | 2.1 |
| 36 | DG | 177 | GLY | 2.1 |
| 42 | DQ | 87 | LYS | 2.1 |
| 31 | DA | 318 | C | 2.1 |
| 12 | AL | 26 | ALA | 2.1 |
| 35 | BF | 7 | TYR | 2.1 |
| 5 | CE | 7 | GLU | 2.1 |
| 13 | AM | 73 | GLU | 2.1 |
| 45 | DT | 11 | GLU | 2.1 |
| 2 | AB | 209 | ARG | 2.1 |
| 3 | AC | 157 | ILE | 2.1 |
| 5 | CE | 121 | LYS | 2.1 |
| 28 | D6 | 46 | HIS | 2.1 |
| 1 | AA | 393 | A | 2.1 |
| 1 | AA | 1302 | U | 2.1 |
| 41 | BP | 99 | LEU | 2.1 |
| 1 | AA | 324 | G | 2.1 |
| 1 | AA | 391 | G | 2.1 |
| 1 | AA | 460 | G | 2.1 |
| 1 | AA | 1309 | G | 2.1 |
| 1 | CA | 1303 | C | 2.1 |
| 31 | BA | 1110 | G | 2.1 |
| 36 | DG | 30 | GLU | 2.1 |
| 41 | BP | 149 | GLU | 2.1 |
| 47 | DV | 60 | GLU | 2.1 |
| 8 | AH | 115 | SER | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | CI | 10 | ARG | 2.1 |
| 12 | CL | 100 | ILE | 2.1 |
| 18 | CR | 86 | VAL | 2.1 |
| 38 | BI | 121 | LYS | 2.1 |
| 38 | DI | 113 | ARG | 2.1 |
| 48 | DW | 113 | LYS | 2.1 |
| 8 | CH | 130 | GLY | 2.1 |
| 9 | CI | 69 | GLY | 2.1 |
| 51 | DZ | 55 | HIS | 2.1 |
| 5 | CE | 16 | THR | 2.1 |
| 4 | AD | 10 | ARG | 2.1 |
| 10 | CJ | 39 | PRO | 2.1 |
| 14 | AN | 34 | TYR | 2.1 |
| 22 | B0 | 4 | LYS | 2.1 |
| 35 | DF | 19 | GLU | 2.1 |
| 38 | DI | 80 | PRO | 2.1 |
| 1 | AA | 1228 | C | 2.1 |
| 1 | CA | 1336 | C | 2.1 |
| 6 | CF | 88 | VAL | 2.1 |
| 3 | CC | 49 | SER | 2.1 |
| 1 | AA | 1343 | G | 2.1 |
| 1 | CA | 954 | G | 2.1 |
| 9 | AI | 115 | GLY | 2.1 |
| 10 | CJ | 35 | SER | 2.1 |
| 2 | CB | 24 | TRP | 2.1 |
| 7 | AG | 20 | ASP | 2.1 |
| 7 | AG | 110 | GLN | 2.1 |
| 14 | AN | 58 | LYS | 2.1 |
| 1 | AA | 65 | U | 2.1 |
| 1 | CA | 1000 | U | 2.1 |
| 1 | CA | 1065 | U | 2.1 |
| 36 | BG | 92 | VAL | 2.1 |
| 23 | B1 | 80 | LEU | 2.1 |
| 37 | DH | 31 | GLY | 2.1 |
| 1 | CA | 1314 | C | 2.1 |
| 11 | CK | 110 | ASP | 2.1 |
| 31 | BA | 1577 | C | 2.1 |
| 3 | AC | 172 | ARG | 2.0 |
| 31 | BA | 1466 | G | 2.0 |
| 7 | CG | 100 | ALA | 2.0 |
| 13 | AM | 43 | THR | 2.0 |
| 36 | DG | 40 | ASN | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | AI | 63 | ILE | 2.0 |
| 19 | AS | 20 | LEU | 2.0 |
| 44 | DS | 35 | ILE | 2.0 |
| 1 | AA | 1225 | A | 2.0 |
| 1 | CA | 1280 | A | 2.0 |
| 10 | CJ | 80 | LYS | 2.0 |
| 13 | CM | 79 | LYS | 2.0 |
| 13 | AM | 101 | GLN | 2.0 |
| 16 | CP | 11 | SER | 2.0 |
| 18 | CR | 63 | GLN | 2.0 |
| 44 | BS | 52 | SER | 2.0 |
| 1 | CA | 1119 | C | 2.0 |
| 5 | AE | 122 | GLU | 2.0 |
| 41 | DP | 120 | ALA | 2.0 |
| 20 | AT | 53 | LEU | 2.0 |
| 49 | BX | 3 | THR | 2.0 |
| 1 | CA | 1373 | G | 2.0 |
| 31 | DA | 1940 | U | 2.0 |
| 4 | AD | 35 | ARG | 2.0 |
| 21 | AU | 10 | ARG | 2.0 |
| 47 | BV | 66 | ARG | 2.0 |
| 51 | BZ | 80 | ARG | 2.0 |
| 17 | CQ | 24 | GLU | 2.0 |
| 15 | CO | 60 | VAL | 2.0 |
| 16 | AP | 20 | VAL | 2.0 |
| 29 | B7 | 46 | VAL | 2.0 |
| 30 | B8 | 64 | TYR | 2.0 |
| 31 | BA | 918 | A | 2.0 |
| 1 | CA | 701 | C | 2.0 |
| 4 | AD | 135 | LEU | 2.0 |
| 17 | CQ | 98 | LEU | 2.0 |
| 5 | AE | 127 | ASN | 2.0 |
| 7 | AG | 41 | ARG | 2.0 |
| 13 | CM | 114 | ARG | 2.0 |
| 28 | B6 | 44 | ARG | 2.0 |
| 28 | D6 | 26 | ASN | 2.0 |
| 42 | DQ | 88 | GLY | 2.0 |
| 50 | BY | 86 | ARG | 2.0 |
| 1 | AA | 473 | G | 2.0 |
| 1 | AA | 698 | G | 2.0 |
| 1 | CA | 1081 | G | 2.0 |
| 1 | CA | 1273 | G | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | CF | 94 | GLN | 2.0 |
| 3 | CC | 154 | SER | 2.0 |
| 30 | D8 | 31 | HIS | 2.0 |
| 31 | BA | 2207 | G | 2.0 |
| 36 | DG | 12 | TYR | 2.0 |
| 45 | DT | 117 | ASP | 2.0 |
| 18 | CR | 21 | LYS | 2.0 |
| 20 | AT | 65 | LYS | 2.0 |
| 51 | DZ | 37 | VAL | 2.0 |
| 1 | AA | 16 | A | 2.0 |
| 1 | AA | 1268 | A | 2.0 |
| 14 | CN | 3 | ARG | 2.0 |
| 34 | BE | 61 | ARG | 2.0 |
| 36 | BG | 44 | GLY | 2.0 |
| 36 | DG | 154 | GLY | 2.0 |
| 1 | AA | 435 | C | 2.0 |
| 1 | CA | 1366 | C | 2.0 |
| 4 | AD | 93 | PHE | 2.0 |
| 7 | CG | 109 | ASN | 2.0 |
| 38 | DI | 1 | MET | 2.0 |
| 44 | BS | 107 | GLU | 2.0 |
| 51 | DZ | 94 | GLU | 2.0 |
| 1 | AA | 434 | U | 2.0 |
| 2 | AB | 219 | VAL | 2.0 |
| 9 | CI | 32 | ASP | 2.0 |
| 46 | DU | 110 | VAL | 2.0 |
| 28 | D6 | 50 | ARG | 2.0 |
| 47 | DV | 62 | LEU | 2.0 |
| 31 | BA | 1740 | G | 2.0 |
| 47 | BV | 75 | PHE | 2.0 |
| 18 | AR | 19 | LYS | 2.0 |
| 23 | D1 | 34 | THR | 2.0 |
| 31 | DA | 1877 | A | 2.0 |
| 32 | DB | 52 | A | 2.0 |
| 1 | AA | 67 | C | 2.0 |
| 1 | AA | 217 | C | 2.0 |
| 1 | AA | 1237 | C | 2.0 |
| 1 | AA | 1403 | C | 2.0 |
| 38 | DI | 54 | GLN | 2.0 |
| 9 | AI | 44 | VAL | 2.0 |
| 12 | AL | 120 | TYR | 2.0 |
| 16 | CP | 18 | ARG | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 37 | DH | 17 | VAL | 2.0 |
| 38 | DI | 140 | LEU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3324 | 1/1 | 0.42 | 0.46 | 69,69,69,69 | 0 |
| 52 | MG | DA | 3162 | 1/1 | 0.47 | 0.40 | 51,51,51,51 | 0 |
| 52 | MG | AA | 1645 | 1/1 | 0.62 | 0.57 | 75,75,75,75 | 0 |
| 52 | MG | BA | 3358 | 1/1 | 0.62 | 0.58 | 80,80,80,80 | 0 |
| 52 | MG | DA | 3276 | 1/1 | 0.63 | 0.47 | 65,65,65,65 | 0 |
| 52 | MG | DA | 3246 | 1/1 | 0.64 | 0.20 | 67,67,67,67 | 0 |
| 52 | MG | BA | 3319 | 1/1 | 0.65 | 0.42 | 64,64,64,64 | 0 |
| 52 | MG | AA | 1635 | 1/1 | 0.67 | 0.17 | 69,69,69,69 | 0 |
| 52 | MG | DA | 3205 | 1/1 | 0.69 | 0.51 | 62,62,62,62 | 0 |
| 52 | MG | BA | 3206 | 1/1 | 0.70 | 0.98 | 57,57,57,57 | 0 |
| 52 | MG | AA | 1642 | 1/1 | 0.71 | 0.46 | 73,73,73,73 | 0 |
| 52 | MG | AA | 1650 | 1/1 | 0.71 | 0.35 | 60,60,60,60 | 0 |
| 52 | MG | CA | 1613 | 1/1 | 0.71 | 0.55 | 68,68,68,68 | 0 |
| 52 | MG | CA | 1628 | 1/1 | 0.72 | 0.51 | 73,73,73,73 | 0 |
| 52 | MG | BA | 3257 | 1/1 | 0.72 | 0.25 | 23,23,23,23 | 0 |
| 52 | MG | BA | 3208 | 1/1 | 0.73 | 0.36 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3328 | 1/1 | 0.74 | 0.22 | 81,81,81,81 | 0 |
| 52 | MG | DA | 3304 | 1/1 | 0.74 | 0.15 | 65,65,65,65 | 0 |
| 52 | MG | DA | 3291 | 1/1 | 0.74 | 0.44 | 62,62,62,62 | 0 |
| 52 | MG | DA | 3247 | 1/1 | 0.74 | 0.44 | 76,76,76,76 | 0 |
| 52 | MG | DA | 3144 | 1/1 | 0.74 | 0.34 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | AA | 1634 | 1/1 | 0.74 | 0.56 | 55,55,55,55 | 0 |
| 52 | MG | CA | 1649 | 1/1 | 0.74 | 0.19 | 63,63,63,63 | 0 |
| 52 | MG | BA | 3327 | 1/1 | 0.75 | 0.53 | 48,48,48,48 | 0 |
| 52 | MG | DA | 3264 | 1/1 | 0.75 | 0.53 | 58,58,58,58 | 0 |
| 52 | MG | AA | 1613 | 1/1 | 0.75 | 0.22 | 76,76,76,76 | 0 |
| 52 | MG | DA | 3231 | 1/1 | 0.75 | 0.49 | 58,58,58,58 | 0 |
| 52 | MG | AA | 1644 | 1/1 | 0.76 | 0.36 | 87,87,87,87 | 0 |
| 52 | MG | DA | 3309 | 1/1 | 0.76 | 0.66 | 62,62,62,62 | 0 |
| 52 | MG | BA | 3248 | 1/1 | 0.76 | 0.38 | 46,46,46,46 | 0 |
| 52 | MG | CA | 1604 | 1/1 | 0.76 | 0.21 | 88,88,88,88 | 0 |
| 52 | MG | DA | 3170 | 1/1 | 0.76 | 0.33 | 61,61,61,61 | 0 |
| 52 | MG | BA | 3245 | 1/1 | 0.76 | 0.45 | 56,56,56,56 | 0 |
| 52 | MG | BA | 3304 | 1/1 | 0.77 | 0.58 | 55,55,55,55 | 0 |
| 52 | MG | DA | 3278 | 1/1 | 0.77 | 1.25 | 74,74,74,74 | 0 |
| 52 | MG | BA | 3074 | 1/1 | 0.77 | 0.60 | 60,60,60,60 | 0 |
| 52 | MG | CA | 1630 | 1/1 | 0.77 | 0.53 | 73,73,73,73 | 0 |
| 52 | MG | DA | 3316 | 1/1 | 0.77 | 0.71 | 60,60,60,60 | 0 |
| 52 | MG | BA | 3151 | 1/1 | 0.77 | 0.48 | 54,54,54,54 | 0 |
| 52 | MG | DA | 3261 | 1/1 | 0.77 | 0.22 | 63,63,63,63 | 0 |
| 52 | MG | DA | 3306 | 1/1 | 0.78 | 0.20 | 69,69,69,69 | 0 |
| 52 | MG | CA | 1635 | 1/1 | 0.78 | 0.45 | 77,77,77,77 | 0 |
| 52 | MG | BA | 3330 | 1/1 | 0.78 | 0.29 | 72,72,72,72 | 0 |
| 52 | MG | DA | 3280 | 1/1 | 0.78 | 0.67 | 64,64,64,64 | 0 |
| 52 | MG | DA | 3069 | 1/1 | 0.78 | 0.28 | 65,65,65,65 | 0 |
| 52 | MG | BA | 3175 | 1/1 | 0.79 | 0.40 | 62,62,62,62 | 0 |
| 52 | MG | DA | 3191 | 1/1 | 0.79 | 0.55 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3154 | 1/1 | 0.80 | 0.40 | 79,79,79,79 | 0 |
