



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:07 pm BST

PDB ID : 4V9S
Title : Crystal structure of antibiotic GE82832 bound to 70S ribosome
Authors : Bulkley, D.P.; Brandi, L.; Polikanov, Y.S.; Fabbretti, A.; O'Connor, M.;
Gualerzi, C.O.; Steitz, T.A.
Deposited on : 2013-12-05
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

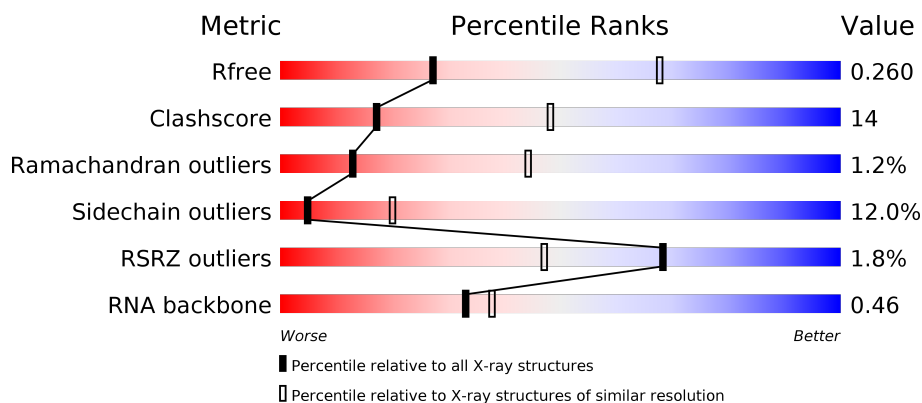
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | AA | 1522 | <div> <div>2%</div> <div> <div>36%</div> <div>43%</div> <div>17%</div> <div>• •</div> </div> </div> |
| 1 | CA | 1522 | <div> <div>2%</div> <div> <div>34%</div> <div>43%</div> <div>18%</div> <div>• •</div> </div> </div> |
| 2 | AB | 256 | <div> <div>3%</div> <div> <div>38%</div> <div>39%</div> <div>11%</div> <div>• 10%</div> </div> </div> |
| 2 | CB | 256 | <div> <div>5%</div> <div> <div>36%</div> <div>44%</div> <div>10%</div> <div>10%</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 | 162 | |
| 5 | CE | 162 | |
| 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 | 132 | |
| 12 | CL | 132 | |
| 13 | AM | 126 | |
| 13 | CM | 126 | |
| 14 | AN | 61 | |
| 14 | CN | 61 | |
| 15 | AO | 89 | |






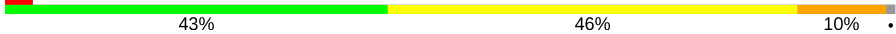



















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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | CO | 89 | |
| 16 | AP | 88 | |
| 16 | CP | 88 | |
| 17 | AQ | 105 | |
| 17 | CQ | 105 | |
| 18 | AR | 88 | |
| 18 | CR | 88 | |
| 19 | AS | 93 | |
| 19 | CS | 93 | |
| 20 | AT | 106 | |
| 20 | CT | 106 | |
| 21 | AU | 27 | |
| 21 | CU | 27 | |
| 22 | AV | 24 | |
| 22 | CV | 24 | |
| 23 | AX | 77 | |
| 23 | CX | 77 | |
| 24 | AW | 10 | |
| 24 | CW | 10 | |
| 25 | BA | 2915 | |
| 25 | DA | 2915 | |
| 26 | BB | 122 | |
| 26 | DB | 122 | |
| 27 | BD | 276 | |
| 27 | DD | 276 | |









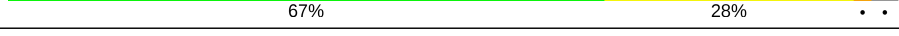


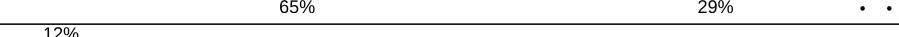

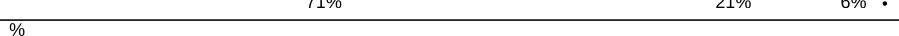


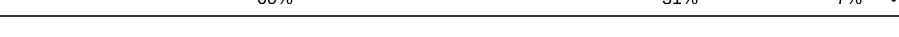

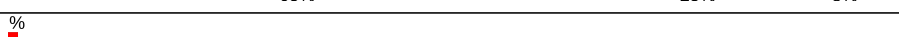
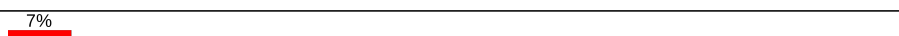

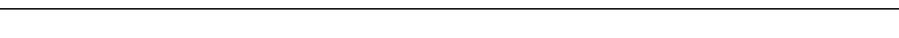
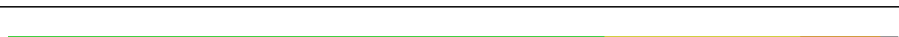


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | BE | 206 |  |
| 28 | DE | 206 |  |
| 29 | BF | 210 |  |
| 29 | DF | 210 |  |
| 30 | BG | 182 |  |
| 30 | DG | 182 |  |
| 31 | BH | 180 |  |
| 31 | DH | 180 |  |
| 32 | BI | 148 |  |
| 32 | DI | 148 |  |
| 33 | BN | 140 |  |
| 33 | DN | 140 |  |
| 34 | BO | 122 |  |
| 34 | DO | 122 |  |
| 35 | BP | 150 |  |
| 35 | DP | 150 |  |
| 36 | BQ | 141 |  |
| 36 | DQ | 141 |  |
| 37 | BR | 118 |  |
| 37 | DR | 118 |  |
| 38 | BS | 112 |  |
| 38 | DS | 112 |  |
| 39 | BT | 146 |  |
| 39 | DT | 146 |  |
| 40 | BU | 118 |  |

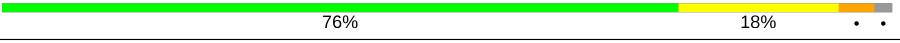


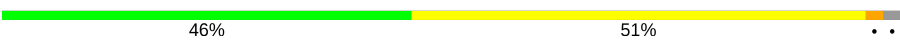


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 40 | DU | 118 |  |
| 41 | BV | 101 |  |
| 41 | DV | 101 |  |
| 42 | BW | 113 |  |
| 42 | DW | 113 |  |
| 43 | BX | 96 |  |
| 43 | DX | 96 |  |
| 44 | BY | 110 |  |
| 44 | DY | 110 |  |
| 45 | BZ | 206 |  |
| 45 | DZ | 206 |  |
| 46 | B0 | 85 |  |
| 46 | D0 | 85 |  |
| 47 | B1 | 98 |  |
| 47 | D1 | 98 |  |
| 48 | B2 | 72 |  |
| 48 | D2 | 72 |  |
| 49 | B3 | 60 |  |
| 49 | D3 | 60 |  |
| 50 | B4 | 71 |  |
| 50 | D4 | 71 |  |
| 51 | B5 | 60 |  |
| 51 | D5 | 60 |  |
| 52 | B6 | 54 |  |
| 52 | D6 | 54 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 53 | B7 | 49 |  |
| 53 | D7 | 49 |  |
| 54 | B8 | 65 |  |
| 54 | D8 | 65 |  |
| 55 | B9 | 37 |  |
| 55 | D9 | 37 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24 | 2QY | CW | 10 | - | - | X | - |
| 24 | MVA | CW | 9 | - | - | X | - |
| 56 | MG | AA | 3028 | - | - | - | X |
| 56 | MG | AA | 3035 | - | - | - | X |
| 56 | MG | AA | 3037 | - | - | - | X |
| 56 | MG | AA | 3043 | - | - | - | X |
| 56 | MG | AA | 3051 | - | - | - | X |
| 56 | MG | AA | 3079 | - | - | - | X |
| 56 | MG | AA | 3089 | - | - | - | X |
| 56 | MG | AA | 3093 | - | - | - | X |
| 56 | MG | AA | 3100 | - | - | - | X |
| 56 | MG | AA | 3114 | - | - | - | X |
| 56 | MG | AA | 3116 | - | - | - | X |
| 56 | MG | AA | 3120 | - | - | - | X |
| 56 | MG | AA | 3147 | - | - | - | X |
| 56 | MG | B1 | 3001 | - | - | - | X |
| 56 | MG | BA | 3065 | - | - | - | X |
| 56 | MG | BA | 3069 | - | - | - | X |
| 56 | MG | BA | 3085 | - | - | - | X |
| 56 | MG | BA | 3087 | - | - | - | X |
| 56 | MG | BA | 3089 | - | - | - | X |
| 56 | MG | BA | 3094 | - | - | - | X |
| 56 | MG | BA | 3160 | - | - | - | X |
| 56 | MG | BA | 3231 | - | - | - | X |
| 56 | MG | BA | 3247 | - | - | - | X |
| 56 | MG | BA | 3295 | - | - | - | X |
| 56 | MG | BA | 3297 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | BA | 3622 | - | - | - | X |
| 56 | MG | BA | 3699 | - | - | - | X |
| 56 | MG | CA | 3016 | - | - | - | X |
| 56 | MG | CA | 3024 | - | - | - | X |
| 56 | MG | CA | 3030 | - | - | - | X |
| 56 | MG | CA | 3038 | - | - | - | X |
| 56 | MG | CA | 3041 | - | - | - | X |
| 56 | MG | CA | 3042 | - | - | - | X |
| 56 | MG | CA | 3053 | - | - | - | X |
| 56 | MG | CA | 3135 | - | - | - | X |
| 56 | MG | DA | 3064 | - | - | - | X |
| 56 | MG | DA | 3098 | - | - | - | X |
| 56 | MG | DA | 3103 | - | - | - | X |
| 56 | MG | DA | 3125 | - | - | - | X |
| 56 | MG | DA | 3186 | - | - | - | X |
| 56 | MG | DA | 3427 | - | - | - | X |
| 56 | MG | DA | 3438 | - | - | - | X |
| 56 | MG | DA | 3464 | - | - | - | X |
| 56 | MG | DA | 3545 | - | - | - | X |
| 56 | MG | DA | 3581 | - | - | - | X |
| 56 | MG | DA | 3615 | - | - | - | X |
| 56 | MG | DW | 202 | - | - | - | X |
| 59 | FME | CX | 101 | - | - | - | X |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 286321 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1498 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32196 | 14328 | 5966 | 10404 | 1498 | | | |
| 1 | CA | 1503 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32312 | 14381 | 5990 | 10438 | 1503 | | | |

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1846 | 1179 | 331 | 331 | 5 | | | |
| 2 | CB | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1825 | 1167 | 326 | 327 | 5 | | | |

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | AC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 976 | 302 | 273 | 1 | | | |
| 3 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1542 | 968 | 300 | 273 | 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 |
| | | | 1659 | 1040 | 326 | 286 | 7 | | | |
| 4 | CD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1674 | 1050 | 333 | 284 | 7 | | | |

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 213 | 198 | 4 | | | |
| 5 | CE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 716 | 214 | 199 | 4 | | | |

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 511 | 143 | 149 | 3 | | | |
| 6 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 146 | 151 | 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 |
| | | | 1231 | 766 | 243 | 216 | 6 | | | |
| 7 | CG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1235 | 769 | 244 | 216 | 6 | | | |

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1088 | 689 | 206 | 191 | 2 | | | |
| 8 | CH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1088 | 689 | 206 | 191 | 2 | | | |

- 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 |
| | | | 983 | 623 | 193 | 167 | | | | |
| 9 | CI | 127 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 978 | 619 | 190 | 169 | | | | |

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 10 | AJ | 97 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 709 | 440 | 138 | 131 | | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10 | CJ | 96 | Total | C | N | O | | | |
| | | | 714 | 445 | 138 | 131 | 0 | 0 | 0 |

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 11 | AK | 114 | Total | C | N | O | S | | |
| | | | 829 | 516 | 155 | 155 | 3 | 0 | 0 |
| 11 | CK | 114 | Total | C | N | O | S | | |
| | | | 833 | 519 | 156 | 155 | 3 | 0 | 0 |

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 12 | AL | 122 | Total | C | N | O | S | | |
| | | | 930 | 585 | 185 | 159 | 1 | 0 | 0 |
| 12 | CL | 122 | Total | C | N | O | S | | |
| | | | 930 | 585 | 185 | 159 | 1 | 0 | 0 |

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 13 | AM | 123 | Total | C | N | O | S | | |
| | | | 958 | 592 | 198 | 166 | 2 | 0 | 0 |
| 13 | CM | 122 | Total | C | N | O | S | | |
| | | | 950 | 586 | 197 | 165 | 2 | 0 | 0 |

- 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 | | |
| | | | 492 | 312 | 104 | 72 | 4 | 0 | 0 |
| 14 | CN | 60 | Total | C | N | O | S | | |
| | | | 492 | 312 | 104 | 72 | 4 | 0 | 0 |

- 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 | | |
| | | | 728 | 456 | 144 | 126 | 2 | 0 | 0 |
| 15 | CO | 88 | Total | C | N | O | S | | |
| | | | 728 | 456 | 144 | 126 | 2 | 0 | 0 |

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 433 | 134 | 113 | 1 | | | |
| 16 | CP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 677 | 430 | 133 | 113 | 1 | | | |

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

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

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | AR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 555 | 355 | 108 | 92 | | | |
| 18 | CR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 555 | 355 | 108 | 92 | | | |

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 652 | 417 | 120 | 113 | 2 | | | |
| 19 | CS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 646 | 412 | 119 | 113 | 2 | | | |

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 728 | 446 | 156 | 124 | 2 | | | |
| 20 | CT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 727 | 446 | 155 | 124 | 2 | | | |

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |
| 21 | CU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |

- Molecule 22 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 22 | AV | 7 | Total | C | N | O | P | 0 | 0 | 1 |
| | | | 114 | 49 | 22 | 37 | 6 | | | |
| 22 | CV | 6 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 113 | 49 | 22 | 36 | 6 | | | |

- Molecule 23 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23 | AX | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1623 | 723 | 294 | 530 | 76 | | | |
| 23 | CX | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1623 | 723 | 294 | 530 | 76 | | | |

- Molecule 24 is a protein called GE82832.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 24 | AW | 10 | Total | C | N | O | 0 | 0 | 0 |
| | | | 93 | 67 | 10 | 16 | | | |
| 24 | CW | 10 | Total | C | N | O | 0 | 0 | 0 |
| | | | 93 | 67 | 10 | 16 | | | |

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25 | BA | 2731 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 58834 | 26185 | 11020 | 18899 | 2730 | | | |
| 25 | DA | 2714 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 58458 | 26018 | 10942 | 18786 | 2712 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26 | BB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26 | DB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27 | BD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |
| 27 | DD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 985 | 298 | 270 | 6 | | | |
| 28 | DE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 985 | 298 | 270 | 6 | | | |

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | BF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1584 | 1009 | 298 | 275 | 2 | | | |
| 29 | DF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1580 | 1007 | 297 | 274 | 2 | | | |

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1425 | 914 | 256 | 251 | 4 | | | |
| 30 | DG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1424 | 911 | 258 | 251 | 4 | | | |

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | BH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |
| 31 | DH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1085 | 693 | 189 | 202 | 1 | | | |
| 32 | DI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1061 | 680 | 186 | 194 | 1 | | | |

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |
| 33 | DN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1135 | 706 | 230 | 196 | 3 | | | |
| 35 | DP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1135 | 706 | 230 | 196 | 3 | | | |

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 37 | DR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 553 | 175 | 149 | | | | |
| 38 | DS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 870 | 549 | 173 | 148 | | | | |

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | BT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1091 | 680 | 225 | 185 | 1 | | | |
| 39 | DT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1083 | 675 | 224 | 183 | 1 | | | |

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |
| 40 | DU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |
| 41 | DV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 557 | 174 | 153 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | DW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 557 | 174 | 153 | 2 | | | |

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |
| 43 | DX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |
| 44 | DY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BZ | 171 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1349 | 862 | 243 | 242 | 2 | | | |
| 45 | DZ | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1360 | 870 | 243 | 245 | 2 | | | |

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | B0 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 404 | 139 | 109 | 1 | | | |
| 46 | D0 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 404 | 139 | 109 | 1 | | | |

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | B1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |
| 47 | D1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | B2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |
| 48 | D2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49 | B3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 49 | D3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 464 | 296 | 90 | 78 | | | |

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | B4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 551 | 348 | 99 | 99 | 5 | | | |
| 50 | D4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 531 | 338 | 97 | 91 | 5 | | | |

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |
| 51 | D5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |
| 52 | D6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 279 | 91 | 75 | 4 | | | |

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53 | B7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 53 | D7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 511 | 328 | 99 | 82 | 2 | | | |
| 54 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55 | B9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 55 | D9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | B4 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | BA | 738 | Total | Mg | 0 | 0 |
| | | | 738 | 738 | | |
| 56 | AK | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DQ | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 56 | D3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DF | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 56 | B8 | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | BE | 10 | Total | Mg | 0 | 0 |
| | | | 10 | 10 | | |
| 56 | B1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | AN | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | BP | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | AX | 9 | Total 9 | Mg 9 | 0 | 0 |
| 56 | DN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | CA | 172 | Total 172 | Mg 172 | 0 | 0 |
| 56 | B5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BB | 18 | Total 18 | Mg 18 | 0 | 0 |
| 56 | D8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | B9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BF | 8 | Total 8 | Mg 8 | 0 | 0 |
| 56 | AV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | B2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AA | 221 | Total 221 | Mg 221 | 0 | 0 |
| 56 | BQ | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | CQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | CX | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | DV | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | AM | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BU | 8 | Total 8 | Mg 8 | 0 | 0 |

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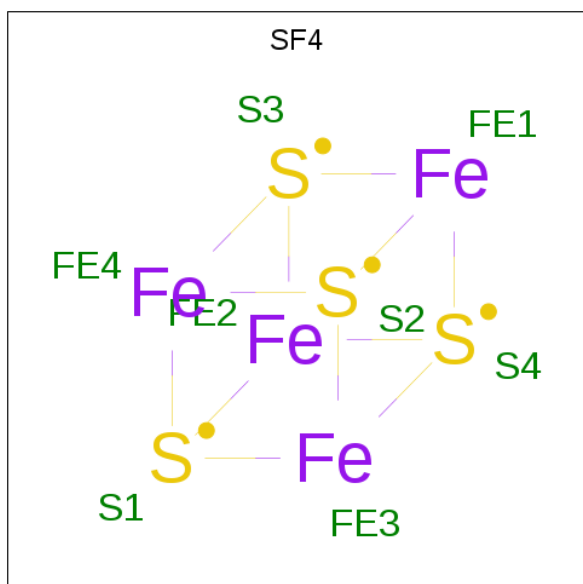
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | DR | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | AD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BN | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | CT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | D0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BG | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | BY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DE | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | B3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | BR | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | DA | 653 | Total 653 | Mg 653 | 0 | 0 |
| 56 | DW | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | B7 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | CF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BV | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | DO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BZ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | D5 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | BD | 12 | Total 12 | Mg 12 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56 | B0 | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | CE | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | BW | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 56 | DD | 8 | Total | Mg | 0 | 0 |
| | | | 8 | 8 | | |
| 56 | AF | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DB | 12 | Total | Mg | 0 | 0 |
| | | | 12 | 12 | | |

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 57 | AD | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 57 | CD | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

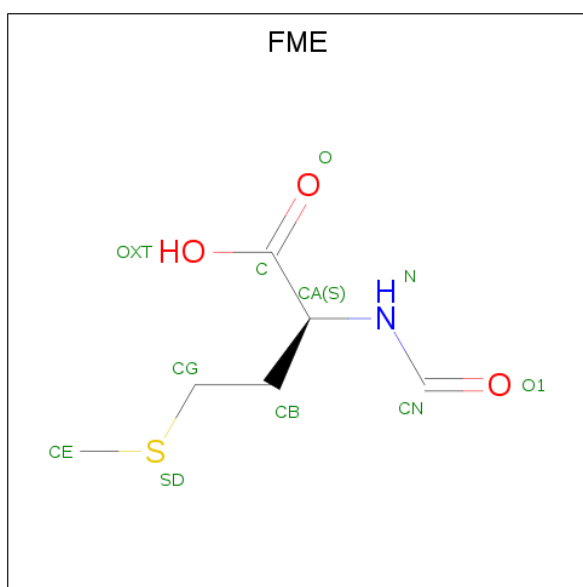
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58 | B5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 58 | B4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | CN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | BY | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | B9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | DY | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | D5 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | D4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | AN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | D6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | B6 | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 59 | AX | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 10 | 6 | 1 | 2 | 1 | | |
| 59 | CX | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 10 | 6 | 1 | 2 | 1 | | |

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 60 | BA | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | DA | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 61 | AA | 148 | Total | O | 0 | 0 |
| | | | 148 | 148 | | |
| 61 | AD | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | AE | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 61 | AJ | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | AL | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | AP | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | AU | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | AV | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | AX | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | BA | 1092 | Total | O | 0 | 0 |
| | | | 1092 | 1092 | | |
| 61 | BB | 26 | Total | O | 0 | 0 |
| | | | 26 | 26 | | |
| 61 | BD | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |
| 61 | BE | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 61 | BF | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | BG | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BN | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BO | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BP | 15 | Total 15 | O 15 | 0 | 0 |
| 61 | BQ | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BR | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BT | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BU | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | BV | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BW | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BX | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | B0 | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | B1 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | B5 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | B7 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | B8 | 8 | Total 8 | O 8 | 0 | 0 |
| 61 | CA | 187 | Total 187 | O 187 | 0 | 0 |
| 61 | CE | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | CN | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CT | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CX | 2 | Total 2 | O 2 | 0 | 0 |

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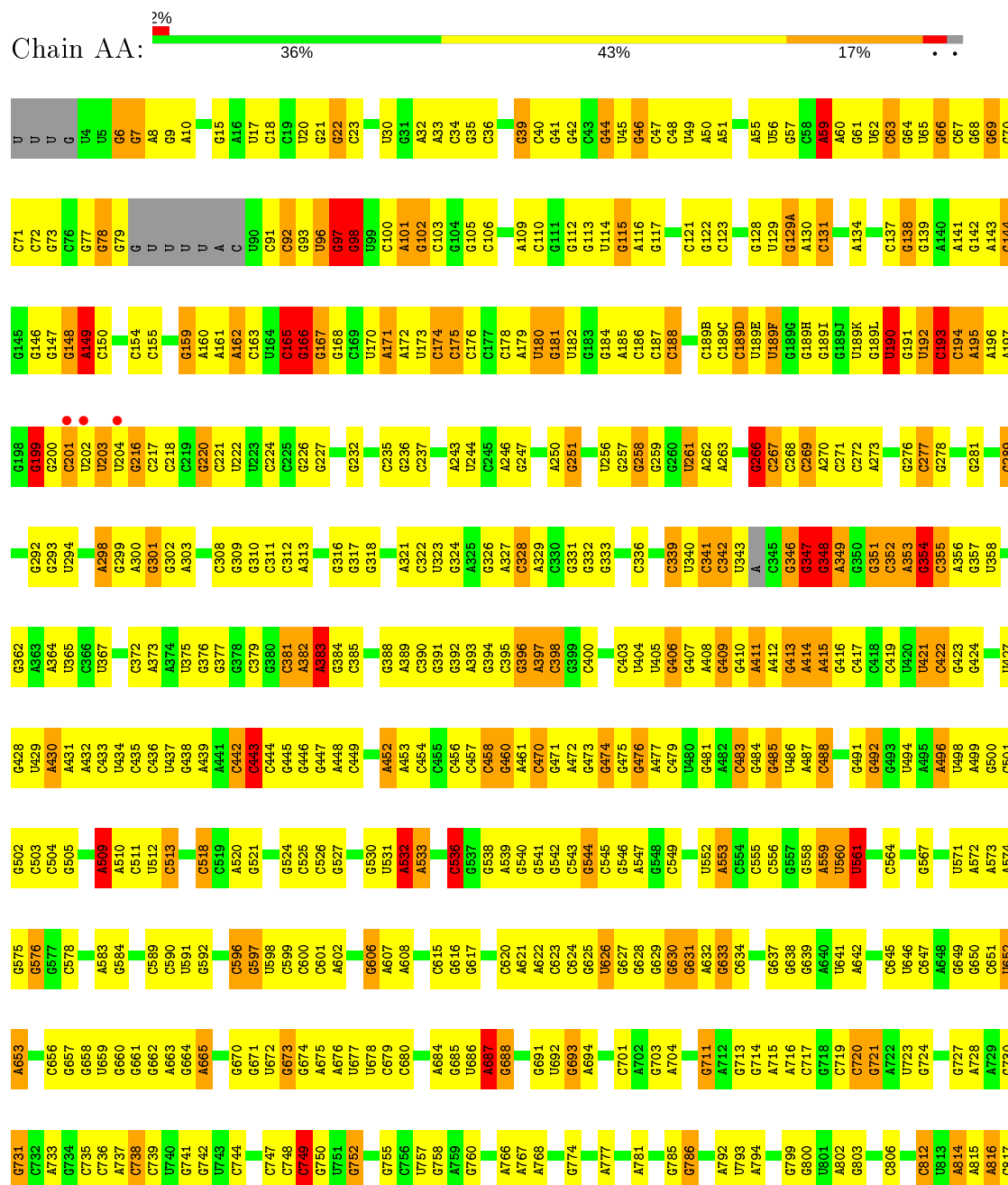
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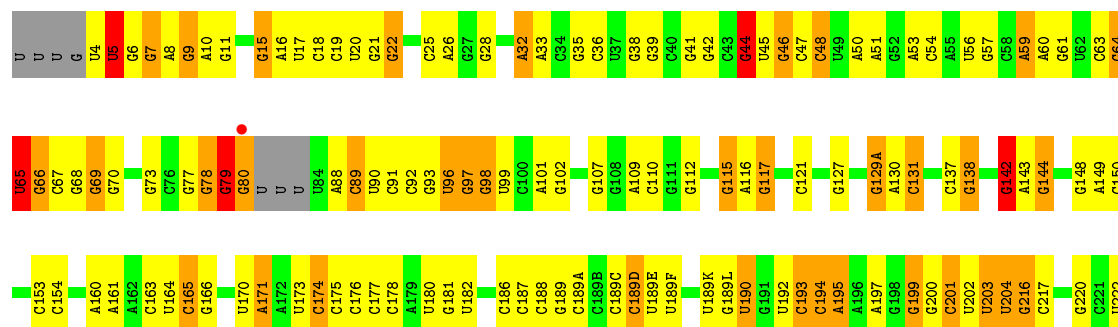
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | DA | 902 | Total 902 | O 902 | 0 | 0 |
| 61 | DB | 7 | Total 7 | O 7 | 0 | 0 |
| 61 | DD | 8 | Total 8 | O 8 | 0 | 0 |
| 61 | DE | 13 | Total 13 | O 13 | 0 | 0 |
| 61 | DF | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | DO | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DP | 14 | Total 14 | O 14 | 0 | 0 |
| 61 | DQ | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | DU | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | DV | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DX | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DY | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | D0 | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | D1 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D7 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | D8 | 4 | Total 4 | O 4 | 0 | 0 |

3 Residue-property plots

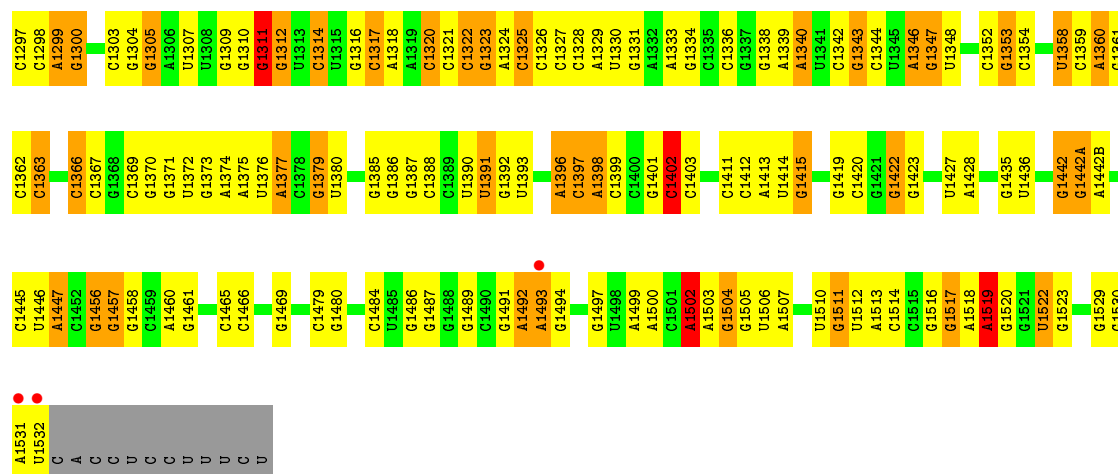
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S Ribosomal RNA