| 52 | MG | DA | 3105 | 1/1 | 0.80 | 0.20 | 43,43,43,43 | 0 |
| 52 | MG | DA | 3223 | 1/1 | 0.80 | 0.18 | 41,41,41,41 | 0 |
| 52 | MG | AA | 1651 | 1/1 | 0.80 | 0.70 | 57,57,57,57 | 0 |
| 52 | MG | CA | 1646 | 1/1 | 0.80 | 0.33 | 59,59,59,59 | 0 |
| 52 | MG | BA | 3273 | 1/1 | 0.81 | 0.41 | 42,42,42,42 | 0 |
| 52 | MG | DA | 3252 | 1/1 | 0.81 | 0.50 | 54,54,54,54 | 0 |
| 52 | MG | AA | 1611 | 1/1 | 0.81 | 0.15 | 82,82,82,82 | 0 |
| 52 | MG | D3 | 101 | 1/1 | 0.81 | 0.65 | 52,52,52,52 | 0 |
| 52 | MG | DA | 3199 | 1/1 | 0.81 | 0.18 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3238 | 1/1 | 0.81 | 0.22 | 40,40,40,40 | 0 |
| 52 | MG | BA | 3361 | 1/1 | 0.81 | 0.09 | 60,60,60,60 | 0 |
| 52 | MG | BA | 3317 | 1/1 | 0.81 | 0.39 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3140 | 1/1 | 0.81 | 0.17 | 46,46,46,46 | 0 |
| 52 | MG | DA | 3090 | 1/1 | 0.81 | 0.29 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3311 | 1/1 | 0.81 | 1.02 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | AA | 1628 | 1/1 | 0.82 | 0.51 | 70,70,70,70 | 0 |
| 52 | MG | DA | 3005 | 1/1 | 0.82 | 0.16 | 63,63,63,63 | 0 |
| 52 | MG | AA | 1653 | 1/1 | 0.82 | 0.08 | 61,61,61,61 | 0 |
| 52 | MG | BA | 3342 | 1/1 | 0.82 | 0.30 | 38,38,38,38 | 0 |
| 52 | MG | CA | 1637 | 1/1 | 0.82 | 0.42 | 61,61,61,61 | 0 |
| 52 | MG | DA | 3300 | 1/1 | 0.82 | 0.88 | 64,64,64,64 | 0 |
| 52 | MG | DA | 3298 | 1/1 | 0.83 | 0.17 | 46,46,46,46 | 0 |
| 52 | MG | DA | 3283 | 1/1 | 0.83 | 0.58 | 67,67,67,67 | 0 |
| 52 | MG | DA | 3320 | 1/1 | 0.83 | 0.67 | 68,68,68,68 | 0 |
| 52 | MG | DA | 3163 | 1/1 | 0.83 | 0.53 | 59,59,59,59 | 0 |
| 52 | MG | DA | 3325 | 1/1 | 0.83 | 0.50 | 67,67,67,67 | 0 |
| 52 | MG | DA | 3166 | 1/1 | 0.83 | 0.43 | 54,54,54,54 | 0 |
| 52 | MG | DA | 3243 | 1/1 | 0.83 | 0.14 | 41,41,41,41 | 0 |
| 52 | MG | CA | 1638 | 1/1 | 0.83 | 0.32 | 61,61,61,61 | 0 |
| 52 | MG | DA | 3047 | 1/1 | 0.83 | 0.45 | 36,36,36,36 | 0 |
| 52 | MG | AA | 1624 | 1/1 | 0.83 | 0.43 | 58,58,58,58 | 0 |
| 52 | MG | DF | 301 | 1/1 | 0.83 | 0.34 | 57,57,57,57 | 0 |
| 52 | MG | CA | 1602 | 1/1 | 0.83 | 0.67 | 55,55,55,55 | 0 |
| 52 | MG | DA | 3301 | 1/1 | 0.83 | 0.74 | 54,54,54,54 | 0 |
| 52 | MG | DA | 3040 | 1/1 | 0.83 | 0.78 | 50,50,50,50 | 0 |
| 52 | MG | DA | 3277 | 1/1 | 0.83 | 0.43 | 76,76,76,76 | 0 |
| 52 | MG | BA | 3265 | 1/1 | 0.83 | 0.26 | 41,41,41,41 | 0 |
| 52 | MG | AA | 1607 | 1/1 | 0.84 | 0.54 | 58,58,58,58 | 0 |
| 52 | MG | BA | 3239 | 1/1 | 0.84 | 0.32 | 50,50,50,50 | 0 |
| 52 | MG | BA | 3336 | 1/1 | 0.84 | 0.79 | 69,69,69,69 | 0 |
| 52 | MG | DA | 3123 | 1/1 | 0.84 | 0.19 | 57,57,57,57 | 0 |
| 52 | MG | AA | 1638 | 1/1 | 0.84 | 0.28 | 67,67,67,67 | 0 |
| 52 | MG | DA | 3208 | 1/1 | 0.84 | 0.27 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3220 | 1/1 | 0.84 | 0.51 | 40,40,40,40 | 0 |
| 52 | MG | AA | 1604 | 1/1 | 0.84 | 0.31 | 73,73,73,73 | 0 |
| 52 | MG | DA | 3267 | 1/1 | 0.84 | 0.34 | 49,49,49,49 | 0 |
| 52 | MG | DA | 3143 | 1/1 | 0.84 | 0.28 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3083 | 1/1 | 0.84 | 0.38 | 35,35,35,35 | 0 |
| 52 | MG | DA | 3141 | 1/1 | 0.84 | 0.81 | 70,70,70,70 | 0 |
| 52 | MG | AA | 1621 | 1/1 | 0.84 | 0.47 | 50,50,50,50 | 0 |
| 52 | MG | DA | 3305 | 1/1 | 0.84 | 0.23 | 83,83,83,83 | 0 |
| 52 | MG | DA | 3219 | 1/1 | 0.84 | 0.64 | 57,57,57,57 | 0 |
| 52 | MG | BA | 3321 | 1/1 | 0.85 | 0.28 | 48,48,48,48 | 0 |
| 52 | MG | BB | 204 | 1/1 | 0.85 | 0.39 | 43,43,43,43 | 0 |
| 52 | MG | DA | 3279 | 1/1 | 0.85 | 0.29 | 59,59,59,59 | 0 |
| 52 | MG | DA | 3131 | 1/1 | 0.85 | 0.17 | 82,82,82,82 | 0 |
| 52 | MG | DA | 3294 | 1/1 | 0.85 | 0.52 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | AA | 1609 | 1/1 | 0.85 | 0.39 | 50,50,50,50 | 0 |
| 52 | MG | BA | 3341 | 1/1 | 0.85 | 0.12 | 70,70,70,70 | 0 |
| 52 | MG | BA | 3235 | 1/1 | 0.85 | 0.47 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3352 | 1/1 | 0.85 | 0.55 | 62,62,62,62 | 0 |
| 52 | MG | DQ | 201 | 1/1 | 0.85 | 0.24 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3328 | 1/1 | 0.85 | 0.46 | 56,56,56,56 | 0 |
| 52 | MG | BA | 3297 | 1/1 | 0.85 | 0.40 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3206 | 1/1 | 0.85 | 0.57 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3360 | 1/1 | 0.85 | 0.09 | 64,64,64,64 | 0 |
| 52 | MG | BA | 3357 | 1/1 | 0.85 | 0.28 | 71,71,71,71 | 0 |
| 52 | MG | DA | 3260 | 1/1 | 0.85 | 0.24 | 65,65,65,65 | 0 |
| 52 | MG | BA | 3345 | 1/1 | 0.85 | 0.32 | 48,48,48,48 | 0 |
| 52 | MG | DA | 3262 | 1/1 | 0.85 | 0.21 | 57,57,57,57 | 0 |
| 52 | MG | BA | 3350 | 1/1 | 0.85 | 0.21 | 65,65,65,65 | 0 |
| 52 | MG | BA | 3344 | 1/1 | 0.85 | 0.44 | 60,60,60,60 | 0 |
| 52 | MG | DA | 3268 | 1/1 | 0.86 | 0.39 | 52,52,52,52 | 0 |
| 52 | MG | DA | 3318 | 1/1 | 0.86 | 0.10 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3097 | 1/1 | 0.86 | 0.48 | 54,54,54,54 | 0 |
| 52 | MG | BA | 3130 | 1/1 | 0.86 | 0.45 | 55,55,55,55 | 0 |
| 52 | MG | DA | 3116 | 1/1 | 0.86 | 0.28 | 62,62,62,62 | 0 |
| 52 | MG | DA | 3092 | 1/1 | 0.86 | 0.53 | 40,40,40,40 | 0 |
| 52 | MG | DA | 3130 | 1/1 | 0.86 | 0.26 | 59,59,59,59 | 0 |
| 52 | MG | BA | 3332 | 1/1 | 0.86 | 0.43 | 40,40,40,40 | 0 |
| 52 | MG | BA | 3183 | 1/1 | 0.86 | 0.27 | 54,54,54,54 | 0 |
| 52 | MG | BA | 3236 | 1/1 | 0.86 | 0.37 | 25,25,25,25 | 0 |
| 52 | MG | BA | 3281 | 1/1 | 0.86 | 0.88 | 61,61,61,61 | 0 |
| 52 | MG | BA | 3254 | 1/1 | 0.86 | 0.35 | 55,55,55,55 | 0 |
| 52 | MG | DA | 3178 | 1/1 | 0.86 | 0.33 | 58,58,58,58 | 0 |
| 52 | MG | BA | 3312 | 1/1 | 0.86 | 0.10 | 40,40,40,40 | 0 |
| 52 | MG | DA | 3212 | 1/1 | 0.86 | 0.35 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3289 | 1/1 | 0.86 | 0.71 | 65,65,65,65 | 0 |
| 52 | MG | DA | 3271 | 1/1 | 0.86 | 0.50 | 61,61,61,61 | 0 |
| 52 | MG | DA | 3085 | 1/1 | 0.87 | 0.12 | 22,22,22,22 | 0 |
| 52 | MG | BA | 3298 | 1/1 | 0.87 | 0.43 | 59,59,59,59 | 0 |
| 52 | MG | BA | 3042 | 1/1 | 0.87 | 0.35 | 14,14,14,14 | 0 |
| 52 | MG | CA | 1608 | 1/1 | 0.87 | 0.37 | 74,74,74,74 | 0 |
| 52 | MG | BA | 3152 | 1/1 | 0.87 | 0.13 | 55,55,55,55 | 0 |
| 52 | MG | BA | 3270 | 1/1 | 0.87 | 0.11 | 66,66,66,66 | 0 |
| 52 | MG | DA | 3189 | 1/1 | 0.87 | 0.56 | 42,42,42,42 | 0 |
| 52 | MG | D7 | 101 | 1/1 | 0.87 | 0.28 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3284 | 1/1 | 0.87 | 0.81 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3233 | 1/1 | 0.87 | 0.20 | 21,21,21,21 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3190 | 1/1 | 0.87 | 0.54 | 43,43,43,43 | 0 |
| 52 | MG | DA | 3323 | 1/1 | 0.87 | 0.10 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3229 | 1/1 | 0.87 | 0.34 | 52,52,52,52 | 0 |
| 52 | MG | AA | 1612 | 1/1 | 0.87 | 0.65 | 70,70,70,70 | 0 |
| 52 | MG | CA | 1624 | 1/1 | 0.87 | 0.28 | 55,55,55,55 | 0 |
| 52 | MG | BA | 3187 | 1/1 | 0.87 | 0.41 | 48,48,48,48 | 0 |
| 52 | MG | BA | 3112 | 1/1 | 0.87 | 0.20 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3355 | 1/1 | 0.87 | 0.26 | 64,64,64,64 | 0 |
| 52 | MG | DA | 3319 | 1/1 | 0.88 | 0.18 | 40,40,40,40 | 0 |
| 52 | MG | BA | 3353 | 1/1 | 0.88 | 0.30 | 26,26,26,26 | 0 |
| 52 | MG | BA | 3288 | 1/1 | 0.88 | 0.27 | 65,65,65,65 | 0 |
| 52 | MG | DA | 3193 | 1/1 | 0.88 | 0.24 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3056 | 1/1 | 0.88 | 0.14 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3271 | 1/1 | 0.88 | 0.44 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3240 | 1/1 | 0.88 | 0.43 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3021 | 1/1 | 0.88 | 0.41 | 22,22,22,22 | 0 |
| 52 | MG | BA | 3179 | 1/1 | 0.88 | 0.52 | 41,41,41,41 | 0 |
| 52 | MG | BA | 3054 | 1/1 | 0.88 | 0.20 | 47,47,47,47 | 0 |
| 52 | MG | BA | 3159 | 1/1 | 0.88 | 0.59 | 43,43,43,43 | 0 |
| 52 | MG | BA | 3114 | 1/1 | 0.88 | 0.36 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3016 | 1/1 | 0.88 | 0.60 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3049 | 1/1 | 0.88 | 0.42 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3289 | 1/1 | 0.88 | 0.23 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3165 | 1/1 | 0.88 | 0.18 | 44,44,44,44 | 0 |
| 52 | MG | AA | 1646 | 1/1 | 0.88 | 0.23 | 51,51,51,51 | 0 |
| 52 | MG | AA | 1616 | 1/1 | 0.88 | 0.26 | 76,76,76,76 | 0 |
| 52 | MG | BA | 3174 | 1/1 | 0.88 | 0.36 | 40,40,40,40 | 0 |
| 52 | MG | BA | 3362 | 1/1 | 0.88 | 0.10 | 70,70,70,70 | 0 |
| 52 | MG | BP | 203 | 1/1 | 0.88 | 0.72 | 55,55,55,55 | 0 |
| 52 | MG | AA | 1648 | 1/1 | 0.88 | 0.19 | 82,82,82,82 | 0 |
| 52 | MG | BA | 3285 | 1/1 | 0.88 | 0.40 | 59,59,59,59 | 0 |
| 52 | MG | BA | 3202 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 52 | MG | BA | 3356 | 1/1 | 0.88 | 0.37 | 60,60,60,60 | 0 |
| 52 | MG | BA | 3085 | 1/1 | 0.89 | 0.14 | 8,8,8,8 | 0 |
| 52 | MG | DA | 3270 | 1/1 | 0.89 | 0.33 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3178 | 1/1 | 0.89 | 0.40 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3026 | 1/1 | 0.89 | 0.36 | 66,66,66,66 | 0 |
| 52 | MG | BA | 3090 | 1/1 | 0.89 | 0.45 | 18,18,18,18 | 0 |
| 52 | MG | DA | 3083 | 1/1 | 0.89 | 0.50 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3195 | 1/1 | 0.89 | 0.38 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3346 | 1/1 | 0.89 | 0.24 | 60,60,60,60 | 0 |
| 52 | MG | AA | 1608 | 1/1 | 0.89 | 0.32 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3307 | 1/1 | 0.89 | 0.28 | 41,41,41,41 | 0 |
| 52 | MG | BA | 3286 | 1/1 | 0.89 | 0.38 | 30,30,30,30 | 0 |
| 52 | MG | BA | 3314 | 1/1 | 0.89 | 0.35 | 49,49,49,49 | 0 |
| 52 | MG | CA | 1610 | 1/1 | 0.89 | 0.16 | 90,90,90,90 | 0 |
| 52 | MG | BA | 3093 | 1/1 | 0.89 | 0.44 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3213 | 1/1 | 0.89 | 0.35 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3237 | 1/1 | 0.89 | 0.13 | 46,46,46,46 | 0 |
| 52 | MG | CA | 1636 | 1/1 | 0.89 | 1.11 | 76,76,76,76 | 0 |
| 52 | MG | CA | 1607 | 1/1 | 0.89 | 0.52 | 58,58,58,58 | 0 |
| 52 | MG | BA | 3164 | 1/1 | 0.89 | 0.26 | 30,30,30,30 | 0 |
| 52 | MG | CA | 1625 | 1/1 | 0.89 | 0.22 | 54,54,54,54 | 0 |
| 52 | MG | BA | 3037 | 1/1 | 0.89 | 0.55 | 22,22,22,22 | 0 |
| 52 | MG | DA | 3236 | 1/1 | 0.89 | 0.61 | 43,43,43,43 | 0 |
| 52 | MG | AA | 1652 | 1/1 | 0.89 | 0.42 | 66,66,66,66 | 0 |
| 52 | MG | BA | 3026 | 1/1 | 0.89 | 0.34 | 48,48,48,48 | 0 |
| 52 | MG | DA | 3232 | 1/1 | 0.89 | 0.22 | 50,50,50,50 | 0 |
| 52 | MG | CA | 1643 | 1/1 | 0.89 | 0.57 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3286 | 1/1 | 0.89 | 0.41 | 47,47,47,47 | 0 |
| 52 | MG | DB | 201 | 1/1 | 0.89 | 0.46 | 58,58,58,58 | 0 |
| 52 | MG | BA | 3313 | 1/1 | 0.89 | 0.31 | 38,38,38,38 | 0 |
| 52 | MG | AA | 1643 | 1/1 | 0.89 | 0.65 | 59,59,59,59 | 0 |
| 52 | MG | DA | 3164 | 1/1 | 0.89 | 0.24 | 49,49,49,49 | 0 |
| 52 | MG | AA | 1615 | 1/1 | 0.89 | 0.29 | 49,49,49,49 | 0 |
| 52 | MG | BA | 3249 | 1/1 | 0.89 | 0.66 | 63,63,63,63 | 0 |
| 52 | MG | DA | 3311 | 1/1 | 0.89 | 0.20 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3139 | 1/1 | 0.89 | 0.50 | 60,60,60,60 | 0 |
| 52 | MG | DA | 3153 | 1/1 | 0.89 | 0.47 | 54,54,54,54 | 0 |
| 52 | MG | DA | 3125 | 1/1 | 0.89 | 0.12 | 45,45,45,45 | 0 |
| 52 | MG | DA | 3159 | 1/1 | 0.89 | 0.49 | 48,48,48,48 | 0 |
| 53 | ZN | AN | 101 | 1/1 | 0.90 | 0.15 | 157,157,157,157 | 0 |
| 52 | MG | BA | 3290 | 1/1 | 0.90 | 0.18 | 46,46,46,46 | 0 |
| 52 | MG | CA | 1626 | 1/1 | 0.90 | 0.35 | 65,65,65,65 | 0 |
| 52 | MG | BA | 3003 | 1/1 | 0.90 | 0.89 | 52,52,52,52 | 0 |
| 52 | MG | BA | 3196 | 1/1 | 0.90 | 0.20 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3043 | 1/1 | 0.90 | 0.22 | 42,42,42,42 | 0 |
| 52 | MG | AA | 1617 | 1/1 | 0.90 | 0.33 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3048 | 1/1 | 0.90 | 0.41 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3302 | 1/1 | 0.90 | 0.39 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3325 | 1/1 | 0.90 | 0.69 | 58,58,58,58 | 0 |
| 52 | MG | DA | 3147 | 1/1 | 0.90 | 0.43 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3302 | 1/1 | 0.90 | 0.39 | 64,64,64,64 | 0 |
| 52 | MG | BA | 3264 | 1/1 | 0.90 | 0.14 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3313 | 1/1 | 0.90 | 0.28 | 66,66,66,66 | 0 |
| 52 | MG | BA | 3001 | 1/1 | 0.90 | 0.41 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3263 | 1/1 | 0.90 | 0.29 | 26,26,26,26 | 0 |
| 52 | MG | BA | 3088 | 1/1 | 0.90 | 0.47 | 34,34,34,34 | 0 |
| 52 | MG | CA | 1620 | 1/1 | 0.90 | 0.29 | 58,58,58,58 | 0 |
| 52 | MG | DA | 3089 | 1/1 | 0.90 | 0.46 | 29,29,29,29 | 0 |
| 52 | MG | BA | 3126 | 1/1 | 0.90 | 0.31 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3166 | 1/1 | 0.90 | 0.29 | 47,47,47,47 | 0 |
| 52 | MG | DA | 3136 | 1/1 | 0.90 | 0.42 | 33,33,33,33 | 0 |
| 52 | MG | D5 | 101 | 1/1 | 0.90 | 0.44 | 35,35,35,35 | 0 |
| 52 | MG | CA | 1627 | 1/1 | 0.90 | 0.64 | 75,75,75,75 | 0 |
| 52 | MG | AA | 1630 | 1/1 | 0.90 | 0.51 | 51,51,51,51 | 0 |
| 52 | MG | DA | 3239 | 1/1 | 0.90 | 0.27 | 29,29,29,29 | 0 |
| 52 | MG | BA | 3331 | 1/1 | 0.90 | 0.30 | 49,49,49,49 | 0 |
| 52 | MG | BA | 3251 | 1/1 | 0.90 | 0.10 | 40,40,40,40 | 0 |
| 52 | MG | DA | 3194 | 1/1 | 0.90 | 0.36 | 47,47,47,47 | 0 |
| 52 | MG | BA | 3162 | 1/1 | 0.90 | 0.52 | 60,60,60,60 | 0 |
| 52 | MG | DA | 3222 | 1/1 | 0.90 | 0.57 | 44,44,44,44 | 0 |
| 52 | MG | CA | 1621 | 1/1 | 0.90 | 0.36 | 54,54,54,54 | 0 |
| 52 | MG | DA | 3273 | 1/1 | 0.90 | 0.93 | 52,52,52,52 | 0 |
| 52 | MG | CA | 1612 | 1/1 | 0.90 | 0.21 | 68,68,68,68 | 0 |
| 52 | MG | DA | 3001 | 1/1 | 0.90 | 0.32 | 56,56,56,56 | 0 |
| 52 | MG | BA | 3305 | 1/1 | 0.90 | 0.29 | 43,43,43,43 | 0 |
| 52 | MG | DA | 3046 | 1/1 | 0.90 | 0.44 | 48,48,48,48 | 0 |
| 52 | MG | AA | 1654 | 1/1 | 0.90 | 0.25 | 69,69,69,69 | 0 |
| 52 | MG | D0 | 101 | 1/1 | 0.90 | 0.14 | 46,46,46,46 | 0 |
| 52 | MG | DA | 3209 | 1/1 | 0.90 | 0.97 | 58,58,58,58 | 0 |
| 52 | MG | BA | 3318 | 1/1 | 0.91 | 0.51 | 40,40,40,40 | 0 |
| 52 | MG | AA | 1606 | 1/1 | 0.91 | 0.43 | 89,89,89,89 | 0 |
| 52 | MG | DA | 3065 | 1/1 | 0.91 | 0.22 | 39,39,39,39 | 0 |
| 52 | MG | DX | 101 | 1/1 | 0.91 | 0.34 | 63,63,63,63 | 0 |
| 52 | MG | DA | 3249 | 1/1 | 0.91 | 0.31 | 51,51,51,51 | 0 |
| 52 | MG | DA | 3021 | 1/1 | 0.91 | 0.30 | 48,48,48,48 | 0 |
| 52 | MG | DA | 3122 | 1/1 | 0.91 | 0.28 | 48,48,48,48 | 0 |
| 52 | MG | AA | 1639 | 1/1 | 0.91 | 0.27 | 49,49,49,49 | 0 |
| 52 | MG | BA | 3291 | 1/1 | 0.91 | 0.19 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3185 | 1/1 | 0.91 | 0.59 | 53,53,53,53 | 0 |
| 52 | MG | AA | 1610 | 1/1 | 0.91 | 0.17 | 41,41,41,41 | 0 |
| 52 | MG | BA | 3147 | 1/1 | 0.91 | 0.60 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3214 | 1/1 | 0.91 | 0.12 | 12,12,12,12 | 0 |
| 52 | MG | DA | 3242 | 1/1 | 0.91 | 0.21 | 53,53,53,53 | 0 |
| 52 | MG | DA | 3210 | 1/1 | 0.91 | 0.20 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | BA | 3347 | 1/1 | 0.91 | 0.17 | 43,43,43,43 | 0 |
| 52 | MG | DA | 3214 | 1/1 | 0.91 | 0.37 | 48,48,48,48 | 0 |
| 52 | MG | BA | 3310 | 1/1 | 0.91 | 0.45 | 59,59,59,59 | 0 |
| 52 | MG | DA | 3233 | 1/1 | 0.91 | 0.57 | 52,52,52,52 | 0 |
| 52 | MG | BF | 301 | 1/1 | 0.91 | 0.23 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3069 | 1/1 | 0.91 | 0.36 | 45,45,45,45 | 0 |
| 52 | MG | DA | 3109 | 1/1 | 0.91 | 0.34 | 42,42,42,42 | 0 |
| 54 | K | DA | 3329 | 1/1 | 0.91 | 0.18 | 55,55,55,55 | 0 |