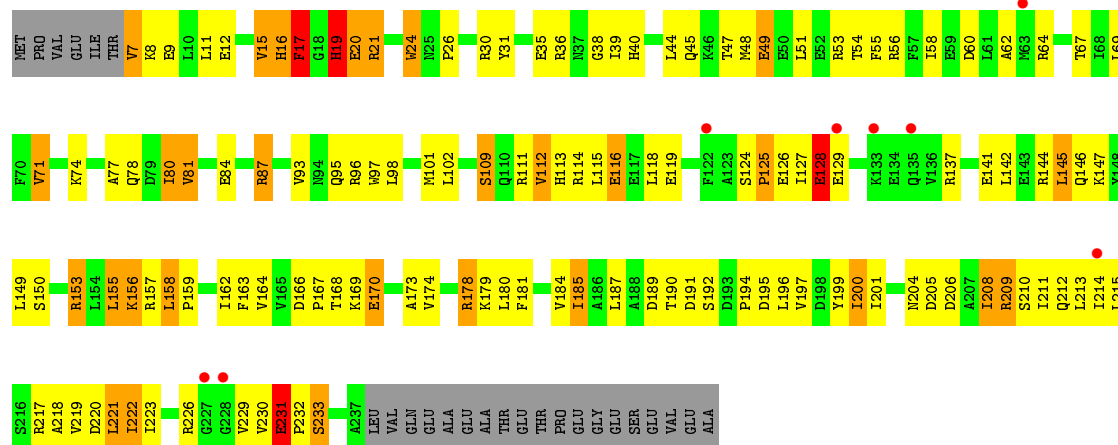




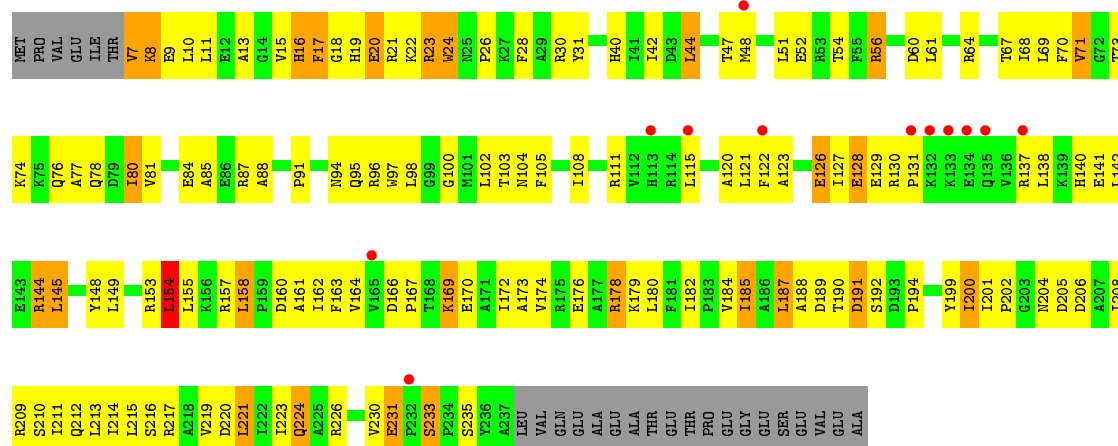
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|-------|-------|-------|--------|-------|------|------|------|------|------|------|------|------|------|------|
| C1228 | A1168 | A1105 | C985 | A1041 | A919 | C834 | G752 | C680 | A608 | G538 | C454 | G388 | C308 | U223 |
| A1169 | A1169 | G1106 | A986 | G1042 | U920 | U835 | A753 | G683 | A609 | A539 | C455 | A389 | C308 | |
| C1233 | G1171 | C1107 | | C1043 | U921 | G836 | G754 | G684 | G610 | G540 | C456 | C390 | G316 | G226 |
| U1235 | C1172 | C1108 | C989 | A1044 | G922 | G837 | G755 | A684 | G611 | G541 | C457 | G391 | G316 | G227 |
| A1236 | G1173 | C1109 | C990 | | A923 | G838 | G756 | G685 | G615 | G542 | C458 | G392 | | A228 |
| C1237 | G1174 | A1110 | U991 | G1047 | C924 | U839 | U757 | U686 | G616 | C543 | G460 | A393 | A321 | U229 |
| A1238 | G1175 | C1112 | U992 | G1048 | G925 | C840 | G758 | A687 | | G544 | A461 | | C922 | |
| A1239 | A1176 | C1113 | G993 | | G926 | U841 | G759 | G688 | U619 | C545 | C470 | G396 | U323 | G232 |
| G1240 | C1116 | | U994 | C1051 | G927 | C848 | A759 | G689 | C620 | G546 | C471 | A397 | G324 | C233 |
| U1241 | G1117 | C1114 | C995 | U1052 | G928 | C849 | A760 | G690 | A621 | G547 | A472 | C398 | A325 | C234 |
| C1242 | A1178 | C1115 | U996 | G1053 | | U850 | A761 | G691 | G622 | G399 | G473 | C399 | G326 | C235 |
| C1243 | A1180 | C1116 | U997 | C1054 | C931 | G851 | A768 | U692 | C623 | U551 | G474 | C400 | A327 | G236 |
| C1244 | A1181 | C1117 | G998 | U1055 | C932 | G852 | G769 | G693 | C624 | U552 | G475 | C401 | G328 | C237 |
| A1245 | G1182 | C1118 | C999 | U1056 | G933 | G855 | G774 | A694 | G625 | A553 | | G402 | A329 | |
| C1246 | A1183 | G1120 | U1000 | G1057 | C934 | G858 | G775 | C701 | U626 | C554 | G484 | C403 | C330 | A243 |
| | G1184 | U1121 | A1001 | G1058 | A935 | G859 | A776 | A711 | G627 | C555 | G485 | U404 | G331 | U244 |
| C1249 | G1185 | A1122 | G1001A | C1059 | C936 | A859 | A777 | A704 | G628 | C556 | U486 | U405 | G332 | C245 |
| A1250 | G1186 | A1123 | G1002 | C1060 | A937 | A860 | | U705 | G629 | G557 | A487 | G406 | G333 | A246 |
| A1251 | G1187 | G1124 | G1003 | U1061 | A938 | G861 | C783 | A706 | G630 | G558 | C488 | G407 | | G247 |
| A1252 | G1188 | U1125 | A1004 | G1062 | G939 | G862 | | G708 | G631 | G559 | A489 | | C337 | |
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| | G1190 | C1127 | C1006 | U1064 | G941 | G868 | G785 | G710 | G633 | U561 | G491 | G410 | C339 | G251 |
| | A1191 | C1128 | C1007 | C1065 | G942 | G869 | G786 | G711 | G634 | C562 | G492 | A411 | U340 | U252 |
| U1257 | C1192 | U1129 | G1008 | C1066 | | | | G712 | G635 | A563 | G493 | A412 | C341 | U253 |
| G1258 | G1193 | A1130 | C1009 | A1067 | G947 | A872 | A790 | A713 | | C564 | U494 | G413 | C342 | G254 |
| C1259 | U1194 | G1131 | G1010 | G1068 | C948 | A873 | G791 | A714 | G638 | U565 | A495 | A414 | U343 | G255 |
| C1260 | A1195 | C1132 | G1011 | C1069 | | A874 | A792 | G713 | G639 | A496 | | A415 | A344 | |
| A1261 | G1196 | U1133 | U1012 | U1070 | G951 | G874 | U793 | G714 | G640 | G568 | | C345 | A346 | G258 |
| C1262 | U1197 | G1134 | G1013 | C1071 | U952 | C875 | A794 | A715 | U641 | U571 | G500 | C418 | G347 | U261 |
| C1263 | G1197 | U1135 | G1014 | G1072 | G953 | G876 | | A716 | A642 | A572 | C501 | C419 | | A262 |
| C1264 | G1198 | U1136 | A1015 | U1073 | G954 | G877 | C797 | | | A573 | G502 | | G350 | A263 |
| U1199 | U1199 | C1137 | A1016 | G1074 | U955 | G878 | G798 | G719 | U646 | | C503 | C422 | G351 | G264 |
| C1200 | C1200 | G1138 | G1017 | C1075 | U956 | C879 | G799 | G720 | G647 | G576 | C504 | G423 | C352 | G265 |
| A1201 | G1201 | C1139 | C1018 | U1076 | U957 | C880 | G800 | A648 | G649 | G577 | G505 | G424 | A353 | G266 |
| A1268 | G1202 | C1140 | U1019 | G1077 | A958 | G881 | U801 | A722 | G650 | G578 | G426 | G425 | G354 | C267 |
| C1203 | C1203 | G1141 | U1020 | U1078 | A959 | C882 | A802 | U723 | G651 | G579 | U427 | G426 | C355 | C268 |
| A1204 | U1204 | G1142 | G1021 | G1079 | U960 | | G803 | G724 | C651 | A509 | G427 | G428 | | C269 |
| U1205 | U1205 | G1143 | U1022 | A1080 | U961 | G885 | U804 | G725 | U652 | A510 | G428 | U429 | U358 | A270 |
| G1206 | G1206 | C1144 | G1023 | G1081 | | G890 | C805 | C726 | A653 | C511 | U429 | U430 | U359 | C271 |
| C1207 | G1207 | G1145 | G1024 | | A964 | U891 | C806 | G727 | A654 | C512 | A431 | | | |
| C1208 | C1208 | U1146 | U1025 | U1084 | A965 | U892 | | G730 | C656 | C513 | A432 | A363 | G276 | G277 |
| C1209 | C1209 | A1147 | G1026 | U1085 | G966 | A892 | C811 | G731 | | C514 | C433 | A364 | A364 | |
| C1210 | C1210 | U1148 | C1027 | U1086 | C967 | C893 | U812 | G732 | G660 | C515 | U434 | U365 | U365 | G281 |
| U1211 | U1211 | G1149 | G1028 | G1087 | A968 | G894 | U813 | A733 | G661 | C516 | C435 | C366 | C366 | A282 |
| U1212 | U1212 | U1150 | C1029 | U1088 | A969 | | A814 | A734 | G662 | C517 | U436 | U367 | | C283 |
| A1213 | A1213 | A1151 | G1030 | G1089 | C970 | C899 | A815 | G735 | A663 | G518 | U437 | | C372 | G284 |
| C1214 | C1214 | A1152 | G1030A | U1090 | G971 | A900 | A816 | C736 | G664 | C519 | G438 | | A373 | |
| C1215 | G1215 | C1153 | C1030B | U1091 | C972 | A901 | C817 | C736 | C590 | G520 | G439 | | A374 | |
| G1283 | G1216 | G1154 | G1030C | A1092 | G973 | G902 | G818 | A737 | A665 | U591 | G439 | | A373 | |
| C1284 | C1217 | G1155 | A1030D | A1093 | A974 | | | C738 | G666 | C525 | A441 | | A374 | U287 |
| U1218 | C1218 | G1156 | G1031 | U1094 | A975 | G906 | G821 | C739 | G667 | G527 | C442 | | U375 | A288 |
| U1219 | U1219 | A1157 | A976 | U1095 | G976 | A907 | | U740 | | C528 | C443 | | G376 | G289 |
| G1220 | G1220 | C1158 | A977 | C1032 | A977 | A908 | C826 | G741 | G671 | G597 | C444 | | G377 | |
| A1287 | A1287 | G1159 | U978 | G1034 | A978 | | U827 | G742 | U672 | U598 | G445 | | | G292 |
| A1288 | A1288 | C1160 | C979 | A1035 | C979 | A913 | U828 | | G673 | C599 | G446 | | G380 | G293 |
| A1289 | G1222 | C1161 | A914 | G1036 | C980 | A914 | G829 | C745 | G674 | C600 | G447 | | C381 | |
| G1290 | C1223 | A1161 | A915 | U981 | G981 | A915 | G830 | | U677 | A535 | A448 | | A382 | G297 |
| G1291 | G1224 | C1162 | A916 | C1037 | U982 | G916 | G831 | | U678 | A536 | | | A383 | A298 |
| U1292 | A1225 | C1163 | A1101 | C1038 | U983 | G917 | U831 | | G332 | G606 | | | G384 | G299 |
| G1293 | G1226 | C1103 | A1102 | C1039 | A983 | G917 | U833 | | C679 | A452 | | | A384 | A300 |
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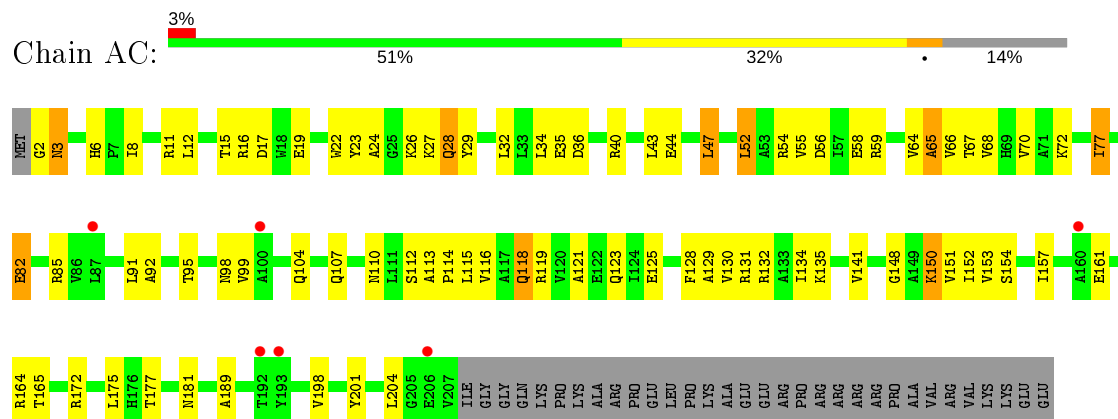
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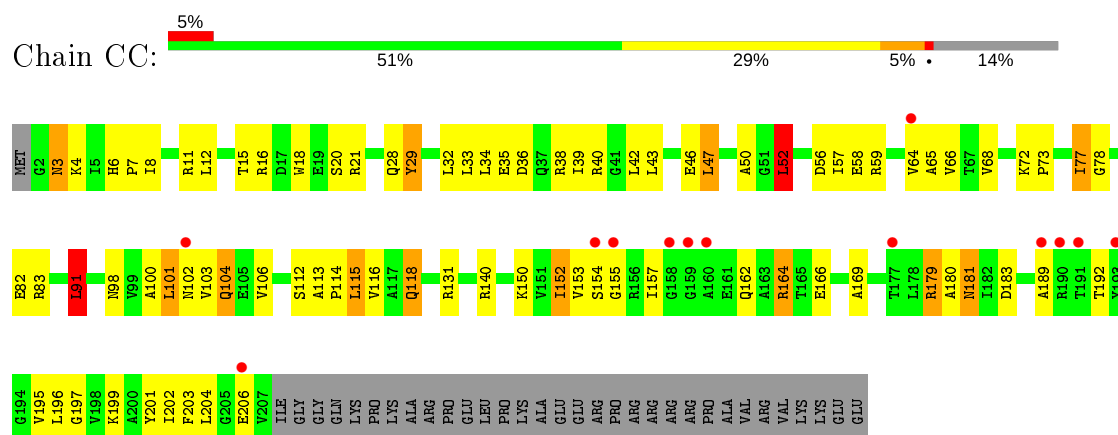
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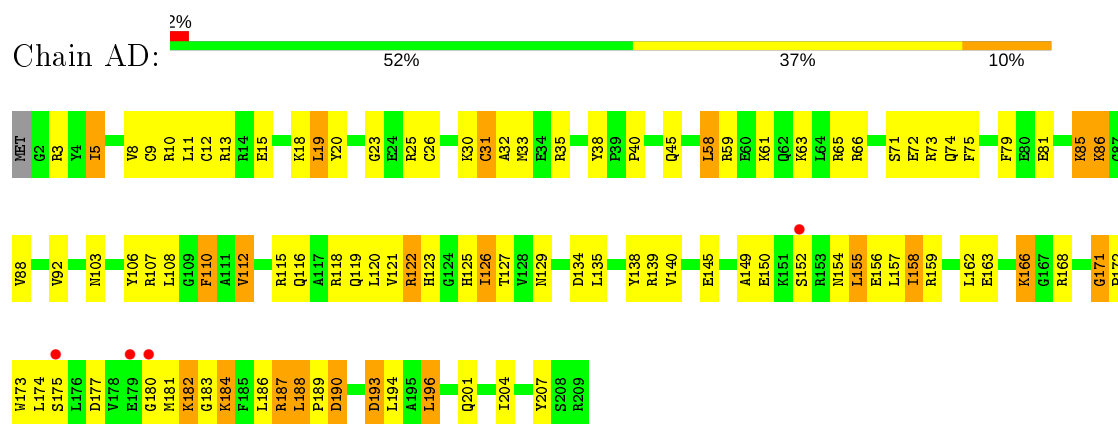
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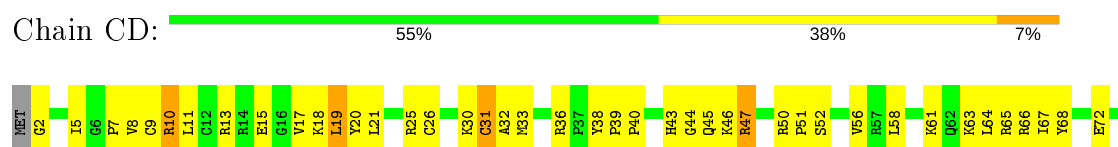
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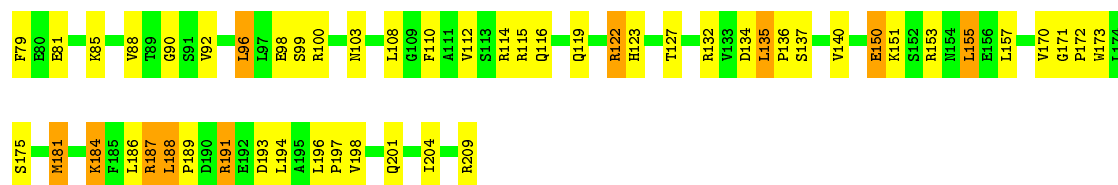


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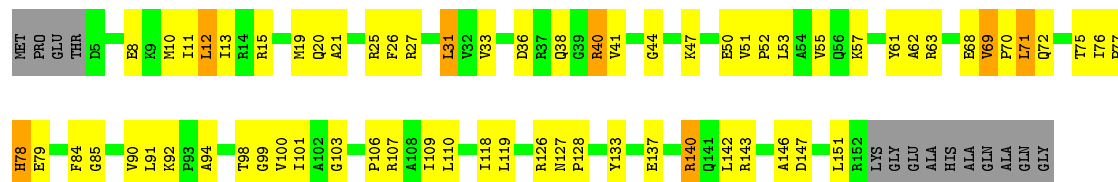
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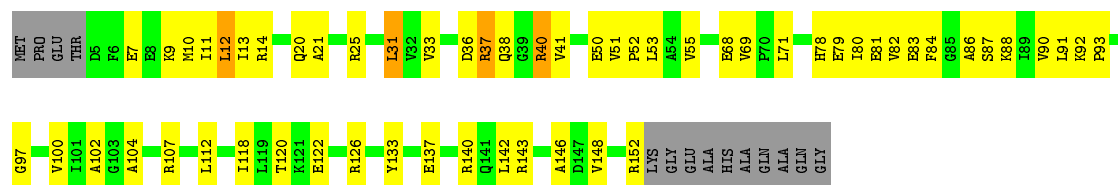
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Chain AE: 50% 37% 9%



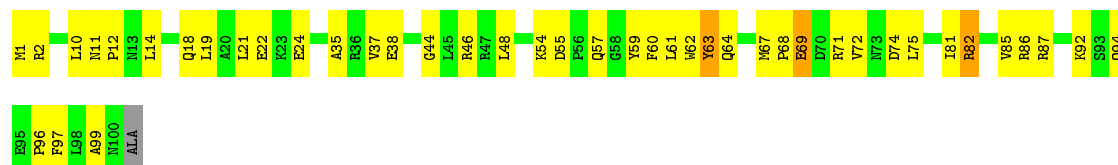
• Molecule 5: 30S Ribosomal Protein S5

Chain CE: 56% 33% 9%



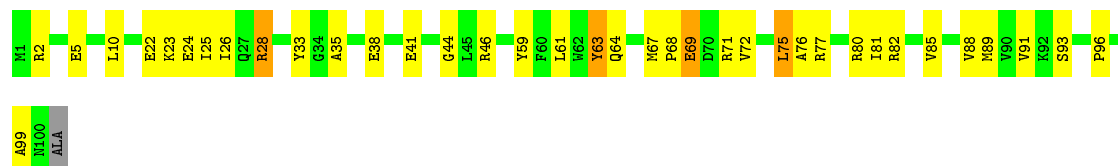
• Molecule 6: 30S Ribosomal Protein S6

Chain AF: 56% 40% 9%



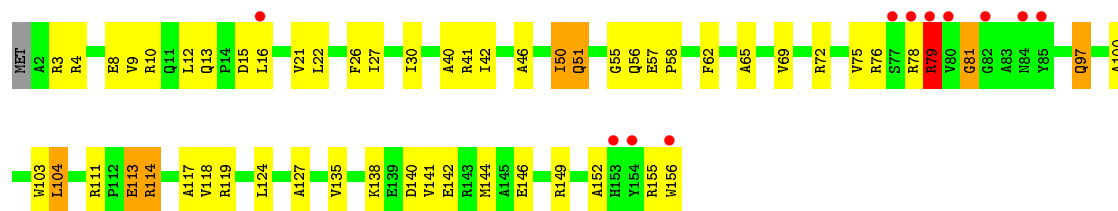
• Molecule 6: 30S Ribosomal Protein S6

Chain CF: 62% 33% 9%

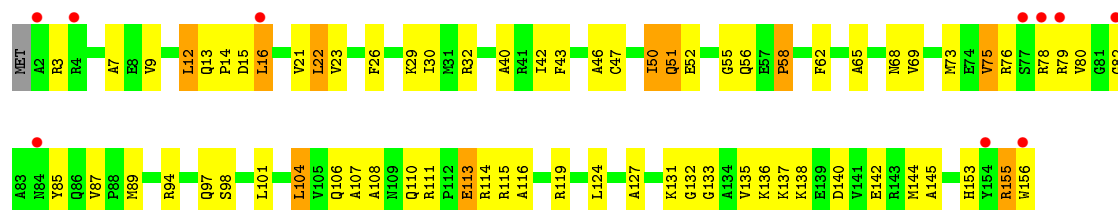


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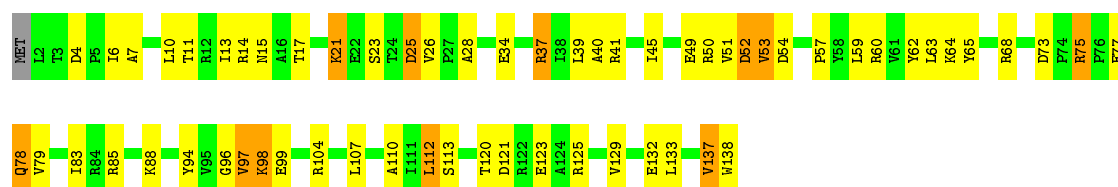
Chain AG: 63% 31% 9%



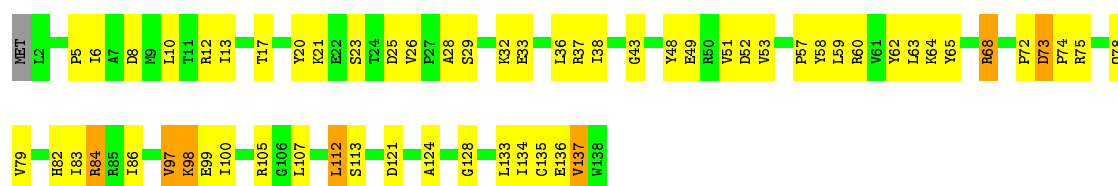
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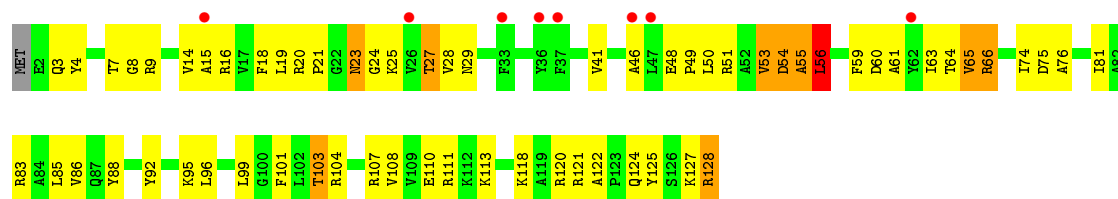
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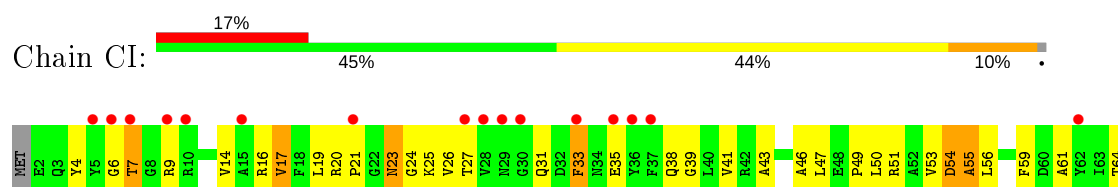
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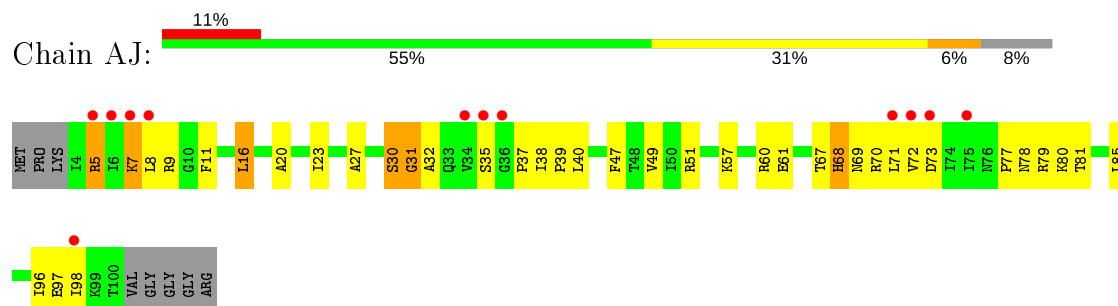
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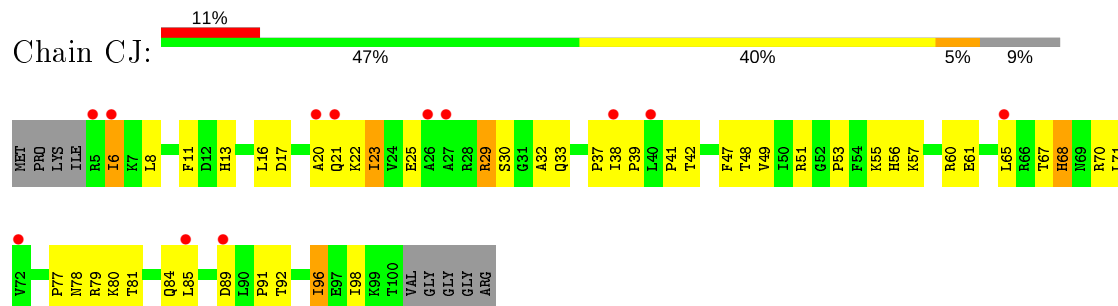
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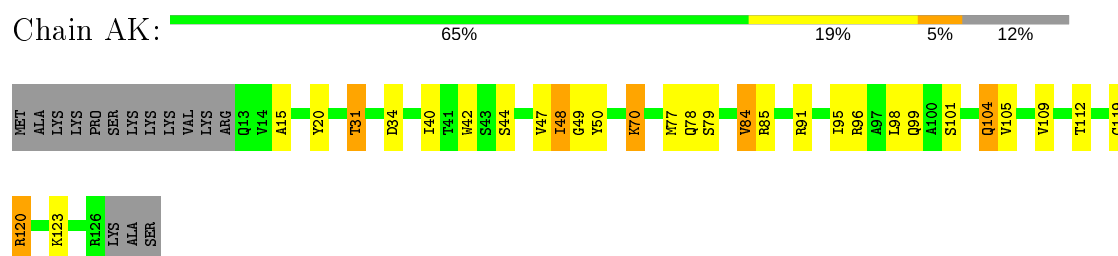
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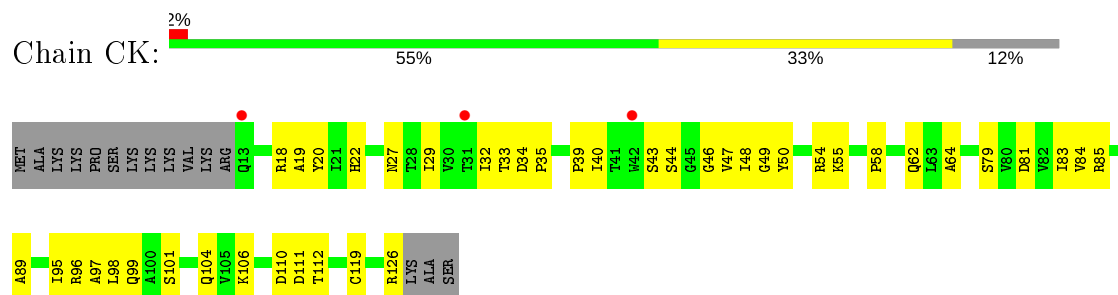
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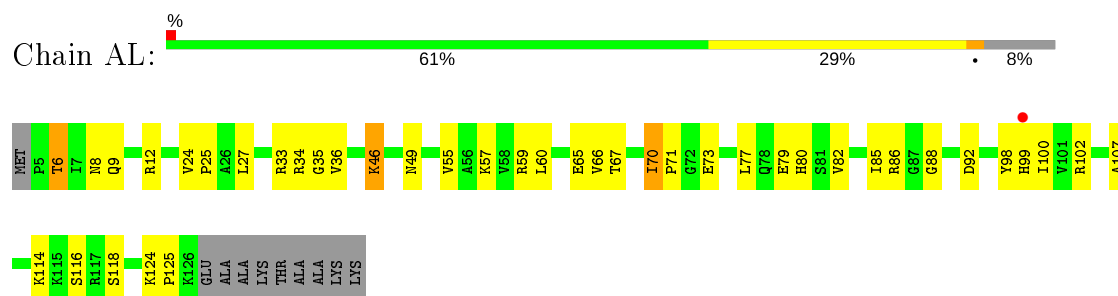
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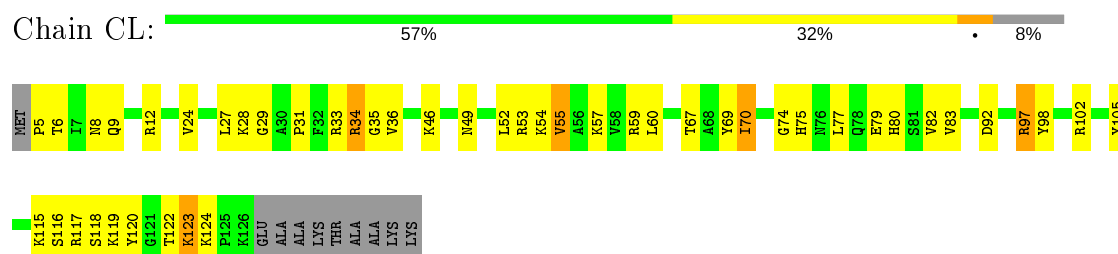
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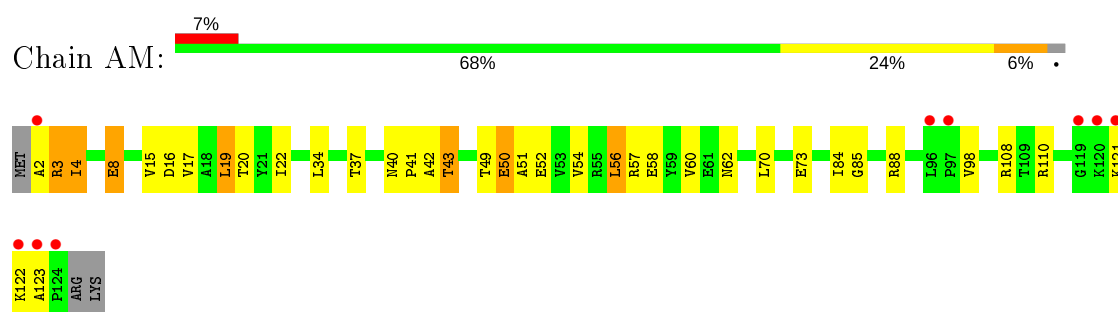
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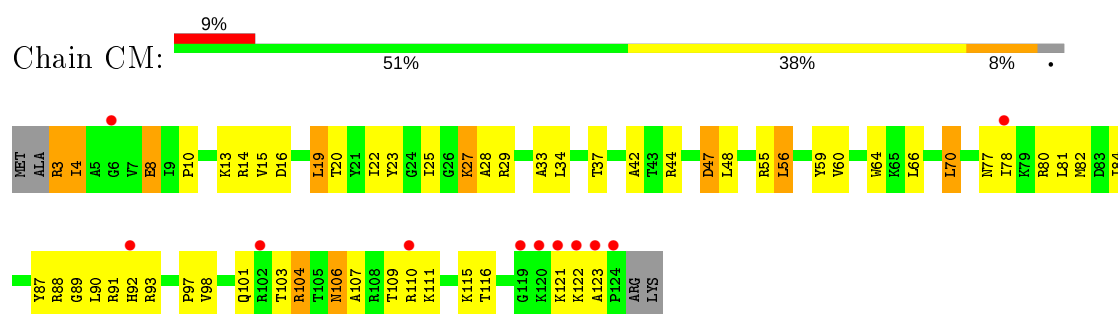
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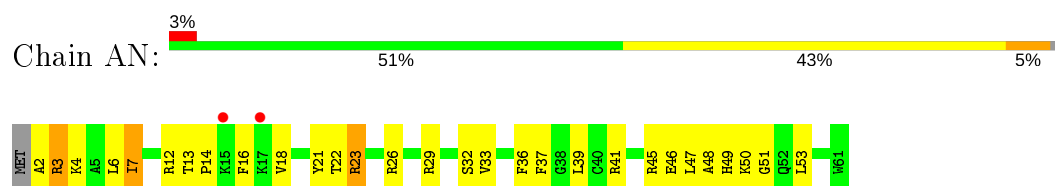
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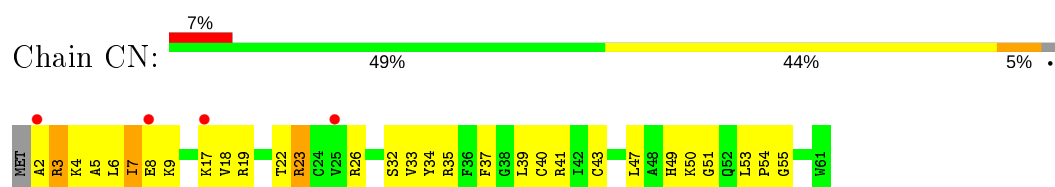
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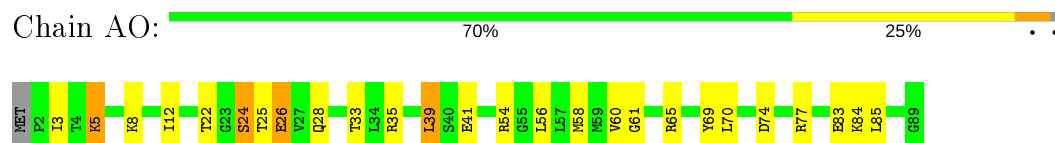
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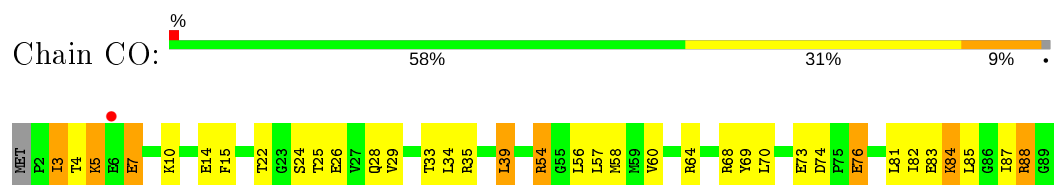
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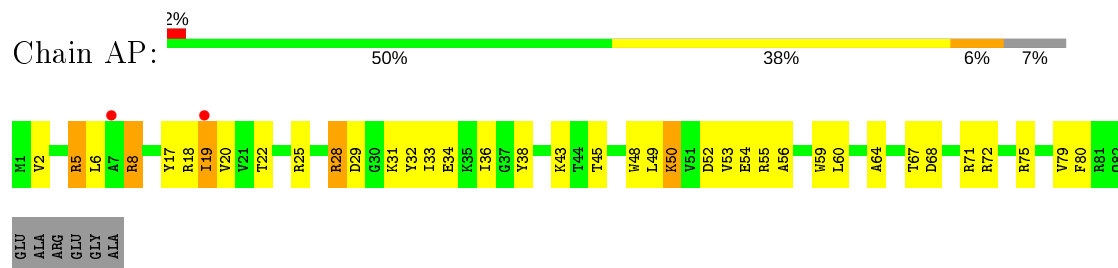
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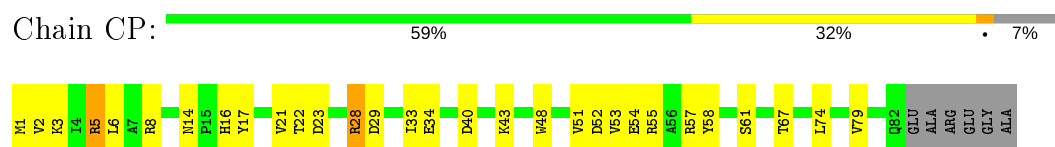
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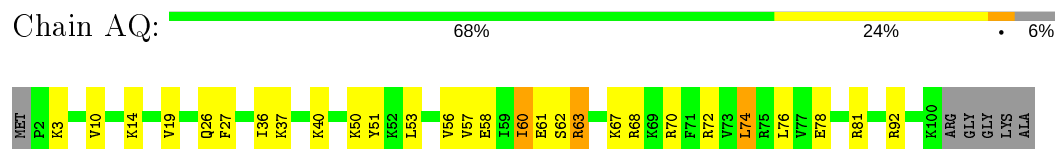
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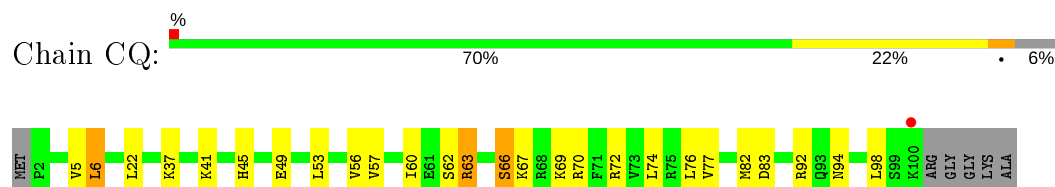
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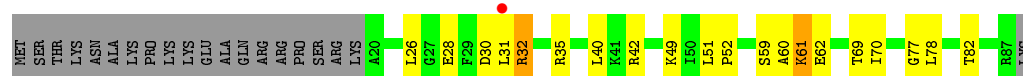
• Molecule 17: 30S Ribosomal Protein S17



• Molecule 17: 30S Ribosomal Protein S17



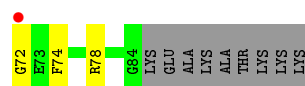
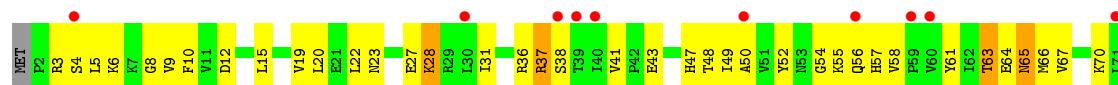
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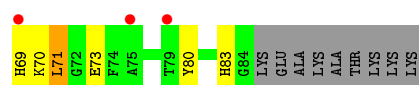
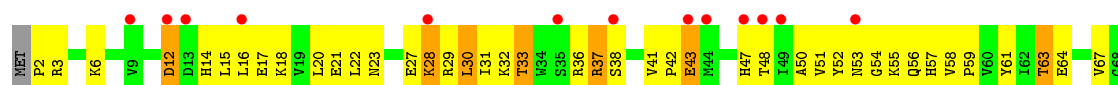
- Molecule 18: 30S Ribosomal Protein S18



- Molecule 19: 30S Ribosomal Protein S19



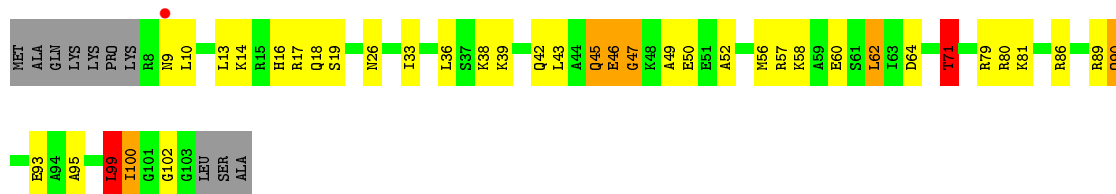
- Molecule 19: 30S Ribosomal Protein S19



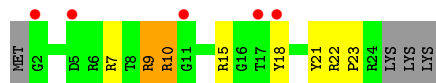
- Molecule 20: 30S Ribosomal Protein S20



- Molecule 20: 30S Ribosomal Protein S20



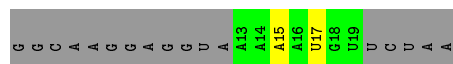
• Molecule 21: 30S Ribosomal Protein THX



• Molecule 21: 30S Ribosomal Protein THX



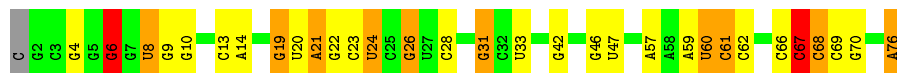
• Molecule 22: mRNA



• Molecule 22: mRNA



• Molecule 23: P-site tRNA



• Molecule 23: P-site tRNA





- Molecule 24: GE82832

Chain AW:  10% 80% 10%



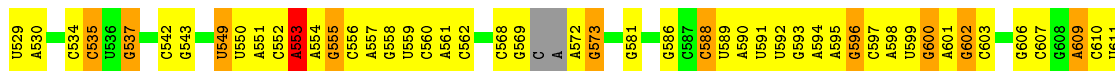
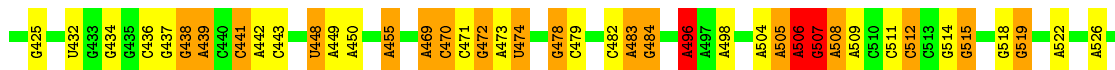
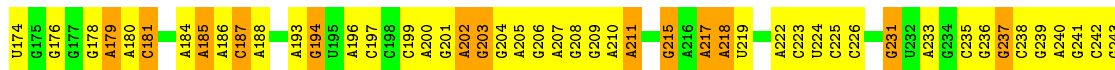
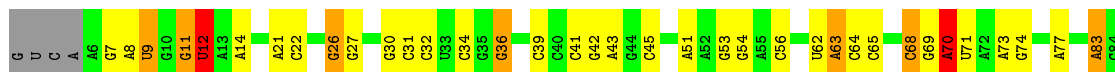
- Molecule 24: GE82832

Chain CW: 



- Molecule 25: 23S Ribosomal RNA

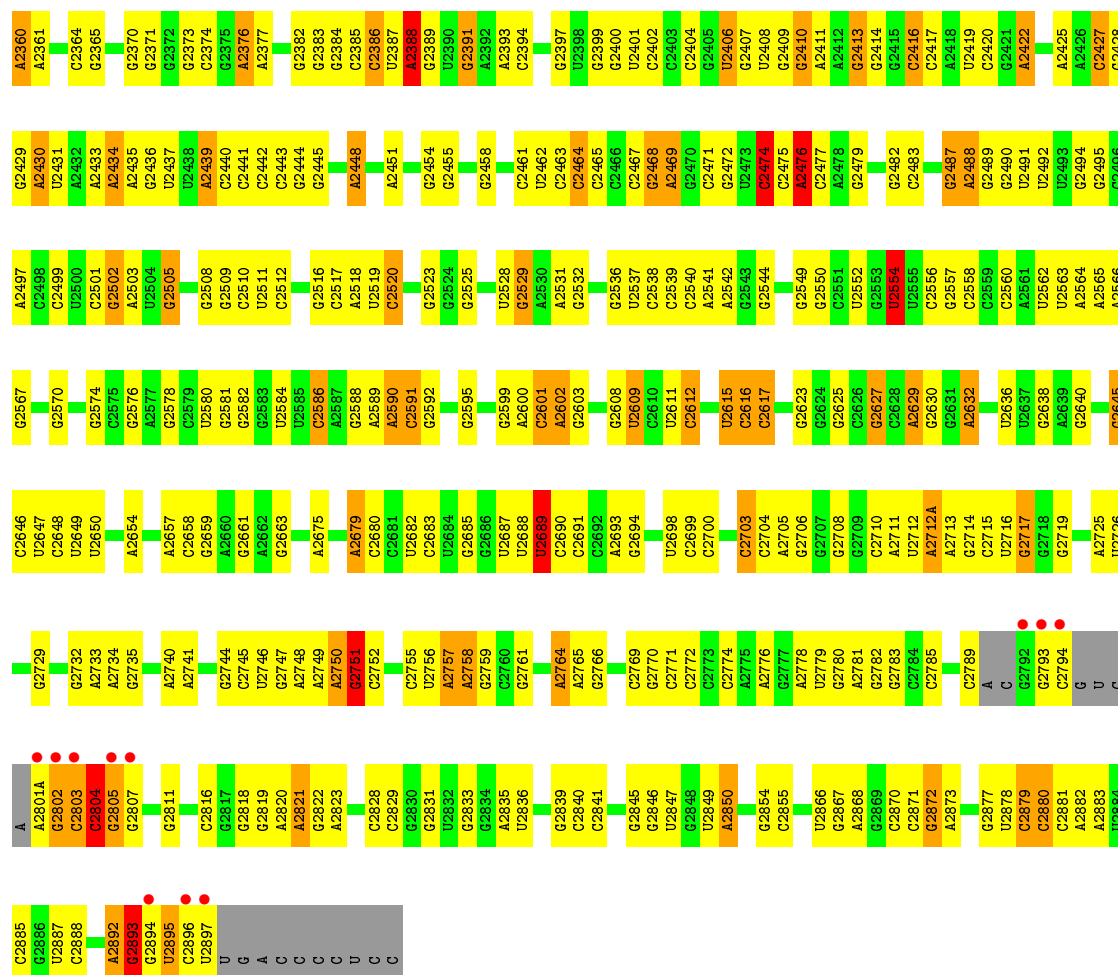
Chain BA:



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| C2059 | G2060 | A1959 | G1858 | G1787 | C1707 | A1614 | G1529 | A1430 | A1347 | G1248 | G1156 | A1096 | G1019 | A937 | A851 |
| G2061 | G2062 | A1960 | G1859 | G1788 | G1708 | G1615 | G1530 | C1432 | G1356 | A1249 | G1158 | C1098 | C1020 | C938 | G852 |
| C2063 | C2064 | C1963 | G1870 | A1790 | C1709 | A1617 | A1536 | U1440 | U1359 | C1252 | G1168 | C | G1024 | C940 | U857 |
| A2065 | U1977 | U1977 | G1871 | A1791 | G1710 | A1618 | G1537 | A1441 | C1360 | A1255 | G1171 | G | A1029 | U841 | U858 |
| C2066 | C2067 | U1985 | C1874 | A1793 | A1712 | U1625 | A1539 | U1442 | C1361 | U1256 | A1174 | G | A1030 | A942 | C859 |
| C2067 | G2070 | C1986 | A1878 | G1795 | A1715 | G1628 | A1540 | C1444 | A1363 | C1263 | A1175 | G | C1032 | C943 | U860 |
| G2071 | G2071 | C1987 | A1879 | G1800 | A1716 | C1629 | A1541 | G1454 | C1366 | A1265 | U1176 | U | A1034 | A947 | G864 |
| G2074 | G2074 | C1988 | U1882 | A1804 | A1717 | A1630 | A1542 | G1459 | A1367 | C1266 | G1177 | G | G1035 | C948 | G865 |
| A2075 | A2075 | C1989 | A1887 | C1805 | C1720 | A1632 | U1543 | U1460 | G1370 | G1273 | C1180 | C | A1036 | C949 | A866 |
| A2076 | C2077 | A1988 | A1879 | C1806 | G1721 | A1633 | C1547 | U1461 | G1373 | G1277 | G1181 | C | G1039 | C950 | G870 |
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| G2078 | A2080 | A1990 | A1890 | U1808 | C1724 | G1640 | C1550 | G1463 | G1377 | G1285 | A1183 | U | G1043 | A956 | U874 |
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| A2082 | A2083 | C2001 | C1901 | U1810 | U1735 | U1648 | C1552 | A1465 | G1378 | U1286 | A1186 | A | U1045 | G962 | A876 |
| A2084 | C2087 | C2011 | C1904 | A1815 | U1736 | U1648 | A1553 | G1467 | C1379 | A1287 | A1187 | A | A1046 | A963 | G877 |
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| G2091 | A2092 | G2019 | C1911 | C1821 | G1744 | G1653 | U1556 | G1471 | A1383 | G1296 | G1190 | G | C1051 | G974 | A882 |
| A2093 | G2094 | G2022 | C1913 | G1823 | G1745 | A1654 | A1557 | C1472 | G1384 | C1297 | G1195 | C | C1054 | G977 | U886 |
| C2095 | U2096 | G2026 | C1914 | G1824 | G1746 | C1661 | G1558 | A1473 | G1385 | G1298 | C1199 | C | A1055 | A978 | G892 |
| U2101 | G2102 | A2035 | C1914 | G1825 | A1747 | A1662 | U1569 | G1475 | U1387 | A1299 | G1200 | U | U1058 | U982 | C893 |
| C2103 | A2104 | A2036 | G1919 | U1826 | A1748 | A1664 | U1574 | A1480 | G1389 | G1303 | A1201 | U | C1059 | C985 | U894 |
| G2105 | C2106 | C2037 | U1920 | C1827 | G1749 | G1665 | A1575 | C1483 | G1390 | C1304 | A1202 | C | U1069 | A986 | U905 |
| C2107 | C2107 | U2039 | G1921 | U1828 | G1751 | G1666 | A1576 | G1487 | A1395 | A1308 | G1210 | U | A1066 | A987 | G902 |
| U2108 | G2109 | G2040 | A1922 | U1829 | G1752 | U1667 | G1576 | A1491 | U1398 | A1311 | U1211 | A | G1067 | G988 | G903 |
| G2110 | C2110 | A2041 | G1925 | G1831 | U1753 | G1668 | C1577 | A1496 | G1402 | U1313 | G1216 | G | U1070 | G989 | C904 |
| G2115 | G2116 | C2043 | A1935 | A1832 | C1757 | A1679 | C1578 | G1497 | U1403 | A1314 | G1217 | A | U1072 | G992 | A908 |
| C2117 | C2118 | U2044 | C1936 | G1845 | G1758 | G1680 | G | A1500 | G1404 | A1315 | G1218 | U | A1073 | G993 | G909 |
| U2119 | U2120 | A1937 | U1937 | G1846 | C1759 | A1681 | U | U1501 | A1405 | C1316 | A1219 | U | A1074 | C994 | A910 |
| U2121 | C2122 | G2045 | A1938 | A1846 | U1760 | C1682 | A | G1502 | A1406 | G1317 | U1220 | C | A1075 | G998 | G911 |
| G2122 | G2122 | U2046 | U1939 | G1847 | A1770 | C1683 | C | G1503 | G1410 | A1320 | A1221 | G | G1076 | A998 | C912 |
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| A2053 | G2115 | A2053 | A1852 | G1853 | G1779 | A1699 | C1597 | G1517 | U1418 | G1327 | G1230 | C | C1086 | A1004 | G927 |
| G2116 | C2117 | U2054 | G1778 | G1854 | C1780 | A1699 | U1604 | G1518 | C1421 | U1338 | G1231 | U | C1087 | A1005 | G928 |
| C2118 | C2119 | A1954 | G1781 | G1855 | A1701 | A1699 | A1605 | G1519 | C1422 | U1339 | G1232 | C | G1088 | G1007 | G929 |
| U2120 | C2122 | U2056 | C1782 | A1702 | G1608 | A1699 | A1605 | G1520 | C1423 | U1340 | A1234 | A | C1089 | U1008 | G930 |
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| C2122 | C2122 | U2056 | C1782 | A1702 | G1608 | A1699 | A1605 | G1522 | A1426 | C1343 | G1240 | U | G1153 | A994 | G933 |
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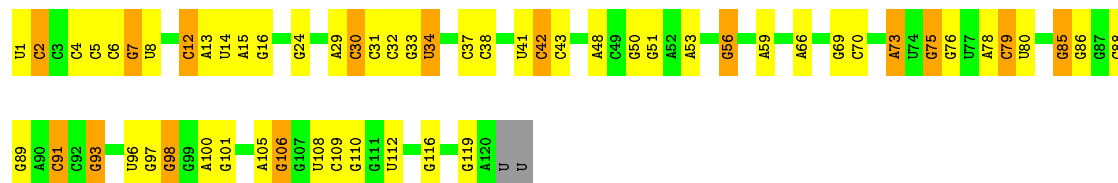
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| G1222 | C1152 | A957 | C893 | C755 | G674 | G618 | G554 | G469 | C376 | A300 | C249 |
| G1223 | G1153 | U958 | C894 | C825 | G675 | G619 | U957 | A470 | G386 | G301 | G250 |
| | G1154 | A959 | U895 | G760 | A676 | G620 | C560 | A471 | | C302 | A251 |
| | A1155 | A960 | A896 | U761 | U827 | | | A472 | | U303 | G252 |
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| G1228 | G1161 | U963 | A899 | A764 | C679 | | G565 | G476 | C392 | G308 | A255 |
| C1229 | C1162 | G966 | A900 | G765 | G680 | A627 | U966 | A477 | C393 | G309 | C263 |
| C1230 | U1033 | C967 | C902 | G766 | G681 | | A667 | A478 | A479 | A310 | C264 |
| | U1034 | C970 | C903 | U773 | A682 | A631 | U568 | A480 | A311 | A265 | G265 |
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| G1236 | U1165 | G972 | C905 | G771 | U688 | A633 | G570 | G482 | | G315 | |
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| A1253 | U | A | C913 | A782 | A706 | G647 | C580 | U504 | G410 | | U271K |
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| G1187 | C1118 | C | C925 | A793 | G723 | C | C591 | U525 | U339 | | G272 |
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| G1192 | C1123 | U | U930 | C797 | A727 | C | C595 | G442 | G344 | | |
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| G1197 | U1129 | U | C935 | A802 | G731 | C | G600 | U448 | | | A278 |
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| U1199 | G1131 | G | U937 | A804 | G733 | C | A532 | C451 | G351 | | A282 |
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| A1204 | G1136 | C | A942 | G808 | C737 | A655 | C505 | G455 | C287 | | C288 |
| U1205 | G1137 | A | A943 | G809 | G738 | G656 | U606 | A456 | G363C | | A289 |
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| A1210 | C1139 | C | G946 | U811 | U740 | C658 | A608 | G538 | G366 | | G291 |
| C1291 | C1140 | C | G948 | U812 | G741 | C659 | G610 | C540 | A460 | | C292 |
| U1292 | G1141 | A | C949 | C812 | | G660 | | G545 | C370 | | A293 |
| C1293 | U1142 | U | C950 | U813 | U747 | | | C | A371 | | |
| A1294 | G1143 | C | G951 | C814 | G748 | G663 | U614 | A | G461 | | |
| G1215 | U1144 | U | C952 | C815 | C749 | | U614A | A | G465 | | G372 |
| G1216 | A1145 | C | A953 | C816 | | U667 | G614B | | A466 | | U373 |
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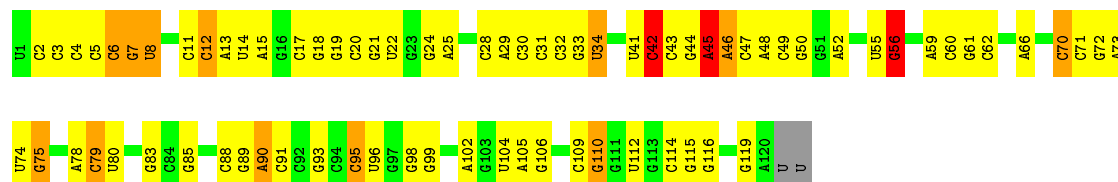
• Molecule 26: 5S Ribosomal RNA

Chain BB: 51% 35% 12%



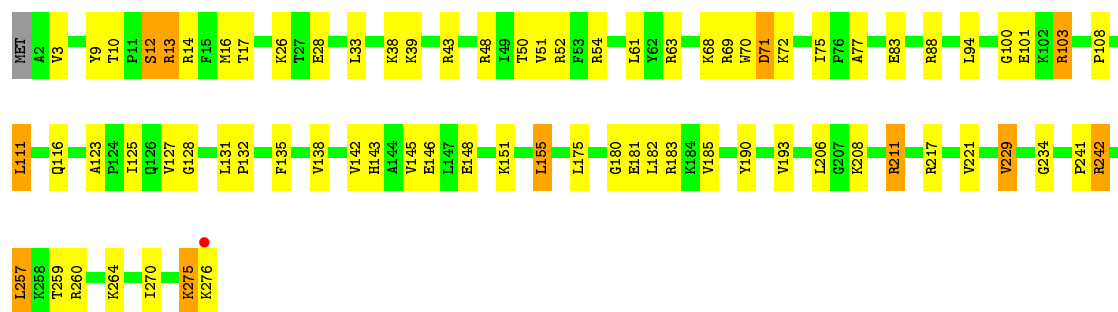
• Molecule 26: 5S Ribosomal RNA

Chain DB: 36% 50% 10%



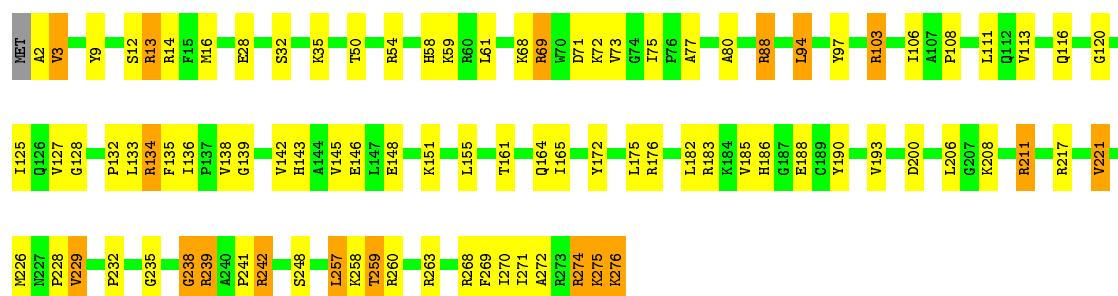
• Molecule 27: 50S Ribosomal Protein L2

Chain BD:  72% 24% .



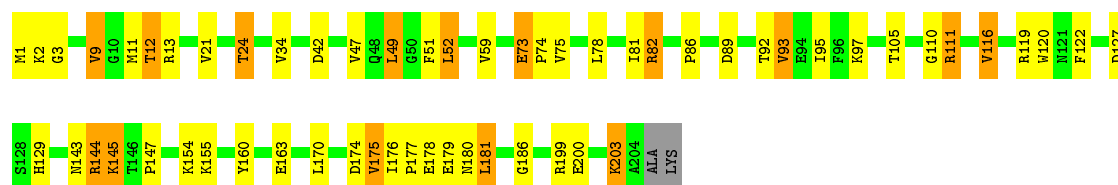
• Molecule 27: 50S Ribosomal Protein L2

Chain DD:  66% 27% 7%



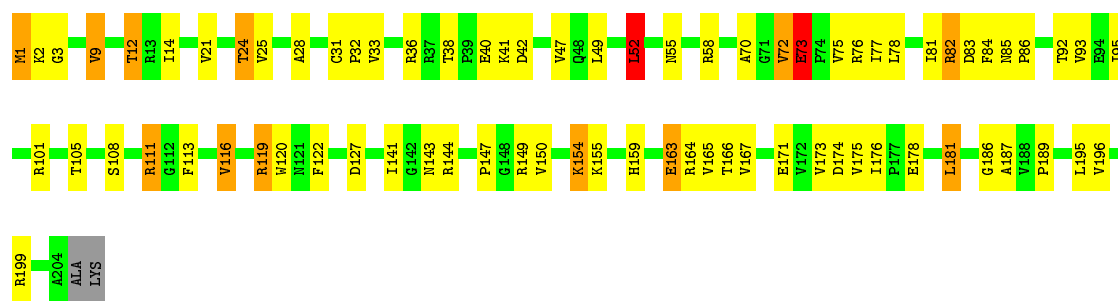
• Molecule 28: 50S Ribosomal Protein L3

Chain BE:  71% 21% 7% .

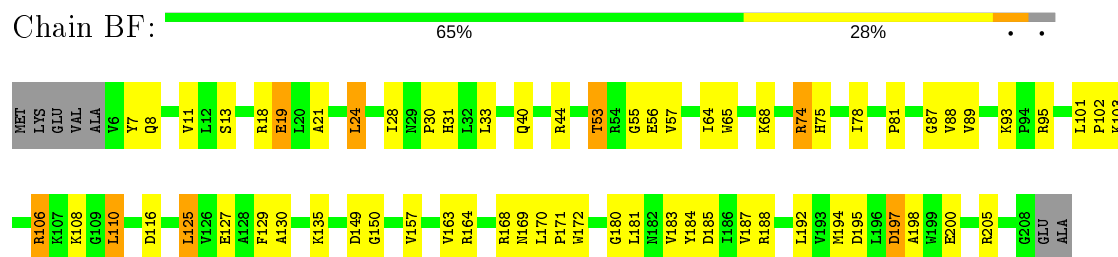


• Molecule 28: 50S Ribosomal Protein L3

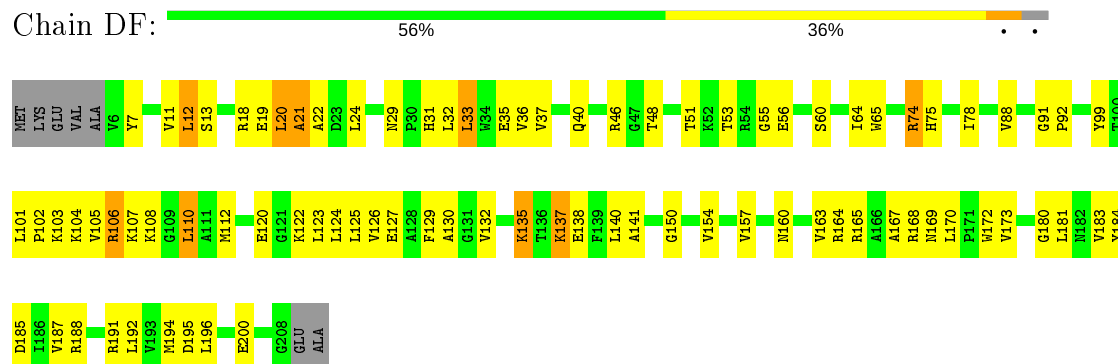
Chain DE:  62% 30% 6% ..



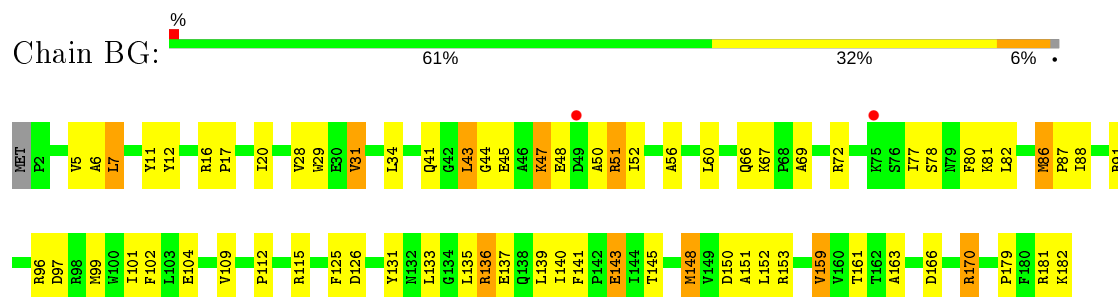
• Molecule 29: 50S Ribosomal Protein L4



• Molecule 29: 50S Ribosomal Protein L4



• Molecule 30: 50S Ribosomal Protein L5

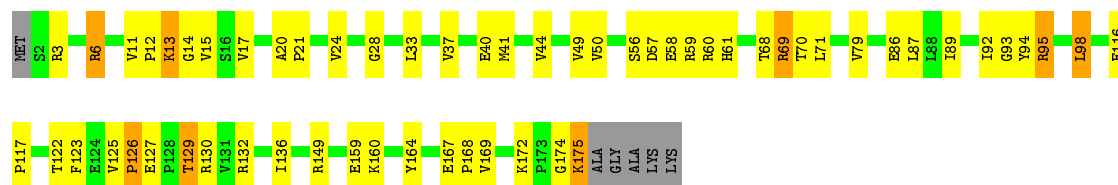


• Molecule 30: 50S Ribosomal Protein L5

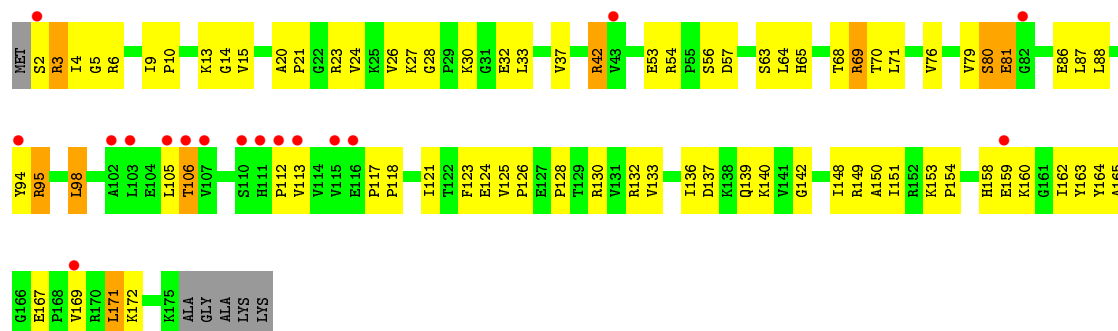


• Molecule 31: 50S Ribosomal Protein L6

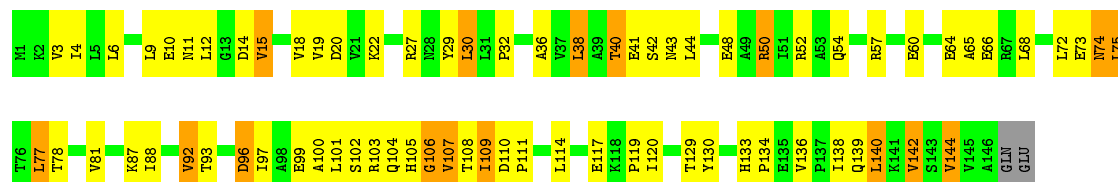




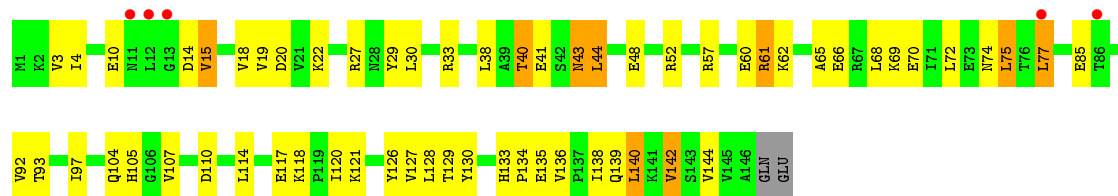
• Molecule 31: 50S Ribosomal Protein L6



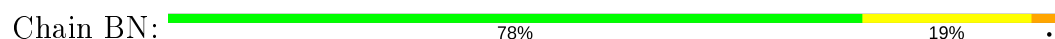
• Molecule 32: 50S Ribosomal Protein L9



• Molecule 32: 50S Ribosomal Protein L9

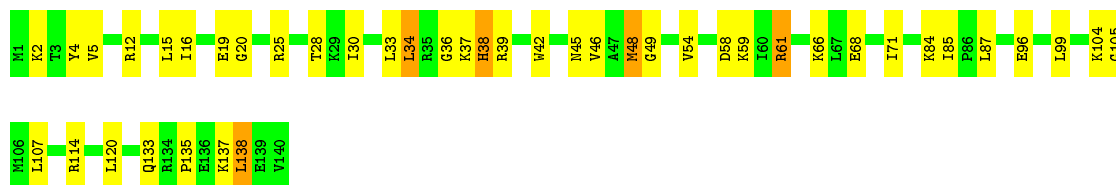


• Molecule 33: 50S Ribosomal Protein L13



• Molecule 33: 50S Ribosomal Protein L13

Chain DN:  69% 27% .



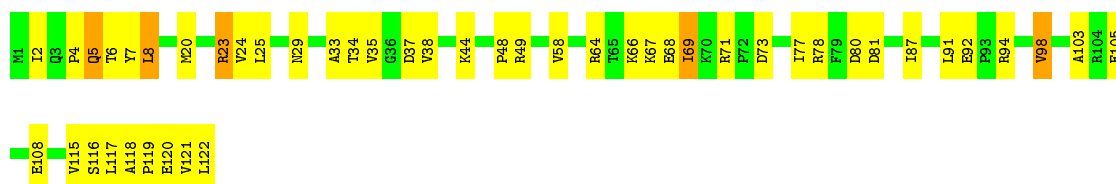
- Molecule 34: 50S Ribosomal Protein L14

Chain BO:  72% 25% ..



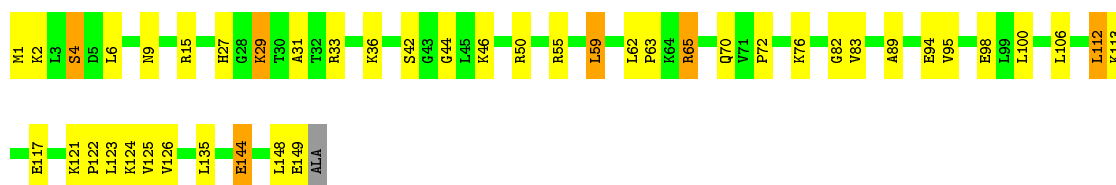
- Molecule 34: 50S Ribosomal Protein L14

Chain DO:  61% 34% .



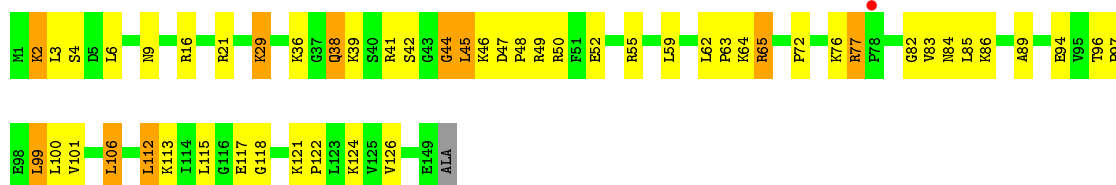
- Molecule 35: 50S Ribosomal Protein L15

Chain BP:  70% 25% ..



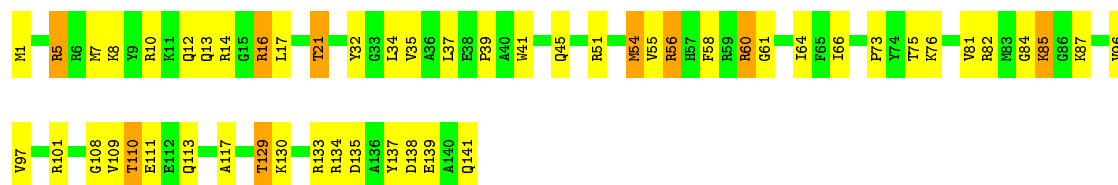
- Molecule 35: 50S Ribosomal Protein L15

Chain DP:  65% 28% 7% .

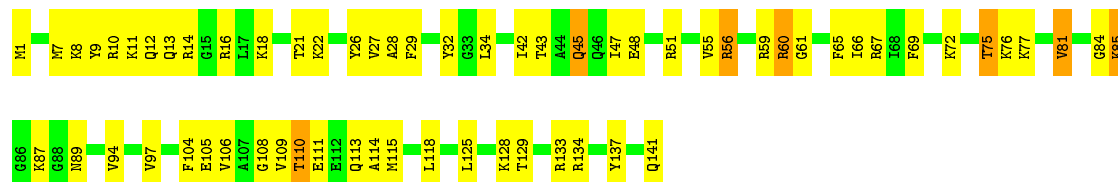


- Molecule 36: 50S Ribosomal Protein L16

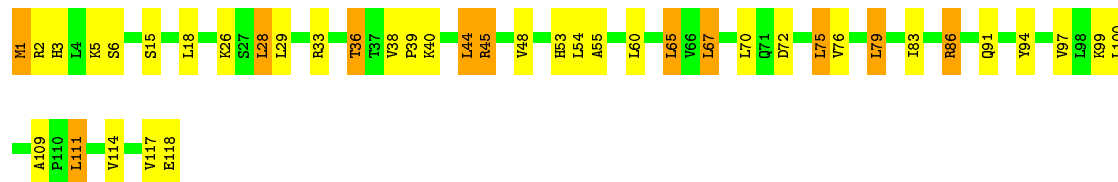
Chain BQ:  62% 31% 6%



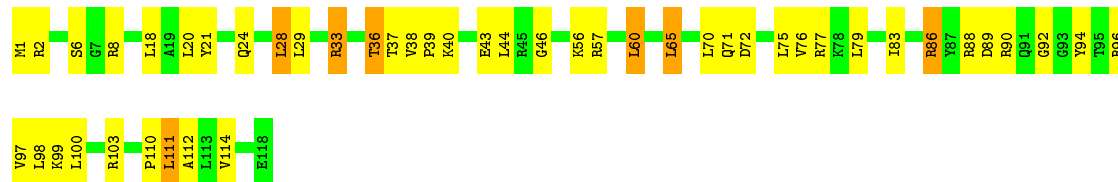
• Molecule 36: 50S Ribosomal Protein L16



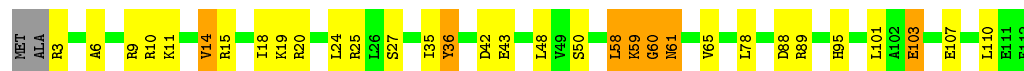
• Molecule 37: 50S Ribosomal Protein L17



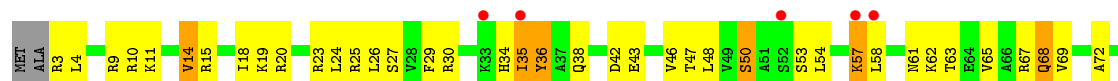
• Molecule 37: 50S Ribosomal Protein L17

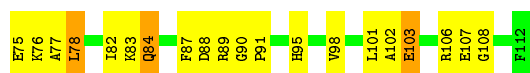


• Molecule 38: 50S Ribosomal Protein L18



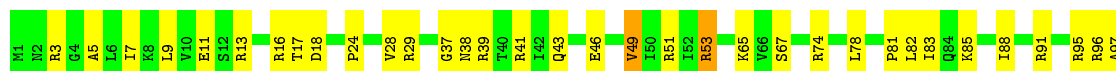
• Molecule 38: 50S Ribosomal Protein L18





• Molecule 39: 50S Ribosomal Protein L19

Chain BT: 62% 26% 10%



• Molecule 39: 50S Ribosomal Protein L19

Chain DT: 60% 27% 10%



• Molecule 40: 50S Ribosomal Protein L20

Chain BU: 69% 25% 5%



• Molecule 40: 50S Ribosomal Protein L20

Chain DU: 66% 27% 5%

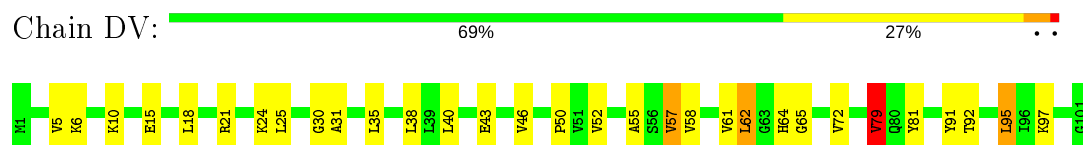


• Molecule 41: 50S Ribosomal Protein L21

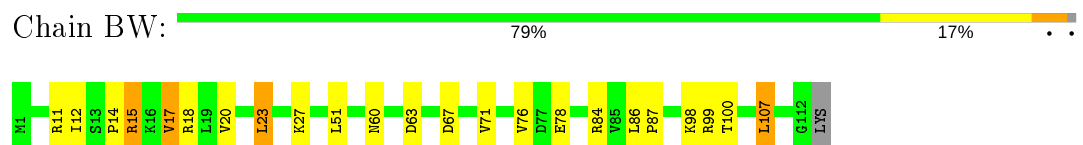
Chain BV: 81% 14% 5%



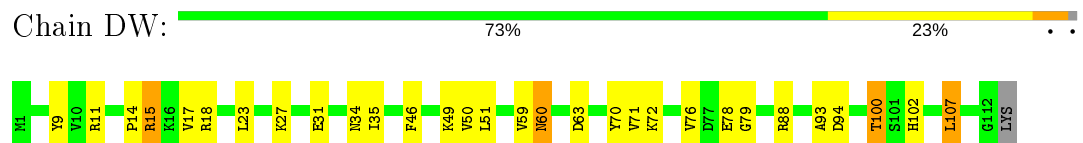
- Molecule 41: 50S Ribosomal Protein L21



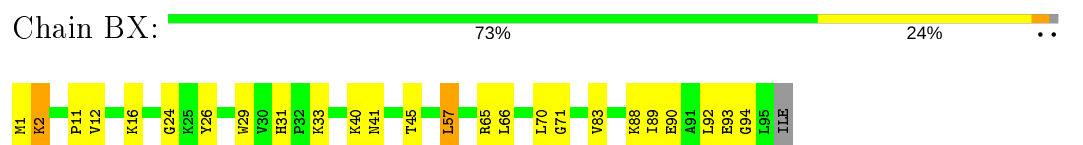
- Molecule 42: 50S Ribosomal Protein L22



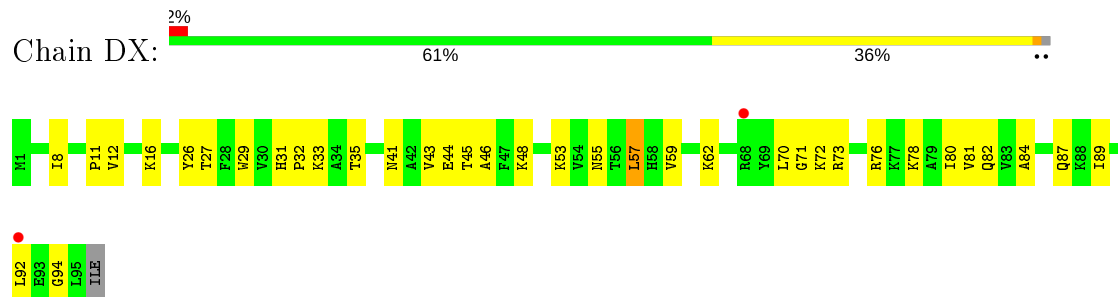
- Molecule 42: 50S Ribosomal Protein L22



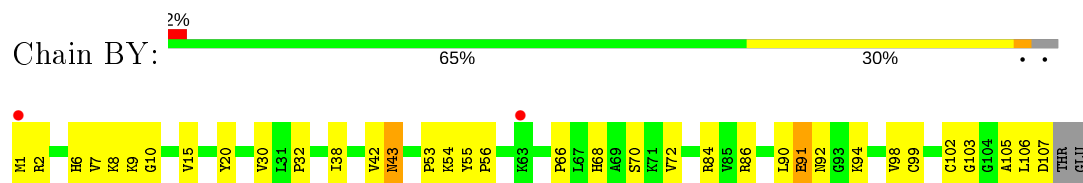
- Molecule 43: 50S Ribosomal Protein L23



- Molecule 43: 50S Ribosomal Protein L23

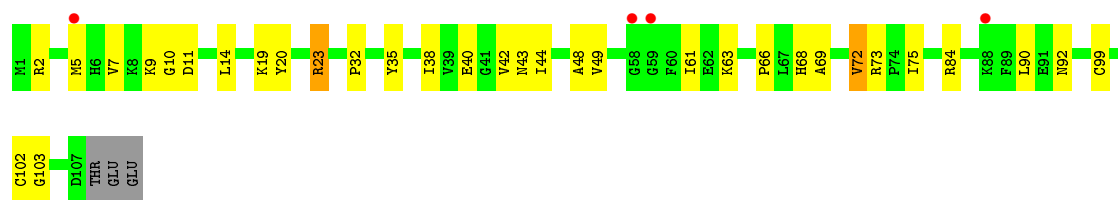


- Molecule 44: 50S Ribosomal Protein L24

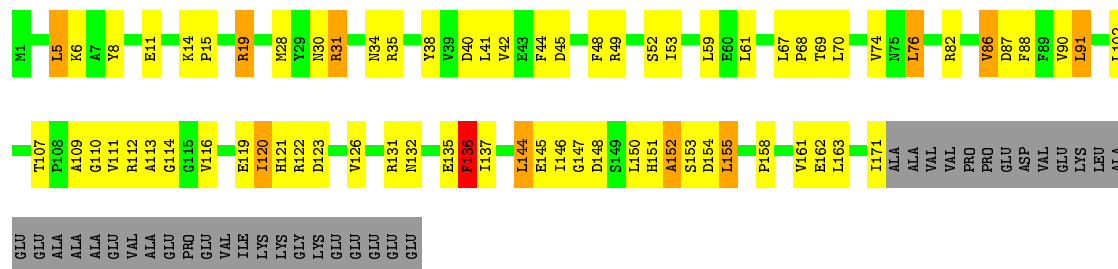


- Molecule 44: 50S Ribosomal Protein L24

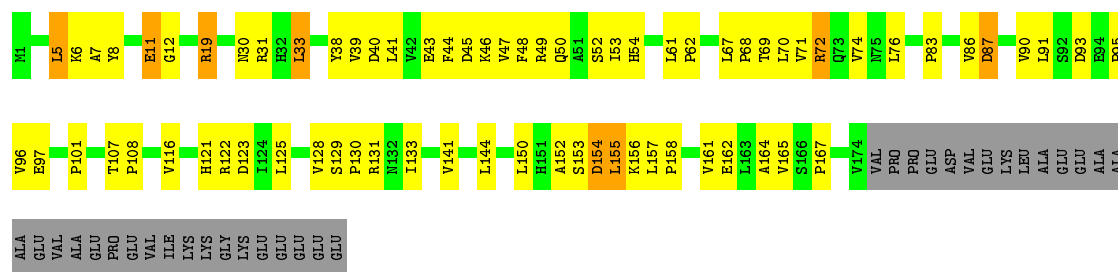




- Molecule 45: 50S Ribosomal Protein L25



- Molecule 45: 50S Ribosomal Protein L25



- Molecule 46: 50S Ribosomal Protein L27

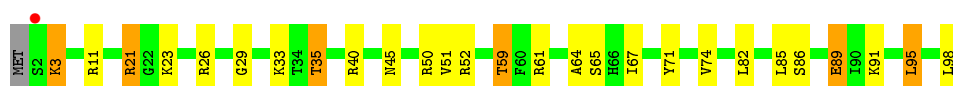


- Molecule 46: 50S Ribosomal Protein L27



- Molecule 47: 50S Ribosomal Protein L28

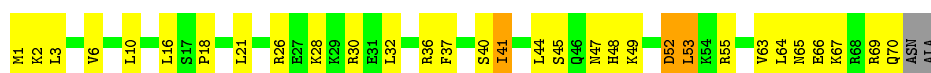




- Molecule 47: 50S Ribosomal Protein L28



- Molecule 48: 50S Ribosomal Protein L29



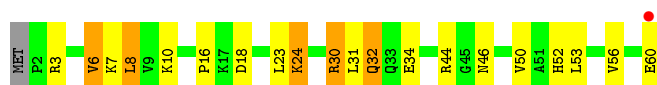
- Molecule 48: 50S Ribosomal Protein L29



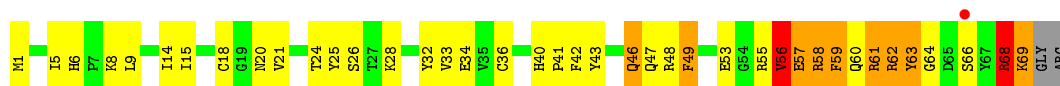
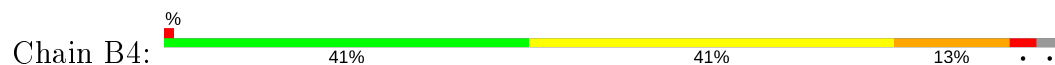
- Molecule 49: 50S Ribosomal Protein L30



- Molecule 49: 50S Ribosomal Protein L30

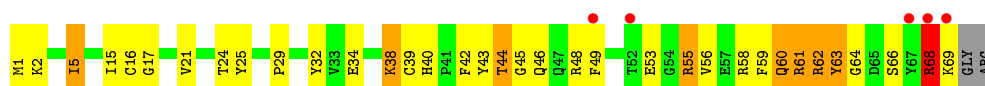


- Molecule 50: 50S Ribosomal Protein L31



- Molecule 50: 50S Ribosomal Protein L31





- Molecule 51: 50S Ribosomal Protein L32



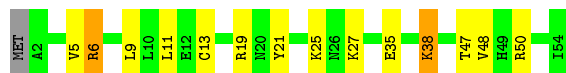
- Molecule 51: 50S Ribosomal Protein L32