| 52 | MG | DA | 3275 | 1/1 | 0.91 | 0.39 | 60,60,60,60 | 0 |
| 52 | MG | BA | 3303 | 1/1 | 0.91 | 0.20 | 65,65,65,65 | 0 |
| 52 | MG | CA | 1614 | 1/1 | 0.91 | 0.12 | 71,71,71,71 | 0 |
| 52 | MG | BA | 3348 | 1/1 | 0.91 | 0.35 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3211 | 1/1 | 0.91 | 0.28 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3128 | 1/1 | 0.91 | 0.30 | 39,39,39,39 | 0 |
| 52 | MG | DA | 3207 | 1/1 | 0.91 | 0.28 | 56,56,56,56 | 0 |
| 52 | MG | CA | 1639 | 1/1 | 0.91 | 1.02 | 70,70,70,70 | 0 |
| 52 | MG | DA | 3137 | 1/1 | 0.91 | 0.42 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3181 | 1/1 | 0.91 | 0.43 | 35,35,35,35 | 0 |
| 52 | MG | DA | 3282 | 1/1 | 0.91 | 0.15 | 48,48,48,48 | 0 |
| 52 | MG | DA | 3017 | 1/1 | 0.91 | 0.34 | 34,34,34,34 | 0 |
| 52 | MG | DA | 3288 | 1/1 | 0.91 | 0.36 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3349 | 1/1 | 0.91 | 0.39 | 33,33,33,33 | 0 |
| 52 | MG | DA | 3120 | 1/1 | 0.91 | 0.30 | 55,55,55,55 | 0 |
| 52 | MG | BA | 3268 | 1/1 | 0.91 | 0.43 | 39,39,39,39 | 0 |
| 53 | ZN | CN | 101 | 1/1 | 0.91 | 0.18 | 139,139,139,139 | 0 |
| 52 | MG | DA | 3255 | 1/1 | 0.91 | 0.20 | 50,50,50,50 | 0 |
| 52 | MG | DA | 3224 | 1/1 | 0.91 | 0.45 | 54,54,54,54 | 0 |
| 52 | MG | BA | 3053 | 1/1 | 0.91 | 0.48 | 27,27,27,27 | 0 |
| 52 | MG | CA | 1601 | 1/1 | 0.91 | 0.17 | 72,72,72,72 | 0 |
| 52 | MG | BA | 3223 | 1/1 | 0.91 | 0.25 | 41,41,41,41 | 0 |
| 52 | MG | DB | 203 | 1/1 | 0.92 | 0.38 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3294 | 1/1 | 0.92 | 0.13 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3061 | 1/1 | 0.92 | 0.29 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3110 | 1/1 | 0.92 | 0.61 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3237 | 1/1 | 0.92 | 0.62 | 40,40,40,40 | 0 |
| 52 | MG | DA | 3327 | 1/1 | 0.92 | 0.15 | 60,60,60,60 | 0 |
| 52 | MG | BA | 3274 | 1/1 | 0.92 | 0.46 | 36,36,36,36 | 0 |
| 52 | MG | CA | 1622 | 1/1 | 0.92 | 0.39 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3034 | 1/1 | 0.92 | 0.34 | 61,61,61,61 | 0 |
| 52 | MG | AA | 1629 | 1/1 | 0.92 | 0.22 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3157 | 1/1 | 0.92 | 0.60 | 52,52,52,52 | 0 |
| 52 | MG | DA | 3074 | 1/1 | 0.92 | 0.54 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3154 | 1/1 | 0.92 | 0.18 | 49,49,49,49 | 0 |
| 52 | MG | BX | 101 | 1/1 | 0.92 | 0.24 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3158 | 1/1 | 0.92 | 0.14 | 53,53,53,53 | 0 |
| 52 | MG | DA | 3081 | 1/1 | 0.92 | 0.78 | 48,48,48,48 | 0 |
| 52 | MG | BA | 3282 | 1/1 | 0.92 | 0.36 | 55,55,55,55 | 0 |
| 52 | MG | BA | 3269 | 1/1 | 0.92 | 0.36 | 43,43,43,43 | 0 |
| 52 | MG | BA | 3155 | 1/1 | 0.92 | 0.23 | 55,55,55,55 | 0 |
| 52 | MG | BA | 3258 | 1/1 | 0.92 | 0.39 | 30,30,30,30 | 0 |
| 52 | MG | BA | 3061 | 1/1 | 0.92 | 0.32 | 27,27,27,27 | 0 |
| 52 | MG | DA | 3002 | 1/1 | 0.92 | 0.48 | 29,29,29,29 | 0 |
| 52 | MG | DA | 3230 | 1/1 | 0.92 | 0.32 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3014 | 1/1 | 0.92 | 0.40 | 56,56,56,56 | 0 |
| 52 | MG | CA | 1632 | 1/1 | 0.92 | 0.29 | 63,63,63,63 | 0 |
| 52 | MG | DA | 3221 | 1/1 | 0.92 | 0.54 | 40,40,40,40 | 0 |
| 52 | MG | DU | 201 | 1/1 | 0.92 | 0.21 | 60,60,60,60 | 0 |
| 52 | MG | DA | 3308 | 1/1 | 0.92 | 0.22 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3293 | 1/1 | 0.92 | 0.48 | 62,62,62,62 | 0 |
| 52 | MG | DA | 3312 | 1/1 | 0.92 | 0.23 | 55,55,55,55 | 0 |
| 52 | MG | CA | 1644 | 1/1 | 0.92 | 0.40 | 62,62,62,62 | 0 |
| 52 | MG | BA | 3276 | 1/1 | 0.92 | 0.31 | 17,17,17,17 | 0 |
| 52 | MG | BA | 3231 | 1/1 | 0.92 | 0.24 | 35,35,35,35 | 0 |
| 52 | MG | CA | 1648 | 1/1 | 0.92 | 0.79 | 70,70,70,70 | 0 |
| 52 | MG | DA | 3107 | 1/1 | 0.92 | 0.41 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3133 | 1/1 | 0.92 | 0.68 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3104 | 1/1 | 0.92 | 0.54 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3333 | 1/1 | 0.92 | 0.15 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3059 | 1/1 | 0.92 | 0.28 | 26,26,26,26 | 0 |
| 52 | MG | BB | 205 | 1/1 | 0.92 | 0.12 | 64,64,64,64 | 0 |
| 52 | MG | DA | 3295 | 1/1 | 0.92 | 0.13 | 46,46,46,46 | 0 |
| 52 | MG | DA | 3080 | 1/1 | 0.92 | 0.75 | 46,46,46,46 | 0 |
| 52 | MG | DB | 202 | 1/1 | 0.92 | 0.39 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3315 | 1/1 | 0.92 | 0.94 | 52,52,52,52 | 0 |
| 52 | MG | BA | 3338 | 1/1 | 0.92 | 0.53 | 50,50,50,50 | 0 |
| 52 | MG | AA | 1640 | 1/1 | 0.92 | 0.42 | 67,67,67,67 | 0 |
| 52 | MG | BA | 3188 | 1/1 | 0.92 | 0.17 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3197 | 1/1 | 0.92 | 0.51 | 46,46,46,46 | 0 |
| 52 | MG | DA | 3112 | 1/1 | 0.92 | 0.28 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3258 | 1/1 | 0.92 | 0.23 | 52,52,52,52 | 0 |
| 52 | MG | DA | 3127 | 1/1 | 0.92 | 0.27 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3105 | 1/1 | 0.92 | 0.59 | 34,34,34,34 | 0 |
| 52 | MG | DA | 3152 | 1/1 | 0.92 | 0.33 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3101 | 1/1 | 0.92 | 0.14 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | BB | 201 | 1/1 | 0.92 | 0.49 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3246 | 1/1 | 0.92 | 0.58 | 46,46,46,46 | 0 |
| 52 | MG | DA | 3117 | 1/1 | 0.92 | 0.26 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3176 | 1/1 | 0.92 | 0.39 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3135 | 1/1 | 0.92 | 0.43 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3242 | 1/1 | 0.92 | 0.51 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3240 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 52 | MG | DA | 3167 | 1/1 | 0.93 | 0.17 | 44,44,44,44 | 0 |
| 52 | MG | DA | 3248 | 1/1 | 0.93 | 0.32 | 82,82,82,82 | 0 |
| 55 | ERY | BA | 3364 | 51/51 | 0.93 | 0.39 | 94,94,94,94 | 0 |
| 52 | MG | DA | 3321 | 1/1 | 0.93 | 0.13 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3004 | 1/1 | 0.93 | 0.43 | 28,28,28,28 | 0 |
| 52 | MG | CA | 1634 | 1/1 | 0.93 | 0.19 | 63,63,63,63 | 0 |
| 52 | MG | BA | 3075 | 1/1 | 0.93 | 0.41 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3217 | 1/1 | 0.93 | 0.21 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3015 | 1/1 | 0.93 | 0.32 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3218 | 1/1 | 0.93 | 0.49 | 27,27,27,27 | 0 |
| 52 | MG | DA | 3297 | 1/1 | 0.93 | 0.24 | 21,21,21,21 | 0 |
| 52 | MG | CA | 1605 | 1/1 | 0.93 | 0.20 | 84,84,84,84 | 0 |
| 52 | MG | BA | 3197 | 1/1 | 0.93 | 0.56 | 47,47,47,47 | 0 |
| 52 | MG | DA | 3057 | 1/1 | 0.93 | 0.30 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3071 | 1/1 | 0.93 | 0.48 | 33,33,33,33 | 0 |
| 52 | MG | DA | 3126 | 1/1 | 0.93 | 0.30 | 42,42,42,42 | 0 |
| 52 | MG | DA | 3051 | 1/1 | 0.93 | 0.45 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3095 | 1/1 | 0.93 | 0.22 | 39,39,39,39 | 0 |
| 52 | MG | DA | 3266 | 1/1 | 0.93 | 0.18 | 74,74,74,74 | 0 |
| 52 | MG | BA | 3064 | 1/1 | 0.93 | 0.42 | 52,52,52,52 | 0 |
| 52 | MG | DA | 3161 | 1/1 | 0.93 | 0.67 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3257 | 1/1 | 0.93 | 0.46 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3243 | 1/1 | 0.93 | 0.32 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3290 | 1/1 | 0.93 | 0.24 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3117 | 1/1 | 0.93 | 0.15 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3334 | 1/1 | 0.93 | 0.30 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3228 | 1/1 | 0.93 | 0.29 | 21,21,21,21 | 0 |
| 52 | MG | CA | 1609 | 1/1 | 0.93 | 0.11 | 34,34,34,34 | 0 |