- Molecule 52: 50S Ribosomal Protein L33



- Molecule 52: 50S Ribosomal Protein L33



- Molecule 53: 50S Ribosomal Protein L34



- Molecule 53: 50S Ribosomal Protein L34

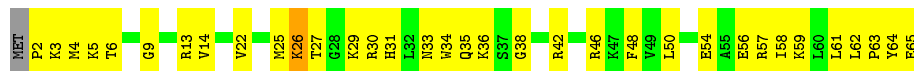


- Molecule 54: 50S Ribosomal Protein L35

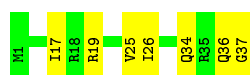
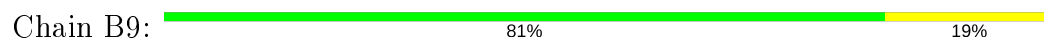




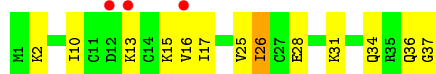
- Molecule 54: 50S Ribosomal Protein L35



- Molecule 55: 50S Ribosomal Protein L36



- Molecule 55: 50S Ribosomal Protein L36



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.68Å 450.64Å 622.54Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.68 – 3.10 49.68 – 3.10 | Depositor EDS |
| % Data completeness (in resolution range) | 98.2 (49.68-3.10) 98.2 (49.68-3.10) | Depositor EDS |
| R_{merge} | 0.20 | Depositor |
| R_{sym} | 0.25 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.32 (at 3.12Å) | Xtriage |
| Refinement program | PHENIX 1.8.2_1309 | Depositor |
| R, R_{free} | 0.203 , 0.260 0.203 , 0.260 | Depositor DCC |
| R_{free} test set | 51894 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 71.0 | Xtriage |
| Anisotropy | 0.077 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 67.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 286321 | wwPDB-VP |
| Average B, all atoms (Å ²) | 62.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: MG, K, 2QZ, ZN, 2QY, MVA, 004, FME, 2R3, SF4, 2R1

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 | 0.75 | 2/36038 (0.0%) | 1.31 | 240/56244 (0.4%) |
| 1 | CA | 0.75 | 10/36170 (0.0%) | 1.36 | 314/56452 (0.6%) |
| 2 | AB | 0.49 | 0/1881 | 0.77 | 1/2542 (0.0%) |
| 2 | CB | 0.54 | 0/1860 | 0.79 | 1/2518 (0.0%) |
| 3 | AC | 0.47 | 0/1576 | 0.65 | 0/2130 |
| 3 | CC | 0.51 | 0/1566 | 0.71 | 2/2119 (0.1%) |
| 4 | AD | 0.49 | 0/1689 | 0.73 | 0/2267 |
| 4 | CD | 0.49 | 0/1704 | 0.70 | 1/2284 (0.0%) |
| 5 | AE | 0.47 | 0/1145 | 0.70 | 0/1543 |
| 5 | CE | 0.50 | 0/1149 | 0.71 | 0/1548 |
| 6 | AF | 0.47 | 0/819 | 0.69 | 0/1111 |
| 6 | CF | 0.52 | 0/829 | 0.74 | 1/1123 (0.1%) |
| 7 | AG | 0.48 | 0/1250 | 0.67 | 1/1679 (0.1%) |
| 7 | CG | 0.50 | 0/1254 | 0.71 | 1/1683 (0.1%) |
| 8 | AH | 0.45 | 0/1108 | 0.66 | 0/1494 |
| 8 | CH | 0.48 | 0/1108 | 0.69 | 0/1494 |
| 9 | AI | 0.46 | 0/1002 | 0.72 | 0/1346 |
| 9 | CI | 0.56 | 0/997 | 0.75 | 1/1343 (0.1%) |
| 10 | AJ | 0.47 | 0/722 | 0.68 | 0/982 |
| 10 | CJ | 0.51 | 0/727 | 0.68 | 0/988 |
| 11 | AK | 0.44 | 0/844 | 0.62 | 0/1145 |
| 11 | CK | 0.46 | 0/848 | 0.66 | 0/1149 |
| 12 | AL | 0.52 | 0/946 | 0.69 | 0/1274 |
| 12 | CL | 0.51 | 0/946 | 0.73 | 0/1274 |
| 13 | AM | 0.46 | 0/969 | 0.69 | 0/1302 |
| 13 | CM | 0.49 | 0/961 | 0.66 | 0/1291 |
| 14 | AN | 0.51 | 0/501 | 0.67 | 0/664 |
| 14 | CN | 0.54 | 0/501 | 0.68 | 0/664 |
| 15 | AO | 0.47 | 0/739 | 0.72 | 0/985 |
| 15 | CO | 0.46 | 0/739 | 0.73 | 0/985 |
| 16 | AP | 0.45 | 0/697 | 0.71 | 0/939 |
| 16 | CP | 0.47 | 0/693 | 0.65 | 0/935 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.48 | 0/836 | 0.66 | 0/1117 |
| 17 | CQ | 0.49 | 0/836 | 0.68 | 0/1117 |
| 18 | AR | 0.49 | 0/560 | 0.72 | 0/746 |
| 18 | CR | 0.51 | 0/560 | 0.75 | 1/746 (0.1%) |
| 19 | AS | 0.47 | 0/667 | 0.68 | 0/900 |
| 19 | CS | 0.54 | 0/661 | 0.82 | 2/893 (0.2%) |
| 20 | AT | 0.51 | 0/730 | 0.76 | 0/965 |
| 20 | CT | 0.44 | 0/729 | 0.68 | 0/965 |
| 21 | AU | 0.45 | 0/203 | 0.65 | 0/266 |
| 21 | CU | 0.51 | 0/203 | 0.68 | 0/266 |
| 22 | AV | 0.94 | 0/127 | 1.36 | 2/198 (1.0%) |
| 22 | CV | 0.86 | 0/126 | 1.29 | 0/195 |
| 23 | AX | 0.85 | 5/1813 (0.3%) | 1.59 | 36/2825 (1.3%) |
| 23 | CX | 0.88 | 4/1813 (0.2%) | 1.81 | 40/2825 (1.4%) |
| 24 | AW | 0.50 | 0/20 | 0.80 | 0/23 |
| 24 | CW | 0.43 | 0/20 | 0.70 | 0/23 |
| 25 | BA | 1.06 | 33/65892 (0.1%) | 1.42 | 649/102850 (0.6%) |
| 25 | DA | 0.79 | 9/65466 (0.0%) | 1.39 | 590/102184 (0.6%) |
| 26 | BB | 0.82 | 0/2878 | 1.26 | 11/4490 (0.2%) |
| 26 | DB | 0.89 | 0/2878 | 1.39 | 18/4490 (0.4%) |
| 27 | BD | 0.67 | 1/2186 (0.0%) | 0.78 | 1/2944 (0.0%) |
| 27 | DD | 0.61 | 2/2186 (0.1%) | 0.77 | 1/2944 (0.0%) |
| 28 | BE | 0.69 | 0/1592 | 0.75 | 0/2149 |
| 28 | DE | 0.55 | 0/1592 | 0.77 | 1/2149 (0.0%) |
| 29 | BF | 0.69 | 0/1619 | 0.76 | 0/2193 |
| 29 | DF | 0.53 | 0/1615 | 0.77 | 1/2188 (0.0%) |
| 30 | BG | 0.46 | 0/1450 | 0.70 | 0/1959 |
| 30 | DG | 0.55 | 0/1449 | 0.74 | 0/1958 |
| 31 | BH | 0.60 | 0/1356 | 0.70 | 0/1834 |
| 31 | DH | 0.56 | 0/1356 | 0.70 | 0/1834 |
| 32 | BI | 0.49 | 0/1100 | 0.74 | 1/1501 (0.1%) |
| 32 | DI | 0.48 | 0/1076 | 0.77 | 0/1471 |
| 33 | BN | 0.65 | 0/1144 | 0.73 | 0/1543 |
| 33 | DN | 0.50 | 0/1144 | 0.72 | 0/1543 |
| 34 | BO | 0.65 | 0/943 | 0.73 | 1/1269 (0.1%) |
| 34 | DO | 0.54 | 0/943 | 0.73 | 1/1269 (0.1%) |
| 35 | BP | 0.62 | 0/1152 | 0.77 | 0/1533 |
| 35 | DP | 0.53 | 0/1152 | 0.80 | 1/1533 (0.1%) |
| 36 | BQ | 0.64 | 0/1143 | 0.76 | 0/1527 |
| 36 | DQ | 0.60 | 0/1143 | 0.79 | 0/1527 |
| 37 | BR | 0.59 | 0/982 | 0.78 | 0/1312 |
| 37 | DR | 0.49 | 0/982 | 0.71 | 0/1312 |
| 38 | BS | 0.54 | 0/887 | 0.77 | 0/1180 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DS | 0.47 | 0/880 | 0.72 | 0/1172 |
| 39 | BT | 0.59 | 0/1105 | 0.79 | 1/1477 (0.1%) |
| 39 | DT | 0.50 | 0/1097 | 0.72 | 0/1468 |
| 40 | BU | 0.71 | 1/977 (0.1%) | 0.73 | 0/1301 |
| 40 | DU | 0.54 | 0/977 | 0.71 | 1/1301 (0.1%) |
| 41 | BV | 0.68 | 0/782 | 0.74 | 1/1049 (0.1%) |
| 41 | DV | 0.55 | 0/782 | 0.71 | 0/1049 |
| 42 | BW | 0.74 | 0/897 | 0.74 | 0/1205 |
| 42 | DW | 0.56 | 0/897 | 0.72 | 0/1205 |
| 43 | BX | 0.66 | 0/764 | 0.96 | 3/1025 (0.3%) |
| 43 | DX | 0.55 | 0/764 | 0.75 | 1/1025 (0.1%) |
| 44 | BY | 0.64 | 0/819 | 0.78 | 0/1095 |
| 44 | DY | 0.54 | 0/819 | 0.74 | 0/1095 |
| 45 | BZ | 0.56 | 0/1379 | 0.75 | 0/1873 |
| 45 | DZ | 0.53 | 0/1390 | 0.71 | 0/1890 |
| 46 | B0 | 0.63 | 0/662 | 0.81 | 2/881 (0.2%) |
| 46 | D0 | 0.54 | 0/662 | 0.73 | 0/881 |
| 47 | B1 | 0.61 | 0/762 | 0.74 | 0/1014 |
| 47 | D1 | 0.51 | 0/762 | 0.75 | 1/1014 (0.1%) |
| 48 | B2 | 0.61 | 0/590 | 0.79 | 0/781 |
| 48 | D2 | 0.48 | 0/590 | 0.66 | 0/781 |
| 49 | B3 | 0.70 | 0/474 | 0.76 | 0/635 |
| 49 | D3 | 0.45 | 0/469 | 0.67 | 0/630 |
| 50 | B4 | 0.58 | 0/564 | 0.79 | 0/759 |
| 50 | D4 | 0.59 | 0/544 | 0.86 | 1/735 (0.1%) |
| 51 | B5 | 0.66 | 0/469 | 0.78 | 0/635 |
| 51 | D5 | 0.53 | 0/469 | 0.74 | 1/635 (0.2%) |
| 52 | B6 | 0.67 | 0/460 | 0.64 | 0/613 |
| 52 | D6 | 0.53 | 0/456 | 0.70 | 0/608 |
| 53 | B7 | 0.79 | 0/426 | 0.78 | 0/561 |
| 53 | D7 | 0.62 | 0/426 | 0.76 | 1/561 (0.2%) |
| 54 | B8 | 0.70 | 0/519 | 0.71 | 0/684 |
| 54 | D8 | 0.55 | 0/525 | 0.75 | 0/691 |
| 55 | B9 | 0.69 | 0/310 | 0.76 | 0/407 |
| 55 | D9 | 0.60 | 0/310 | 0.79 | 0/407 |
| All | All | 0.79 | 67/305966 (0.0%) | 1.24 | 1933/457396 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | AB | 0 | 3 |
| 4 | CD | 0 | 1 |
| 7 | AG | 0 | 1 |
| 23 | CX | 1 | 0 |
| 24 | AW | 0 | 1 |
| 24 | CW | 0 | 1 |
| 27 | DD | 0 | 1 |
| 38 | BS | 0 | 1 |
| 45 | BZ | 0 | 1 |
| 50 | B4 | 0 | 1 |
| All | All | 1 | 11 |

All (67) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|--------|-------------|----------|
| 23 | AX | 76 | A | N7-C5 | -11.16 | 1.32 | 1.39 |
| 1 | CA | 1154 | G | C6-N1 | -11.02 | 1.31 | 1.39 |
| 1 | CA | 1154 | G | N1-C2 | -10.69 | 1.29 | 1.37 |
| 25 | BA | 1188 | A | N9-C4 | -10.29 | 1.31 | 1.37 |
| 1 | CA | 1119 | C | N3-C4 | -10.20 | 1.26 | 1.33 |
| 25 | BA | 2299 | A | N9-C4 | -9.27 | 1.32 | 1.37 |
| 23 | CX | 76 | A | N7-C5 | -8.97 | 1.33 | 1.39 |
| 25 | BA | 1067 | A | N9-C4 | -8.63 | 1.32 | 1.37 |
| 23 | CX | 76 | A | C5-C6 | -8.11 | 1.33 | 1.41 |
| 25 | DA | 528 | A | N9-C4 | -7.89 | 1.33 | 1.37 |
| 1 | CA | 1492 | A | N9-C4 | 7.83 | 1.42 | 1.37 |
| 25 | BA | 1222 | A | N9-C4 | 7.65 | 1.42 | 1.37 |
| 23 | AX | 76 | A | C5-C6 | -7.63 | 1.34 | 1.41 |
| 1 | CA | 1154 | G | N7-C5 | -7.45 | 1.34 | 1.39 |
| 25 | BA | 1234 | A | N9-C4 | -6.96 | 1.33 | 1.37 |
| 23 | CX | 76 | A | C5-C4 | -6.68 | 1.34 | 1.38 |
| 25 | BA | 1188 | A | N3-C4 | -6.67 | 1.30 | 1.34 |
| 25 | DA | 2287 | A | N9-C4 | -6.63 | 1.33 | 1.37 |
| 40 | BU | 69 | CYS | CB-SG | -6.61 | 1.71 | 1.82 |
| 25 | BA | 2601 | A | N9-C4 | -6.59 | 1.33 | 1.37 |
| 25 | DA | 2207 | G | N7-C5 | -6.42 | 1.35 | 1.39 |
| 23 | AX | 22 | G | N7-C5 | 6.40 | 1.43 | 1.39 |
| 27 | DD | 28 | GLU | CG-CD | 6.36 | 1.61 | 1.51 |
| 25 | BA | 1605 | A | N9-C4 | -6.13 | 1.34 | 1.37 |
| 25 | BA | 2444 | A | C5-C6 | -6.13 | 1.35 | 1.41 |
| 1 | CA | 1154 | G | C5-C4 | 6.05 | 1.42 | 1.38 |
| 25 | DA | 1142(A) | A | N9-C4 | -6.03 | 1.34 | 1.37 |
| 25 | DA | 2320 | A | N9-C4 | 6.01 | 1.41 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 25 | DA | 2725 | A | N9-C4 | -5.99 | 1.34 | 1.37 |
| 1 | CA | 1154 | G | N9-C4 | 5.94 | 1.42 | 1.38 |
| 23 | AX | 46 | G | C6-N1 | 5.78 | 1.43 | 1.39 |
| 25 | BA | 978 | A | N9-C4 | -5.77 | 1.34 | 1.37 |
| 25 | BA | 657 | A | N9-C4 | -5.77 | 1.34 | 1.37 |
| 25 | BA | 178 | G | N7-C5 | -5.64 | 1.35 | 1.39 |
| 1 | CA | 1119 | C | N1-C2 | 5.58 | 1.45 | 1.40 |
| 25 | BA | 1425 | A | N9-C4 | -5.57 | 1.34 | 1.37 |
| 25 | BA | 354 | A | N9-C4 | -5.49 | 1.34 | 1.37 |
| 25 | BA | 2527 | C | N1-C6 | -5.48 | 1.33 | 1.37 |
| 25 | BA | 552 | C | N3-C4 | -5.46 | 1.30 | 1.33 |
| 25 | BA | 782 | A | N3-C4 | -5.42 | 1.31 | 1.34 |
| 25 | DA | 530 | G | N9-C8 | 5.42 | 1.41 | 1.37 |
| 25 | BA | 506 | A | N7-C5 | -5.42 | 1.36 | 1.39 |
| 1 | CA | 1154 | G | C8-N7 | -5.40 | 1.27 | 1.30 |
| 25 | BA | 2803 | A | N9-C4 | 5.38 | 1.41 | 1.37 |
| 25 | BA | 1153 | G | N9-C4 | 5.35 | 1.42 | 1.38 |
| 25 | BA | 2509 | A | N3-C4 | -5.31 | 1.31 | 1.34 |
| 25 | BA | 2039 | U | C2-N3 | -5.30 | 1.34 | 1.37 |
| 1 | AA | 1124 | G | N9-C4 | 5.29 | 1.42 | 1.38 |
| 23 | CX | 22 | G | N7-C5 | 5.27 | 1.42 | 1.39 |
| 1 | AA | 1531 | A | N9-C4 | 5.25 | 1.41 | 1.37 |
| 27 | DD | 28 | GLU | CB-CG | 5.21 | 1.62 | 1.52 |
| 25 | BA | 840 | A | N7-C5 | -5.21 | 1.36 | 1.39 |
| 25 | BA | 1234 | A | N3-C4 | -5.20 | 1.31 | 1.34 |
| 25 | DA | 2599 | G | C6-N1 | -5.20 | 1.35 | 1.39 |
| 25 | BA | 840 | A | C5-C6 | -5.18 | 1.36 | 1.41 |
| 25 | BA | 1076 | G | C6-N1 | -5.17 | 1.35 | 1.39 |
| 25 | DA | 784 | A | N9-C4 | -5.17 | 1.34 | 1.37 |
| 25 | BA | 186 | A | N3-C4 | -5.17 | 1.31 | 1.34 |
| 1 | CA | 998 | G | N7-C5 | 5.16 | 1.42 | 1.39 |
| 25 | BA | 781 | A | N9-C4 | -5.16 | 1.34 | 1.37 |
| 25 | BA | 1818 | A | C6-N1 | -5.04 | 1.32 | 1.35 |
| 27 | BD | 28 | GLU | CG-CD | 5.04 | 1.59 | 1.51 |
| 25 | BA | 1030 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 25 | BA | 990 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 25 | BA | 2598 | C | N1-C6 | -5.02 | 1.34 | 1.37 |
| 23 | AX | 14 | A | N7-C5 | -5.01 | 1.36 | 1.39 |
| 25 | BA | 2080 | A | N3-C4 | -5.01 | 1.31 | 1.34 |