| 52 | MG | DA | 3168 | 1/1 | 0.93 | 0.36 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3201 | 1/1 | 0.93 | 0.78 | 51,51,51,51 | 0 |
| 52 | MG | DA | 3245 | 1/1 | 0.93 | 0.25 | 38,38,38,38 | 0 |
| 52 | MG | CA | 1606 | 1/1 | 0.93 | 0.59 | 44,44,44,44 | 0 |
| 52 | MG | DA | 3172 | 1/1 | 0.93 | 0.42 | 56,56,56,56 | 0 |
| 52 | MG | CA | 1616 | 1/1 | 0.93 | 0.49 | 67,67,67,67 | 0 |
| 52 | MG | DA | 3202 | 1/1 | 0.93 | 0.30 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | CA | 1615 | 1/1 | 0.93 | 0.37 | 69,69,69,69 | 0 |
| 52 | MG | DA | 3124 | 1/1 | 0.93 | 0.19 | 42,42,42,42 | 0 |
| 52 | MG | DA | 3004 | 1/1 | 0.93 | 0.36 | 29,29,29,29 | 0 |
| 52 | MG | BA | 3150 | 1/1 | 0.93 | 0.32 | 40,40,40,40 | 0 |
| 52 | MG | BA | 3278 | 1/1 | 0.93 | 0.24 | 39,39,39,39 | 0 |
| 52 | MG | DA | 3165 | 1/1 | 0.93 | 0.46 | 35,35,35,35 | 0 |
| 52 | MG | CA | 1619 | 1/1 | 0.93 | 0.47 | 47,47,47,47 | 0 |
| 52 | MG | DA | 3108 | 1/1 | 0.93 | 0.39 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3225 | 1/1 | 0.93 | 0.14 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3283 | 1/1 | 0.93 | 0.23 | 33,33,33,33 | 0 |
| 52 | MG | BR | 201 | 1/1 | 0.93 | 0.48 | 24,24,24,24 | 0 |
| 52 | MG | DA | 3103 | 1/1 | 0.93 | 0.69 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3225 | 1/1 | 0.93 | 0.12 | 20,20,20,20 | 0 |
| 52 | MG | BA | 3244 | 1/1 | 0.93 | 0.23 | 60,60,60,60 | 0 |
| 52 | MG | DA | 3218 | 1/1 | 0.93 | 0.29 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3012 | 1/1 | 0.93 | 0.40 | 25,25,25,25 | 0 |
| 52 | MG | DA | 3049 | 1/1 | 0.93 | 0.49 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3115 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 52 | MG | BA | 3138 | 1/1 | 0.93 | 0.53 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3253 | 1/1 | 0.93 | 0.74 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3300 | 1/1 | 0.93 | 0.54 | 48,48,48,48 | 0 |
| 52 | MG | BA | 3293 | 1/1 | 0.93 | 0.37 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3310 | 1/1 | 0.93 | 0.58 | 56,56,56,56 | 0 |
| 52 | MG | BA | 3127 | 1/1 | 0.93 | 0.55 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3158 | 1/1 | 0.93 | 0.39 | 30,30,30,30 | 0 |
| 52 | MG | AA | 1641 | 1/1 | 0.93 | 0.24 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3200 | 1/1 | 0.93 | 0.42 | 46,46,46,46 | 0 |
| 52 | MG | DA | 3244 | 1/1 | 0.93 | 0.22 | 32,32,32,32 | 0 |
| 52 | MG | CA | 1603 | 1/1 | 0.93 | 0.36 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3220 | 1/1 | 0.93 | 0.28 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3048 | 1/1 | 0.93 | 0.47 | 23,23,23,23 | 0 |
| 52 | MG | DA | 3182 | 1/1 | 0.93 | 0.13 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3146 | 1/1 | 0.93 | 0.33 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3111 | 1/1 | 0.93 | 0.21 | 17,17,17,17 | 0 |
| 52 | MG | DA | 3326 | 1/1 | 0.93 | 0.30 | 52,52,52,52 | 0 |
| 55 | ERY | DA | 3330 | 51/51 | 0.93 | 0.33 | 94,94,94,94 | 0 |
| 52 | MG | DA | 3064 | 1/1 | 0.93 | 0.46 | 47,47,47,47 | 0 |
| 52 | MG | BQ | 202 | 1/1 | 0.94 | 0.25 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3299 | 1/1 | 0.94 | 0.39 | 57,57,57,57 | 0 |
| 52 | MG | BA | 3022 | 1/1 | 0.94 | 0.20 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3251 | 1/1 | 0.94 | 0.17 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3177 | 1/1 | 0.94 | 0.33 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3031 | 1/1 | 0.94 | 0.08 | 62,62,62,62 | 0 |
| 52 | MG | BA | 3215 | 1/1 | 0.94 | 0.58 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3102 | 1/1 | 0.94 | 0.63 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3146 | 1/1 | 0.94 | 0.43 | 52,52,52,52 | 0 |
| 52 | MG | BA | 3142 | 1/1 | 0.94 | 0.60 | 33,33,33,33 | 0 |
| 52 | MG | CA | 1633 | 1/1 | 0.94 | 0.55 | 48,48,48,48 | 0 |
| 52 | MG | AA | 1631 | 1/1 | 0.94 | 0.67 | 70,70,70,70 | 0 |
| 52 | MG | DA | 3175 | 1/1 | 0.94 | 0.29 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3329 | 1/1 | 0.94 | 0.29 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3089 | 1/1 | 0.94 | 0.30 | 12,12,12,12 | 0 |
| 52 | MG | BA | 3039 | 1/1 | 0.94 | 0.51 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3144 | 1/1 | 0.94 | 0.59 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3142 | 1/1 | 0.94 | 0.55 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3292 | 1/1 | 0.94 | 0.18 | 54,54,54,54 | 0 |
| 52 | MG | DA | 3204 | 1/1 | 0.94 | 0.47 | 53,53,53,53 | 0 |
| 52 | MG | B5 | 102 | 1/1 | 0.94 | 0.42 | 56,56,56,56 | 0 |
| 52 | MG | AA | 1632 | 1/1 | 0.94 | 0.63 | 68,68,68,68 | 0 |
| 52 | MG | DA | 3100 | 1/1 | 0.94 | 0.35 | 37,37,37,37 | 0 |
| 52 | MG | CA | 1642 | 1/1 | 0.94 | 0.32 | 55,55,55,55 | 0 |
| 52 | MG | BP | 201 | 1/1 | 0.94 | 0.54 | 39,39,39,39 | 0 |
| 52 | MG | DA | 3150 | 1/1 | 0.94 | 0.71 | 72,72,72,72 | 0 |
| 52 | MG | AA | 1637 | 1/1 | 0.94 | 0.57 | 53,53,53,53 | 0 |
| 52 | MG | DA | 3097 | 1/1 | 0.94 | 0.25 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3316 | 1/1 | 0.94 | 0.33 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3037 | 1/1 | 0.94 | 0.70 | 35,35,35,35 | 0 |
| 52 | MG | AA | 1619 | 1/1 | 0.94 | 0.36 | 49,49,49,49 | 0 |
| 52 | MG | B5 | 101 | 1/1 | 0.94 | 0.44 | 40,40,40,40 | 0 |
| 52 | MG | CA | 1629 | 1/1 | 0.94 | 0.17 | 67,67,67,67 | 0 |
| 52 | MG | DA | 3151 | 1/1 | 0.94 | 0.60 | 47,47,47,47 | 0 |
| 52 | MG | DA | 3250 | 1/1 | 0.94 | 0.52 | 41,41,41,41 | 0 |
| 52 | MG | BA | 3259 | 1/1 | 0.94 | 0.31 | 23,23,23,23 | 0 |
| 52 | MG | CA | 1645 | 1/1 | 0.94 | 0.88 | 64,64,64,64 | 0 |
| 52 | MG | DA | 3018 | 1/1 | 0.94 | 0.24 | 23,23,23,23 | 0 |
| 52 | MG | DA | 3274 | 1/1 | 0.94 | 0.11 | 36,36,36,36 | 0 |
| 52 | MG | BA | 3200 | 1/1 | 0.94 | 0.55 | 36,36,36,36 | 0 |
| 52 | MG | BA | 3032 | 1/1 | 0.94 | 0.38 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3227 | 1/1 | 0.94 | 0.54 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3110 | 1/1 | 0.94 | 0.47 | 36,36,36,36 | 0 |
| 52 | MG | BA | 3337 | 1/1 | 0.94 | 0.72 | 47,47,47,47 | 0 |
| 52 | MG | AA | 1620 | 1/1 | 0.94 | 0.59 | 51,51,51,51 | 0 |
| 52 | MG | DA | 3253 | 1/1 | 0.94 | 0.17 | 58,58,58,58 | 0 |
| 52 | MG | DA | 3285 | 1/1 | 0.94 | 0.12 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DP | 201 | 1/1 | 0.94 | 0.32 | 27,27,27,27 | 0 |
| 52 | MG | DA | 3039 | 1/1 | 0.94 | 0.64 | 53,53,53,53 | 0 |
| 52 | MG | BA | 3051 | 1/1 | 0.94 | 0.36 | 17,17,17,17 | 0 |
| 52 | MG | BA | 3326 | 1/1 | 0.94 | 0.54 | 37,37,37,37 | 0 |
| 52 | MG | CA | 1640 | 1/1 | 0.94 | 0.25 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3308 | 1/1 | 0.94 | 0.19 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3188 | 1/1 | 0.94 | 0.30 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3101 | 1/1 | 0.94 | 0.49 | 43,43,43,43 | 0 |
| 52 | MG | CA | 1647 | 1/1 | 0.94 | 0.38 | 66,66,66,66 | 0 |
| 52 | MG | DA | 3067 | 1/1 | 0.94 | 0.38 | 49,49,49,49 | 0 |
| 52 | MG | DA | 3114 | 1/1 | 0.94 | 0.27 | 47,47,47,47 | 0 |
| 52 | MG | DA | 3054 | 1/1 | 0.94 | 0.28 | 43,43,43,43 | 0 |
| 52 | MG | DA | 3181 | 1/1 | 0.94 | 0.45 | 44,44,44,44 | 0 |
| 52 | MG | BP | 202 | 1/1 | 0.94 | 0.21 | 0,0,0,0 | 0 |
| 52 | MG | DA | 3032 | 1/1 | 0.94 | 0.42 | 25,25,25,25 | 0 |
| 52 | MG | AA | 1603 | 1/1 | 0.94 | 0.31 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3170 | 1/1 | 0.94 | 0.68 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3169 | 1/1 | 0.94 | 0.23 | 35,35,35,35 | 0 |
| 52 | MG | DA | 3128 | 1/1 | 0.94 | 0.29 | 47,47,47,47 | 0 |
| 52 | MG | B0 | 101 | 1/1 | 0.94 | 0.18 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3106 | 1/1 | 0.94 | 0.76 | 63,63,63,63 | 0 |
| 52 | MG | BA | 3229 | 1/1 | 0.94 | 0.73 | 45,45,45,45 | 0 |
| 52 | MG | DA | 3174 | 1/1 | 0.94 | 0.14 | 67,67,67,67 | 0 |
| 52 | MG | BA | 3307 | 1/1 | 0.94 | 0.42 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3185 | 1/1 | 0.94 | 0.26 | 46,46,46,46 | 0 |
| 53 | ZN | AD | 301 | 1/1 | 0.94 | 0.28 | 120,120,120,120 | 0 |
| 52 | MG | BA | 3068 | 1/1 | 0.94 | 0.53 | 35,35,35,35 | 0 |
| 52 | MG | AA | 1605 | 1/1 | 0.94 | 0.30 | 69,69,69,69 | 0 |
| 52 | MG | DA | 3254 | 1/1 | 0.94 | 0.17 | 68,68,68,68 | 0 |
| 52 | MG | DA | 3156 | 1/1 | 0.94 | 0.18 | 39,39,39,39 | 0 |
| 52 | MG | DA | 3138 | 1/1 | 0.94 | 0.48 | 47,47,47,47 | 0 |
| 52 | MG | BA | 3160 | 1/1 | 0.94 | 0.77 | 62,62,62,62 | 0 |
| 52 | MG | DA | 3038 | 1/1 | 0.94 | 0.51 | 26,26,26,26 | 0 |
| 52 | MG | DA | 3256 | 1/1 | 0.94 | 0.41 | 82,82,82,82 | 0 |
| 52 | MG | DA | 3082 | 1/1 | 0.94 | 0.34 | 47,47,47,47 | 0 |
| 52 | MG | DA | 3179 | 1/1 | 0.95 | 0.72 | 39,39,39,39 | 0 |
| 52 | MG | DA | 3139 | 1/1 | 0.95 | 0.52 | 44,44,44,44 | 0 |
| 52 | MG | DA | 3186 | 1/1 | 0.95 | 0.66 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3234 | 1/1 | 0.95 | 0.56 | 53,53,53,53 | 0 |
| 52 | MG | DA | 3056 | 1/1 | 0.95 | 0.22 | 14,14,14,14 | 0 |
| 52 | MG | AA | 1627 | 1/1 | 0.95 | 0.19 | 51,51,51,51 | 0 |
| 52 | MG | DA | 3241 | 1/1 | 0.95 | 0.43 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | BA | 3041 | 1/1 | 0.95 | 0.30 | 24,24,24,24 | 0 |
| 52 | MG | DA | 3013 | 1/1 | 0.95 | 0.50 | 18,18,18,18 | 0 |
| 52 | MG | DA | 3281 | 1/1 | 0.95 | 0.61 | 51,51,51,51 | 0 |
| 52 | MG | DA | 3063 | 1/1 | 0.95 | 0.41 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3098 | 1/1 | 0.95 | 0.23 | 39,39,39,39 | 0 |
| 52 | MG | AA | 1647 | 1/1 | 0.95 | 0.38 | 62,62,62,62 | 0 |
| 52 | MG | BA | 3343 | 1/1 | 0.95 | 0.24 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3058 | 1/1 | 0.95 | 0.30 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3279 | 1/1 | 0.95 | 0.29 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3322 | 1/1 | 0.95 | 0.43 | 48,48,48,48 | 0 |
| 52 | MG | BA | 3029 | 1/1 | 0.95 | 0.24 | 16,16,16,16 | 0 |
| 52 | MG | BD | 301 | 1/1 | 0.95 | 0.36 | 25,25,25,25 | 0 |
| 52 | MG | AA | 1618 | 1/1 | 0.95 | 0.11 | 59,59,59,59 | 0 |
| 52 | MG | AA | 1602 | 1/1 | 0.95 | 0.59 | 41,41,41,41 | 0 |
| 52 | MG | BA | 3099 | 1/1 | 0.95 | 0.26 | 21,21,21,21 | 0 |
| 52 | MG | DR | 201 | 1/1 | 0.95 | 0.44 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3230 | 1/1 | 0.95 | 0.09 | 21,21,21,21 | 0 |
| 52 | MG | BA | 3031 | 1/1 | 0.95 | 0.32 | 50,50,50,50 | 0 |
| 52 | MG | BB | 202 | 1/1 | 0.95 | 0.34 | 26,26,26,26 | 0 |
| 52 | MG | DA | 3259 | 1/1 | 0.95 | 0.28 | 49,49,49,49 | 0 |
| 52 | MG | BA | 3062 | 1/1 | 0.95 | 0.10 | 19,19,19,19 | 0 |
| 52 | MG | DA | 3098 | 1/1 | 0.95 | 0.33 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3323 | 1/1 | 0.95 | 0.20 | 32,32,32,32 | 0 |
| 52 | MG | DA | 3094 | 1/1 | 0.95 | 0.56 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3287 | 1/1 | 0.95 | 0.33 | 44,44,44,44 | 0 |
| 52 | MG | AA | 1614 | 1/1 | 0.95 | 0.40 | 49,49,49,49 | 0 |
| 52 | MG | BA | 3157 | 1/1 | 0.95 | 0.49 | 22,22,22,22 | 0 |
| 52 | MG | BA | 3002 | 1/1 | 0.95 | 0.45 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3296 | 1/1 | 0.95 | 0.22 | 43,43,43,43 | 0 |
| 52 | MG | BA | 3340 | 1/1 | 0.95 | 0.34 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3280 | 1/1 | 0.95 | 0.21 | 33,33,33,33 | 0 |
| 52 | MG | DA | 3227 | 1/1 | 0.95 | 0.63 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3320 | 1/1 | 0.95 | 0.48 | 50,50,50,50 | 0 |
| 52 | MG | DA | 3088 | 1/1 | 0.95 | 0.35 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3247 | 1/1 | 0.95 | 0.32 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3359 | 1/1 | 0.95 | 0.27 | 52,52,52,52 | 0 |
| 52 | MG | BA | 3192 | 1/1 | 0.95 | 0.25 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3120 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3082 | 1/1 | 0.95 | 0.35 | 33,33,33,33 | 0 |
| 52 | MG | DA | 3135 | 1/1 | 0.95 | 0.38 | 29,29,29,29 | 0 |
| 52 | MG | DA | 3119 | 1/1 | 0.95 | 0.21 | 50,50,50,50 | 0 |
| 52 | MG | DA | 3315 | 1/1 | 0.95 | 0.40 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | CA | 1617 | 1/1 | 0.95 | 0.50 | 54,54,54,54 | 0 |
| 52 | MG | DA | 3099 | 1/1 | 0.95 | 0.51 | 42,42,42,42 | 0 |
| 52 | MG | CA | 1650 | 1/1 | 0.95 | 0.25 | 58,58,58,58 | 0 |
| 52 | MG | BA | 3354 | 1/1 | 0.95 | 0.27 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3081 | 1/1 | 0.95 | 0.41 | 23,23,23,23 | 0 |
| 52 | MG | DA | 3009 | 1/1 | 0.95 | 0.40 | 49,49,49,49 | 0 |
| 52 | MG | DA | 3075 | 1/1 | 0.95 | 0.37 | 36,36,36,36 | 0 |
| 52 | MG | BA | 3221 | 1/1 | 0.95 | 0.54 | 29,29,29,29 | 0 |
| 52 | MG | DA | 3007 | 1/1 | 0.95 | 0.28 | 53,53,53,53 | 0 |
| 52 | MG | DA | 3198 | 1/1 | 0.95 | 0.19 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3226 | 1/1 | 0.95 | 0.23 | 40,40,40,40 | 0 |
| 52 | MG | BA | 3161 | 1/1 | 0.95 | 0.31 | 43,43,43,43 | 0 |
| 52 | MG | BA | 3077 | 1/1 | 0.95 | 0.18 | 21,21,21,21 | 0 |
| 52 | MG | DA | 3022 | 1/1 | 0.95 | 0.37 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3222 | 1/1 | 0.95 | 0.38 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3335 | 1/1 | 0.95 | 0.17 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3275 | 1/1 | 0.95 | 0.36 | 40,40,40,40 | 0 |
| 52 | MG | DA | 3228 | 1/1 | 0.95 | 0.12 | 52,52,52,52 | 0 |
| 52 | MG | BA | 3261 | 1/1 | 0.95 | 0.08 | 27,27,27,27 | 0 |
| 52 | MG | BA | 3013 | 1/1 | 0.95 | 0.43 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3116 | 1/1 | 0.96 | 0.18 | 55,55,55,55 | 0 |
| 52 | MG | BA | 3339 | 1/1 | 0.96 | 0.08 | 53,53,53,53 | 0 |
| 52 | MG | BA | 3203 | 1/1 | 0.96 | 0.38 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3109 | 1/1 | 0.96 | 0.40 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3006 | 1/1 | 0.96 | 0.54 | 30,30,30,30 | 0 |
| 52 | MG | BA | 3086 | 1/1 | 0.96 | 0.25 | 24,24,24,24 | 0 |
| 52 | MG | DA | 3303 | 1/1 | 0.96 | 0.13 | 47,47,47,47 | 0 |
| 52 | MG | DA | 3145 | 1/1 | 0.96 | 0.20 | 59,59,59,59 | 0 |
| 52 | MG | DA | 3045 | 1/1 | 0.96 | 0.39 | 29,29,29,29 | 0 |
| 52 | MG | BA | 3080 | 1/1 | 0.96 | 0.59 | 17,17,17,17 | 0 |
| 52 | MG | BA | 3199 | 1/1 | 0.96 | 0.30 | 20,20,20,20 | 0 |
| 52 | MG | BA | 3232 | 1/1 | 0.96 | 0.15 | 4,4,4,4 | 0 |
| 52 | MG | BA | 3009 | 1/1 | 0.96 | 0.39 | 27,27,27,27 | 0 |
| 52 | MG | DA | 3077 | 1/1 | 0.96 | 0.19 | 33,33,33,33 | 0 |
| 52 | MG | DA | 3121 | 1/1 | 0.96 | 0.80 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3182 | 1/1 | 0.96 | 0.32 | 43,43,43,43 | 0 |
| 52 | MG | DA | 3296 | 1/1 | 0.96 | 0.44 | 55,55,55,55 | 0 |
| 52 | MG | BA | 3277 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 52 | MG | BA | 3309 | 1/1 | 0.96 | 0.29 | 55,55,55,55 | 0 |
| 52 | MG | DA | 3028 | 1/1 | 0.96 | 0.36 | 36,36,36,36 | 0 |
| 52 | MG | BA | 3095 | 1/1 | 0.96 | 0.38 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3121 | 1/1 | 0.96 | 0.44 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | BA | 3046 | 1/1 | 0.96 | 0.31 | 28,28,28,28 | 0 |
| 52 | MG | AA | 1622 | 1/1 | 0.96 | 0.64 | 63,63,63,63 | 0 |
| 52 | MG | AA | 1633 | 1/1 | 0.96 | 0.06 | 39,39,39,39 | 0 |
| 52 | MG | DA | 3093 | 1/1 | 0.96 | 0.53 | 48,48,48,48 | 0 |
| 52 | MG | BA | 3067 | 1/1 | 0.96 | 0.54 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3260 | 1/1 | 0.96 | 0.28 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3096 | 1/1 | 0.96 | 0.26 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3141 | 1/1 | 0.96 | 0.48 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3190 | 1/1 | 0.96 | 0.38 | 23,23,23,23 | 0 |
| 52 | MG | DA | 3052 | 1/1 | 0.96 | 0.44 | 40,40,40,40 | 0 |