All (1933) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 23 | CX | 76 | A | O4'-C1'-N9 | 38.71 | 139.17 | 108.20 |
| 1 | CA | 1119 | C | N1-C2-O2 | 32.56 | 138.44 | 118.90 |
| 1 | CA | 1154 | G | C5-C6-O6 | 28.63 | 145.78 | 128.60 |
| 1 | CA | 1154 | G | N3-C2-N2 | 25.05 | 137.43 | 119.90 |
| 1 | CA | 1154 | G | N1-C2-N2 | -22.71 | 95.76 | 116.20 |
| 1 | CA | 1119 | C | N3-C2-O2 | -21.96 | 106.53 | 121.90 |
| 23 | CX | 76 | A | C2-N3-C4 | 19.79 | 120.49 | 110.60 |
| 23 | CX | 76 | A | N1-C2-N3 | -19.05 | 119.78 | 129.30 |
| 23 | AX | 76 | A | C2-N3-C4 | 18.48 | 119.84 | 110.60 |
| 23 | AX | 76 | A | N1-C2-N3 | -17.90 | 120.35 | 129.30 |
| 1 | CA | 1119 | C | C2-N3-C4 | 17.09 | 128.45 | 119.90 |
| 1 | CA | 1154 | G | C5-C6-N1 | -17.07 | 102.97 | 111.50 |
| 1 | CA | 1119 | C | C2-N1-C1' | 16.03 | 136.44 | 118.80 |
| 43 | BX | 65 | ARG | NE-CZ-NH2 | 15.41 | 128.00 | 120.30 |
| 23 | AX | 76 | A | O4'-C1'-N9 | 15.35 | 120.48 | 108.20 |
| 1 | CA | 1154 | G | C6-N1-C2 | 14.89 | 134.03 | 125.10 |
| 23 | AX | 8 | U | C2-N3-C4 | 14.86 | 135.91 | 127.00 |
| 1 | CA | 1119 | C | C5-C4-N4 | 14.60 | 130.42 | 120.20 |
| 1 | CA | 1154 | G | N1-C6-O6 | -14.49 | 111.20 | 119.90 |
| 25 | BA | 1067 | A | C2-N3-C4 | -14.43 | 103.38 | 110.60 |
| 1 | CA | 999 | C | N1-C2-O2 | 13.32 | 126.89 | 118.90 |
| 1 | CA | 1154 | G | C4-N9-C1' | 12.75 | 143.07 | 126.50 |
| 25 | DA | 528 | A | C2-N3-C4 | -12.60 | 104.30 | 110.60 |
| 25 | BA | 2058 | C | O5'-P-OP1 | -12.50 | 94.45 | 105.70 |
| 23 | CX | 8 | U | C2-N3-C4 | 12.28 | 134.37 | 127.00 |
| 1 | CA | 1119 | C | N3-C4-N4 | -12.22 | 109.45 | 118.00 |
| 1 | CA | 1119 | C | C6-N1-C2 | -12.18 | 115.43 | 120.30 |
| 25 | BA | 139 | A | N7-C8-N9 | 12.11 | 119.86 | 113.80 |
| 25 | DA | 945 | A | N1-C6-N6 | 11.58 | 125.55 | 118.60 |
| 25 | BA | 139 | A | C5-N7-C8 | -11.57 | 98.12 | 103.90 |
| 1 | CA | 1119 | C | C6-N1-C1' | -11.45 | 107.07 | 120.80 |
| 43 | BX | 65 | ARG | NE-CZ-NH1 | -11.42 | 114.59 | 120.30 |
| 1 | CA | 1154 | G | C8-N9-C1' | -11.28 | 112.34 | 127.00 |
| 25 | BA | 1188 | A | C2-N3-C4 | -11.10 | 105.05 | 110.60 |
| 1 | AA | 1125 | U | N1-C2-O2 | 11.09 | 130.56 | 122.80 |
| 23 | CX | 76 | A | N3-C4-C5 | -10.90 | 119.17 | 126.80 |
| 23 | CX | 8 | U | C5-C6-N1 | 10.69 | 128.04 | 122.70 |
| 26 | BB | 91 | C | C6-N1-C2 | 10.59 | 124.53 | 120.30 |
| 23 | AX | 46 | G | C6-N1-C2 | -10.39 | 118.86 | 125.10 |
| 1 | CA | 1004 | A | O4'-C1'-N9 | 10.33 | 116.47 | 108.20 |
| 25 | BA | 990 | A | C5-N7-C8 | -10.27 | 98.77 | 103.90 |
| 25 | BA | 1098 | C | C6-N1-C2 | -10.25 | 116.20 | 120.30 |
| 23 | CX | 76 | A | C5-N7-C8 | 10.25 | 109.02 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 25 | BA | 2835 | C | O5'-P-OP1 | -10.24 | 96.48 | 105.70 |
| 23 | CX | 76 | A | N7-C8-N9 | -10.24 | 108.68 | 113.80 |
| 23 | AX | 76 | A | N7-C8-N9 | -10.15 | 108.72 | 113.80 |
| 1 | AA | 1125 | U | N1-C2-N3 | -10.09 | 108.85 | 114.90 |
| 25 | DA | 856 | C | C6-N1-C2 | -10.03 | 116.29 | 120.30 |
| 25 | BA | 201 | G | O5'-P-OP2 | -9.99 | 96.71 | 105.70 |
| 23 | CX | 46 | G | C6-N1-C2 | -9.84 | 119.20 | 125.10 |
| 1 | CA | 1119 | C | C5-C6-N1 | 9.74 | 125.87 | 121.00 |
| 25 | DA | 1698 | A | N1-C6-N6 | 9.70 | 124.42 | 118.60 |
| 1 | CA | 927 | G | C5-C6-O6 | 9.70 | 134.42 | 128.60 |
| 25 | DA | 205 | G | C8-N9-C4 | 9.64 | 110.26 | 106.40 |
| 25 | BA | 990 | A | C2-N3-C4 | -9.64 | 105.78 | 110.60 |
| 25 | BA | 1067 | A | C5-N7-C8 | -9.61 | 99.10 | 103.90 |
| 1 | CA | 1154 | G | C5-N7-C8 | 9.58 | 109.09 | 104.30 |
| 25 | DA | 2084 | C | C6-N1-C2 | 9.51 | 124.10 | 120.30 |
| 23 | AX | 76 | A | C5-N7-C8 | 9.49 | 108.64 | 103.90 |
| 25 | DA | 1823 | G | O5'-P-OP2 | -9.46 | 97.19 | 105.70 |
| 25 | BA | 724 | A | O5'-P-OP2 | -9.43 | 97.22 | 105.70 |
| 25 | BA | 1440 | U | O5'-P-OP1 | -9.40 | 97.24 | 105.70 |
| 25 | BA | 1020 | C | C6-N1-C2 | 9.38 | 124.05 | 120.30 |
| 25 | BA | 607 | C | C6-N1-C2 | 9.38 | 124.05 | 120.30 |
| 25 | BA | 537 | G | O4'-C1'-N9 | 9.35 | 115.68 | 108.20 |
| 25 | DA | 1021 | A | C2-N3-C4 | -9.26 | 105.97 | 110.60 |
| 23 | AX | 8 | U | C5-C4-O4 | 9.26 | 131.45 | 125.90 |
| 23 | AX | 14 | A | C5-N7-C8 | 9.19 | 108.49 | 103.90 |
| 25 | BA | 2299 | A | C2-N3-C4 | -9.15 | 106.03 | 110.60 |
| 1 | AA | 1127 | G | N3-C4-N9 | 9.14 | 131.48 | 126.00 |
| 23 | AX | 22 | G | C5-N7-C8 | -9.09 | 99.76 | 104.30 |
| 25 | DA | 2253 | G | N1-C6-O6 | 9.03 | 125.32 | 119.90 |
| 23 | CX | 22 | G | C5-N7-C8 | -9.03 | 99.79 | 104.30 |
| 25 | BA | 1225 | C | C6-N1-C2 | 8.99 | 123.89 | 120.30 |
| 25 | DA | 2503 | A | C5-C6-N6 | -8.97 | 116.52 | 123.70 |
| 25 | BA | 354 | A | C2-N3-C4 | -8.94 | 106.13 | 110.60 |
| 25 | BA | 139 | A | C8-N9-C4 | -8.93 | 102.23 | 105.80 |
| 26 | DB | 115 | G | C8-N9-C4 | 8.93 | 109.97 | 106.40 |
| 25 | DA | 2207 | G | C6-C5-N7 | -8.92 | 125.05 | 130.40 |
| 25 | BA | 1216 | G | C8-N9-C4 | -8.90 | 102.84 | 106.40 |
| 25 | DA | 915 | C | C6-N1-C2 | -8.87 | 116.75 | 120.30 |
| 23 | AX | 14 | A | C4-C5-C6 | 8.85 | 121.42 | 117.00 |
| 25 | DA | 1269 | A | N1-C6-N6 | 8.84 | 123.91 | 118.60 |
| 23 | AX | 76 | A | N3-C4-C5 | -8.83 | 120.62 | 126.80 |
| 25 | DA | 1204 | A | C2-N3-C4 | -8.80 | 106.20 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 25 | BA | 934 | A | O4'-C1'-N9 | 8.80 | 115.24 | 108.20 |
| 25 | DA | 970 | C | N1-C2-O2 | -8.78 | 113.63 | 118.90 |
| 1 | CA | 1154 | G | C4-C5-C6 | 8.76 | 124.06 | 118.80 |
| 25 | DA | 2804 | C | C6-N1-C2 | -8.75 | 116.80 | 120.30 |
| 25 | DA | 1698 | A | C6-C5-N7 | -8.74 | 126.18 | 132.30 |
| 25 | BA | 930 | G | O4'-C1'-N9 | 8.72 | 115.18 | 108.20 |
| 25 | DA | 2188 | C | C6-N1-C2 | -8.68 | 116.83 | 120.30 |
| 25 | DA | 1698 | A | C2-N3-C4 | -8.66 | 106.27 | 110.60 |
| 1 | AA | 1030(B) | C | C2-N1-C1' | 8.62 | 128.28 | 118.80 |
| 25 | DA | 530 | G | C8-N9-C4 | -8.62 | 102.95 | 106.40 |
| 25 | BA | 1686 | U | O5'-P-OP2 | -8.60 | 97.96 | 105.70 |
| 1 | CA | 1003 | G | N3-C4-C5 | -8.57 | 124.32 | 128.60 |
| 25 | BA | 1314 | A | C8-N9-C4 | 8.55 | 109.22 | 105.80 |
| 25 | BA | 1067 | A | N3-C4-C5 | 8.55 | 132.79 | 126.80 |
| 1 | AA | 1036 | G | C4-N9-C1' | 8.55 | 137.61 | 126.50 |
| 23 | CX | 46 | G | N3-C2-N2 | -8.53 | 113.93 | 119.90 |
| 25 | BA | 2105 | G | C5-C6-O6 | -8.49 | 123.51 | 128.60 |
| 1 | CA | 1260 | C | C6-N1-C2 | -8.48 | 116.91 | 120.30 |
| 25 | BA | 507 | G | O4'-C1'-N9 | 8.45 | 114.96 | 108.20 |
| 1 | AA | 166 | G | C8-N9-C4 | -8.43 | 103.03 | 106.40 |
| 25 | BA | 1665 | G | O5'-P-OP2 | -8.41 | 98.13 | 105.70 |
| 7 | CG | 22 | LEU | CA-CB-CG | 8.39 | 134.60 | 115.30 |
| 25 | DA | 1791 | A | O5'-P-OP1 | -8.39 | 98.15 | 105.70 |
| 1 | CA | 998 | G | C6-C5-N7 | 8.37 | 135.42 | 130.40 |
| 1 | CA | 1154 | G | C2-N3-C4 | -8.36 | 107.72 | 111.90 |
| 25 | BA | 2630 | G | N3-C4-C5 | -8.35 | 124.42 | 128.60 |
| 25 | DA | 249 | C | C6-N1-C2 | 8.34 | 123.64 | 120.30 |
| 25 | DA | 1489 | U | N3-C2-O2 | -8.34 | 116.36 | 122.20 |
| 23 | AX | 46 | G | C5-C6-N1 | 8.31 | 115.66 | 111.50 |
| 1 | CA | 999 | C | N3-C2-O2 | -8.30 | 116.09 | 121.90 |
| 25 | BA | 1188 | A | O5'-P-OP1 | -8.29 | 98.24 | 105.70 |
| 25 | DA | 945 | A | C2-N3-C4 | -8.29 | 106.46 | 110.60 |
| 25 | DA | 528 | A | N1-C2-N3 | 8.27 | 133.44 | 129.30 |
| 25 | BA | 837 | C | O5'-P-OP2 | -8.27 | 98.26 | 105.70 |
| 25 | BA | 1067 | A | C5-C6-N1 | -8.27 | 113.57 | 117.70 |
| 1 | CA | 1122 | U | C2-N1-C1' | 8.26 | 127.61 | 117.70 |
| 25 | DA | 1937 | A | N1-C6-N6 | 8.26 | 123.56 | 118.60 |
| 25 | DA | 1284 | A | N1-C6-N6 | 8.25 | 123.55 | 118.60 |
| 1 | CA | 1154 | G | N3-C4-C5 | -8.24 | 124.48 | 128.60 |
| 25 | BA | 2701 | U | P-O3'-C3' | 8.23 | 129.58 | 119.70 |
| 25 | BA | 1072 | U | N1-C2-O2 | 8.23 | 128.56 | 122.80 |
| 25 | BA | 2830 | A | N1-C6-N6 | 8.23 | 123.54 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | DA | 945 | A | C6-C5-N7 | -8.23 | 126.54 | 132.30 |
| 25 | BA | 194 | G | C8-N9-C4 | 8.22 | 109.69 | 106.40 |
| 1 | CA | 1154 | G | C4-C5-N7 | -8.21 | 107.52 | 110.80 |
| 25 | DA | 37 | C | C6-N1-C2 | 8.19 | 123.58 | 120.30 |
| 25 | DA | 1489 | U | C2-N1-C1' | 8.19 | 127.53 | 117.70 |
| 1 | CA | 1311 | G | N3-C4-N9 | -8.19 | 121.09 | 126.00 |
| 25 | BA | 553 | A | C2-N3-C4 | -8.18 | 106.51 | 110.60 |
| 1 | CA | 841 | U | C5-C6-N1 | 8.18 | 126.79 | 122.70 |
| 25 | BA | 2298 | A | N1-C2-N3 | 8.18 | 133.39 | 129.30 |
| 25 | BA | 1985 | U | C2-N1-C1' | 8.17 | 127.50 | 117.70 |
| 1 | CA | 1012 | U | N1-C2-O2 | -8.17 | 117.08 | 122.80 |
| 25 | DA | 2039 | C | C6-N1-C2 | -8.16 | 117.04 | 120.30 |
| 1 | AA | 1036 | G | C8-N9-C1' | -8.15 | 116.41 | 127.00 |
| 23 | AX | 8 | U | N1-C2-N3 | -8.15 | 110.01 | 114.90 |
| 25 | BA | 990 | A | C4-C5-N7 | 8.10 | 114.75 | 110.70 |
| 1 | CA | 1396 | A | O5'-P-OP1 | -8.10 | 98.42 | 105.70 |
| 25 | DA | 933 | A | C5-N7-C8 | -8.09 | 99.86 | 103.90 |
| 25 | DA | 1380 | G | O5'-P-OP2 | -8.08 | 98.43 | 105.70 |
| 25 | DA | 1786 | A | O4'-C1'-N9 | 8.07 | 114.66 | 108.20 |
| 25 | DA | 249 | C | O5'-P-OP2 | -8.07 | 98.44 | 105.70 |
| 1 | AA | 896 | C | C6-N1-C2 | 8.01 | 123.50 | 120.30 |
| 25 | DA | 1284 | A | O5'-P-OP2 | -8.01 | 98.49 | 105.70 |
| 25 | BA | 2331 | G | N3-C4-C5 | 8.00 | 132.60 | 128.60 |
| 25 | BA | 133 | G | N3-C4-C5 | 8.00 | 132.60 | 128.60 |
| 25 | DA | 945 | A | C4-C5-N7 | 8.00 | 114.70 | 110.70 |
| 25 | BA | 254 | A | N7-C8-N9 | 7.99 | 117.80 | 113.80 |
| 25 | BA | 1700 | G | P-O3'-C3' | 7.98 | 129.28 | 119.70 |
| 25 | BA | 1216 | G | N7-C8-N9 | 7.98 | 117.09 | 113.10 |
| 25 | DA | 2503 | A | N1-C6-N6 | 7.97 | 123.39 | 118.60 |
| 1 | CA | 1037 | C | C6-N1-C2 | -7.97 | 117.11 | 120.30 |
| 25 | DA | 330 | A | C2-N3-C4 | -7.96 | 106.62 | 110.60 |
| 25 | BA | 552 | C | N3-C2-O2 | -7.96 | 116.33 | 121.90 |
| 25 | BA | 254 | A | C8-N9-C4 | -7.96 | 102.62 | 105.80 |
| 1 | CA | 1141 | C | C2-N1-C1' | -7.96 | 110.05 | 118.80 |
| 25 | BA | 2331 | G | C2-N3-C4 | -7.94 | 107.93 | 111.90 |
| 25 | BA | 2835 | C | N1-C2-O2 | -7.88 | 114.17 | 118.90 |
| 23 | CX | 39 | C | C6-N1-C2 | -7.88 | 117.15 | 120.30 |
| 25 | BA | 288 | U | O4'-C1'-N1 | 7.87 | 114.50 | 108.20 |
| 25 | BA | 12 | U | N3-C2-O2 | -7.86 | 116.70 | 122.20 |
| 25 | DA | 898 | C | C5-C6-N1 | 7.86 | 124.93 | 121.00 |
| 25 | BA | 2725 | A | O5'-P-OP1 | -7.85 | 98.64 | 105.70 |
| 25 | BA | 2830 | A | C4-C5-N7 | 7.85 | 114.62 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 25 | DA | 1236 | G | O5'-P-OP1 | -7.85 | 98.64 | 105.70 |
| 1 | CA | 1149 | C | C6-N1-C2 | -7.84 | 117.16 | 120.30 |
| 25 | DA | 1934 | C | C6-N1-C2 | 7.84 | 123.44 | 120.30 |
| 1 | AA | 193 | C | C5-C6-N1 | 7.84 | 124.92 | 121.00 |
| 1 | AA | 1125 | U | C2-N3-C4 | 7.84 | 131.70 | 127.00 |
| 23 | AX | 8 | U | N1-C2-O2 | 7.83 | 128.28 | 122.80 |
| 23 | CX | 14 | A | C5-N7-C8 | 7.79 | 107.79 | 103.90 |
| 25 | DA | 1640 | C | N1-C2-O2 | 7.78 | 123.56 | 118.90 |
| 25 | BA | 2734 | A | O5'-P-OP1 | -7.77 | 98.71 | 105.70 |
| 25 | BA | 978 | A | C5-N7-C8 | -7.77 | 100.02 | 103.90 |
| 1 | AA | 1030(B) | C | N1-C2-O2 | 7.76 | 123.56 | 118.90 |
| 25 | DA | 2207 | G | N1-C6-O6 | 7.76 | 124.56 | 119.90 |
| 25 | BA | 733 | G | C5-C6-O6 | -7.76 | 123.94 | 128.60 |
| 25 | BA | 2265 | G | N1-C6-O6 | 7.76 | 124.55 | 119.90 |
| 1 | AA | 1530 | G | N1-C6-O6 | 7.73 | 124.54 | 119.90 |
| 1 | AA | 1158 | C | C4-C5-C6 | 7.71 | 121.25 | 117.40 |
| 1 | CA | 1017 | G | C6-N1-C2 | 7.71 | 129.72 | 125.10 |
| 1 | CA | 1183 | A | P-O3'-C3' | 7.71 | 128.95 | 119.70 |
| 25 | BA | 2876 | U | C5-C6-N1 | -7.70 | 118.85 | 122.70 |
| 34 | DO | 8 | LEU | CA-CB-CG | 7.69 | 132.98 | 115.30 |
| 1 | CA | 1484 | C | C6-N1-C2 | 7.67 | 123.37 | 120.30 |
| 25 | BA | 2830 | A | N9-C4-C5 | -7.67 | 102.73 | 105.80 |
| 1 | AA | 1131 | G | C6-C5-N7 | -7.65 | 125.81 | 130.40 |
| 25 | DA | 1372 | U | C5-C4-O4 | -7.64 | 121.32 | 125.90 |
| 25 | DA | 735 | A | C8-N9-C4 | 7.64 | 108.85 | 105.80 |
| 25 | DA | 912 | C | C6-N1-C2 | -7.63 | 117.25 | 120.30 |
| 25 | BA | 961 | C | N1-C2-O2 | 7.63 | 123.48 | 118.90 |
| 25 | BA | 484 | G | N9-C4-C5 | 7.62 | 108.45 | 105.40 |
| 25 | BA | 1188 | A | N3-C4-C5 | 7.62 | 132.14 | 126.80 |
| 25 | BA | 990 | A | N7-C8-N9 | 7.62 | 117.61 | 113.80 |
| 25 | DA | 1118 | C | C6-N1-C2 | -7.62 | 117.25 | 120.30 |
| 1 | CA | 1133 | G | C5-C6-O6 | 7.61 | 133.17 | 128.60 |
| 25 | DA | 2273 | A | C8-N9-C4 | 7.61 | 108.84 | 105.80 |
| 25 | DA | 1703 | G | N1-C6-O6 | 7.61 | 124.46 | 119.90 |
| 25 | BA | 2607 | G | O5'-P-OP1 | -7.61 | 98.86 | 105.70 |
| 1 | CA | 1033 | G | N9-C4-C5 | -7.59 | 102.36 | 105.40 |
| 25 | DA | 448 | U | O5'-P-OP1 | -7.59 | 98.87 | 105.70 |
| 25 | BA | 1067 | A | N3-C4-N9 | -7.58 | 121.33 | 127.40 |
| 25 | DA | 948 | G | N3-C4-C5 | 7.58 | 132.39 | 128.60 |
| 25 | BA | 2250 | G | O5'-P-OP1 | -7.57 | 98.89 | 105.70 |
| 25 | BA | 139 | A | C4-C5-N7 | 7.56 | 114.48 | 110.70 |
| 25 | BA | 990 | A | C6-C5-N7 | -7.56 | 127.01 | 132.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | CX | 76 | A | N9-C4-C5 | 7.55 | 108.82 | 105.80 |
| 25 | BA | 1327 | G | N1-C6-O6 | 7.54 | 124.42 | 119.90 |
| 25 | BA | 2092 | G | N9-C4-C5 | -7.51 | 102.40 | 105.40 |
| 1 | CA | 299 | G | N1-C6-O6 | 7.50 | 124.40 | 119.90 |
| 25 | BA | 1222 | A | C8-N9-C4 | -7.49 | 102.80 | 105.80 |
| 1 | CA | 998 | G | N1-C6-O6 | -7.49 | 115.41 | 119.90 |
| 25 | BA | 1719 | C | N3-C4-C5 | -7.48 | 118.91 | 121.90 |
| 25 | BA | 2608 | U | C5-C6-N1 | -7.48 | 118.96 | 122.70 |
| 25 | BA | 1067 | A | N1-C6-N6 | 7.48 | 123.09 | 118.60 |
| 1 | AA | 1137 | C | C6-N1-C2 | -7.48 | 117.31 | 120.30 |
| 25 | DA | 573 | G | N1-C6-O6 | -7.48 | 115.41 | 119.90 |
| 1 | AA | 188 | C | C6-N1-C2 | -7.47 | 117.31 | 120.30 |
| 25 | DA | 1372 | U | N3-C4-O4 | 7.47 | 124.63 | 119.40 |
| 1 | CA | 927 | G | N1-C6-O6 | -7.47 | 115.42 | 119.90 |
| 1 | CA | 1054 | C | C2-N1-C1' | 7.45 | 127.00 | 118.80 |
| 25 | BA | 1093 | G | N3-C4-C5 | -7.44 | 124.88 | 128.60 |
| 26 | DB | 6 | C | C6-N1-C2 | 7.43 | 123.27 | 120.30 |
| 25 | BA | 1800 | G | N1-C6-O6 | 7.43 | 124.36 | 119.90 |
| 25 | BA | 2015 | U | O5'-P-OP1 | -7.43 | 99.01 | 105.70 |
| 1 | AA | 476 | G | O4'-C1'-N9 | 7.43 | 114.14 | 108.20 |
| 25 | DA | 1489 | U | N1-C2-O2 | 7.43 | 128.00 | 122.80 |
| 23 | CX | 76 | A | C4-C5-N7 | -7.42 | 106.99 | 110.70 |
| 25 | BA | 1153 | G | N3-C4-C5 | -7.42 | 124.89 | 128.60 |
| 25 | BA | 2262 | G | O5'-P-OP2 | -7.41 | 99.03 | 105.70 |
| 25 | DA | 2253 | G | C4-C5-N7 | 7.40 | 113.76 | 110.80 |
| 1 | AA | 1124 | G | C8-N9-C4 | -7.40 | 103.44 | 106.40 |
| 25 | BA | 1093 | G | N3-C4-N9 | 7.40 | 130.44 | 126.00 |
| 23 | AX | 22 | G | N3-C4-N9 | -7.40 | 121.56 | 126.00 |
| 25 | BA | 215 | G | O4'-C1'-N9 | 7.39 | 114.11 | 108.20 |
| 23 | AX | 76 | A | C5-C6-N1 | 7.39 | 121.39 | 117.70 |
| 25 | BA | 2081 | A | C8-N9-C4 | 7.39 | 108.75 | 105.80 |
| 25 | DA | 1404 | C | O5'-P-OP2 | -7.38 | 99.06 | 105.70 |
| 1 | CA | 998 | G | C4-C5-N7 | -7.38 | 107.85 | 110.80 |
| 25 | BA | 990 | A | N1-C6-N6 | 7.38 | 123.03 | 118.60 |
| 25 | BA | 1766 | G | C4-C5-N7 | 7.36 | 113.74 | 110.80 |
| 25 | DA | 2805 | G | N1-C6-O6 | -7.35 | 115.49 | 119.90 |
| 25 | DA | 1022 | G | N3-C4-N9 | -7.34 | 121.59 | 126.00 |
| 25 | BA | 2515 | A | N1-C2-N3 | -7.33 | 125.64 | 129.30 |
| 1 | AA | 1124 | G | N3-C4-C5 | -7.33 | 124.94 | 128.60 |
| 1 | CA | 1154 | G | N3-C4-N9 | 7.31 | 130.38 | 126.00 |
| 25 | BA | 2299 | A | N3-C4-C5 | 7.30 | 131.91 | 126.80 |
| 25 | DA | 1696 | G | O5'-P-OP2 | -7.30 | 99.13 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 25 | DA | 827 | U | N3-C2-O2 | 7.29 | 127.31 | 122.20 |
| 1 | CA | 1141 | C | C6-N1-C1' | 7.29 | 129.55 | 120.80 |
| 25 | DA | 2805 | G | N9-C4-C5 | 7.28 | 108.31 | 105.40 |
| 1 | AA | 738 | C | C6-N1-C2 | -7.27 | 117.39 | 120.30 |
| 23 | AX | 22 | G | C4-C5-C6 | -7.27 | 114.44 | 118.80 |
| 25 | DA | 2805 | G | C4-C5-N7 | -7.27 | 107.89 | 110.80 |
| 25 | BA | 2627 | U | O5'-P-OP1 | -7.25 | 99.17 | 105.70 |
| 1 | CA | 998 | G | C5-C6-O6 | 7.24 | 132.95 | 128.60 |
| 25 | DA | 1142(A) | A | C2-N3-C4 | -7.24 | 106.98 | 110.60 |
| 51 | D5 | 58 | LEU | CA-CB-CG | 7.24 | 131.95 | 115.30 |
| 1 | AA | 728 | A | O5'-P-OP2 | -7.23 | 99.19 | 105.70 |
| 1 | CA | 927 | G | C4-C5-N7 | -7.23 | 107.91 | 110.80 |
| 25 | DA | 2261 | C | C6-N1-C2 | 7.23 | 123.19 | 120.30 |
| 25 | BA | 201 | G | O5'-P-OP1 | 7.22 | 119.37 | 110.70 |
| 25 | BA | 2331 | G | C5-N7-C8 | -7.22 | 100.69 | 104.30 |
| 25 | DA | 687 | C | N3-C4-C5 | 7.21 | 124.78 | 121.90 |
| 1 | AA | 1030(B) | C | C6-N1-C2 | -7.21 | 117.42 | 120.30 |
| 25 | DA | 2207 | G | C4-C5-C6 | 7.21 | 123.12 | 118.80 |
| 25 | DA | 476 | G | O5'-P-OP2 | -7.21 | 99.22 | 105.70 |
| 25 | DA | 2374 | C | C6-N1-C2 | 7.21 | 123.18 | 120.30 |
| 25 | BA | 2298 | A | C4-C5-C6 | 7.20 | 120.60 | 117.00 |
| 1 | AA | 1028 | C | C6-N1-C2 | -7.19 | 117.42 | 120.30 |
| 25 | DA | 205 | G | N7-C8-N9 | -7.18 | 109.51 | 113.10 |
| 25 | BA | 2092 | G | C8-N9-C4 | 7.18 | 109.27 | 106.40 |
| 25 | DA | 1204 | A | O4'-C1'-N9 | 7.17 | 113.94 | 108.20 |
| 25 | DA | 2574 | G | N1-C6-O6 | 7.17 | 124.20 | 119.90 |
| 25 | DA | 2463 | C | C6-N1-C2 | 7.17 | 123.17 | 120.30 |
| 1 | CA | 1038 | C | C2-N3-C4 | 7.16 | 123.48 | 119.90 |
| 1 | CA | 1492 | A | C8-N9-C4 | -7.16 | 102.94 | 105.80 |
| 25 | BA | 1054 | C | N1-C2-O2 | 7.16 | 123.20 | 118.90 |
| 25 | BA | 1745 | A | C2-N3-C4 | -7.15 | 107.02 | 110.60 |
| 25 | BA | 2701 | U | N3-C2-O2 | -7.15 | 117.19 | 122.20 |
| 25 | BA | 2058 | C | O5'-P-OP2 | 7.15 | 119.28 | 110.70 |
| 1 | CA | 1113 | C | C6-N1-C2 | -7.15 | 117.44 | 120.30 |
| 25 | BA | 2028 | C | O5'-P-OP1 | -7.15 | 99.27 | 105.70 |
| 25 | BA | 733 | G | C4-C5-N7 | 7.14 | 113.66 | 110.80 |
| 25 | BA | 834 | U | O5'-P-OP1 | -7.14 | 99.27 | 105.70 |
| 25 | BA | 553 | A | C6-N1-C2 | 7.14 | 122.88 | 118.60 |
| 23 | AX | 4 | G | C8-N9-C4 | 7.14 | 109.25 | 106.40 |
| 25 | BA | 1076 | G | N1-C2-N2 | -7.13 | 109.78 | 116.20 |
| 25 | BA | 706 | C | C6-N1-C2 | 7.12 | 123.15 | 120.30 |
| 23 | CX | 76 | A | C4-C5-C6 | 7.12 | 120.56 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | BA | 1605 | A | C2-N3-C4 | -7.11 | 107.04 | 110.60 |
| 25 | BA | 852 | G | O5'-P-OP1 | -7.11 | 99.31 | 105.70 |
| 25 | BA | 1077 | G | N1-C6-O6 | -7.10 | 115.64 | 119.90 |
| 25 | DA | 2588 | G | O5'-P-OP1 | -7.10 | 99.31 | 105.70 |
| 25 | BA | 2229 | A | O4'-C1'-N9 | 7.10 | 113.88 | 108.20 |
| 25 | BA | 1249 | A | O4'-C1'-N9 | 7.09 | 113.88 | 108.20 |
| 25 | DA | 528 | A | N3-C4-C5 | 7.09 | 131.77 | 126.80 |
| 25 | DA | 2805 | G | C8-N9-C4 | -7.09 | 103.56 | 106.40 |
| 1 | CA | 1126 | U | C5-C6-N1 | 7.08 | 126.24 | 122.70 |
| 1 | AA | 1026 | G | C4-N9-C1' | 7.07 | 135.69 | 126.50 |
| 25 | DA | 2321 | G | N9-C4-C5 | -7.07 | 102.57 | 105.40 |
| 25 | BA | 2556 | G | N1-C6-O6 | 7.07 | 124.14 | 119.90 |
| 25 | DA | 129 | C | C6-N1-C2 | 7.07 | 123.13 | 120.30 |
| 25 | BA | 1068 | G | N3-C4-N9 | -7.07 | 121.76 | 126.00 |
| 25 | DA | 1284 | A | N9-C4-C5 | -7.06 | 102.98 | 105.80 |
| 25 | DA | 2253 | G | C6-C5-N7 | -7.04 | 126.17 | 130.40 |
| 25 | DA | 2523 | G | O5'-P-OP2 | -7.04 | 99.37 | 105.70 |
| 25 | BA | 1067 | A | N7-C8-N9 | 7.03 | 117.32 | 113.80 |
| 25 | BA | 103 | C | O5'-P-OP2 | -7.01 | 99.39 | 105.70 |
| 25 | DA | 2253 | G | C5-C6-O6 | -7.01 | 124.39 | 128.60 |
| 25 | BA | 473 | A | O5'-P-OP1 | -7.01 | 99.39 | 105.70 |
| 1 | CA | 927 | G | N9-C4-C5 | 7.01 | 108.20 | 105.40 |
| 25 | BA | 1098 | C | C5-C6-N1 | 7.01 | 124.50 | 121.00 |
| 1 | CA | 1033 | G | C4-C5-N7 | 7.01 | 113.60 | 110.80 |
| 1 | AA | 1531 | A | O4'-C1'-N9 | -7.01 | 102.59 | 108.20 |
| 25 | BA | 733 | G | N1-C6-O6 | 7.01 | 124.10 | 119.90 |
| 1 | CA | 1157 | A | N1-C6-N6 | -7.00 | 114.40 | 118.60 |
| 23 | CX | 14 | A | C4-C5-C6 | 7.00 | 120.50 | 117.00 |
| 25 | BA | 602 | G | N1-C6-O6 | 7.00 | 124.10 | 119.90 |
| 25 | BA | 2589 | A | C8-N9-C4 | -7.00 | 103.00 | 105.80 |
| 25 | BA | 122 | G | O5'-P-OP2 | -6.99 | 99.41 | 105.70 |
| 25 | DA | 2298 | A | C6-N1-C2 | 6.99 | 122.79 | 118.60 |
| 25 | DA | 214 | G | O4'-C1'-N9 | 6.98 | 113.78 | 108.20 |
| 25 | BA | 1871 | G | N1-C6-O6 | -6.98 | 115.71 | 119.90 |
| 25 | BA | 852 | G | C5-C6-N1 | 6.97 | 114.99 | 111.50 |
| 25 | BA | 753 | A | C2-N3-C4 | -6.97 | 107.11 | 110.60 |
| 23 | AX | 46 | G | C5-C6-O6 | -6.97 | 124.42 | 128.60 |
| 25 | BA | 1006 | C | O5'-P-OP2 | -6.97 | 99.43 | 105.70 |
| 25 | BA | 2577 | A | O5'-P-OP1 | -6.97 | 99.43 | 105.70 |
| 25 | BA | 1719 | C | C6-N1-C2 | -6.96 | 117.52 | 120.30 |
| 25 | BA | 1844 | G | C8-N9-C4 | 6.96 | 109.18 | 106.40 |
| 25 | BA | 819 | C | C6-N1-C2 | 6.94 | 123.08 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | DA | 467 | G | C8-N9-C4 | 6.94 | 109.17 | 106.40 |
| 1 | AA | 1131 | G | N7-C8-N9 | 6.93 | 116.56 | 113.10 |
| 25 | DA | 2007 | C | C6-N1-C2 | 6.93 | 123.07 | 120.30 |
| 25 | DA | 1204 | A | N1-C6-N6 | 6.92 | 122.75 | 118.60 |
| 25 | DA | 2427 | C | C6-N1-C2 | 6.92 | 123.07 | 120.30 |
| 25 | BA | 1188 | A | N3-C4-N9 | -6.92 | 121.86 | 127.40 |
| 25 | DA | 981 | A | C5-C6-N6 | 6.91 | 129.23 | 123.70 |
| 25 | BA | 2081 | A | N7-C8-N9 | -6.91 | 110.34 | 113.80 |
| 1 | CA | 1259 | C | C6-N1-C2 | -6.91 | 117.53 | 120.30 |
| 25 | BA | 2804 | C | C6-N1-C2 | -6.90 | 117.54 | 120.30 |
| 25 | DA | 1339 | G | O5'-P-OP1 | -6.90 | 99.49 | 105.70 |
| 25 | DA | 1783 | A | C8-N9-C4 | 6.90 | 108.56 | 105.80 |
| 25 | DA | 2298 | A | N1-C2-N3 | -6.90 | 125.85 | 129.30 |
| 25 | BA | 2331 | G | C4-C5-N7 | 6.89 | 113.56 | 110.80 |
| 1 | AA | 199 | G | C8-N9-C4 | 6.89 | 109.16 | 106.40 |
| 1 | AA | 383 | A | C5-N7-C8 | 6.89 | 107.35 | 103.90 |
| 1 | CA | 1000 | U | C5-C6-N1 | 6.89 | 126.14 | 122.70 |
| 25 | DA | 1251 | C | N1-C2-O2 | -6.89 | 114.77 | 118.90 |
| 25 | BA | 555 | G | C4-C5-N7 | 6.88 | 113.55 | 110.80 |
| 1 | CA | 79 | G | C5-C6-O6 | 6.88 | 132.73 | 128.60 |
| 1 | AA | 476 | G | C4-N9-C1' | 6.88 | 135.44 | 126.50 |
| 25 | DA | 1022 | G | N3-C2-N2 | -6.88 | 115.08 | 119.90 |
| 1 | AA | 1007 | C | C5-C6-N1 | 6.88 | 124.44 | 121.00 |
| 1 | CA | 1119 | C | N1-C2-N3 | -6.88 | 114.39 | 119.20 |
| 25 | DA | 933 | A | N7-C8-N9 | 6.88 | 117.24 | 113.80 |
| 25 | DA | 1653 | G | C4-N9-C1' | 6.88 | 135.44 | 126.50 |
| 1 | CA | 1017 | G | C5-C6-O6 | 6.87 | 132.72 | 128.60 |
| 25 | BA | 2549 | U | C5-C4-O4 | 6.87 | 130.02 | 125.90 |
| 1 | CA | 525 | C | C5-C6-N1 | 6.87 | 124.43 | 121.00 |
| 1 | AA | 443 | C | C2-N1-C1' | 6.86 | 126.35 | 118.80 |
| 25 | BA | 1462 | G | O4'-C1'-N9 | 6.86 | 113.69 | 108.20 |
| 1 | AA | 97 | G | O4'-C1'-N9 | 6.86 | 113.69 | 108.20 |
| 1 | AA | 921 | U | C2-N3-C4 | 6.85 | 131.11 | 127.00 |
| 25 | DA | 2689 | U | P-O3'-C3' | 6.85 | 127.92 | 119.70 |
| 1 | AA | 1397 | C | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 25 | BA | 1588 | G | N3-C4-C5 | -6.84 | 125.18 | 128.60 |
| 25 | BA | 2551 | C | C6-N1-C2 | 6.84 | 123.03 | 120.30 |
| 25 | DA | 2829 | C | C6-N1-C2 | 6.83 | 123.03 | 120.30 |
| 25 | DA | 1328 | G | C5-C6-O6 | -6.83 | 124.50 | 128.60 |
| 1 | AA | 720 | C | C6-N1-C2 | -6.83 | 117.57 | 120.30 |
| 25 | DA | 2206 | G | C4-N9-C1' | -6.83 | 117.62 | 126.50 |
| 1 | CA | 1054 | C | C6-N1-C2 | -6.83 | 117.57 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | DA | 148 | C | C6-N1-C2 | 6.83 | 123.03 | 120.30 |
| 1 | AA | 1396 | A | C6-N1-C2 | 6.82 | 122.69 | 118.60 |
| 25 | DA | 2048 | G | C5-C6-O6 | 6.82 | 132.69 | 128.60 |
| 1 | CA | 1163 | C | C5-C6-N1 | 6.82 | 124.41 | 121.00 |
| 25 | DA | 294 | A | N1-C6-N6 | -6.82 | 114.51 | 118.60 |
| 25 | BA | 2105 | G | N1-C6-O6 | 6.82 | 123.99 | 119.90 |
| 25 | DA | 1432 | C | C6-N1-C2 | 6.82 | 123.03 | 120.30 |
| 25 | DA | 2345 | G | C5-C6-O6 | 6.81 | 132.69 | 128.60 |
| 1 | CA | 117 | G | N3-C4-N9 | 6.81 | 130.09 | 126.00 |
| 25 | BA | 555 | G | N3-C4-C5 | 6.80 | 132.00 | 128.60 |
| 25 | BA | 2299 | A | N3-C4-N9 | -6.80 | 121.96 | 127.40 |
| 1 | CA | 1054 | C | P-O3'-C3' | 6.80 | 127.86 | 119.70 |
| 25 | DA | 2313 | C | N1-C2-O2 | 6.79 | 122.97 | 118.90 |
| 1 | AA | 893 | C | N1-C2-O2 | 6.79 | 122.97 | 118.90 |
| 25 | DA | 2751 | G | N3-C4-C5 | -6.79 | 125.21 | 128.60 |
| 1 | AA | 509 | A | C8-N9-C4 | -6.78 | 103.09 | 105.80 |
| 1 | AA | 63 | C | N1-C2-O2 | 6.78 | 122.97 | 118.90 |
| 25 | BA | 824 | A | N1-C2-N3 | 6.77 | 132.68 | 129.30 |
| 1 | CA | 1042 | G | C6-N1-C2 | 6.76 | 129.16 | 125.10 |
| 25 | BA | 841 | G | C5-C6-O6 | 6.76 | 132.65 | 128.60 |
| 25 | BA | 1314 | A | N7-C8-N9 | -6.75 | 110.42 | 113.80 |
| 25 | BA | 2444 | A | N1-C6-N6 | 6.75 | 122.65 | 118.60 |
| 25 | BA | 553 | A | N3-C4-C5 | 6.75 | 131.52 | 126.80 |
| 1 | AA | 1285 | A | P-O3'-C3' | 6.74 | 127.79 | 119.70 |
| 25 | BA | 2014 | G | P-O3'-C3' | 6.74 | 127.79 | 119.70 |
| 1 | AA | 1397 | C | C2-N1-C1' | 6.74 | 126.21 | 118.80 |
| 25 | DA | 524 | U | O5'-P-OP2 | -6.74 | 99.64 | 105.70 |
| 1 | CA | 1502 | A | O5'-P-OP2 | -6.73 | 99.64 | 105.70 |
| 25 | DA | 2010 | G | O5'-P-OP2 | 6.73 | 118.78 | 110.70 |
| 25 | BA | 1843 | A | O5'-P-OP1 | -6.72 | 99.65 | 105.70 |
| 1 | CA | 848 | C | C5-C6-N1 | 6.72 | 124.36 | 121.00 |
| 1 | AA | 1395 | C | C2-N3-C4 | 6.72 | 123.26 | 119.90 |
| 25 | DA | 741 | G | O5'-P-OP1 | -6.72 | 99.65 | 105.70 |
| 1 | CA | 979 | C | C6-N1-C2 | -6.72 | 117.61 | 120.30 |
| 25 | DA | 110 | G | C8-N9-C4 | 6.72 | 109.09 | 106.40 |
| 25 | DA | 1721 | G | N3-C4-N9 | 6.71 | 130.03 | 126.00 |
| 1 | CA | 1258 | G | O4'-C1'-N9 | 6.71 | 113.57 | 108.20 |
| 25 | DA | 2520 | C | N3-C4-C5 | 6.71 | 124.58 | 121.90 |
| 1 | CA | 1003 | G | N3-C4-N9 | 6.71 | 130.03 | 126.00 |
| 1 | CA | 1033 | G | N1-C6-O6 | 6.71 | 123.93 | 119.90 |
| 25 | DA | 219 | G | N3-C4-C5 | -6.71 | 125.25 | 128.60 |
| 25 | DA | 1489 | U | C4-C5-C6 | 6.70 | 123.72 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3 | CC | 52 | LEU | CA-CB-CG | 6.70 | 130.72 | 115.30 |
| 25 | DA | 784 | A | C8-N9-C4 | 6.70 | 108.48 | 105.80 |
| 1 | CA | 1126 | U | C2-N1-C1' | 6.69 | 125.73 | 117.70 |
| 1 | CA | 1135 | U | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 25 | DA | 738 | G | N3-C4-C5 | -6.67 | 125.26 | 128.60 |
| 1 | AA | 1502 | A | O5'-P-OP2 | -6.67 | 99.69 | 105.70 |
| 1 | CA | 1023 | G | N3-C4-N9 | 6.67 | 130.00 | 126.00 |
| 26 | DB | 42 | C | O5'-P-OP1 | -6.67 | 99.70 | 105.70 |
| 1 | CA | 1456 | G | C8-N9-C4 | 6.67 | 109.07 | 106.40 |
| 25 | BA | 1327 | G | C5-C6-O6 | -6.67 | 124.60 | 128.60 |
| 1 | CA | 1311 | G | C6-C5-N7 | 6.67 | 134.40 | 130.40 |
| 25 | BA | 831 | A | O4'-C1'-N9 | 6.66 | 113.53 | 108.20 |
| 25 | DA | 2360 | A | C8-N9-C4 | 6.66 | 108.46 | 105.80 |
| 25 | BA | 555 | G | C2-N3-C4 | -6.66 | 108.57 | 111.90 |
| 25 | DA | 827 | U | N1-C2-O2 | -6.65 | 118.14 | 122.80 |
| 25 | BA | 1093 | G | C4-N9-C1' | 6.65 | 135.14 | 126.50 |
| 25 | BA | 2448 | G | N3-C2-N2 | -6.64 | 115.25 | 119.90 |
| 25 | DA | 1992 | G | C8-N9-C4 | -6.64 | 103.74 | 106.40 |
| 25 | BA | 43 | A | C2-N3-C4 | -6.64 | 107.28 | 110.60 |
| 25 | DA | 1281 | G | O5'-P-OP2 | 6.64 | 118.67 | 110.70 |
| 25 | DA | 2286 | A | N1-C6-N6 | 6.64 | 122.58 | 118.60 |
| 25 | BA | 2228 | G | OP1-P-O3' | 6.64 | 119.80 | 105.20 |
| 25 | BA | 2551 | C | C5-C6-N1 | -6.64 | 117.68 | 121.00 |
| 25 | DA | 776 | G | C8-N9-C4 | -6.64 | 103.75 | 106.40 |
| 25 | DA | 945 | A | O4'-C1'-N9 | 6.64 | 113.51 | 108.20 |
| 25 | DA | 933 | A | C4-C5-N7 | 6.63 | 114.02 | 110.70 |
| 25 | DA | 945 | A | C5-N7-C8 | -6.63 | 100.59 | 103.90 |
| 25 | DA | 2388 | A | O4'-C1'-N9 | 6.63 | 113.50 | 108.20 |
| 26 | DB | 104 | U | C6-N1-C2 | 6.63 | 124.98 | 121.00 |
| 25 | BA | 2260 | C | O5'-P-OP2 | -6.62 | 99.74 | 105.70 |
| 1 | CA | 726 | C | O5'-P-OP1 | -6.62 | 99.74 | 105.70 |
| 25 | BA | 2550 | C | C6-N1-C2 | 6.62 | 122.95 | 120.30 |
| 25 | DA | 1395 | A | O4'-C1'-N9 | 6.62 | 113.50 | 108.20 |
| 1 | AA | 1493 | A | P-O3'-C3' | 6.61 | 127.64 | 119.70 |
| 1 | CA | 1180 | A | O4'-C1'-N9 | 6.61 | 113.48 | 108.20 |
| 25 | BA | 254 | A | C5-N7-C8 | -6.60 | 100.60 | 103.90 |
| 25 | DA | 63 | U | N3-C4-O4 | -6.60 | 114.78 | 119.40 |
| 25 | DA | 1489 | U | C6-N1-C1' | -6.60 | 111.96 | 121.20 |
| 1 | CA | 1286 | A | C8-N9-C4 | -6.60 | 103.16 | 105.80 |
| 25 | BA | 805 | C | C6-N1-C2 | -6.59 | 117.66 | 120.30 |
| 1 | CA | 1123 | A | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 25 | DA | 2218 | U | N3-C2-O2 | -6.59 | 117.58 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | DA | 482 | A | O5'-P-OP2 | -6.59 | 99.77 | 105.70 |
| 25 | DA | 2050 | C | C6-N1-C2 | 6.59 | 122.94 | 120.30 |
| 25 | DA | 2388 | A | C2-N3-C4 | 6.59 | 113.89 | 110.60 |
| 25 | DA | 451 | C | C6-N1-C2 | 6.59 | 122.94 | 120.30 |
| 1 | AA | 193 | C | C6-N1-C2 | -6.58 | 117.67 | 120.30 |
| 1 | AA | 458 | C | C2-N1-C1' | 6.58 | 126.04 | 118.80 |
| 25 | BA | 2298 | A | C6-C5-N7 | -6.58 | 127.69 | 132.30 |
| 25 | DA | 945 | A | N9-C4-C5 | -6.58 | 103.17 | 105.80 |
| 25 | DA | 2805 | G | O4'-C1'-N9 | 6.58 | 113.46 | 108.20 |
| 25 | BA | 418 | G | C5-C6-O6 | -6.57 | 124.66 | 128.60 |
| 25 | BA | 148 | C | C6-N1-C2 | 6.57 | 122.93 | 120.30 |
| 25 | DA | 826 | U | C5-C6-N1 | -6.57 | 119.41 | 122.70 |
| 25 | DA | 2253 | G | N9-C4-C5 | -6.57 | 102.77 | 105.40 |
| 1 | CA | 1003 | G | C4-N9-C1' | 6.57 | 135.04 | 126.50 |
| 1 | CA | 999 | C | C6-N1-C1' | -6.57 | 112.92 | 120.80 |
| 25 | BA | 717 | A | O4'-C1'-N9 | -6.56 | 102.95 | 108.20 |
| 25 | BA | 2331 | G | O4'-C1'-N9 | 6.55 | 113.44 | 108.20 |
| 1 | CA | 899 | C | C6-N1-C2 | 6.55 | 122.92 | 120.30 |
| 1 | AA | 1137 | C | C5-C6-N1 | 6.55 | 124.28 | 121.00 |
| 25 | DA | 2287 | A | C2-N3-C4 | -6.55 | 107.33 | 110.60 |
| 25 | DA | 2501 | C | N3-C4-C5 | 6.55 | 124.52 | 121.90 |
| 25 | BA | 2054 | G | N3-C4-C5 | 6.54 | 131.87 | 128.60 |
| 25 | DA | 2512 | C | C6-N1-C2 | 6.54 | 122.92 | 120.30 |
| 1 | AA | 266 | G | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 25 | BA | 1483 | C | C6-N1-C2 | -6.54 | 117.68 | 120.30 |
| 25 | DA | 2560 | C | C6-N1-C2 | 6.54 | 122.92 | 120.30 |
| 25 | BA | 176 | G | N1-C6-O6 | 6.54 | 123.82 | 119.90 |
| 25 | DA | 2061 | G | C8-N9-C4 | 6.53 | 109.01 | 106.40 |
| 25 | BA | 666 | C | C6-N1-C2 | -6.51 | 117.69 | 120.30 |
| 1 | AA | 1127 | G | C5-N7-C8 | 6.51 | 107.56 | 104.30 |
| 1 | CA | 1023 | G | N3-C2-N2 | 6.51 | 124.46 | 119.90 |
| 25 | BA | 660 | C | C6-N1-C2 | -6.51 | 117.70 | 120.30 |
| 25 | DA | 1681 | G | N3-C4-C5 | 6.50 | 131.85 | 128.60 |
| 25 | BA | 176 | G | C4-C5-N7 | 6.49 | 113.40 | 110.80 |
| 1 | CA | 1502 | A | N1-C2-N3 | 6.49 | 132.54 | 129.30 |
| 1 | CA | 1502 | A | C5-N7-C8 | -6.49 | 100.66 | 103.90 |
| 25 | DA | 1257 | C | C6-N1-C2 | -6.48 | 117.71 | 120.30 |
| 26 | BB | 98 | G | O5'-P-OP2 | -6.48 | 99.87 | 105.70 |
| 25 | BA | 781 | A | N1-C6-N6 | 6.47 | 122.48 | 118.60 |
| 2 | CB | 154 | LEU | CA-CB-CG | 6.47 | 130.19 | 115.30 |
| 25 | BA | 2544 | G | N1-C6-O6 | 6.47 | 123.78 | 119.90 |
| 25 | DA | 1022 | G | C8-N9-C1' | 6.47 | 135.41 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | DA | 987 | G | C5-C6-O6 | -6.47 | 124.72 | 128.60 |
| 23 | AX | 8 | U | N3-C4-C5 | -6.46 | 110.72 | 114.60 |
| 1 | AA | 382 | A | N1-C6-N6 | -6.46 | 114.72 | 118.60 |
| 1 | AA | 1125 | U | C4-C5-C6 | -6.46 | 115.83 | 119.70 |
| 1 | CA | 65 | U | P-O3'-C3' | 6.46 | 127.45 | 119.70 |
| 1 | AA | 470 | C | N1-C2-O2 | 6.46 | 122.77 | 118.90 |
| 23 | AX | 22 | G | N3-C4-C5 | 6.46 | 131.83 | 128.60 |
| 1 | CA | 1260 | C | C5-C6-N1 | 6.46 | 124.23 | 121.00 |
| 25 | DA | 530 | G | N3-C4-N9 | -6.45 | 122.13 | 126.00 |
| 25 | BA | 1263 | C | O5'-P-OP2 | -6.45 | 99.90 | 105.70 |
| 25 | BA | 271 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 25 | DA | 1635 | G | N1-C6-O6 | 6.44 | 123.77 | 119.90 |
| 25 | BA | 2638 | C | C6-N1-C2 | 6.44 | 122.88 | 120.30 |
| 25 | DA | 1142 | U | N1-C2-O2 | 6.44 | 127.31 | 122.80 |
| 25 | DA | 933 | A | N1-C6-N6 | 6.44 | 122.46 | 118.60 |
| 25 | BA | 2253 | A | O5'-P-OP1 | -6.43 | 99.91 | 105.70 |
| 1 | CA | 1163 | C | C2-N3-C4 | 6.43 | 123.12 | 119.90 |
| 25 | BA | 139 | A | O4'-C1'-N9 | 6.43 | 113.35 | 108.20 |
| 25 | DA | 2805 | G | N3-C4-C5 | -6.43 | 125.38 | 128.60 |
| 25 | BA | 1423 | G | N1-C6-O6 | -6.42 | 116.05 | 119.90 |
| 25 | BA | 1742 | G | C6-C5-N7 | -6.42 | 126.55 | 130.40 |
| 1 | CA | 1036 | G | C5-C6-N1 | -6.42 | 108.29 | 111.50 |
| 1 | AA | 1206 | G | C5-C6-O6 | -6.42 | 124.75 | 128.60 |
| 23 | CX | 46 | G | C5-C6-N1 | 6.41 | 114.71 | 111.50 |
| 25 | DA | 216 | A | C2-N3-C4 | -6.41 | 107.40 | 110.60 |
| 1 | AA | 165 | C | C6-N1-C2 | -6.41 | 117.74 | 120.30 |
| 25 | BA | 2673 | G | N3-C4-C5 | -6.41 | 125.40 | 128.60 |
| 1 | AA | 532 | A | OP1-P-O3' | 6.40 | 119.29 | 105.20 |
| 25 | DA | 1021 | A | N1-C2-N3 | 6.40 | 132.50 | 129.30 |
| 25 | BA | 2227 | G | C4-N9-C1' | -6.40 | 118.18 | 126.50 |
| 25 | BA | 2891 | C | C6-N1-C2 | -6.40 | 117.74 | 120.30 |
| 25 | DA | 2544 | G | N1-C6-O6 | 6.40 | 123.74 | 119.90 |
| 22 | AV | 17 | U | C5-C4-O4 | 6.40 | 129.74 | 125.90 |
| 25 | DA | 2313 | C | N3-C2-O2 | -6.40 | 117.42 | 121.90 |
| 25 | BA | 2630 | G | N3-C4-N9 | 6.40 | 129.84 | 126.00 |
| 25 | BA | 352 | U | O5'-P-OP2 | -6.40 | 99.94 | 105.70 |
| 1 | AA | 63 | C | N3-C2-O2 | -6.39 | 117.42 | 121.90 |
| 1 | CA | 1042 | G | C8-N9-C4 | 6.39 | 108.96 | 106.40 |
| 43 | DX | 57 | LEU | CA-CB-CG | 6.39 | 130.00 | 115.30 |
| 1 | CA | 1132 | C | C6-N1-C2 | -6.39 | 117.74 | 120.30 |
| 25 | DA | 2512 | C | N3-C2-O2 | 6.39 | 126.37 | 121.90 |
| 1 | AA | 458 | C | N1-C2-O2 | 6.39 | 122.73 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | BA | 2830 | A | C6-C5-N7 | -6.39 | 127.83 | 132.30 |
| 1 | AA | 841 | U | C6-N1-C2 | -6.39 | 117.17 | 121.00 |
| 25 | BA | 1045 | U | O5'-P-OP2 | -6.38 | 99.95 | 105.70 |
| 25 | BA | 2026 | G | C2-N3-C4 | -6.38 | 108.71 | 111.90 |
| 25 | DA | 1698 | A | C4-C5-N7 | 6.38 | 113.89 | 110.70 |
| 25 | BA | 2331 | G | N3-C4-N9 | -6.38 | 122.17 | 126.00 |
| 25 | BA | 1312 | G | C8-N9-C4 | 6.38 | 108.95 | 106.40 |
| 25 | BA | 1919 | G | N1-C6-O6 | 6.38 | 123.73 | 119.90 |
| 1 | CA | 1033 | G | C6-N1-C2 | 6.38 | 128.93 | 125.10 |
| 1 | CA | 1169 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 25 | DA | 2850 | A | OP1-P-OP2 | -6.37 | 110.04 | 119.60 |
| 1 | AA | 1058 | G | C5-C6-O6 | -6.37 | 124.78 | 128.60 |
| 25 | BA | 2280 | A | O5'-P-OP1 | -6.36 | 99.97 | 105.70 |
| 1 | AA | 1024 | G | C4-N9-C1' | 6.36 | 134.76 | 126.50 |
| 25 | DA | 2574 | G | C5-C6-O6 | -6.36 | 124.78 | 128.60 |
| 25 | BA | 978 | A | N7-C8-N9 | 6.35 | 116.98 | 113.80 |
| 25 | BA | 1812 | C | C6-N1-C2 | 6.35 | 122.84 | 120.30 |
| 25 | DA | 63 | U | C5-C4-O4 | 6.35 | 129.71 | 125.90 |
| 25 | DA | 1022 | G | C4-N9-C1' | -6.35 | 118.24 | 126.50 |
| 1 | CA | 1511 | G | N1-C6-O6 | 6.35 | 123.71 | 119.90 |
| 1 | AA | 496 | A | C8-N9-C4 | -6.34 | 103.26 | 105.80 |
| 25 | BA | 568 | C | C6-N1-C2 | 6.34 | 122.84 | 120.30 |
| 1 | CA | 1122 | U | C6-N1-C1' | -6.34 | 112.32 | 121.20 |
| 25 | DA | 31 | C | C6-N1-C2 | -6.34 | 117.76 | 120.30 |
| 1 | AA | 443 | C | C6-N1-C1' | -6.34 | 113.19 | 120.80 |
| 1 | CA | 1012 | U | N1-C2-N3 | 6.33 | 118.70 | 114.90 |
| 26 | DB | 95 | C | C6-N1-C2 | 6.33 | 122.83 | 120.30 |
| 25 | BA | 2442 | A | N1-C6-N6 | -6.33 | 114.80 | 118.60 |
| 1 | AA | 800 | G | C8-N9-C4 | -6.33 | 103.87 | 106.40 |
| 25 | BA | 2701 | U | C6-N1-C2 | -6.33 | 117.20 | 121.00 |
| 1 | CA | 754 | C | C2-N1-C1' | 6.32 | 125.75 | 118.80 |
| 23 | CX | 22 | G | C4-C5-C6 | -6.32 | 115.01 | 118.80 |
| 25 | BA | 342 | C | C6-N1-C2 | -6.32 | 117.77 | 120.30 |
| 1 | CA | 1402 | C | C6-N1-C2 | -6.32 | 117.77 | 120.30 |
| 1 | CA | 1311 | G | N3-C4-C5 | 6.32 | 131.76 | 128.60 |
| 26 | DB | 8 | U | C5-C6-N1 | 6.31 | 125.86 | 122.70 |
| 35 | DP | 44 | GLY | N-CA-C | -6.31 | 97.31 | 113.10 |
| 25 | BA | 2094 | G | C6-C5-N7 | -6.31 | 126.61 | 130.40 |
| 25 | DA | 1681 | G | C2-N3-C4 | -6.31 | 108.74 | 111.90 |
| 25 | DA | 2279 | G | C8-N9-C4 | 6.31 | 108.92 | 106.40 |
| 1 | AA | 1054 | C | P-O3'-C3' | 6.31 | 127.27 | 119.70 |
| 1 | CA | 1391 | U | C5-C4-O4 | 6.30 | 129.68 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | AA | 1029 | C | C2-N1-C1' | -6.30 | 111.87 | 118.80 |
| 25 | BA | 733 | G | C6-C5-N7 | -6.30 | 126.62 | 130.40 |
| 25 | BA | 781 | A | C2-N3-C4 | -6.30 | 107.45 | 110.60 |
| 1 | CA | 967 | C | C6-N1-C2 | 6.30 | 122.82 | 120.30 |
| 1 | CA | 1227 | A | N7-C8-N9 | 6.30 | 116.95 | 113.80 |
| 25 | DA | 1284 | A | C5-C6-N6 | -6.30 | 118.66 | 123.70 |
| 25 | BA | 2631 | C | C6-N1-C2 | 6.29 | 122.82 | 120.30 |
| 1 | CA | 908 | A | O5'-P-OP2 | -6.29 | 100.04 | 105.70 |
| 25 | DA | 528 | A | N1-C6-N6 | 6.29 | 122.38 | 118.60 |
| 25 | DA | 1363 | C | C5-C6-N1 | -6.29 | 117.85 | 121.00 |
| 25 | BA | 484 | G | C8-N9-C4 | -6.29 | 103.88 | 106.40 |
| 25 | DA | 2070 | G | N1-C6-O6 | -6.28 | 116.13 | 119.90 |
| 25 | BA | 849 | A | C8-N9-C4 | -6.28 | 103.29 | 105.80 |
| 1 | CA | 999 | C | C2-N1-C1' | 6.28 | 125.70 | 118.80 |
| 25 | DA | 1600 | C | O5'-P-OP2 | -6.28 | 100.05 | 105.70 |
| 1 | AA | 227 | G | C8-N9-C4 | 6.27 | 108.91 | 106.40 |
| 25 | DA | 2617 | C | O5'-P-OP1 | -6.27 | 100.05 | 105.70 |
| 25 | BA | 1779 | G | C8-N9-C4 | -6.27 | 103.89 | 106.40 |
| 25 | DA | 2048 | G | N1-C6-O6 | -6.27 | 116.14 | 119.90 |
| 25 | DA | 271(Y) | U | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 1 | AA | 383 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 1 | CA | 528 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 25 | DA | 2357 | U | O5'-P-OP2 | -6.26 | 100.06 | 105.70 |
| 1 | CA | 1272 | G | C5-C6-O6 | 6.26 | 132.35 | 128.60 |
| 25 | DA | 2554 | U | O5'-P-OP2 | -6.25 | 100.07 | 105.70 |
| 25 | BA | 405 | C | C6-N1-C2 | 6.25 | 122.80 | 120.30 |
| 25 | BA | 474 | U | N3-C2-O2 | -6.25 | 117.82 | 122.20 |
| 1 | CA | 117 | G | C8-N9-C1' | -6.25 | 118.87 | 127.00 |
| 1 | CA | 1500 | A | N1-C6-N6 | 6.25 | 122.35 | 118.60 |
| 25 | BA | 2638 | C | N3-C4-C5 | 6.24 | 124.40 | 121.90 |
| 1 | AA | 1127 | G | N3-C4-C5 | -6.24 | 125.48 | 128.60 |
| 26 | DB | 115 | G | N9-C4-C5 | -6.24 | 102.90 | 105.40 |
| 25 | BA | 2283 | G | N3-C4-N9 | 6.24 | 129.74 | 126.00 |
| 25 | DA | 2406 | U | O4'-C1'-N1 | -6.24 | 103.21 | 108.20 |
| 1 | AA | 167 | G | C4-N9-C1' | 6.23 | 134.60 | 126.50 |
| 25 | DA | 1698 | A | N1-C2-N3 | 6.23 | 132.41 | 129.30 |
| 1 | AA | 1127 | G | C8-N9-C4 | 6.22 | 108.89 | 106.40 |
| 25 | BA | 1779 | G | N7-C8-N9 | 6.22 | 116.21 | 113.10 |
| 25 | BA | 1926 | G | N1-C6-O6 | -6.22 | 116.17 | 119.90 |
| 1 | CA | 509 | A | C8-N9-C4 | -6.22 | 103.31 | 105.80 |
| 1 | AA | 175 | C | C6-N1-C2 | -6.21 | 117.81 | 120.30 |
| 1 | AA | 1067 | A | P-O3'-C3' | 6.21 | 127.16 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | CA | 5 | U | C6-N1-C2 | -6.21 | 117.27 | 121.00 |
| 1 | CA | 967 | C | N3-C2-O2 | 6.21 | 126.25 | 121.90 |
| 25 | DA | 614 | U | C5-C4-O4 | 6.21 | 129.63 | 125.90 |
| 25 | DA | 2751 | G | C4-N9-C1' | 6.21 | 134.57 | 126.50 |
| 26 | BB | 93 | G | C8-N9-C4 | -6.21 | 103.92 | 106.40 |
| 25 | BA | 1832 | G | N1-C6-O6 | 6.20 | 123.62 | 119.90 |
| 1 | CA | 354 | G | C6-C5-N7 | -6.20 | 126.68 | 130.40 |
| 25 | BA | 1629 | C | C5-C6-N1 | -6.20 | 117.90 | 121.00 |
| 1 | AA | 1515 | C | N3-C4-C5 | -6.19 | 119.42 | 121.90 |
| 25 | BA | 77 | A | N1-C6-N6 | 6.19 | 122.32 | 118.60 |
| 1 | AA | 1150 | U | C2-N3-C4 | 6.19 | 130.71 | 127.00 |
| 25 | BA | 2298 | A | N7-C8-N9 | 6.19 | 116.90 | 113.80 |
| 25 | DA | 566 | U | C5-C6-N1 | -6.19 | 119.61 | 122.70 |
| 25 | DA | 2520 | C | C6-N1-C2 | 6.19 | 122.78 | 120.30 |
| 25 | DA | 2053 | G | C8-N9-C4 | 6.18 | 108.87 | 106.40 |
| 25 | DA | 1558 | A | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 1 | CA | 1064 | G | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 25 | BA | 1343 | C | OP1-P-O3' | 6.18 | 118.79 | 105.20 |
| 1 | AA | 1131 | G | C4-C5-N7 | 6.17 | 113.27 | 110.80 |
| 25 | BA | 595 | A | N1-C6-N6 | -6.17 | 114.90 | 118.60 |
| 25 | DA | 154(A) | C | N1-C2-O2 | 6.17 | 122.60 | 118.90 |
| 25 | DA | 1363 | C | C6-N1-C2 | 6.17 | 122.77 | 120.30 |
| 25 | DA | 2298 | A | N9-C4-C5 | -6.16 | 103.33 | 105.80 |
| 25 | BA | 39 | C | O5'-P-OP2 | -6.16 | 100.16 | 105.70 |
| 19 | CS | 16 | LEU | CA-CB-CG | 6.16 | 129.47 | 115.30 |
| 1 | AA | 488 | C | C6-N1-C2 | -6.16 | 117.84 | 120.30 |
| 25 | BA | 1255 | A | C8-N9-C4 | -6.15 | 103.34 | 105.80 |
| 25 | BA | 2403 | G | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 25 | DA | 2591 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 25 | DA | 130 | C | N3-C4-C5 | 6.15 | 124.36 | 121.90 |
| 1 | CA | 818 | G | C8-N9-C4 | 6.15 | 108.86 | 106.40 |
| 25 | BA | 1067 | A | C4-C5-N7 | 6.14 | 113.77 | 110.70 |
| 25 | DA | 1790 | C | P-O3'-C3' | 6.14 | 127.07 | 119.70 |
| 25 | DA | 2042 | A | C8-N9-C4 | 6.14 | 108.25 | 105.80 |
| 25 | BA | 859 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 25 | BA | 842 | C | N1-C2-O2 | 6.13 | 122.58 | 118.90 |
| 25 | BA | 994 | C | C6-N1-C2 | 6.13 | 122.75 | 120.30 |
| 25 | DA | 75 | G | C8-N9-C4 | -6.13 | 103.95 | 106.40 |
| 1 | AA | 347 | G | C4-N9-C1' | 6.13 | 134.47 | 126.50 |
| 25 | BA | 1725 | G | C8-N9-C4 | -6.13 | 103.95 | 106.40 |
| 25 | BA | 1067 | A | N1-C2-N3 | 6.13 | 132.37 | 129.30 |
| 25 | DA | 414 | C | O5'-P-OP2 | -6.13 | 100.18 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | AA | 1026 | G | N3-C4-C5 | -6.13 | 125.54 | 128.60 |
| 1 | AA | 1531 | A | C8-N9-C4 | -6.13 | 103.35 | 105.80 |
| 1 | CA | 1122 | U | C5-C4-O4 | -6.13 | 122.22 | 125.90 |
| 25 | BA | 2624 | C | O5'-P-OP1 | -6.12 | 100.19 | 105.70 |
| 1 | AA | 226 | G | C8-N9-C4 | 6.12 | 108.85 | 106.40 |
| 1 | AA | 536 | C | O5'-P-OP2 | -6.12 | 100.19 | 105.70 |
| 25 | DA | 2207 | G | C4-N9-C1' | 6.12 | 134.45 | 126.50 |
| 25 | BA | 892 | G | O4'-C1'-N9 | 6.11 | 113.09 | 108.20 |
| 23 | CX | 46 | G | N9-C4-C5 | 6.11 | 107.84 | 105.40 |
| 25 | DA | 2623 | G | N1-C6-O6 | 6.11 | 123.57 | 119.90 |
| 1 | AA | 1530 | G | C5-C6-O6 | -6.11 | 124.94 | 128.60 |
| 25 | BA | 840 | A | N1-C6-N6 | 6.11 | 122.26 | 118.60 |
| 25 | BA | 2298 | A | C8-N9-C4 | -6.10 | 103.36 | 105.80 |
| 25 | DA | 1239 | G | N1-C6-O6 | 6.10 | 123.56 | 119.90 |
| 25 | BA | 139 | A | C6-C5-N7 | -6.10 | 128.03 | 132.30 |
| 25 | BA | 2807 | C | C5-C6-N1 | 6.10 | 124.05 | 121.00 |
| 1 | CA | 1002 | G | N3-C2-N2 | -6.10 | 115.63 | 119.90 |
| 25 | BA | 590 | A | C2-N3-C4 | -6.09 | 107.55 | 110.60 |
| 25 | BA | 873 | U | OP2-P-O3' | 6.09 | 118.61 | 105.20 |
| 25 | DA | 133 | C | O5'-P-OP2 | -6.09 | 100.22 | 105.70 |
| 25 | DA | 141 | A | N7-C8-N9 | 6.09 | 116.85 | 113.80 |
| 1 | CA | 894 | G | N3-C4-C5 | 6.09 | 131.65 | 128.60 |
| 25 | BA | 834 | U | N1-C2-N3 | 6.09 | 118.55 | 114.90 |
| 1 | CA | 1149 | C | C5-C6-N1 | 6.08 | 124.04 | 121.00 |
| 25 | DA | 2084 | C | C5-C6-N1 | -6.08 | 117.96 | 121.00 |
| 1 | CA | 736 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 25 | DA | 2321 | G | C8-N9-C1' | -6.08 | 119.09 | 127.00 |
| 1 | AA | 1030(A) | G | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 25 | DA | 2218 | U | N1-C2-O2 | 6.08 | 127.06 | 122.80 |
| 26 | BB | 30 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 1 | CA | 915 | A | C8-N9-C4 | 6.07 | 108.23 | 105.80 |
| 25 | DA | 991 | C | O5'-P-OP1 | 6.07 | 117.98 | 110.70 |
| 1 | CA | 1137 | C | P-O3'-C3' | 6.07 | 126.98 | 119.70 |
| 1 | CA | 1484 | C | C5-C6-N1 | -6.06 | 117.97 | 121.00 |
| 25 | BA | 56 | C | C2-N3-C4 | 6.06 | 122.93 | 119.90 |
| 25 | DA | 1721 | G | N3-C2-N2 | 6.06 | 124.14 | 119.90 |
| 1 | CA | 1154 | G | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 25 | DA | 1531 | C | C5-C6-N1 | 6.06 | 124.03 | 121.00 |
| 25 | BA | 332 | G | C6-C5-N7 | -6.06 | 126.77 | 130.40 |
| 25 | DA | 1122 | G | O5'-P-OP2 | -6.06 | 100.25 | 105.70 |
| 25 | BA | 2077 | C | C2-N3-C4 | 6.05 | 122.93 | 119.90 |
| 1 | AA | 383 | A | C8-N9-C1' | -6.05 | 116.81 | 127.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | CA | 1002 | G | C5-C6-O6 | 6.05 | 132.23 | 128.60 |
| 25 | BA | 1298 | G | N3-C2-N2 | -6.05 | 115.67 | 119.90 |
| 1 | AA | 1030(B) | C | N3-C2-O2 | -6.05 | 117.67 | 121.90 |
| 25 | BA | 12 | U | C6-N1-C2 | -6.05 | 117.37 | 121.00 |
| 25 | BA | 2107 | C | O5'-P-OP2 | -6.05 | 100.26 | 105.70 |
| 25 | BA | 332 | G | C4-C5-N7 | 6.04 | 113.22 | 110.80 |
| 25 | BA | 552 | C | N3-C4-N4 | -6.04 | 113.77 | 118.00 |
| 25 | DA | 801 | G | O5'-P-OP2 | -6.04 | 100.26 | 105.70 |
| 25 | BA | 535 | C | C6-N1-C2 | -6.04 | 117.88 | 120.30 |
| 1 | AA | 1127 | G | N9-C4-C5 | -6.04 | 102.98 | 105.40 |
| 25 | DA | 94(A) | G | C8-N9-C4 | -6.04 | 103.98 | 106.40 |
| 25 | BA | 254 | A | C6-C5-N7 | -6.03 | 128.08 | 132.30 |
| 25 | DA | 1653 | G | C8-N9-C1' | -6.03 | 119.16 | 127.00 |
| 23 | CX | 8 | U | N1-C2-N3 | -6.03 | 111.28 | 114.90 |
| 25 | BA | 1718 | U | N1-C2-O2 | -6.03 | 118.58 | 122.80 |
| 26 | BB | 91 | C | N3-C4-C5 | 6.03 | 124.31 | 121.90 |
| 25 | DA | 2540 | C | C6-N1-C2 | 6.03 | 122.71 | 120.30 |
| 1 | CA | 299 | G | N9-C4-C5 | -6.03 | 102.99 | 105.40 |
| 25 | DA | 2335 | A | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 25 | BA | 588 | C | N1-C2-O2 | 6.02 | 122.51 | 118.90 |
| 25 | BA | 2830 | A | C5-N7-C8 | -6.02 | 100.89 | 103.90 |
| 25 | BA | 783 | C | N1-C2-O2 | -6.02 | 115.29 | 118.90 |
| 1 | CA | 1044 | A | C6-N1-C2 | 6.02 | 122.21 | 118.60 |
| 25 | DA | 461 | C | N3-C2-O2 | 6.02 | 126.11 | 121.90 |
| 25 | BA | 978 | A | O4'-C1'-N9 | 6.01 | 113.01 | 108.20 |
| 25 | BA | 2236 | G | C8-N9-C4 | 6.01 | 108.81 | 106.40 |
| 25 | DA | 1763 | G | O5'-P-OP2 | -6.01 | 100.29 | 105.70 |
| 1 | CA | 992 | U | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 25 | BA | 876 | A | O5'-P-OP2 | -6.00 | 100.30 | 105.70 |
| 25 | BA | 1076 | G | N3-C2-N2 | 6.00 | 124.10 | 119.90 |
| 25 | BA | 2650 | G | C8-N9-C4 | -6.00 | 104.00 | 106.40 |
| 1 | CA | 1042 | G | N1-C2-N3 | -6.00 | 120.30 | 123.90 |
| 25 | DA | 482 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 25 | DA | 971 | C | N1-C2-O2 | -6.00 | 115.30 | 118.90 |
| 25 | BA | 2462 | A | N1-C6-N6 | 6.00 | 122.20 | 118.60 |
| 25 | DA | 141 | A | C5-N7-C8 | -6.00 | 100.90 | 103.90 |
| 1 | AA | 218 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 1 | AA | 1493 | A | O5'-P-OP1 | 6.00 | 117.89 | 110.70 |
| 25 | BA | 2228 | G | P-O3'-C3' | 5.99 | 126.89 | 119.70 |
| 25 | DA | 680 | G | N1-C6-O6 | 5.99 | 123.50 | 119.90 |
| 25 | DA | 2751 | G | N3-C4-N9 | 5.99 | 129.59 | 126.00 |
| 23 | CX | 34 | C | C6-N1-C2 | -5.98 | 117.91 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | DA | 807 | U | O5'-P-OP2 | 5.98 | 117.87 | 110.70 |
| 1 | CA | 841 | U | C6-N1-C2 | -5.98 | 117.41 | 121.00 |
| 23 | CX | 22 | G | N7-C8-N9 | 5.97 | 116.09 | 113.10 |
| 25 | DA | 2090 | G | N1-C6-O6 | -5.97 | 116.32 | 119.90 |
| 1 | AA | 890 | G | O4'-C1'-N9 | 5.97 | 112.97 | 108.20 |
| 25 | BA | 2110 | G | N3-C4-C5 | 5.97 | 131.59 | 128.60 |
| 1 | AA | 1286 | A | C8-N9-C4 | -5.97 | 103.41 | 105.80 |
| 25 | BA | 2515 | A | C2-N3-C4 | 5.97 | 113.58 | 110.60 |
| 25 | DA | 627 | A | C8-N9-C4 | 5.96 | 108.19 | 105.80 |
| 25 | BA | 348 | A | O5'-P-OP1 | -5.96 | 100.33 | 105.70 |
| 1 | AA | 1131 | G | N1-C6-O6 | 5.96 | 123.47 | 119.90 |
| 1 | AA | 1201 | A | P-O3'-C3' | 5.96 | 126.85 | 119.70 |
| 25 | BA | 89 | U | N3-C2-O2 | -5.96 | 118.03 | 122.20 |
| 1 | CA | 1028 | C | C5-C6-N1 | 5.96 | 123.98 | 121.00 |
| 25 | DA | 53 | A | C8-N9-C4 | 5.96 | 108.18 | 105.80 |
| 1 | AA | 738 | C | C5-C6-N1 | 5.96 | 123.98 | 121.00 |
| 1 | AA | 1127 | G | N7-C8-N9 | -5.96 | 110.12 | 113.10 |
| 1 | AA | 1150 | U | N3-C4-C5 | -5.96 | 111.03 | 114.60 |
| 26 | DB | 74 | U | C5-C4-O4 | 5.96 | 129.47 | 125.90 |
| 25 | BA | 1800 | G | O5'-P-OP2 | -5.96 | 100.34 | 105.70 |
| 1 | AA | 1007 | C | C2-N1-C1' | 5.95 | 125.35 | 118.80 |
| 25 | DA | 141 | A | C2-N3-C4 | -5.95 | 107.62 | 110.60 |
| 1 | CA | 1169 | A | N1-C6-N6 | 5.95 | 122.17 | 118.60 |
| 25 | BA | 1072 | U | C2-N1-C1' | 5.95 | 124.84 | 117.70 |
| 25 | DA | 1573 | G | C8-N9-C4 | 5.95 | 108.78 | 106.40 |
| 25 | DA | 2617 | C | C6-N1-C2 | 5.95 | 122.68 | 120.30 |
| 1 | CA | 308 | C | C6-N1-C2 | 5.95 | 122.68 | 120.30 |
| 25 | DA | 1325 | G | C6-C5-N7 | -5.95 | 126.83 | 130.40 |
| 25 | BA | 70 | A | P-O3'-C3' | 5.95 | 126.83 | 119.70 |
| 1 | AA | 92 | C | C5-C6-N1 | 5.94 | 123.97 | 121.00 |
| 25 | BA | 354 | A | C5-N7-C8 | -5.94 | 100.93 | 103.90 |
| 26 | BB | 80 | U | C5-C4-O4 | 5.94 | 129.47 | 125.90 |
| 25 | DA | 2351 | G | N3-C4-N9 | 5.94 | 129.57 | 126.00 |
| 25 | DA | 901 | A | N7-C8-N9 | 5.94 | 116.77 | 113.80 |
| 25 | BA | 1555 | C | C6-N1-C2 | -5.94 | 117.92 | 120.30 |
| 25 | BA | 2080 | A | OP2-P-O3' | 5.94 | 118.27 | 105.20 |
| 1 | AA | 476 | G | C8-N9-C1' | -5.94 | 119.28 | 127.00 |
| 1 | AA | 1026 | G | C8-N9-C1' | -5.94 | 119.28 | 127.00 |
| 25 | BA | 2372 | A | C2-N3-C4 | -5.94 | 107.63 | 110.60 |
| 1 | AA | 122 | G | C8-N9-C4 | 5.93 | 108.77 | 106.40 |
| 25 | DA | 1129 | A | N1-C6-N6 | -5.93 | 115.04 | 118.60 |
| 25 | DA | 210 | C | C2-N1-C1' | -5.93 | 112.28 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | DA | 1673 | U | C5-C4-O4 | -5.93 | 122.34 | 125.90 |
| 25 | BA | 1072 | U | N3-C2-O2 | -5.92 | 118.05 | 122.20 |
| 1 | CA | 1312 | G | N9-C4-C5 | 5.92 | 107.77 | 105.40 |
| 25 | DA | 1648 | C | O5'-P-OP1 | 5.92 | 117.81 | 110.70 |
| 25 | BA | 1240 | G | N9-C4-C5 | 5.92 | 107.77 | 105.40 |
| 25 | BA | 2735 | G | N3-C4-N9 | 5.92 | 129.55 | 126.00 |
| 23 | AX | 8 | U | C5-C6-N1 | 5.92 | 125.66 | 122.70 |
| 25 | BA | 2835 | C | N3-C2-O2 | 5.92 | 126.04 | 121.90 |
| 25 | BA | 1423 | G | C5-C6-O6 | 5.91 | 132.15 | 128.60 |
| 1 | CA | 916 | G | C8-N9-C4 | -5.91 | 104.03 | 106.40 |
| 25 | DA | 633 | A | N1-C6-N6 | 5.91 | 122.15 | 118.60 |
| 25 | DA | 1640 | C | C2-N1-C1' | 5.91 | 125.30 | 118.80 |
| 25 | BA | 1757 | C | C6-N1-C2 | 5.91 | 122.66 | 120.30 |
| 1 | AA | 383 | A | C4-N9-C1' | 5.91 | 136.93 | 126.30 |
| 25 | DA | 2351 | G | N3-C4-C5 | -5.91 | 125.65 | 128.60 |
| 25 | BA | 2026 | G | OP2-P-O3' | 5.90 | 118.19 | 105.20 |
| 25 | DA | 2805 | G | C5-C6-O6 | 5.90 | 132.14 | 128.60 |
| 1 | CA | 204 | U | C2-N1-C1' | 5.90 | 124.78 | 117.70 |
| 7 | AG | 81 | GLY | N-CA-C | 5.90 | 127.85 | 113.10 |
| 25 | BA | 176 | G | C6-C5-N7 | -5.90 | 126.86 | 130.40 |
| 1 | CA | 337 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 25 | DA | 176 | G | C8-N9-C4 | 5.90 | 108.76 | 106.40 |
| 23 | CX | 20 | U | C2-N1-C1' | 5.89 | 124.77 | 117.70 |
| 25 | BA | 1249 | A | C2-N3-C4 | -5.89 | 107.66 | 110.60 |
| 25 | BA | 2268 | G | C4-C5-N7 | 5.88 | 113.15 | 110.80 |
| 1 | CA | 1125 | U | C2-N1-C1' | 5.88 | 124.76 | 117.70 |
| 25 | DA | 1368 | G | O5'-P-OP2 | -5.88 | 100.41 | 105.70 |
| 1 | AA | 1502 | A | N7-C8-N9 | 5.88 | 116.74 | 113.80 |
| 25 | BA | 2354 | C | C6-N1-C2 | -5.88 | 117.95 | 120.30 |
| 25 | BA | 119 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 25 | BA | 670 | C | C5-C6-N1 | 5.88 | 123.94 | 121.00 |
| 25 | DA | 1257 | C | N3-C4-C5 | -5.88 | 119.55 | 121.90 |
| 1 | AA | 1171 | G | N3-C4-C5 | -5.88 | 125.66 | 128.60 |
| 1 | CA | 998 | G | N3-C4-N9 | -5.88 | 122.47 | 126.00 |
| 25 | DA | 454 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 25 | BA | 2601 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 9 | CI | 105 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | AA | 1181 | G | C6-N1-C2 | 5.87 | 128.62 | 125.10 |
| 25 | BA | 2258 | G | N9-C4-C5 | -5.87 | 103.05 | 105.40 |
| 25 | DA | 2033 | A | C2-N3-C4 | 5.87 | 113.53 | 110.60 |
| 25 | BA | 2506 | G | C8-N9-C4 | 5.87 | 108.75 | 106.40 |
| 25 | DA | 2273 | A | N7-C8-N9 | -5.87 | 110.87 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | BA | 1959 | A | C8-N9-C4 | 5.87 | 108.15 | 105.80 |
| 23 | AX | 76 | A | C5-C6-N6 | -5.86 | 119.01 | 123.70 |
| 1 | CA | 917 | G | C8-N9-C4 | -5.86 | 104.06 | 106.40 |
| 25 | BA | 1377 | A | C2-N3-C4 | -5.86 | 107.67 | 110.60 |
| 25 | DA | 945 | A | C5-C6-N6 | -5.86 | 119.02 | 123.70 |
| 25 | DA | 1698 | A | C4-C5-C6 | 5.85 | 119.93 | 117.00 |
| 1 | AA | 97 | G | N3-C4-C5 | -5.85 | 125.67 | 128.60 |
| 1 | CA | 901 | A | N1-C6-N6 | -5.85 | 115.09 | 118.60 |
| 1 | CA | 1169 | A | C6-C5-N7 | -5.85 | 128.21 | 132.30 |
| 25 | DA | 735 | A | N7-C8-N9 | -5.85 | 110.88 | 113.80 |
| 1 | AA | 1127 | G | C4-C5-C6 | 5.84 | 122.31 | 118.80 |
| 25 | DA | 459 | U | N3-C2-O2 | -5.84 | 118.11 | 122.20 |
| 1 | AA | 990 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 25 | DA | 2032 | G | N1-C6-O6 | -5.84 | 116.40 | 119.90 |
| 25 | BA | 621 | G | O5'-P-OP2 | -5.84 | 100.44 | 105.70 |
| 25 | DA | 2324 | C | N3-C4-C5 | 5.84 | 124.24 | 121.90 |
| 25 | BA | 279 | G | N7-C8-N9 | 5.84 | 116.02 | 113.10 |
| 1 | AA | 841 | U | C5-C6-N1 | 5.83 | 125.62 | 122.70 |
| 25 | DA | 948 | G | C8-N9-C4 | 5.83 | 108.73 | 106.40 |
| 47 | D1 | 85 | LEU | CA-CB-CG | 5.83 | 128.72 | 115.30 |
| 25 | BA | 1093 | G | C8-N9-C1' | -5.83 | 119.42 | 127.00 |
| 1 | AA | 1054 | C | N3-C2-O2 | -5.83 | 117.82 | 121.90 |
| 25 | BA | 2105 | G | N9-C4-C5 | -5.83 | 103.07 | 105.40 |
| 1 | CA | 1311 | G | C4-N9-C1' | -5.83 | 118.92 | 126.50 |
| 25 | DA | 2330 | G | N1-C6-O6 | 5.83 | 123.40 | 119.90 |
| 25 | BA | 903 | C | C6-N1-C2 | -5.83 | 117.97 | 120.30 |
| 1 | CA | 1271 | G | C5-C6-O6 | -5.83 | 125.11 | 128.60 |
| 25 | BA | 1461 | U | C5-C4-O4 | 5.82 | 129.39 | 125.90 |
| 1 | CA | 117 | G | C6-C5-N7 | -5.82 | 126.91 | 130.40 |
| 1 | AA | 1125 | U | P-O3'-C3' | 5.82 | 126.69 | 119.70 |
| 25 | BA | 2876 | U | C4-C5-C6 | 5.82 | 123.19 | 119.70 |
| 1 | CA | 1286 | A | N7-C8-N9 | 5.82 | 116.71 | 113.80 |
| 25 | DA | 2024 | G | C8-N9-C4 | 5.82 | 108.73 | 106.40 |
| 25 | BA | 1719 | C | N3-C4-N4 | 5.82 | 122.07 | 118.00 |
| 23 | CX | 18 | G | N3-C4-C5 | 5.82 | 131.51 | 128.60 |
| 25 | DA | 2679 | A | O5'-P-OP2 | -5.82 | 100.47 | 105.70 |
| 25 | DA | 2287 | A | N3-C4-C5 | 5.82 | 130.87 | 126.80 |
| 1 | CA | 1000 | U | C2-N3-C4 | 5.81 | 130.49 | 127.00 |
| 1 | CA | 1157 | A | C6-C5-N7 | 5.81 | 136.37 | 132.30 |
| 1 | AA | 884 | U | O5'-P-OP2 | -5.81 | 100.47 | 105.70 |
| 1 | AA | 1131 | G | C4-N9-C1' | 5.81 | 134.06 | 126.50 |
| 25 | BA | 1154 | U | N1-C2-O2 | 5.81 | 126.87 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | BA | 1663 | C | C2-N3-C4 | -5.81 | 116.99 | 119.90 |
| 25 | BA | 2729 | U | N3-C2-O2 | -5.81 | 118.13 | 122.20 |