| 52 | MG | AA | 1625 | 1/1 | 0.96 | 0.40 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3058 | 1/1 | 0.96 | 0.35 | 48,48,48,48 | 0 |
| 52 | MG | DA | 3134 | 1/1 | 0.96 | 0.19 | 67,67,67,67 | 0 |
| 52 | MG | BA | 3038 | 1/1 | 0.96 | 0.43 | 14,14,14,14 | 0 |
| 52 | MG | DA | 3203 | 1/1 | 0.96 | 0.51 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3191 | 1/1 | 0.96 | 0.32 | 21,21,21,21 | 0 |
| 52 | MG | DA | 3035 | 1/1 | 0.96 | 0.36 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3015 | 1/1 | 0.96 | 0.29 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3267 | 1/1 | 0.96 | 0.48 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3255 | 1/1 | 0.96 | 0.10 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3168 | 1/1 | 0.96 | 0.24 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3210 | 1/1 | 0.96 | 0.34 | 33,33,33,33 | 0 |
| 52 | MG | DA | 3033 | 1/1 | 0.96 | 0.28 | 43,43,43,43 | 0 |
| 52 | MG | DA | 3087 | 1/1 | 0.96 | 0.21 | 34,34,34,34 | 0 |
| 52 | MG | BE | 301 | 1/1 | 0.96 | 0.41 | 25,25,25,25 | 0 |
| 52 | MG | DA | 3176 | 1/1 | 0.96 | 0.44 | 44,44,44,44 | 0 |
| 52 | MG | DA | 3079 | 1/1 | 0.96 | 0.23 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3140 | 1/1 | 0.96 | 0.41 | 52,52,52,52 | 0 |
| 52 | MG | CA | 1611 | 1/1 | 0.96 | 0.42 | 65,65,65,65 | 0 |
| 52 | MG | DA | 3041 | 1/1 | 0.96 | 0.30 | 31,31,31,31 | 0 |
| 52 | MG | DE | 301 | 1/1 | 0.96 | 0.29 | 23,23,23,23 | 0 |
| 52 | MG | BA | 3030 | 1/1 | 0.96 | 0.22 | 15,15,15,15 | 0 |
| 52 | MG | AA | 1649 | 1/1 | 0.96 | 0.68 | 62,62,62,62 | 0 |
| 52 | MG | BA | 3306 | 1/1 | 0.96 | 0.33 | 52,52,52,52 | 0 |
| 52 | MG | DA | 3238 | 1/1 | 0.96 | 0.08 | 59,59,59,59 | 0 |
| 52 | MG | BA | 3149 | 1/1 | 0.96 | 0.27 | 19,19,19,19 | 0 |
| 52 | MG | CA | 1631 | 1/1 | 0.96 | 0.09 | 73,73,73,73 | 0 |
| 52 | MG | DA | 3072 | 1/1 | 0.96 | 0.73 | 58,58,58,58 | 0 |
| 52 | MG | BA | 3224 | 1/1 | 0.96 | 0.48 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3091 | 1/1 | 0.96 | 0.46 | 31,31,31,31 | 0 |
| 52 | MG | AA | 1636 | 1/1 | 0.96 | 0.28 | 44,44,44,44 | 0 |
| 52 | MG | DA | 3086 | 1/1 | 0.96 | 0.18 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | BB | 207 | 1/1 | 0.96 | 0.26 | 62,62,62,62 | 0 |
| 52 | MG | BA | 3212 | 1/1 | 0.96 | 0.52 | 26,26,26,26 | 0 |
| 52 | MG | CA | 1623 | 1/1 | 0.96 | 0.26 | 62,62,62,62 | 0 |
| 52 | MG | BA | 3292 | 1/1 | 0.96 | 0.56 | 56,56,56,56 | 0 |
| 52 | MG | BA | 3076 | 1/1 | 0.96 | 0.23 | 21,21,21,21 | 0 |
| 52 | MG | BA | 3131 | 1/1 | 0.96 | 0.32 | 21,21,21,21 | 0 |
| 52 | MG | BA | 3351 | 1/1 | 0.96 | 0.28 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3123 | 1/1 | 0.96 | 0.39 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3322 | 1/1 | 0.96 | 0.31 | 50,50,50,50 | 0 |
| 52 | MG | BA | 3108 | 1/1 | 0.96 | 0.53 | 42,42,42,42 | 0 |
| 52 | MG | DA | 3173 | 1/1 | 0.96 | 0.44 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3027 | 1/1 | 0.96 | 0.51 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3102 | 1/1 | 0.96 | 0.37 | 23,23,23,23 | 0 |
| 52 | MG | BA | 3207 | 1/1 | 0.96 | 0.35 | 27,27,27,27 | 0 |
| 52 | MG | DA | 3129 | 1/1 | 0.96 | 0.16 | 54,54,54,54 | 0 |
| 52 | MG | BA | 3324 | 1/1 | 0.96 | 0.40 | 40,40,40,40 | 0 |
| 52 | MG | DA | 3183 | 1/1 | 0.96 | 0.57 | 56,56,56,56 | 0 |
| 52 | MG | DA | 3155 | 1/1 | 0.96 | 0.37 | 30,30,30,30 | 0 |
| 52 | MG | BA | 3198 | 1/1 | 0.97 | 0.44 | 36,36,36,36 | 0 |
| 52 | MG | BA | 3072 | 1/1 | 0.97 | 0.55 | 39,39,39,39 | 0 |
| 52 | MG | DA | 3113 | 1/1 | 0.97 | 0.28 | 52,52,52,52 | 0 |
| 52 | MG | DA | 3314 | 1/1 | 0.97 | 0.06 | 58,58,58,58 | 0 |
| 52 | MG | DA | 3060 | 1/1 | 0.97 | 0.30 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3084 | 1/1 | 0.97 | 0.43 | 21,21,21,21 | 0 |
| 52 | MG | BA | 3036 | 1/1 | 0.97 | 0.51 | 19,19,19,19 | 0 |
| 52 | MG | BA | 3284 | 1/1 | 0.97 | 0.23 | 25,25,25,25 | 0 |
| 52 | MG | DA | 3008 | 1/1 | 0.97 | 0.39 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3010 | 1/1 | 0.97 | 0.42 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3103 | 1/1 | 0.97 | 0.27 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3113 | 1/1 | 0.97 | 0.49 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3169 | 1/1 | 0.97 | 0.59 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3163 | 1/1 | 0.97 | 0.37 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3071 | 1/1 | 0.97 | 0.42 | 35,35,35,35 | 0 |
| 52 | MG | DA | 3029 | 1/1 | 0.97 | 0.39 | 45,45,45,45 | 0 |
| 52 | MG | DA | 3055 | 1/1 | 0.97 | 0.26 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3287 | 1/1 | 0.97 | 0.25 | 40,40,40,40 | 0 |
| 52 | MG | DA | 3023 | 1/1 | 0.97 | 0.53 | 38,38,38,38 | 0 |
| 52 | MG | AA | 1601 | 1/1 | 0.97 | 0.16 | 59,59,59,59 | 0 |
| 52 | MG | BA | 3019 | 1/1 | 0.97 | 0.52 | 19,19,19,19 | 0 |
| 52 | MG | DA | 3215 | 1/1 | 0.97 | 0.21 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3008 | 1/1 | 0.97 | 0.36 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3129 | 1/1 | 0.97 | 0.09 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | BA | 3011 | 1/1 | 0.97 | 0.48 | 19,19,19,19 | 0 |
| 52 | MG | BA | 3073 | 1/1 | 0.97 | 0.33 | 20,20,20,20 | 0 |
| 52 | MG | BA | 3118 | 1/1 | 0.97 | 0.48 | 40,40,40,40 | 0 |
| 52 | MG | BA | 3006 | 1/1 | 0.97 | 0.54 | 30,30,30,30 | 0 |
| 52 | MG | BA | 3252 | 1/1 | 0.97 | 0.40 | 30,30,30,30 | 0 |
| 52 | MG | BA | 3189 | 1/1 | 0.97 | 0.51 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3211 | 1/1 | 0.97 | 0.32 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3204 | 1/1 | 0.97 | 0.59 | 43,43,43,43 | 0 |
| 52 | MG | BA | 3033 | 1/1 | 0.97 | 0.20 | 27,27,27,27 | 0 |
| 52 | MG | BA | 3063 | 1/1 | 0.97 | 0.34 | 36,36,36,36 | 0 |
| 52 | MG | BA | 3027 | 1/1 | 0.97 | 0.38 | 19,19,19,19 | 0 |
| 52 | MG | DA | 3118 | 1/1 | 0.97 | 0.37 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3018 | 1/1 | 0.97 | 0.29 | 20,20,20,20 | 0 |
| 52 | MG | DA | 3171 | 1/1 | 0.97 | 0.56 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3226 | 1/1 | 0.97 | 0.41 | 14,14,14,14 | 0 |
| 52 | MG | BB | 203 | 1/1 | 0.97 | 0.06 | 41,41,41,41 | 0 |
| 52 | MG | BQ | 201 | 1/1 | 0.97 | 0.19 | 19,19,19,19 | 0 |
| 52 | MG | DA | 3217 | 1/1 | 0.97 | 0.27 | 23,23,23,23 | 0 |
| 52 | MG | BA | 3045 | 1/1 | 0.97 | 0.40 | 21,21,21,21 | 0 |
| 52 | MG | DA | 3195 | 1/1 | 0.97 | 0.42 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3017 | 1/1 | 0.97 | 0.41 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3184 | 1/1 | 0.97 | 0.22 | 44,44,44,44 | 0 |
| 52 | MG | DA | 3148 | 1/1 | 0.97 | 0.45 | 41,41,41,41 | 0 |
| 54 | K | BA | 3363 | 1/1 | 0.97 | 0.15 | 43,43,43,43 | 0 |
| 52 | MG | BA | 3020 | 1/1 | 0.97 | 0.30 | 18,18,18,18 | 0 |
| 53 | ZN | CD | 301 | 1/1 | 0.97 | 0.27 | 116,116,116,116 | 0 |
| 52 | MG | DA | 3020 | 1/1 | 0.97 | 0.48 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3205 | 1/1 | 0.97 | 0.61 | 43,43,43,43 | 0 |
| 52 | MG | BA | 3094 | 1/1 | 0.97 | 0.61 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3201 | 1/1 | 0.97 | 0.36 | 30,30,30,30 | 0 |
| 52 | MG | BA | 3256 | 1/1 | 0.97 | 0.12 | 39,39,39,39 | 0 |
| 52 | MG | AA | 1623 | 1/1 | 0.97 | 0.33 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3250 | 1/1 | 0.97 | 0.20 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3066 | 1/1 | 0.97 | 0.41 | 40,40,40,40 | 0 |
| 52 | MG | BA | 3091 | 1/1 | 0.97 | 0.17 | 20,20,20,20 | 0 |
| 52 | MG | DA | 3059 | 1/1 | 0.97 | 0.40 | 26,26,26,26 | 0 |
| 52 | MG | DA | 3111 | 1/1 | 0.97 | 0.47 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3184 | 1/1 | 0.97 | 0.33 | 57,57,57,57 | 0 |
| 52 | MG | DA | 3272 | 1/1 | 0.97 | 0.37 | 42,42,42,42 | 0 |