| 25 | DA | 792 | G | C5-C6-N1 | 5.81 | 114.41 | 111.50 |
| 1 | AA | 261 | U | N1-C2-O2 | -5.81 | 118.73 | 122.80 |
| 1 | AA | 1024 | G | N3-C4-C5 | -5.81 | 125.70 | 128.60 |
| 25 | BA | 555 | G | C5-N7-C8 | -5.81 | 101.40 | 104.30 |
| 1 | CA | 353 | A | OP2-P-O3' | 5.81 | 117.98 | 105.20 |
| 1 | CA | 1125 | U | C5-C6-N1 | 5.81 | 125.60 | 122.70 |
| 25 | DA | 1192 | G | C8-N9-C4 | 5.81 | 108.72 | 106.40 |
| 1 | AA | 904 | C | C6-N1-C2 | 5.80 | 122.62 | 120.30 |
| 1 | CA | 117 | G | C4-N9-C1' | 5.80 | 134.05 | 126.50 |
| 1 | AA | 1269 | A | N1-C6-N6 | -5.80 | 115.12 | 118.60 |
| 25 | BA | 2026 | G | N3-C4-C5 | 5.80 | 131.50 | 128.60 |
| 25 | DA | 901 | A | C8-N9-C4 | -5.80 | 103.48 | 105.80 |
| 25 | BA | 990 | A | C5-C6-N1 | -5.80 | 114.80 | 117.70 |
| 1 | AA | 336 | C | N3-C2-O2 | 5.80 | 125.96 | 121.90 |
| 1 | AA | 421 | U | N1-C2-O2 | 5.80 | 126.86 | 122.80 |
| 1 | AA | 1396 | A | C5-C6-N6 | 5.80 | 128.34 | 123.70 |
| 25 | BA | 125 | A | N1-C6-N6 | 5.80 | 122.08 | 118.60 |
| 1 | CA | 691 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 23 | AX | 22 | G | N7-C8-N9 | 5.79 | 116.00 | 113.10 |
| 25 | DA | 1682 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 1 | CA | 1206 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 25 | DA | 1899 | G | N9-C4-C5 | -5.79 | 103.08 | 105.40 |
| 1 | CA | 79 | G | C6-N1-C2 | 5.79 | 128.57 | 125.10 |
| 25 | DA | 205 | G | N9-C4-C5 | -5.79 | 103.09 | 105.40 |
| 25 | BA | 553 | A | C4-C5-N7 | 5.78 | 113.59 | 110.70 |
| 25 | BA | 1255 | A | P-O3'-C3' | 5.78 | 126.64 | 119.70 |
| 25 | DA | 1405 | U | O5'-P-OP2 | -5.78 | 100.50 | 105.70 |
| 1 | AA | 991 | U | P-O3'-C3' | 5.78 | 126.63 | 119.70 |
| 1 | CA | 1149 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 25 | DA | 1413 | G | N1-C6-O6 | 5.78 | 123.37 | 119.90 |
| 1 | AA | 167 | G | N7-C8-N9 | 5.78 | 115.99 | 113.10 |
| 25 | BA | 176 | G | C5-N7-C8 | -5.78 | 101.41 | 104.30 |
| 1 | CA | 1216 | G | N3-C4-C5 | 5.78 | 131.49 | 128.60 |
| 25 | DA | 1325 | G | N3-C4-N9 | 5.77 | 129.46 | 126.00 |
| 1 | CA | 1499 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 25 | DA | 1239 | G | C5-C6-O6 | -5.77 | 125.14 | 128.60 |
| 25 | BA | 2320 | G | N3-C4-C5 | 5.77 | 131.49 | 128.60 |
| 1 | CA | 1044 | A | C5-C6-N6 | 5.77 | 128.32 | 123.70 |
| 1 | AA | 483 | C | C6-N1-C2 | 5.77 | 122.61 | 120.30 |
| 25 | DA | 2010 | G | C8-N9-C4 | -5.77 | 104.09 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | BA | 1578 | C | C5-C6-N1 | 5.77 | 123.88 | 121.00 |
| 25 | BA | 1153 | G | N3-C4-N9 | 5.76 | 129.46 | 126.00 |
| 25 | BA | 2065 | C | N1-C2-O2 | -5.76 | 115.44 | 118.90 |
| 1 | CA | 794 | A | C8-N9-C4 | -5.76 | 103.49 | 105.80 |
| 1 | CA | 398 | C | N3-C4-N4 | -5.76 | 113.97 | 118.00 |
| 25 | DA | 1284 | A | C4-C5-N7 | 5.76 | 113.58 | 110.70 |
| 1 | AA | 1026 | G | N3-C4-N9 | 5.76 | 129.46 | 126.00 |
| 25 | BA | 553 | A | C5-N7-C8 | -5.76 | 101.02 | 103.90 |
| 23 | AX | 14 | A | C5-C6-N1 | -5.76 | 114.82 | 117.70 |
| 25 | BA | 2044 | U | O5'-P-OP1 | -5.76 | 100.52 | 105.70 |
| 26 | BB | 41 | U | C5-C6-N1 | -5.76 | 119.82 | 122.70 |
| 25 | DA | 962 | G | C8-N9-C4 | -5.76 | 104.10 | 106.40 |
| 1 | AA | 1181 | G | N3-C4-C5 | 5.76 | 131.48 | 128.60 |
| 25 | BA | 841 | G | C4-C5-N7 | -5.75 | 108.50 | 110.80 |
| 25 | DA | 467 | G | N7-C8-N9 | -5.75 | 110.22 | 113.10 |
| 25 | DA | 2347 | C | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 25 | BA | 2014 | G | C2'-C3'-O3' | 5.75 | 122.90 | 113.70 |
| 1 | CA | 890 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 25 | BA | 2245 | U | C5-C6-N1 | -5.75 | 119.83 | 122.70 |
| 1 | AA | 1036 | G | N3-C4-N9 | 5.74 | 129.45 | 126.00 |
| 1 | CA | 377 | G | N3-C4-N9 | 5.74 | 129.45 | 126.00 |
| 46 | B0 | 77 | ARG | NE-CZ-NH1 | -5.74 | 117.43 | 120.30 |
| 25 | BA | 1605 | A | N1-C6-N6 | 5.74 | 122.04 | 118.60 |
| 23 | CX | 76 | A | N3-C4-N9 | 5.74 | 131.99 | 127.40 |
| 25 | DA | 2281 | C | O5'-P-OP1 | -5.74 | 100.54 | 105.70 |
| 25 | BA | 1252 | C | O5'-P-OP1 | -5.74 | 100.54 | 105.70 |
| 25 | DA | 2744 | G | C5-C6-O6 | -5.74 | 125.16 | 128.60 |
| 1 | CA | 915 | A | N7-C8-N9 | -5.73 | 110.93 | 113.80 |
| 1 | CA | 721 | G | N1-C6-O6 | 5.73 | 123.34 | 119.90 |
| 25 | DA | 727 | A | C8-N9-C4 | -5.73 | 103.51 | 105.80 |
| 25 | DA | 1027 | A | N9-C4-C5 | -5.73 | 103.51 | 105.80 |
| 1 | CA | 1002 | G | N3-C4-N9 | -5.73 | 122.56 | 126.00 |
| 25 | DA | 557 | U | C5-C6-N1 | -5.73 | 119.84 | 122.70 |
| 25 | DA | 308 | G | O5'-P-OP2 | -5.72 | 100.55 | 105.70 |
| 25 | DA | 981 | A | N1-C6-N6 | -5.72 | 115.17 | 118.60 |
| 23 | AX | 6 | G | N1-C6-O6 | 5.72 | 123.33 | 119.90 |
| 25 | BA | 989 | G | C4-N9-C1' | 5.72 | 133.94 | 126.50 |
| 43 | BX | 57 | LEU | CA-CB-CG | 5.72 | 128.46 | 115.30 |
| 1 | CA | 1028 | C | N3-C2-O2 | 5.72 | 125.90 | 121.90 |
| 25 | DA | 119 | A | N1-C6-N6 | 5.72 | 122.03 | 118.60 |
| 25 | DA | 912 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 1 | AA | 166 | G | N7-C8-N9 | 5.71 | 115.96 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 25 | DA | 2509 | G | C5-C6-N1 | -5.71 | 108.64 | 111.50 |
| 1 | CA | 1157 | A | C4-C5-N7 | -5.71 | 107.84 | 110.70 |
| 25 | DA | 738 | G | O5'-P-OP1 | 5.71 | 117.55 | 110.70 |
| 1 | CA | 997 | U | C2-N3-C4 | 5.71 | 130.43 | 127.00 |
| 25 | BA | 2271 | G | C8-N9-C4 | -5.71 | 104.12 | 106.40 |
| 1 | CA | 1149 | C | C2-N1-C1' | 5.71 | 125.08 | 118.80 |
| 25 | DA | 242 | G | N7-C8-N9 | -5.71 | 110.25 | 113.10 |
| 25 | DA | 1647 | G | O4'-C1'-N9 | -5.71 | 103.63 | 108.20 |
| 1 | AA | 1531 | A | N7-C8-N9 | 5.71 | 116.65 | 113.80 |
| 25 | BA | 2836 | A | C8-N9-C4 | 5.71 | 108.08 | 105.80 |
| 19 | CS | 71 | LEU | CA-CB-CG | 5.71 | 128.42 | 115.30 |
| 25 | DA | 504 | U | N1-C2-O2 | 5.71 | 126.79 | 122.80 |
| 25 | BA | 1694 | G | O5'-P-OP1 | -5.70 | 100.57 | 105.70 |
| 25 | BA | 1742 | G | N3-C4-N9 | 5.70 | 129.42 | 126.00 |
| 25 | DA | 2271 | G | N3-C4-N9 | 5.70 | 129.42 | 126.00 |
| 25 | BA | 990 | A | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 1 | CA | 1134 | G | C8-N9-C4 | -5.70 | 104.12 | 106.40 |
| 25 | DA | 1698 | A | C5-N7-C8 | -5.70 | 101.05 | 103.90 |
| 25 | DA | 560 | C | C6-N1-C2 | 5.70 | 122.58 | 120.30 |
| 25 | DA | 991 | C | O5'-P-OP2 | -5.69 | 100.58 | 105.70 |
| 25 | BA | 295 | C | O5'-P-OP2 | -5.69 | 100.58 | 105.70 |
| 25 | BA | 1222 | A | N7-C8-N9 | 5.69 | 116.65 | 113.80 |
| 46 | B0 | 12 | ASN | N-CA-C | 5.69 | 126.37 | 111.00 |
| 1 | CA | 5 | U | N3-C2-O2 | -5.69 | 118.22 | 122.20 |
| 25 | BA | 2054 | G | N3-C4-N9 | -5.69 | 122.59 | 126.00 |
| 1 | CA | 754 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |
| 1 | CA | 1492 | A | C2-N3-C4 | 5.69 | 113.44 | 110.60 |
| 25 | DA | 2057 | A | C8-N9-C4 | 5.69 | 108.07 | 105.80 |
| 25 | DA | 2725 | A | C2-N3-C4 | -5.69 | 107.76 | 110.60 |
| 25 | DA | 1142(A) | A | N1-C2-N3 | 5.68 | 132.14 | 129.30 |
| 1 | AA | 162 | A | C8-N9-C4 | -5.68 | 103.53 | 105.80 |
| 1 | AA | 1124 | G | C2-N3-C4 | 5.68 | 114.74 | 111.90 |
| 25 | BA | 2608 | U | N1-C2-O2 | -5.68 | 118.82 | 122.80 |
| 25 | DA | 193 | U | N3-C4-O4 | 5.68 | 123.38 | 119.40 |
| 25 | DA | 885 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 25 | DA | 2345 | G | C8-N9-C4 | -5.68 | 104.13 | 106.40 |
| 25 | BA | 1343 | C | OP2-P-O3' | -5.68 | 92.71 | 105.20 |
| 25 | DA | 2794 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 25 | BA | 2902 | G | P-O3'-C3' | 5.68 | 126.51 | 119.70 |
| 1 | CA | 266 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 25 | DA | 795 | C | O5'-P-OP2 | -5.68 | 100.59 | 105.70 |
| 25 | DA | 1926 | U | N3-C2-O2 | -5.68 | 118.23 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | DA | 1328 | G | C4-C5-N7 | 5.67 | 113.07 | 110.80 |
| 1 | AA | 1054 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 25 | BA | 2495 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 25 | BA | 716 | G | C8-N9-C4 | 5.67 | 108.67 | 106.40 |
| 25 | BA | 1766 | G | C5-C6-O6 | -5.67 | 125.20 | 128.60 |
| 25 | DA | 2590 | A | O5'-P-OP2 | 5.67 | 117.50 | 110.70 |
| 25 | BA | 357 | G | C4-N9-C1' | 5.67 | 133.87 | 126.50 |
| 1 | CA | 1277 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 26 | DB | 52 | A | C8-N9-C4 | -5.67 | 103.53 | 105.80 |
| 25 | BA | 2861 | A | OP2-P-O3' | 5.67 | 117.66 | 105.20 |
| 1 | CA | 142 | G | N3-C4-C5 | -5.67 | 125.77 | 128.60 |
| 25 | BA | 36 | G | O5'-P-OP2 | -5.66 | 100.61 | 105.70 |
| 25 | DA | 1377 | G | N3-C4-C5 | -5.66 | 125.77 | 128.60 |
| 25 | BA | 553 | A | C5-C6-N1 | -5.66 | 114.87 | 117.70 |
| 25 | DA | 1363 | C | O5'-P-OP2 | -5.66 | 100.61 | 105.70 |
| 25 | BA | 1850 | A | C8-N9-C4 | 5.66 | 108.06 | 105.80 |
| 25 | DA | 2043 | C | C2-N1-C1' | 5.65 | 125.02 | 118.80 |
| 25 | DA | 2053 | G | N9-C4-C5 | -5.65 | 103.14 | 105.40 |
| 1 | AA | 71 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 25 | BA | 2804 | C | C5-C6-N1 | 5.65 | 123.83 | 121.00 |
| 25 | BA | 185 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 25 | BA | 2056 | U | N3-C4-O4 | 5.65 | 123.35 | 119.40 |
| 25 | BA | 737 | G | N1-C6-O6 | 5.65 | 123.29 | 119.90 |
| 25 | BA | 1700 | G | N3-C4-C5 | -5.64 | 125.78 | 128.60 |
| 1 | CA | 557 | G | N9-C4-C5 | -5.64 | 103.14 | 105.40 |
| 25 | DA | 532 | A | O4'-C1'-N9 | 5.64 | 112.72 | 108.20 |
| 25 | DA | 783 | A | O5'-P-OP2 | -5.64 | 100.62 | 105.70 |
| 25 | DA | 1997 | G | N3-C4-C5 | -5.64 | 125.78 | 128.60 |
| 26 | DB | 45 | A | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 25 | DA | 1115 | G | N3-C4-C5 | 5.64 | 131.42 | 128.60 |
| 25 | BA | 615 | G | N1-C6-O6 | -5.64 | 116.52 | 119.90 |
| 25 | BA | 1807 | G | N1-C6-O6 | 5.64 | 123.28 | 119.90 |
| 25 | DA | 2061 | G | N9-C4-C5 | -5.64 | 103.14 | 105.40 |
| 25 | BA | 2522 | C | C6-N1-C2 | 5.64 | 122.55 | 120.30 |
| 1 | CA | 1484 | C | C2-N1-C1' | -5.64 | 112.60 | 118.80 |
| 1 | CA | 1272 | G | N1-C6-O6 | -5.63 | 116.52 | 119.90 |
| 25 | DA | 1455 | G | N1-C6-O6 | 5.63 | 123.28 | 119.90 |
| 25 | DA | 2440 | C | C5-C4-N4 | 5.63 | 124.14 | 120.20 |
| 25 | DA | 956 | G | C4-N9-C1' | 5.63 | 133.82 | 126.50 |
| 25 | DA | 781 | A | N1-C6-N6 | -5.63 | 115.22 | 118.60 |
| 25 | BA | 103 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 25 | BA | 1667 | U | N3-C4-C5 | -5.62 | 111.22 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | CX | 8 | U | N3-C4-C5 | -5.62 | 111.23 | 114.60 |
| 1 | AA | 526 | C | C6-N1-C2 | 5.62 | 122.55 | 120.30 |
| 25 | DA | 915 | C | N3-C2-O2 | -5.62 | 117.97 | 121.90 |
| 25 | BA | 1153 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 25 | BA | 2272 | C | C5-C6-N1 | -5.62 | 118.19 | 121.00 |
| 1 | CA | 1227 | A | C8-N9-C4 | -5.62 | 103.55 | 105.80 |
| 25 | DA | 768 | G | N1-C6-O6 | 5.62 | 123.27 | 119.90 |
| 25 | DA | 1021 | A | C5-C6-N1 | -5.62 | 114.89 | 117.70 |
| 25 | BA | 1378 | G | C4-C5-N7 | 5.62 | 113.05 | 110.80 |
| 1 | CA | 1189 | C | C6-N1-C2 | 5.62 | 122.55 | 120.30 |
| 25 | BA | 2096 | U | O5'-P-OP1 | -5.62 | 100.65 | 105.70 |
| 25 | DA | 2206 | G | C8-N9-C1' | 5.61 | 134.30 | 127.00 |
| 25 | BA | 120 | G | C5-C6-O6 | -5.61 | 125.23 | 128.60 |
| 25 | DA | 971 | C | N3-C4-N4 | 5.61 | 121.93 | 118.00 |
| 25 | DA | 1269 | A | C5-C6-N1 | -5.61 | 114.90 | 117.70 |
| 25 | DA | 2081 | C | C6-N1-C2 | 5.61 | 122.54 | 120.30 |
| 29 | DF | 12 | LEU | CA-CB-CG | 5.61 | 128.20 | 115.30 |
| 1 | AA | 652 | U | O5'-P-OP1 | -5.61 | 100.66 | 105.70 |
| 25 | BA | 1378 | G | C5-C6-O6 | -5.60 | 125.24 | 128.60 |
| 25 | BA | 1681 | A | C8-N9-C4 | -5.60 | 103.56 | 105.80 |
| 25 | DA | 110 | G | N7-C8-N9 | -5.60 | 110.30 | 113.10 |
| 1 | CA | 399 | G | C8-N9-C4 | 5.60 | 108.64 | 106.40 |
| 25 | BA | 1426 | G | O5'-P-OP2 | -5.60 | 100.66 | 105.70 |
| 1 | CA | 557 | G | N3-C2-N2 | 5.60 | 123.82 | 119.90 |
| 25 | BA | 179 | A | C5-N7-C8 | -5.60 | 101.10 | 103.90 |
| 1 | AA | 340 | U | C6-N1-C2 | 5.60 | 124.36 | 121.00 |
| 25 | BA | 1663 | C | N3-C4-C5 | 5.60 | 124.14 | 121.90 |
| 40 | DU | 74 | LEU | CA-CB-CG | 5.59 | 128.17 | 115.30 |
| 25 | BA | 1188 | A | C5-N7-C8 | -5.59 | 101.10 | 103.90 |
| 1 | CA | 544 | G | N1-C6-O6 | -5.59 | 116.55 | 119.90 |
| 25 | DA | 956 | G | N3-C4-C5 | -5.59 | 125.80 | 128.60 |
| 25 | BA | 1068 | G | N3-C2-N2 | -5.59 | 115.99 | 119.90 |
| 25 | BA | 1390 | G | N1-C6-O6 | 5.59 | 123.25 | 119.90 |
| 25 | DA | 806 | C | N3-C4-C5 | -5.59 | 119.66 | 121.90 |
| 25 | DA | 733 | G | N9-C4-C5 | -5.59 | 103.17 | 105.40 |
| 25 | DA | 912 | C | C5-C6-N1 | 5.59 | 123.79 | 121.00 |
| 25 | BA | 2630 | G | C6-N1-C2 | -5.59 | 121.75 | 125.10 |
| 25 | BA | 2495 | C | C5-C6-N1 | 5.58 | 123.79 | 121.00 |
| 25 | BA | 2239 | A | N9-C4-C5 | 5.58 | 108.03 | 105.80 |
| 25 | DA | 2476 | A | C8-N9-C4 | -5.58 | 103.57 | 105.80 |
| 25 | BA | 1158 | G | C8-N9-C4 | -5.58 | 104.17 | 106.40 |
| 25 | DA | 242 | G | C4-N9-C1' | -5.58 | 119.24 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 25 | DA | 2333 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 1 | CA | 1042 | G | N3-C4-C5 | 5.58 | 131.39 | 128.60 |
| 25 | DA | 2804 | C | N3-C2-O2 | -5.58 | 117.99 | 121.90 |
| 1 | CA | 1279 | A | C5-N7-C8 | -5.58 | 101.11 | 103.90 |
| 1 | CA | 687 | A | P-O3'-C3' | 5.58 | 126.39 | 119.70 |
| 25 | DA | 376 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 25 | BA | 113 | C | O5'-P-OP1 | -5.57 | 100.68 | 105.70 |
| 25 | BA | 403 | C | N3-C4-N4 | -5.57 | 114.10 | 118.00 |
| 25 | BA | 1221 | G | OP1-P-O3' | 5.57 | 117.46 | 105.20 |
| 25 | BA | 2513 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 25 | BA | 1152 | G | O4'-C1'-N9 | -5.57 | 103.74 | 108.20 |
| 25 | DA | 981 | A | C6-N1-C2 | 5.57 | 121.94 | 118.60 |
| 25 | DA | 1328 | G | N9-C4-C5 | -5.57 | 103.17 | 105.40 |
| 1 | CA | 1051 | C | N1-C2-O2 | -5.57 | 115.56 | 118.90 |
| 25 | BA | 94 | G | O5'-P-OP2 | -5.57 | 100.69 | 105.70 |
| 25 | DA | 210 | C | C6-N1-C2 | 5.57 | 122.53 | 120.30 |
| 1 | AA | 1030(B) | C | C5-C6-N1 | 5.57 | 123.78 | 121.00 |
| 25 | BA | 2641 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 1 | CA | 1067 | A | P-O3'-C3' | 5.56 | 126.38 | 119.70 |
| 25 | BA | 514 | G | C4-C5-N7 | -5.56 | 108.58 | 110.80 |
| 3 | CC | 91 | LEU | CA-CB-CG | 5.56 | 128.09 | 115.30 |
| 25 | DA | 2771 | C | O5'-P-OP1 | -5.56 | 100.69 | 105.70 |
| 25 | DA | 2896 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 25 | BA | 2419 | G | C8-N9-C1' | -5.56 | 119.77 | 127.00 |
| 25 | BA | 1659 | G | C5-C6-O6 | 5.56 | 131.94 | 128.60 |
| 25 | BA | 2740 | G | O5'-P-OP2 | -5.56 | 100.70 | 105.70 |
| 25 | DA | 552 | G | N3-C4-C5 | 5.56 | 131.38 | 128.60 |
| 25 | DA | 2464 | C | C5-C6-N1 | -5.56 | 118.22 | 121.00 |
| 25 | BA | 873 | U | OP1-P-O3' | -5.55 | 92.99 | 105.20 |
| 1 | AA | 383 | A | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 1 | CA | 299 | G | C6-C5-N7 | -5.55 | 127.07 | 130.40 |
| 1 | CA | 1124 | G | N3-C4-C5 | -5.55 | 125.83 | 128.60 |
| 25 | BA | 472 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 25 | BA | 105 | C | C6-N1-C2 | 5.55 | 122.52 | 120.30 |
| 25 | BA | 2666 | A | N1-C6-N6 | 5.55 | 121.93 | 118.60 |
| 25 | DA | 1348 | G | C5-C6-O6 | -5.55 | 125.27 | 128.60 |
| 1 | CA | 117 | G | N9-C4-C5 | -5.54 | 103.18 | 105.40 |
| 1 | CA | 1017 | G | C5-C6-N1 | -5.54 | 108.73 | 111.50 |
| 1 | AA | 1127 | G | C8-N9-C1' | -5.54 | 119.80 | 127.00 |
| 1 | AA | 1192 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 25 | BA | 553 | A | O4'-C1'-N9 | -5.54 | 103.77 | 108.20 |
| 25 | BA | 1991 | A | O5'-P-OP2 | 5.54 | 117.35 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 25 | BA | 2103 | C | O5'-P-OP2 | -5.54 | 100.71 | 105.70 |
| 25 | DA | 106 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 1 | CA | 1492 | A | N3-C4-C5 | -5.54 | 122.92 | 126.80 |
| 25 | DA | 2416 | C | N1-C2-O2 | -5.54 | 115.58 | 118.90 |
| 25 | BA | 498 | A | O5'-P-OP1 | 5.54 | 117.34 | 110.70 |
| 25 | BA | 1431 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 25 | BA | 1832 | G | C4-C5-N7 | 5.54 | 113.01 | 110.80 |
| 1 | CA | 365 | U | C5-C6-N1 | -5.54 | 119.93 | 122.70 |
| 25 | DA | 1213 | A | C8-N9-C4 | 5.54 | 108.01 | 105.80 |
| 25 | DA | 2321 | G | C6-N1-C2 | 5.54 | 128.42 | 125.10 |
| 1 | AA | 1298 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 25 | BA | 1075 | A | N1-C6-N6 | 5.53 | 121.92 | 118.60 |
| 25 | BA | 2061 | C | C5-C6-N1 | 5.53 | 123.77 | 121.00 |
| 1 | AA | 1030(B) | C | C6-N1-C1' | -5.53 | 114.16 | 120.80 |
| 1 | CA | 1003 | G | C8-N9-C1' | -5.53 | 119.81 | 127.00 |
| 25 | BA | 1746 | G | C8-N9-C4 | -5.53 | 104.19 | 106.40 |
| 25 | DA | 1769 | G | C8-N9-C4 | -5.53 | 104.19 | 106.40 |
| 25 | DA | 465 | G | C5-C6-O6 | -5.53 | 125.28 | 128.60 |
| 25 | DA | 1926 | U | C5-C4-O4 | 5.53 | 129.22 | 125.90 |
| 25 | BA | 1929 | G | N1-C6-O6 | 5.53 | 123.22 | 119.90 |
| 41 | BV | 82 | ARG | NE-CZ-NH1 | -5.53 | 117.54 | 120.30 |
| 1 | CA | 1279 | A | N7-C8-N9 | 5.53 | 116.56 | 113.80 |
| 1 | CA | 1502 | A | C4-C5-N7 | 5.53 | 113.46 | 110.70 |
| 25 | BA | 1325 | G | O5'-P-OP2 | -5.53 | 100.73 | 105.70 |
| 25 | BA | 1629 | C | C6-N1-C2 | 5.53 | 122.51 | 120.30 |
| 1 | CA | 1011 | G | C4-C5-N7 | -5.53 | 108.59 | 110.80 |
| 1 | AA | 381 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 23 | CX | 9 | G | C4-N9-C1' | -5.52 | 119.32 | 126.50 |
| 1 | AA | 687 | A | P-O3'-C3' | 5.52 | 126.33 | 119.70 |
| 25 | DA | 2595 | G | C8-N9-C4 | 5.52 | 108.61 | 106.40 |
| 1 | AA | 1154 | G | N9-C4-C5 | -5.52 | 103.19 | 105.40 |
| 25 | BA | 271 | U | C2-N1-C1' | -5.52 | 111.08 | 117.70 |
| 25 | BA | 1284 | G | N1-C6-O6 | 5.52 | 123.21 | 119.90 |
| 25 | DA | 277 | C | C2-N1-C1' | 5.52 | 124.87 | 118.80 |
| 23 | AX | 14 | A | C4-C5-N7 | -5.52 | 107.94 | 110.70 |
| 25 | BA | 1343 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 25 | DA | 786 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 26 | DB | 102 | A | C8-N9-C4 | 5.52 | 108.01 | 105.80 |
| 25 | BA | 2094 | G | C4-C5-N7 | 5.52 | 113.01 | 110.80 |
| 25 | BA | 990 | A | C8-N9-C4 | -5.51 | 103.59 | 105.80 |
| 26 | BB | 93 | G | C6-C5-N7 | -5.51 | 127.09 | 130.40 |
| 25 | DA | 1830 | C | C6-N1-C2 | 5.51 | 122.50 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1007 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 1 | CA | 1273 | G | N3-C4-N9 | 5.51 | 129.31 | 126.00 |
| 25 | BA | 179 | A | C5-C6-N6 | -5.51 | 119.29 | 123.70 |
| 4 | CD | 188 | LEU | CA-CB-CG | 5.51 | 127.97 | 115.30 |
| 1 | CA | 265 | G | O4'-C1'-N9 | -5.50 | 103.80 | 108.20 |
| 25 | DA | 508 | G | O5'-P-OP1 | -5.50 | 100.75 | 105.70 |
| 26 | DB | 79 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 25 | DA | 389 | G | C5-C6-O6 | -5.50 | 125.30 | 128.60 |
| 25 | DA | 2744 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 25 | BA | 179 | A | C4-C5-N7 | 5.50 | 113.45 | 110.70 |
| 1 | AA | 913 | A | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 23 | AX | 69 | C | C2-N1-C1' | 5.49 | 124.84 | 118.80 |
| 25 | BA | 68 | C | OP2-P-O3' | 5.49 | 117.29 | 105.20 |
| 25 | DA | 1665 | A | C8-N9-C4 | -5.49 | 103.60 | 105.80 |
| 25 | BA | 1078 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 25 | BA | 1429 | C | C5-C6-N1 | 5.49 | 123.75 | 121.00 |
| 1 | CA | 1183 | A | OP1-P-O3' | 5.49 | 117.28 | 105.20 |
| 1 | CA | 1271 | G | N9-C4-C5 | -5.49 | 103.20 | 105.40 |
| 25 | BA | 592 | U | N1-C2-O2 | -5.49 | 118.96 | 122.80 |
| 25 | BA | 2105 | G | C4-C5-N7 | 5.49 | 113.00 | 110.80 |
| 25 | BA | 2622 | C | O5'-P-OP1 | -5.49 | 100.76 | 105.70 |
| 25 | DA | 1672 | C | C5-C4-N4 | -5.49 | 116.36 | 120.20 |
| 25 | BA | 902 | G | N3-C4-N9 | 5.49 | 129.29 | 126.00 |
| 25 | DA | 1261 | C | O5'-P-OP1 | -5.49 | 100.76 | 105.70 |
| 25 | BA | 827 | G | N3-C4-C5 | -5.48 | 125.86 | 128.60 |
| 25 | BA | 1051 | C | OP1-P-OP2 | 5.48 | 127.82 | 119.60 |
| 25 | BA | 2059 | G | N3-C2-N2 | 5.48 | 123.74 | 119.90 |
| 28 | DE | 72 | VAL | C-N-CA | 5.48 | 135.41 | 121.70 |
| 1 | CA | 300 | A | N1-C6-N6 | -5.48 | 115.31 | 118.60 |
| 25 | DA | 250 | G | C8-N9-C4 | -5.48 | 104.21 | 106.40 |
| 1 | AA | 1058 | G | N9-C4-C5 | -5.48 | 103.21 | 105.40 |
| 25 | BA | 12 | U | N1-C2-O2 | 5.48 | 126.64 | 122.80 |
| 1 | CA | 5 | U | C2-N1-C1' | 5.48 | 124.27 | 117.70 |
| 23 | CX | 18 | G | C8-N9-C4 | 5.48 | 108.59 | 106.40 |
| 25 | DA | 917 | A | OP1-P-O3' | 5.48 | 117.25 | 105.20 |
| 25 | BA | 193 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 1 | AA | 267 | C | O5'-P-OP1 | -5.47 | 100.77 | 105.70 |
| 25 | DA | 1531 | C | C2-N1-C1' | 5.47 | 124.82 | 118.80 |
| 25 | DA | 1982 | C | N3-C4-C5 | -5.47 | 119.71 | 121.90 |
| 1 | AA | 1145 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 25 | BA | 2380 | C | C6-N1-C2 | 5.47 | 122.49 | 120.30 |
| 1 | CA | 1022 | G | N3-C4-N9 | -5.47 | 122.72 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | BA | 2054 | G | C8-N9-C1' | 5.47 | 134.11 | 127.00 |
| 25 | BA | 2601 | A | N3-C4-C5 | 5.47 | 130.63 | 126.80 |
| 25 | BA | 2460 | A | N1-C6-N6 | 5.46 | 121.88 | 118.60 |
| 1 | CA | 1420 | C | C6-N1-C2 | -5.46 | 118.11 | 120.30 |
| 25 | BA | 978 | A | C4-C5-N7 | 5.46 | 113.43 | 110.70 |
| 1 | CA | 354 | G | C4-N9-C1' | 5.46 | 133.60 | 126.50 |
| 25 | DA | 2351 | G | C4-N9-C1' | 5.46 | 133.60 | 126.50 |
| 25 | BA | 235 | C | O5'-P-OP1 | -5.46 | 100.79 | 105.70 |
| 25 | DA | 1336 | A | N1-C6-N6 | -5.46 | 115.32 | 118.60 |
| 25 | DA | 2230 | G | O5'-P-OP1 | -5.46 | 100.79 | 105.70 |
| 25 | DA | 2252 | G | N3-C4-N9 | -5.46 | 122.72 | 126.00 |
| 1 | AA | 922 | G | C6-N1-C2 | 5.46 | 128.38 | 125.10 |
| 25 | BA | 1055 | A | C8-N9-C4 | -5.46 | 103.62 | 105.80 |
| 25 | DA | 1672 | C | C6-N1-C1' | -5.46 | 114.25 | 120.80 |
| 25 | DA | 2532 | G | C5-C6-O6 | -5.46 | 125.32 | 128.60 |
| 25 | BA | 2298 | A | C4-N9-C1' | 5.46 | 136.12 | 126.30 |
| 25 | BA | 2601 | A | C4-C5-C6 | -5.46 | 114.27 | 117.00 |
| 1 | CA | 1420 | C | C5-C6-N1 | 5.46 | 123.73 | 121.00 |
| 1 | CA | 1502 | A | C6-C5-N7 | -5.46 | 128.48 | 132.30 |
| 25 | BA | 1402 | G | C5-C6-O6 | -5.45 | 125.33 | 128.60 |
| 25 | DA | 1004 | C | N1-C2-O2 | -5.45 | 115.63 | 118.90 |
| 25 | DA | 1688 | U | O5'-P-OP2 | -5.45 | 100.79 | 105.70 |
| 25 | BA | 2495 | C | C2-N1-C1' | 5.45 | 124.80 | 118.80 |
| 26 | DB | 104 | U | C5-C6-N1 | -5.45 | 119.97 | 122.70 |
| 25 | BA | 2498 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 25 | DA | 1123 | C | C6-N1-C2 | 5.45 | 122.48 | 120.30 |
| 25 | DA | 1348 | G | N1-C6-O6 | 5.45 | 123.17 | 119.90 |
| 1 | CA | 998 | G | C4-N9-C1' | -5.45 | 119.42 | 126.50 |
| 25 | DA | 193 | U | C5-C4-O4 | -5.45 | 122.63 | 125.90 |
| 25 | DA | 1256 | G | C4-N9-C1' | 5.45 | 133.58 | 126.50 |
| 26 | DB | 56 | G | N3-C4-C5 | -5.45 | 125.88 | 128.60 |
| 25 | DA | 1236 | G | O5'-P-OP2 | 5.45 | 117.24 | 110.70 |
| 1 | CA | 1034 | G | N3-C4-N9 | -5.45 | 122.73 | 126.00 |
| 1 | CA | 1122 | U | C5-C6-N1 | 5.44 | 125.42 | 122.70 |
| 23 | CX | 76 | A | C5-C6-N1 | 5.44 | 120.42 | 117.70 |
| 1 | CA | 1124 | G | O4'-C1'-N9 | 5.44 | 112.56 | 108.20 |
| 25 | BA | 397 | G | N9-C4-C5 | -5.44 | 103.22 | 105.40 |
| 25 | BA | 552 | C | C5-C4-N4 | 5.44 | 124.01 | 120.20 |
| 26 | BB | 79 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 25 | DA | 2623 | G | C5-C6-O6 | -5.44 | 125.33 | 128.60 |
| 1 | AA | 1058 | G | N1-C6-O6 | 5.44 | 123.16 | 119.90 |
| 25 | BA | 828 | A | C2-N3-C4 | 5.44 | 113.32 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | BA | 1858 | C | N3-C2-O2 | -5.44 | 118.09 | 121.90 |
| 25 | BA | 1605 | A | N3-C4-C5 | 5.44 | 130.61 | 126.80 |
| 25 | BA | 2830 | A | C5-C6-N6 | -5.44 | 119.35 | 123.70 |
| 1 | CA | 1290 | G | C8-N9-C4 | -5.44 | 104.22 | 106.40 |
| 25 | BA | 186 | A | C5-N7-C8 | -5.44 | 101.18 | 103.90 |
| 25 | DA | 668 | G | C2-N3-C4 | -5.44 | 109.18 | 111.90 |
| 1 | AA | 1007 | C | C2-N3-C4 | 5.43 | 122.62 | 119.90 |
| 25 | BA | 1207 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 25 | BA | 1538 | G | C8-N9-C4 | 5.43 | 108.57 | 106.40 |
| 25 | DA | 738 | G | C4-N9-C1' | 5.43 | 133.56 | 126.50 |
| 25 | DA | 2207 | G | N3-C4-N9 | 5.43 | 129.26 | 126.00 |
| 25 | BA | 2248 | C | C5-C4-N4 | -5.43 | 116.40 | 120.20 |
| 25 | DA | 2458 | G | N3-C4-N9 | 5.43 | 129.26 | 126.00 |
| 1 | CA | 1126 | U | C6-N1-C2 | -5.43 | 117.74 | 121.00 |
| 25 | BA | 993 | G | N9-C4-C5 | -5.43 | 103.23 | 105.40 |
| 1 | AA | 348 | G | C5-C6-O6 | -5.43 | 125.34 | 128.60 |
| 25 | BA | 839 | G | N3-C2-N2 | 5.43 | 123.70 | 119.90 |
| 1 | CA | 525 | C | N3-C4-N4 | 5.43 | 121.80 | 118.00 |
| 1 | AA | 458 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 1 | CA | 1003 | G | C4-C5-C6 | 5.42 | 122.06 | 118.80 |
| 1 | CA | 1227 | A | C5-N7-C8 | -5.42 | 101.19 | 103.90 |
| 1 | CA | 115 | G | P-O3'-C3' | 5.42 | 126.21 | 119.70 |
| 25 | DA | 242 | G | C6-C5-N7 | 5.42 | 133.65 | 130.40 |
| 25 | DA | 1432 | C | C5-C4-N4 | -5.42 | 116.41 | 120.20 |
| 25 | BA | 125 | A | C5-C6-N6 | -5.42 | 119.36 | 123.70 |
| 25 | DA | 1769 | G | N3-C4-C5 | -5.42 | 125.89 | 128.60 |
| 1 | AA | 1530 | G | C4-C5-N7 | 5.42 | 112.97 | 110.80 |
| 23 | AX | 76 | A | N3-C4-N9 | 5.42 | 131.73 | 127.40 |
| 25 | BA | 1188 | A | C5-C6-N1 | -5.42 | 114.99 | 117.70 |
| 25 | BA | 2331 | G | N1-C6-O6 | 5.42 | 123.15 | 119.90 |
| 1 | CA | 1028 | C | N1-C2-O2 | -5.42 | 115.65 | 118.90 |
| 25 | DA | 133 | C | C6-N1-C2 | 5.42 | 122.47 | 120.30 |
| 25 | DA | 906 | G | N9-C4-C5 | 5.42 | 107.57 | 105.40 |
| 1 | AA | 98 | G | N7-C8-N9 | 5.42 | 115.81 | 113.10 |
| 25 | BA | 1608 | G | C8-N9-C4 | -5.42 | 104.23 | 106.40 |
| 26 | BB | 85 | G | C6-C5-N7 | -5.42 | 127.15 | 130.40 |
| 1 | CA | 794 | A | N7-C8-N9 | 5.41 | 116.51 | 113.80 |
| 25 | BA | 279 | G | C8-N9-C4 | -5.41 | 104.24 | 106.40 |
| 25 | BA | 2460 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 1 | AA | 749 | C | C5-C6-N1 | 5.41 | 123.70 | 121.00 |
| 25 | BA | 254 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 25 | BA | 1985 | U | C6-N1-C1' | -5.41 | 113.63 | 121.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 149 | A | C8-N9-C4 | -5.40 | 103.64 | 105.80 |
| 25 | DA | 242 | G | C8-N9-C4 | 5.40 | 108.56 | 106.40 |
| 25 | BA | 2567 | U | O5'-P-OP1 | -5.40 | 100.84 | 105.70 |
| 25 | BA | 2896 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 1 | CA | 499 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 1 | CA | 1199 | U | C5-C4-O4 | 5.40 | 129.14 | 125.90 |
| 23 | CX | 22 | G | N3-C4-N9 | -5.40 | 122.76 | 126.00 |
| 25 | BA | 311 | C | C6-N1-C2 | 5.40 | 122.46 | 120.30 |
| 25 | BA | 1577 | C | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 25 | DA | 1937 | A | C6-C5-N7 | -5.40 | 128.52 | 132.30 |
| 25 | BA | 2094 | G | N1-C6-O6 | 5.40 | 123.14 | 119.90 |
| 1 | CA | 993 | G | N3-C4-N9 | 5.40 | 129.24 | 126.00 |
| 1 | AA | 1123 | A | C6-N1-C2 | 5.40 | 121.84 | 118.60 |
| 1 | AA | 1149 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 25 | DA | 956 | G | C4-C5-C6 | 5.39 | 122.04 | 118.80 |
| 25 | DA | 970 | C | N3-C2-O2 | 5.39 | 125.68 | 121.90 |
| 25 | BA | 1177 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 25 | DA | 2373 | G | N1-C6-O6 | 5.39 | 123.14 | 119.90 |
| 34 | BO | 8 | LEU | CA-CB-CG | 5.39 | 127.70 | 115.30 |
| 25 | DA | 188 | G | C4-C5-N7 | 5.39 | 112.96 | 110.80 |