| 52 | MG | BB | 206 | 1/1 | 0.97 | 0.59 | 50,50,50,50 | 0 |
| 52 | MG | BA | 3007 | 1/1 | 0.97 | 0.49 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3216 | 1/1 | 0.97 | 0.31 | 26,26,26,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3180 | 1/1 | 0.97 | 0.59 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3016 | 1/1 | 0.97 | 0.43 | 21,21,21,21 | 0 |
| 52 | MG | BA | 3106 | 1/1 | 0.97 | 0.24 | 18,18,18,18 | 0 |
| 52 | MG | DA | 3234 | 1/1 | 0.97 | 0.16 | 46,46,46,46 | 0 |
| 52 | MG | BA | 3143 | 1/1 | 0.97 | 0.46 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3153 | 1/1 | 0.97 | 0.32 | 47,47,47,47 | 0 |
| 52 | MG | B1 | 101 | 1/1 | 0.97 | 0.33 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3219 | 1/1 | 0.97 | 0.55 | 25,25,25,25 | 0 |
| 52 | MG | BA | 3060 | 1/1 | 0.97 | 0.34 | 27,27,27,27 | 0 |
| 52 | MG | DA | 3196 | 1/1 | 0.97 | 0.44 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3266 | 1/1 | 0.97 | 0.23 | 48,48,48,48 | 0 |
| 52 | MG | DA | 3070 | 1/1 | 0.97 | 0.26 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3052 | 1/1 | 0.97 | 0.42 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3119 | 1/1 | 0.97 | 0.30 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3122 | 1/1 | 0.97 | 0.33 | 35,35,35,35 | 0 |
| 52 | MG | DA | 3235 | 1/1 | 0.97 | 0.40 | 40,40,40,40 | 0 |
| 52 | MG | DA | 3068 | 1/1 | 0.97 | 0.61 | 56,56,56,56 | 0 |
| 52 | MG | DA | 3025 | 1/1 | 0.97 | 0.35 | 44,44,44,44 | 0 |
| 52 | MG | DA | 3263 | 1/1 | 0.98 | 0.17 | 45,45,45,45 | 0 |
| 52 | MG | BA | 3167 | 1/1 | 0.98 | 0.48 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3156 | 1/1 | 0.98 | 0.51 | 26,26,26,26 | 0 |
| 52 | MG | BA | 3301 | 1/1 | 0.98 | 0.26 | 41,41,41,41 | 0 |
| 52 | MG | DA | 3044 | 1/1 | 0.98 | 0.39 | 32,32,32,32 | 0 |
| 52 | MG | DA | 3187 | 1/1 | 0.98 | 0.11 | 54,54,54,54 | 0 |
| 52 | MG | DA | 3042 | 1/1 | 0.98 | 0.37 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3262 | 1/1 | 0.98 | 0.18 | 25,25,25,25 | 0 |
| 52 | MG | DA | 3062 | 1/1 | 0.98 | 0.10 | 24,24,24,24 | 0 |
| 52 | MG | DA | 3104 | 1/1 | 0.98 | 0.36 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3030 | 1/1 | 0.98 | 0.33 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3172 | 1/1 | 0.98 | 0.22 | 52,52,52,52 | 0 |
| 52 | MG | BA | 3014 | 1/1 | 0.98 | 0.41 | 29,29,29,29 | 0 |
| 52 | MG | DA | 3192 | 1/1 | 0.98 | 0.32 | 29,29,29,29 | 0 |
| 52 | MG | DA | 3269 | 1/1 | 0.98 | 0.47 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3194 | 1/1 | 0.98 | 0.66 | 47,47,47,47 | 0 |
| 52 | MG | BA | 3043 | 1/1 | 0.98 | 0.20 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3084 | 1/1 | 0.98 | 0.50 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3173 | 1/1 | 0.98 | 0.39 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3023 | 1/1 | 0.98 | 0.50 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3193 | 1/1 | 0.98 | 0.56 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3186 | 1/1 | 0.98 | 0.46 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3066 | 1/1 | 0.98 | 0.39 | 29,29,29,29 | 0 |
| 52 | MG | BA | 3025 | 1/1 | 0.98 | 0.24 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3265 | 1/1 | 0.98 | 0.48 | 47,47,47,47 | 0 |
| 52 | MG | DA | 3076 | 1/1 | 0.98 | 0.28 | 29,29,29,29 | 0 |
| 52 | MG | BA | 3012 | 1/1 | 0.98 | 0.39 | 23,23,23,23 | 0 |
| 52 | MG | BA | 3010 | 1/1 | 0.98 | 0.44 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3044 | 1/1 | 0.98 | 0.38 | 14,14,14,14 | 0 |
| 52 | MG | BA | 3209 | 1/1 | 0.98 | 0.49 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3003 | 1/1 | 0.98 | 0.71 | 41,41,41,41 | 0 |
| 52 | MG | BA | 3171 | 1/1 | 0.98 | 0.58 | 32,32,32,32 | 0 |
| 52 | MG | BA | 3299 | 1/1 | 0.98 | 0.47 | 38,38,38,38 | 0 |
| 52 | MG | BA | 3057 | 1/1 | 0.98 | 0.21 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3092 | 1/1 | 0.98 | 0.34 | 9,9,9,9 | 0 |
| 52 | MG | DA | 3036 | 1/1 | 0.98 | 0.59 | 29,29,29,29 | 0 |
| 52 | MG | DA | 3034 | 1/1 | 0.98 | 0.40 | 51,51,51,51 | 0 |
| 52 | MG | BA | 3148 | 1/1 | 0.98 | 0.46 | 26,26,26,26 | 0 |
| 52 | MG | BA | 3180 | 1/1 | 0.98 | 0.11 | 48,48,48,48 | 0 |
| 52 | MG | BA | 3035 | 1/1 | 0.98 | 0.38 | 26,26,26,26 | 0 |
| 52 | MG | BA | 3137 | 1/1 | 0.98 | 0.40 | 10,10,10,10 | 0 |
| 52 | MG | DA | 3317 | 1/1 | 0.98 | 0.39 | 42,42,42,42 | 0 |
| 52 | MG | BA | 3134 | 1/1 | 0.98 | 0.17 | 36,36,36,36 | 0 |
| 52 | MG | DA | 3132 | 1/1 | 0.98 | 0.43 | 25,25,25,25 | 0 |
| 52 | MG | BA | 3028 | 1/1 | 0.98 | 0.36 | 22,22,22,22 | 0 |
| 52 | MG | BA | 3132 | 1/1 | 0.98 | 0.29 | 18,18,18,18 | 0 |
| 52 | MG | AA | 1626 | 1/1 | 0.98 | 0.33 | 46,46,46,46 | 0 |
| 52 | MG | DA | 3160 | 1/1 | 0.98 | 0.52 | 33,33,33,33 | 0 |
| 52 | MG | BA | 3124 | 1/1 | 0.98 | 0.44 | 10,10,10,10 | 0 |
| 52 | MG | BU | 201 | 1/1 | 0.98 | 0.34 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3107 | 1/1 | 0.98 | 0.18 | 28,28,28,28 | 0 |
| 52 | MG | CA | 1641 | 1/1 | 0.98 | 0.24 | 52,52,52,52 | 0 |
| 52 | MG | BA | 3024 | 1/1 | 0.98 | 0.31 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3136 | 1/1 | 0.98 | 0.24 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3272 | 1/1 | 0.98 | 0.34 | 28,28,28,28 | 0 |
| 52 | MG | DA | 3073 | 1/1 | 0.98 | 0.40 | 31,31,31,31 | 0 |
| 52 | MG | DA | 3078 | 1/1 | 0.98 | 0.41 | 37,37,37,37 | 0 |
| 52 | MG | DA | 3149 | 1/1 | 0.98 | 0.35 | 29,29,29,29 | 0 |
| 52 | MG | BA | 3241 | 1/1 | 0.98 | 0.34 | 26,26,26,26 | 0 |
| 52 | MG | BA | 3070 | 1/1 | 0.98 | 0.29 | 9,9,9,9 | 0 |
| 52 | MG | BA | 3040 | 1/1 | 0.98 | 0.60 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3125 | 1/1 | 0.98 | 0.18 | 18,18,18,18 | 0 |
| 52 | MG | DA | 3011 | 1/1 | 0.98 | 0.53 | 30,30,30,30 | 0 |
| 52 | MG | DA | 3216 | 1/1 | 0.98 | 0.42 | 31,31,31,31 | 0 |
| 52 | MG | BA | 3005 | 1/1 | 0.98 | 0.26 | 24,24,24,24 | 0 |
| 52 | MG | BA | 3145 | 1/1 | 0.98 | 0.45 | 33,33,33,33 | 0 |

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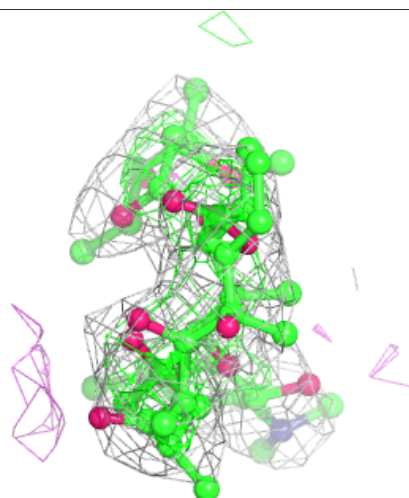
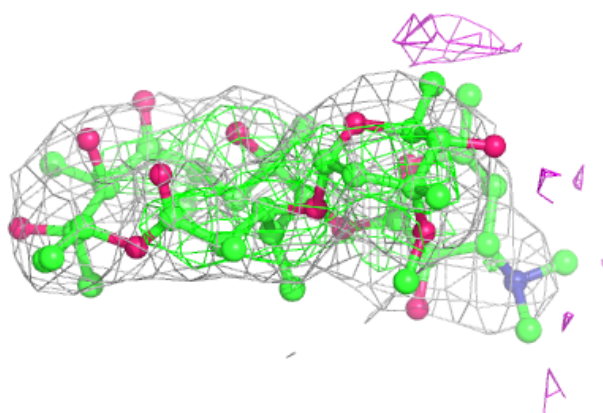
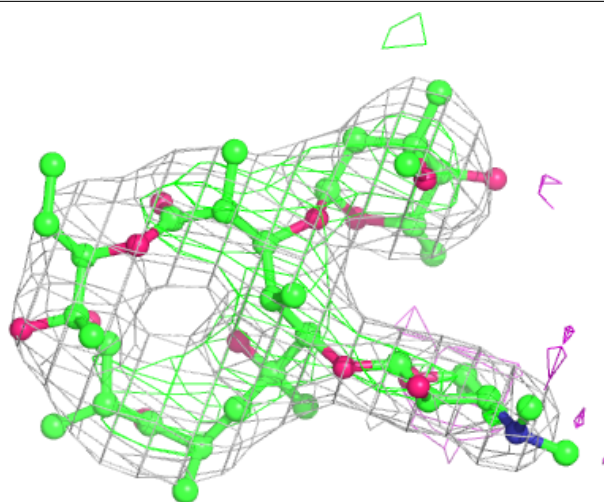
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 52 | MG | DA | 3019 | 1/1 | 0.99 | 0.55 | 21,21,21,21 | 0 |
| 52 | MG | BA | 3055 | 1/1 | 0.99 | 0.32 | 16,16,16,16 | 0 |
| 52 | MG | DA | 3024 | 1/1 | 0.99 | 0.33 | 35,35,35,35 | 0 |
| 52 | MG | BA | 3177 | 1/1 | 0.99 | 0.28 | 38,38,38,38 | 0 |
| 52 | MG | DA | 3050 | 1/1 | 0.99 | 0.35 | 39,39,39,39 | 0 |
| 52 | MG | BA | 3078 | 1/1 | 0.99 | 0.48 | 30,30,30,30 | 0 |
| 52 | MG | BA | 3050 | 1/1 | 0.99 | 0.35 | 27,27,27,27 | 0 |
| 52 | MG | BA | 3079 | 1/1 | 0.99 | 0.16 | 17,17,17,17 | 0 |
| 52 | MG | CA | 1618 | 1/1 | 0.99 | 0.49 | 65,65,65,65 | 0 |
| 52 | MG | BA | 3295 | 1/1 | 0.99 | 0.42 | 34,34,34,34 | 0 |
| 52 | MG | BA | 3100 | 1/1 | 0.99 | 0.35 | 28,28,28,28 | 0 |
| 52 | MG | BA | 3065 | 1/1 | 0.99 | 0.28 | 26,26,26,26 | 0 |
| 52 | MG | BA | 3096 | 1/1 | 0.99 | 0.48 | 19,19,19,19 | 0 |
| 52 | MG | BA | 3047 | 1/1 | 0.99 | 0.56 | 28,28,28,28 | 0 |
| 52 | MG | DA | 3053 | 1/1 | 0.99 | 0.34 | 27,27,27,27 | 0 |
| 52 | MG | DA | 3115 | 1/1 | 0.99 | 0.40 | 44,44,44,44 | 0 |
| 52 | MG | BA | 3213 | 1/1 | 0.99 | 0.16 | 20,20,20,20 | 0 |
| 52 | MG | BA | 3133 | 1/1 | 0.99 | 0.23 | 37,37,37,37 | 0 |
| 52 | MG | BA | 3087 | 1/1 | 0.99 | 0.25 | 18,18,18,18 | 0 |

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

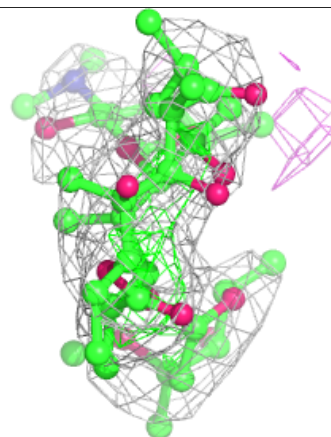
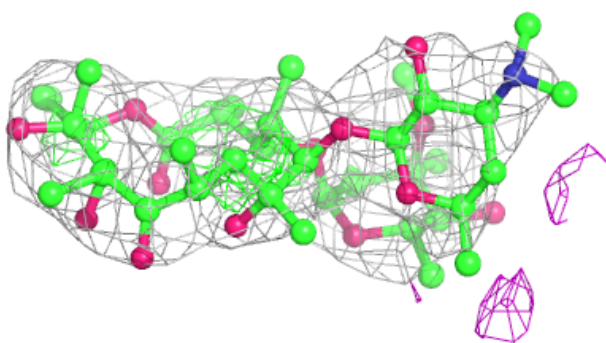
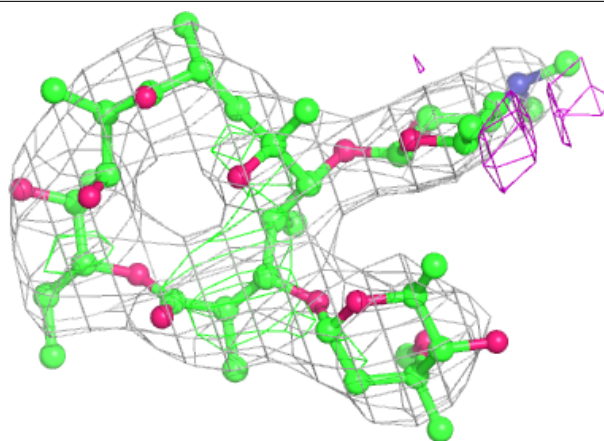
Electron density around ERY BA 3364:

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



Electron density around ERY DA 3330:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.