| 25 | DA | 793 | A | O5'-P-OP2 | -5.39 | 100.85 | 105.70 |
| 1 | CA | 246 | A | C8-N9-C4 | 5.39 | 107.95 | 105.80 |
| 1 | CA | 1125 | U | C6-N1-C2 | -5.39 | 117.77 | 121.00 |
| 1 | CA | 1311 | G | C8-N9-C1' | 5.39 | 134.00 | 127.00 |
| 23 | CX | 45 | G | N3-C4-C5 | 5.39 | 131.29 | 128.60 |
| 25 | DA | 512 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 50 | D4 | 68 | ARG | NE-CZ-NH2 | 5.39 | 122.99 | 120.30 |
| 1 | CA | 1415 | G | O5'-P-OP2 | -5.38 | 100.86 | 105.70 |
| 25 | DA | 2689 | U | N3-C2-O2 | -5.38 | 118.43 | 122.20 |
| 1 | AA | 1502 | A | C6-C5-N7 | -5.38 | 128.53 | 132.30 |
| 25 | BA | 2703 | C | O5'-P-OP1 | -5.38 | 100.86 | 105.70 |
| 1 | CA | 28 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 25 | BA | 187 | C | OP2-P-O3' | 5.38 | 117.03 | 105.20 |
| 25 | BA | 1302 | G | C8-N9-C1' | -5.38 | 120.01 | 127.00 |
| 25 | BA | 2036 | A | N1-C6-N6 | 5.38 | 121.83 | 118.60 |
| 25 | DA | 1430 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 1 | AA | 115 | G | P-O3'-C3' | 5.38 | 126.15 | 119.70 |
| 25 | BA | 181 | C | N3-C4-C5 | 5.38 | 124.05 | 121.90 |
| 1 | CA | 525 | C | C5-C4-N4 | -5.38 | 116.44 | 120.20 |
| 1 | CA | 913 | A | P-O3'-C3' | 5.37 | 126.15 | 119.70 |
| 25 | BA | 1304 | C | C6-N1-C2 | 5.37 | 122.45 | 120.30 |
| 25 | DA | 1021 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 166 | G | N3-C4-C5 | -5.37 | 125.92 | 128.60 |
| 1 | AA | 1139 | G | C6-C5-N7 | 5.37 | 133.62 | 130.40 |
| 1 | CA | 502 | G | OP1-P-O3' | 5.37 | 117.01 | 105.20 |
| 1 | CA | 1366 | C | C2-N3-C4 | 5.37 | 122.58 | 119.90 |
| 1 | CA | 1398 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 25 | DA | 1365 | A | C6-N1-C2 | -5.37 | 115.38 | 118.60 |
| 25 | DA | 2616 | C | N3-C2-O2 | -5.37 | 118.14 | 121.90 |
| 25 | BA | 116 | A | N1-C6-N6 | -5.37 | 115.38 | 118.60 |
| 25 | DA | 530 | G | N7-C8-N9 | 5.37 | 115.78 | 113.10 |
| 1 | AA | 63 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 25 | BA | 1412 | A | N1-C6-N6 | -5.37 | 115.38 | 118.60 |
| 25 | BA | 2059 | G | N3-C4-N9 | 5.37 | 129.22 | 126.00 |
| 1 | CA | 354 | G | N3-C4-N9 | 5.37 | 129.22 | 126.00 |
| 1 | CA | 397 | A | OP2-P-O3' | 5.37 | 117.00 | 105.20 |
| 25 | DA | 2332 | U | C5-C6-N1 | -5.37 | 120.02 | 122.70 |
| 25 | BA | 2476 | C | C6-N1-C2 | 5.36 | 122.44 | 120.30 |
| 25 | DA | 179 | G | C5-C6-O6 | -5.36 | 125.38 | 128.60 |
| 25 | DA | 1607 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 1 | AA | 1007 | C | O4'-C1'-N1 | -5.36 | 103.91 | 108.20 |
| 25 | BA | 716 | G | N1-C6-O6 | -5.36 | 116.68 | 119.90 |
| 1 | CA | 1312 | G | N3-C4-N9 | -5.36 | 122.78 | 126.00 |
| 1 | AA | 71 | C | C5-C6-N1 | 5.36 | 123.68 | 121.00 |
| 1 | CA | 1325 | C | C5-C4-N4 | 5.36 | 123.95 | 120.20 |
| 25 | BA | 2462 | A | N1-C2-N3 | -5.36 | 126.62 | 129.30 |
| 25 | DA | 2325 | G | C8-N9-C4 | -5.36 | 104.26 | 106.40 |
| 25 | BA | 1246 | C | C6-N1-C2 | 5.36 | 122.44 | 120.30 |
| 25 | BA | 1543 | U | N3-C4-O4 | -5.36 | 115.65 | 119.40 |
| 25 | BA | 1298 | G | C4-C5-N7 | -5.35 | 108.66 | 110.80 |
| 25 | BA | 1919 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 32 | BI | 30 | LEU | CA-CB-CG | -5.35 | 102.99 | 115.30 |
| 25 | DA | 907 | U | C5-C6-N1 | 5.35 | 125.38 | 122.70 |
| 25 | BA | 678 | A | C8-N9-C4 | -5.35 | 103.66 | 105.80 |
| 25 | DA | 2275 | C | O4'-C1'-N1 | -5.35 | 103.92 | 108.20 |
| 1 | AA | 561 | U | C6-N1-C2 | 5.35 | 124.21 | 121.00 |
| 25 | BA | 140 | A | N1-C6-N6 | -5.35 | 115.39 | 118.60 |
| 25 | BA | 1370 | G | C8-N9-C4 | 5.35 | 108.54 | 106.40 |
| 25 | BA | 2265 | G | C8-N9-C4 | 5.35 | 108.54 | 106.40 |
| 25 | BA | 2735 | G | N3-C4-C5 | -5.35 | 125.93 | 128.60 |
| 25 | DA | 179 | G | N1-C6-O6 | 5.35 | 123.11 | 119.90 |
| 25 | DA | 1365 | A | N1-C2-N3 | 5.35 | 131.97 | 129.30 |
| 25 | DA | 2503 | A | N3-C4-N9 | 5.35 | 131.68 | 127.40 |
| 25 | DA | 530 | G | N9-C4-C5 | 5.34 | 107.54 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | AA | 1029 | C | C6-N1-C1' | 5.34 | 127.21 | 120.80 |
| 25 | BA | 145 | G | O5'-P-OP2 | -5.34 | 100.89 | 105.70 |
| 1 | CA | 1099 | G | C4-C5-N7 | -5.34 | 108.66 | 110.80 |
| 25 | DA | 116 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 1 | AA | 576 | G | N1-C6-O6 | 5.34 | 123.10 | 119.90 |
| 25 | BA | 1783 | C | C6-N1-C2 | 5.34 | 122.44 | 120.30 |
| 25 | BA | 1977 | U | N1-C2-O2 | -5.34 | 119.06 | 122.80 |
| 1 | CA | 1030(B) | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 25 | DA | 2540 | C | C2-N1-C1' | -5.34 | 112.93 | 118.80 |
| 1 | AA | 561 | U | N1-C2-N3 | -5.34 | 111.70 | 114.90 |
| 25 | DA | 204 | A | OP1-P-O3' | 5.34 | 116.94 | 105.20 |
| 25 | DA | 1210 | A | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 25 | DA | 2586 | C | C5-C6-N1 | 5.34 | 123.67 | 121.00 |
| 26 | DB | 30 | C | C6-N1-C2 | -5.34 | 118.17 | 120.30 |
| 25 | BA | 2513 | C | C2-N1-C1' | -5.33 | 112.93 | 118.80 |
| 25 | DA | 1781 | C | N1-C2-O2 | -5.33 | 115.70 | 118.90 |
| 1 | CA | 266 | G | C5-N7-C8 | -5.33 | 101.63 | 104.30 |
| 25 | DA | 1471 | A | C8-N9-C4 | -5.33 | 103.67 | 105.80 |
| 25 | BA | 1302 | G | N9-C4-C5 | -5.33 | 103.27 | 105.40 |
| 25 | BA | 2634 | C | N3-C2-O2 | 5.33 | 125.63 | 121.90 |
| 25 | BA | 2734 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 1 | CA | 1043 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 1 | CA | 1119 | C | C4-C5-C6 | -5.33 | 114.73 | 117.40 |
| 25 | DA | 1897 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 25 | DA | 2488 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 25 | DA | 2532 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 25 | BA | 405 | C | C5-C4-N4 | -5.33 | 116.47 | 120.20 |
| 1 | CA | 572 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 25 | DA | 811 | U | C5-C6-N1 | -5.33 | 120.04 | 122.70 |
| 25 | BA | 397 | G | N3-C4-N9 | 5.32 | 129.19 | 126.00 |
| 25 | BA | 1723 | A | N1-C6-N6 | -5.32 | 115.41 | 118.60 |
| 25 | BA | 1389 | G | C4-N9-C1' | 5.32 | 133.42 | 126.50 |
| 1 | CA | 1005 | A | OP1-P-O3' | 5.32 | 116.91 | 105.20 |
| 1 | CA | 1063 | C | C6-N1-C2 | -5.32 | 118.17 | 120.30 |
| 1 | AA | 1388 | C | N1-C2-O2 | -5.32 | 115.71 | 118.90 |
| 25 | BA | 354 | A | N3-C4-C5 | 5.32 | 130.52 | 126.80 |
| 25 | BA | 1298 | G | N3-C4-N9 | -5.32 | 122.81 | 126.00 |
| 1 | CA | 615 | C | C6-N1-C2 | -5.32 | 118.17 | 120.30 |
| 25 | DA | 1703 | G | C6-C5-N7 | -5.32 | 127.21 | 130.40 |
| 1 | CA | 1065 | U | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 25 | BA | 2239 | A | C8-N9-C4 | -5.32 | 103.67 | 105.80 |
| 25 | DA | 1181 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | DA | 1930 | G | C4-N9-C1' | -5.32 | 119.59 | 126.50 |
| 1 | AA | 1122 | U | N3-C2-O2 | -5.32 | 118.48 | 122.20 |
| 1 | CA | 701 | C | N3-C2-O2 | -5.32 | 118.18 | 121.90 |
| 25 | BA | 1746 | G | N9-C4-C5 | 5.31 | 107.53 | 105.40 |
| 25 | DA | 1313 | U | C2-N1-C1' | 5.31 | 124.08 | 117.70 |
| 25 | BA | 2011 | G | C8-N9-C4 | 5.31 | 108.52 | 106.40 |
| 25 | DA | 1204 | A | C4-C5-N7 | 5.31 | 113.36 | 110.70 |
| 25 | DA | 2772 | C | C6-N1-C2 | 5.31 | 122.42 | 120.30 |
| 1 | AA | 1067 | A | O4'-C1'-N9 | -5.31 | 103.95 | 108.20 |
| 25 | BA | 139 | A | N1-C6-N6 | 5.31 | 121.79 | 118.60 |
| 25 | BA | 1154 | U | N3-C2-O2 | -5.31 | 118.48 | 122.20 |
| 1 | CA | 984 | C | C2-N3-C4 | 5.31 | 122.55 | 119.90 |
| 25 | DA | 729 | G | N1-C6-O6 | 5.31 | 123.09 | 119.90 |
| 25 | DA | 2755 | C | C5-C6-N1 | 5.31 | 123.66 | 121.00 |
| 1 | AA | 1396 | A | C5-C6-N1 | -5.31 | 115.05 | 117.70 |
| 25 | BA | 2054 | G | C5-N7-C8 | -5.31 | 101.65 | 104.30 |
| 25 | DA | 1254 | A | C8-N9-C4 | -5.31 | 103.68 | 105.80 |
| 1 | CA | 1180 | A | N7-C8-N9 | 5.31 | 116.45 | 113.80 |
| 25 | BA | 2036 | A | N9-C4-C5 | -5.30 | 103.68 | 105.80 |
| 25 | BA | 2370 | G | N1-C6-O6 | -5.30 | 116.72 | 119.90 |
| 25 | BA | 2518 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 1 | CA | 783 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 25 | BA | 478 | G | N3-C4-C5 | -5.30 | 125.95 | 128.60 |
| 25 | DA | 2207 | G | C8-N9-C1' | -5.30 | 120.11 | 127.00 |
| 25 | BA | 410 | U | C2-N1-C1' | -5.30 | 111.34 | 117.70 |
| 25 | BA | 839 | G | O4'-C1'-N9 | -5.30 | 103.96 | 108.20 |
| 25 | DA | 1142 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 25 | BA | 670 | C | C2-N1-C1' | 5.29 | 124.62 | 118.80 |
| 1 | CA | 1205 | U | C6-N1-C2 | -5.29 | 117.82 | 121.00 |
| 1 | AA | 97 | G | N3-C4-N9 | 5.29 | 129.18 | 126.00 |
| 1 | CA | 400 | C | C6-N1-C2 | 5.29 | 122.42 | 120.30 |
| 25 | DA | 1698 | A | N9-C4-C5 | -5.29 | 103.68 | 105.80 |
| 25 | BA | 139 | A | C2-N3-C4 | -5.29 | 107.96 | 110.60 |
| 25 | DA | 2338 | G | C4-N9-C1' | -5.29 | 119.62 | 126.50 |
| 25 | BA | 342 | C | N3-C4-C5 | -5.29 | 119.78 | 121.90 |
| 25 | BA | 1425 | A | OP2-P-O3' | 5.29 | 116.83 | 105.20 |
| 1 | AA | 1131 | G | C5-N7-C8 | -5.29 | 101.66 | 104.30 |
| 25 | BA | 1068 | G | N9-C4-C5 | 5.29 | 107.51 | 105.40 |
| 25 | BA | 1298 | G | N9-C4-C5 | 5.29 | 107.51 | 105.40 |
| 25 | BA | 2495 | C | C6-N1-C2 | -5.29 | 118.19 | 120.30 |
| 1 | CA | 733 | A | O5'-P-OP2 | -5.29 | 100.94 | 105.70 |
| 25 | DA | 1831 | G | C8-N9-C4 | -5.29 | 104.29 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 557 | G | C8-N9-C4 | 5.28 | 108.51 | 106.40 |
| 1 | CA | 1502 | A | N7-C8-N9 | 5.28 | 116.44 | 113.80 |
| 1 | AA | 944 | G | C4-N9-C1' | 5.28 | 133.37 | 126.50 |
| 25 | DA | 1684 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |
| 23 | AX | 46 | G | N3-C2-N2 | -5.28 | 116.20 | 119.90 |
| 25 | DA | 2479 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 25 | BA | 2262 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 1 | CA | 1163 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 25 | DA | 2252 | G | N3-C2-N2 | -5.28 | 116.20 | 119.90 |
| 1 | AA | 1235 | U | C6-N1-C2 | -5.28 | 117.83 | 121.00 |
| 1 | CA | 660 | G | C8-N9-C4 | 5.28 | 108.51 | 106.40 |
| 23 | CX | 24 | U | C6-N1-C2 | -5.28 | 117.83 | 121.00 |
| 25 | DA | 1653 | G | C6-C5-N7 | -5.28 | 127.23 | 130.40 |
| 25 | BA | 1954 | A | O5'-P-OP1 | -5.28 | 100.95 | 105.70 |
| 25 | DA | 1021 | A | C5-N7-C8 | -5.28 | 101.26 | 103.90 |
| 25 | DA | 1281 | G | N3-C4-C5 | 5.27 | 131.24 | 128.60 |
| 25 | BA | 496 | A | OP1-P-O3' | 5.27 | 116.80 | 105.20 |
| 25 | BA | 1066 | A | C8-N9-C4 | -5.27 | 103.69 | 105.80 |
| 25 | DA | 2612 | C | C6-N1-C2 | 5.27 | 122.41 | 120.30 |
| 1 | AA | 998 | G | N3-C4-N9 | -5.27 | 122.84 | 126.00 |
| 1 | AA | 1278 | U | C5-C6-N1 | 5.27 | 125.33 | 122.70 |
| 25 | BA | 2858 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 1 | AA | 422 | C | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 25 | BA | 1009 | C | N3-C4-N4 | 5.27 | 121.69 | 118.00 |
| 25 | DA | 1212 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |
| 1 | AA | 159 | G | C4-N9-C1' | -5.27 | 119.65 | 126.50 |
| 25 | DA | 669 | G | OP1-P-OP2 | -5.27 | 111.70 | 119.60 |
| 25 | DA | 2645 | G | N3-C2-N2 | 5.27 | 123.59 | 119.90 |
| 25 | DA | 1880 | C | C6-N1-C2 | 5.26 | 122.41 | 120.30 |
| 27 | DD | 275 | LYS | N-CA-C | -5.26 | 96.79 | 111.00 |
| 25 | BA | 1421 | C | OP1-P-O3' | 5.26 | 116.78 | 105.20 |
| 1 | CA | 667 | G | N3-C4-C5 | 5.26 | 131.23 | 128.60 |
| 1 | CA | 1004 | A | N1-C6-N6 | -5.26 | 115.44 | 118.60 |
| 25 | DA | 511 | U | N3-C2-O2 | -5.26 | 118.52 | 122.20 |
| 25 | BA | 2291 | G | C8-N9-C4 | 5.26 | 108.50 | 106.40 |
| 25 | BA | 498 | A | O5'-P-OP2 | -5.26 | 100.97 | 105.70 |
| 25 | BA | 1444 | C | OP2-P-O3' | 5.26 | 116.77 | 105.20 |
| 25 | DA | 729 | G | C4-N9-C1' | 5.26 | 133.34 | 126.50 |
| 25 | BA | 1718 | U | N3-C2-O2 | 5.25 | 125.88 | 122.20 |
| 1 | CA | 65 | U | OP2-P-O3' | 5.25 | 116.76 | 105.20 |
| 25 | DA | 1963 | U | C2-N1-C1' | 5.25 | 124.00 | 117.70 |
| 25 | BA | 1314 | A | C2-N3-C4 | -5.25 | 107.97 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 25 | DA | 1270 | C | OP2-P-O3' | 5.25 | 116.75 | 105.20 |
| 25 | BA | 2042 | A | O5'-P-OP1 | -5.25 | 100.97 | 105.70 |
| 1 | CA | 1026 | G | N7-C8-N9 | 5.25 | 115.72 | 113.10 |
| 1 | CA | 1149 | C | N3-C2-O2 | -5.25 | 118.23 | 121.90 |
| 25 | DA | 2491 | U | N1-C2-O2 | 5.25 | 126.47 | 122.80 |
| 1 | CA | 1312 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |
| 25 | DA | 2057 | A | N7-C8-N9 | -5.25 | 111.18 | 113.80 |
| 25 | DA | 1899 | G | OP1-P-O3' | 5.24 | 116.73 | 105.20 |
| 25 | BA | 1308 | A | N1-C6-N6 | 5.24 | 121.74 | 118.60 |
| 25 | DA | 740 | U | O5'-P-OP1 | 5.24 | 116.99 | 110.70 |
| 1 | AA | 1113 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 25 | BA | 88 | G | C8-N9-C4 | -5.24 | 104.31 | 106.40 |
| 25 | BA | 193 | A | N7-C8-N9 | -5.24 | 111.18 | 113.80 |
| 25 | BA | 702 | A | C8-N9-C4 | -5.24 | 103.70 | 105.80 |
| 25 | BA | 912 | C | C6-N1-C2 | 5.24 | 122.39 | 120.30 |
| 25 | BA | 12 | U | C2-N1-C1' | 5.24 | 123.98 | 117.70 |
| 25 | DA | 1997 | G | N3-C4-N9 | 5.24 | 129.14 | 126.00 |
| 22 | AV | 17 | U | C2-N3-C4 | 5.24 | 130.14 | 127.00 |
| 25 | DA | 71 | A | N1-C6-N6 | 5.24 | 121.74 | 118.60 |
| 25 | DA | 2531 | A | C8-N9-C4 | 5.24 | 107.89 | 105.80 |
| 25 | BA | 600 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 25 | DA | 21 | A | C8-N9-C4 | 5.23 | 107.89 | 105.80 |
| 1 | AA | 934 | C | O5'-P-OP1 | -5.23 | 100.99 | 105.70 |
| 1 | AA | 1150 | U | C6-N1-C2 | -5.23 | 117.86 | 121.00 |
| 25 | BA | 180 | A | OP2-P-O3' | 5.23 | 116.70 | 105.20 |
| 1 | CA | 354 | G | C4-C5-N7 | 5.23 | 112.89 | 110.80 |
| 25 | BA | 719 | C | OP2-P-O3' | 5.23 | 116.70 | 105.20 |
| 25 | DA | 1571 | A | N1-C6-N6 | -5.23 | 115.46 | 118.60 |
| 25 | BA | 2684 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 25 | DA | 116 | C | C4-C5-C6 | 5.23 | 120.01 | 117.40 |
| 1 | AA | 98 | G | N3-C4-N9 | 5.22 | 129.13 | 126.00 |
| 25 | BA | 827 | G | C4-C5-C6 | 5.22 | 121.94 | 118.80 |
| 25 | BA | 2062 | C | C6-N1-C2 | 5.22 | 122.39 | 120.30 |
| 25 | BA | 2283 | G | C8-N9-C1' | -5.22 | 120.21 | 127.00 |
| 1 | CA | 44 | G | C4-N9-C1' | 5.22 | 133.29 | 126.50 |
| 25 | DA | 154(A) | C | C2-N1-C1' | 5.22 | 124.55 | 118.80 |
| 1 | AA | 1531 | A | C4-N9-C1' | 5.22 | 135.70 | 126.30 |
| 25 | DA | 1372 | U | C2-N1-C1' | 5.22 | 123.97 | 117.70 |
| 1 | CA | 1080 | A | N1-C6-N6 | -5.22 | 115.47 | 118.60 |
| 25 | DA | 1880 | C | C5-C6-N1 | -5.22 | 118.39 | 121.00 |
| 25 | DA | 1992 | G | C2-N3-C4 | 5.22 | 114.51 | 111.90 |
| 25 | DA | 2374 | C | C5-C6-N1 | -5.22 | 118.39 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 175 | C | C5-C6-N1 | 5.22 | 123.61 | 121.00 |
| 1 | AA | 340 | U | C5-C6-N1 | -5.22 | 120.09 | 122.70 |
| 25 | BA | 194 | G | O5'-P-OP2 | -5.22 | 101.00 | 105.70 |
| 25 | DA | 2601 | C | N3-C4-C5 | 5.22 | 123.99 | 121.90 |
| 25 | BA | 331 | G | O5'-P-OP1 | -5.21 | 101.01 | 105.70 |
| 23 | CX | 35 | A | C5-C6-N6 | 5.21 | 127.87 | 123.70 |
| 1 | AA | 6 | G | N3-C4-N9 | 5.21 | 129.13 | 126.00 |
| 25 | DA | 933 | A | C6-C5-N7 | -5.21 | 128.65 | 132.30 |
| 25 | DA | 1555 | G | N1-C6-O6 | 5.21 | 123.03 | 119.90 |
| 25 | DA | 1970 | A | O4'-C1'-N9 | -5.21 | 104.03 | 108.20 |
| 25 | BA | 733 | G | C5-N7-C8 | -5.21 | 101.69 | 104.30 |
| 1 | AA | 167 | G | C8-N9-C1' | -5.21 | 120.23 | 127.00 |
| 25 | DA | 1797 | C | C5-C6-N1 | -5.21 | 118.40 | 121.00 |
| 1 | AA | 354 | G | O5'-P-OP2 | -5.21 | 101.02 | 105.70 |
| 25 | BA | 231 | G | N3-C4-C5 | 5.21 | 131.20 | 128.60 |
| 25 | BA | 2011 | G | N7-C8-N9 | -5.21 | 110.50 | 113.10 |
| 25 | BA | 2421 | G | N1-C2-N2 | -5.21 | 111.51 | 116.20 |
| 25 | BA | 989 | G | C8-N9-C4 | -5.20 | 104.32 | 106.40 |
| 25 | BA | 1725 | G | N9-C4-C5 | 5.20 | 107.48 | 105.40 |
| 25 | BA | 2285 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 25 | DA | 1897 | G | O5'-P-OP1 | -5.20 | 101.02 | 105.70 |
| 25 | BA | 1187 | U | C5-C6-N1 | 5.20 | 125.30 | 122.70 |
| 25 | DA | 885 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 25 | DA | 1475 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 25 | DA | 2519 | U | C6-N1-C2 | 5.20 | 124.12 | 121.00 |
| 1 | AA | 645 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 25 | DA | 807 | U | C6-N1-C2 | -5.20 | 117.88 | 121.00 |
| 1 | AA | 1276 | G | N3-C4-C5 | -5.20 | 126.00 | 128.60 |
| 25 | BA | 1454 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 25 | BA | 1367 | A | O5'-P-OP1 | -5.19 | 101.03 | 105.70 |
| 25 | DA | 2249 | U | C5-C4-O4 | 5.19 | 129.02 | 125.90 |
| 25 | BA | 665 | C | N1-C2-O2 | -5.19 | 115.79 | 118.90 |
| 25 | BA | 2227 | G | C8-N9-C1' | 5.19 | 133.75 | 127.00 |
| 1 | CA | 1141 | C | C5-C4-N4 | 5.19 | 123.83 | 120.20 |
| 25 | DA | 2877 | G | N3-C4-C5 | 5.19 | 131.19 | 128.60 |
| 53 | D7 | 35 | ARG | NE-CZ-NH1 | -5.19 | 117.70 | 120.30 |
| 1 | AA | 339 | C | C5-C6-N1 | -5.19 | 118.41 | 121.00 |
| 1 | CA | 1226 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 23 | CX | 46 | G | C8-N9-C1' | 5.19 | 133.74 | 127.00 |
| 25 | DA | 1961 | C | C2-N1-C1' | -5.19 | 113.09 | 118.80 |
| 25 | DA | 2010 | G | O5'-P-OP1 | -5.19 | 101.03 | 105.70 |
| 25 | DA | 2878 | U | C6-N1-C2 | -5.19 | 117.89 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | BA | 1220 | U | P-O3'-C3' | 5.19 | 125.92 | 119.70 |
| 23 | CX | 23 | C | O5'-P-OP1 | -5.19 | 101.03 | 105.70 |
| 25 | DA | 1602 | U | O5'-P-OP2 | 5.19 | 116.92 | 110.70 |
| 1 | AA | 496 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 1 | AA | 1127 | G | C6-C5-N7 | -5.18 | 127.29 | 130.40 |
| 1 | CA | 1397 | C | C2-N1-C1' | 5.18 | 124.50 | 118.80 |
| 25 | DA | 1679 | U | C5-C4-O4 | 5.18 | 129.01 | 125.90 |
| 1 | AA | 348 | G | O5'-P-OP1 | 5.18 | 116.92 | 110.70 |
| 25 | BA | 2077 | C | N3-C4-C5 | -5.18 | 119.83 | 121.90 |
| 25 | DA | 792 | G | N3-C4-C5 | -5.18 | 126.01 | 128.60 |
| 25 | BA | 1386 | U | N1-C2-O2 | -5.18 | 119.17 | 122.80 |
| 25 | BA | 2389 | A | C2-N3-C4 | -5.18 | 108.01 | 110.60 |
| 25 | DA | 188 | G | C5-N7-C8 | -5.18 | 101.71 | 104.30 |
| 27 | BD | 111 | LEU | CA-CB-CG | 5.18 | 127.21 | 115.30 |
| 25 | DA | 2227 | A | N1-C6-N6 | -5.18 | 115.49 | 118.60 |
| 25 | DA | 2540 | C | O5'-P-OP2 | -5.18 | 101.04 | 105.70 |
| 25 | BA | 1382 | A | O5'-P-OP2 | -5.17 | 101.04 | 105.70 |
| 25 | BA | 2059 | G | N1-C2-N2 | -5.17 | 111.54 | 116.20 |
| 1 | CA | 1240 | U | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 25 | DA | 13 | A | N1-C6-N6 | -5.17 | 115.50 | 118.60 |
| 25 | DA | 1432 | C | N3-C4-N4 | 5.17 | 121.62 | 118.00 |
| 25 | BA | 242 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 1 | CA | 46 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 1 | CA | 64 | G | C5-C6-N1 | -5.17 | 108.91 | 111.50 |
| 25 | BA | 1035 | G | N3-C4-N9 | 5.17 | 129.10 | 126.00 |
| 25 | DA | 954 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 25 | DA | 2804 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 23 | CX | 9 | G | N3-C4-C5 | 5.17 | 131.19 | 128.60 |
| 25 | DA | 1215 | G | OP1-P-O3' | 5.17 | 116.57 | 105.20 |
| 25 | BA | 1154 | U | C2-N1-C1' | 5.17 | 123.90 | 117.70 |
| 25 | BA | 1852 | A | C8-N9-C4 | -5.17 | 103.73 | 105.80 |
| 1 | CA | 254 | G | OP2-P-O3' | 5.17 | 116.57 | 105.20 |
| 1 | CA | 380 | G | N3-C4-N9 | -5.17 | 122.90 | 126.00 |
| 1 | CA | 1171 | G | N7-C8-N9 | 5.17 | 115.68 | 113.10 |
| 25 | DA | 34 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 25 | BA | 2594 | G | C8-N9-C4 | -5.17 | 104.33 | 106.40 |
| 25 | BA | 962 | G | N3-C4-C5 | -5.16 | 126.02 | 128.60 |
| 25 | BA | 1175 | A | N1-C6-N6 | -5.16 | 115.50 | 118.60 |
| 25 | BA | 2299 | A | C5-N7-C8 | -5.16 | 101.32 | 103.90 |
| 1 | CA | 1036 | G | C4-N9-C1' | 5.16 | 133.21 | 126.50 |
| 25 | BA | 202 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 1 | CA | 1246 | C | N3-C2-O2 | -5.16 | 118.29 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | CX | 26 | G | C6-N1-C2 | 5.16 | 128.20 | 125.10 |
| 25 | DA | 448 | U | C5-C6-N1 | -5.16 | 120.12 | 122.70 |
| 25 | DA | 2320 | A | C2-N3-C4 | 5.16 | 113.18 | 110.60 |
| 25 | BA | 1985 | U | C5-C6-N1 | 5.16 | 125.28 | 122.70 |
| 25 | BA | 2299 | A | O4'-C1'-N9 | -5.16 | 104.07 | 108.20 |
| 25 | DA | 512 | G | C8-N9-C1' | 5.16 | 133.71 | 127.00 |
| 1 | AA | 46 | G | N1-C6-O6 | 5.16 | 122.99 | 119.90 |
| 25 | BA | 2065 | C | N3-C2-O2 | 5.16 | 125.51 | 121.90 |
| 18 | CR | 64 | ARG | NE-CZ-NH2 | -5.16 | 117.72 | 120.30 |
| 25 | DA | 1204 | A | C5-N7-C8 | -5.16 | 101.32 | 103.90 |
| 25 | BA | 639 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 25 | DA | 2512 | C | N1-C2-O2 | -5.15 | 115.81 | 118.90 |
| 25 | BA | 1076 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 25 | BA | 1222 | A | C4-C5-C6 | 5.15 | 119.58 | 117.00 |
| 25 | DA | 2386 | C | N3-C4-C5 | 5.15 | 123.96 | 121.90 |
| 25 | BA | 1019 | G | OP1-P-OP2 | 5.15 | 127.33 | 119.60 |
| 25 | DA | 446 | G | C8-N9-C4 | 5.15 | 108.46 | 106.40 |
| 25 | DA | 645 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 26 | DB | 70 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 25 | BA | 2428 | C | C5-C6-N1 | 5.15 | 123.57 | 121.00 |
| 1 | CA | 800 | G | OP2-P-O3' | 5.15 | 116.53 | 105.20 |
| 25 | DA | 2483 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 25 | BA | 354 | A | N1-C2-N3 | 5.15 | 131.87 | 129.30 |
| 25 | DA | 737 | C | C6-N1-C2 | 5.15 | 122.36 | 120.30 |
| 25 | BA | 2537 | G | O5'-P-OP1 | 5.14 | 116.87 | 110.70 |
| 25 | DA | 1937 | A | N9-C4-C5 | -5.14 | 103.74 | 105.80 |
| 25 | BA | 2061 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 25 | BA | 2544 | G | C5-C6-O6 | -5.14 | 125.52 | 128.60 |
| 25 | BA | 2574 | U | C5-C6-N1 | -5.14 | 120.13 | 122.70 |
| 25 | DA | 1313 | U | C5-C6-N1 | 5.14 | 125.27 | 122.70 |
| 25 | DA | 2321 | G | C6-C5-N7 | -5.14 | 127.32 | 130.40 |
| 1 | AA | 159 | G | N9-C1'-C2' | -5.14 | 106.35 | 112.00 |
| 25 | BA | 1321 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 25 | BA | 1745 | A | N1-C6-N6 | 5.14 | 121.68 | 118.60 |
| 25 | BA | 2608 | U | C6-N1-C2 | 5.14 | 124.08 | 121.00 |
| 25 | DA | 1487 | G | C8-N9-C4 | -5.14 | 104.34 | 106.40 |
| 25 | BA | 332 | G | C8-N9-C1' | -5.14 | 120.32 | 127.00 |
| 1 | CA | 299 | G | C5-C6-O6 | -5.14 | 125.52 | 128.60 |
| 1 | AA | 1506 | U | N3-C4-O4 | 5.13 | 122.99 | 119.40 |
| 25 | BA | 2256 | U | N3-C4-O4 | -5.13 | 115.81 | 119.40 |
| 25 | BA | 2419 | G | C4-N9-C1' | 5.13 | 133.18 | 126.50 |
| 25 | BA | 2566 | U | N1-C2-O2 | -5.13 | 119.21 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 25 | DA | 271(M) | G | N3-C4-C5 | -5.13 | 126.03 | 128.60 |
| 25 | DA | 792 | G | N3-C4-N9 | 5.13 | 129.08 | 126.00 |
| 25 | BA | 30 | G | OP1-P-O3' | 5.13 | 116.49 | 105.20 |
| 1 | AA | 341 | C | C6-N1-C2 | 5.13 | 122.35 | 120.30 |
| 25 | DA | 90 | U | C2-N1-C1' | 5.13 | 123.86 | 117.70 |
| 25 | DA | 1124 | C | N3-C4-C5 | 5.13 | 123.95 | 121.90 |
| 25 | BA | 1153 | G | C2-N3-C4 | 5.13 | 114.47 | 111.90 |
| 1 | CA | 1028 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 1 | CA | 1269 | A | N1-C6-N6 | -5.13 | 115.52 | 118.60 |
| 25 | DA | 762 | U | C2-N1-C1' | 5.13 | 123.86 | 117.70 |
| 25 | DA | 1375 | C | O5'-P-OP1 | -5.13 | 101.08 | 105.70 |
| 25 | DA | 1596 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 25 | DA | 2039 | C | C2-N1-C1' | 5.13 | 124.44 | 118.80 |
| 1 | AA | 578 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 1 | AA | 1150 | U | C5-C6-N1 | 5.13 | 125.26 | 122.70 |
| 25 | BA | 1707 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 25 | DA | 602 | G | N3-C4-N9 | 5.13 | 129.08 | 126.00 |
| 1 | CA | 893 | C | C6-N1-C2 | 5.13 | 122.35 | 120.30 |
| 1 | CA | 1307 | U | C5-C6-N1 | 5.13 | 125.26 | 122.70 |
| 25 | DA | 914 | C | N1-C2-O2 | 5.13 | 121.97 | 118.90 |
| 25 | DA | 1718 | G | C4-N9-C1' | 5.13 | 133.16 | 126.50 |
| 25 | DA | 1966 | A | N1-C6-N6 | -5.13 | 115.53 | 118.60 |
| 25 | DA | 2591 | C | N3-C4-C5 | -5.13 | 119.85 | 121.90 |
| 1 | CA | 1519 | A | C8-N9-C4 | -5.12 | 103.75 | 105.80 |
| 25 | DA | 889 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 1 | AA | 190 | U | C5-C6-N1 | 5.12 | 125.26 | 122.70 |
| 25 | DA | 1017 | G | C4-N9-C1' | 5.12 | 133.16 | 126.50 |
| 25 | DA | 2413 | G | N1-C6-O6 | 5.12 | 122.97 | 119.90 |
| 1 | AA | 781 | A | N9-C4-C5 | -5.12 | 103.75 | 105.80 |
| 1 | AA | 814 | A | OP1-P-O3' | 5.12 | 116.47 | 105.20 |
| 1 | AA | 1435 | G | C5-C6-N1 | -5.12 | 108.94 | 111.50 |
| 25 | BA | 332 | G | C4-N9-C1' | 5.12 | 133.16 | 126.50 |
| 25 | BA | 725 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 25 | DA | 199 | A | C5-C6-N6 | -5.12 | 119.60 | 123.70 |
| 25 | DA | 2474 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 25 | BA | 2258 | G | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 1 | CA | 1502 | A | C2-N3-C4 | -5.12 | 108.04 | 110.60 |
| 25 | BA | 861 | C | C4-C5-C6 | -5.12 | 114.84 | 117.40 |
| 25 | DA | 1115 | G | C4-N9-C1' | -5.12 | 119.85 | 126.50 |
| 1 | CA | 1522 | U | OP2-P-O3' | 5.11 | 116.45 | 105.20 |
| 25 | BA | 2040 | G | O5'-P-OP1 | 5.11 | 116.83 | 110.70 |
| 1 | AA | 1004 | A | P-O3'-C3' | 5.11 | 125.83 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1145 | C | N3-C2-O2 | -5.11 | 118.32 | 121.90 |
| 25 | BA | 2230 | U | N1-C2-O2 | 5.11 | 126.38 | 122.80 |
| 25 | DA | 783 | A | C4-C5-C6 | 5.11 | 119.56 | 117.00 |
| 25 | DA | 1897 | G | C5-C6-O6 | -5.11 | 125.53 | 128.60 |
| 25 | BA | 1483 | C | C2-N1-C1' | 5.11 | 124.42 | 118.80 |
| 25 | BA | 1725 | G | N3-C2-N2 | -5.11 | 116.32 | 119.90 |
| 1 | CA | 865 | A | C8-N9-C4 | -5.11 | 103.76 | 105.80 |
| 25 | DA | 912 | C | N3-C2-O2 | -5.11 | 118.33 | 121.90 |
| 25 | DA | 2893 | G | N9-C4-C5 | -5.11 | 103.36 | 105.40 |
| 1 | AA | 421 | U | N3-C2-O2 | -5.11 | 118.63 | 122.20 |
| 25 | BA | 2621 | U | C6-N1-C2 | 5.11 | 124.06 | 121.00 |
| 1 | CA | 998 | G | N9-C4-C5 | 5.11 | 107.44 | 105.40 |
| 25 | DA | 584 | C | N1-C2-O2 | -5.11 | 115.84 | 118.90 |
| 25 | BA | 418 | G | N1-C6-O6 | 5.10 | 122.96 | 119.90 |
| 25 | DA | 188 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 25 | BA | 515 | G | N1-C6-O6 | 5.10 | 122.96 | 119.90 |
| 25 | BA | 553 | A | O5'-P-OP2 | -5.10 | 101.11 | 105.70 |
| 25 | BA | 1418 | U | C5-C6-N1 | 5.10 | 125.25 | 122.70 |
| 25 | BA | 1429 | C | C5-C4-N4 | -5.10 | 116.63 | 120.20 |
| 25 | DA | 389 | G | N1-C6-O6 | 5.10 | 122.96 | 119.90 |
| 25 | DA | 1363 | C | N3-C4-N4 | -5.10 | 114.43 | 118.00 |
| 25 | DA | 2297 | C | C5-C6-N1 | 5.10 | 123.55 | 121.00 |
| 1 | CA | 833 | U | O5'-P-OP2 | -5.10 | 101.11 | 105.70 |
| 25 | BA | 1718 | U | C5-C6-N1 | 5.10 | 125.25 | 122.70 |
| 25 | BA | 2054 | G | C4-N9-C1' | -5.10 | 119.87 | 126.50 |
| 25 | DA | 560 | C | C5-C6-N1 | -5.10 | 118.45 | 121.00 |
| 25 | DA | 1204 | A | N9-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 1 | AA | 192 | U | C6-N1-C2 | -5.10 | 117.94 | 121.00 |
| 1 | AA | 348 | G | N1-C6-O6 | 5.10 | 122.96 | 119.90 |
| 25 | BA | 772 | G | N3-C4-C5 | -5.10 | 126.05 | 128.60 |
| 25 | DA | 1802 | A | C6-N1-C2 | -5.10 | 115.54 | 118.60 |
| 1 | AA | 840 | C | O4'-C1'-N1 | -5.10 | 104.12 | 108.20 |
| 1 | AA | 1125 | U | C6-N1-C2 | 5.09 | 124.06 | 121.00 |
| 25 | BA | 2735 | G | C8-N9-C1' | -5.09 | 120.38 | 127.00 |
| 25 | DA | 394 | A | O5'-P-OP1 | -5.09 | 101.12 | 105.70 |
| 26 | DB | 79 | C | C6-N1-C2 | -5.09 | 118.26 | 120.30 |
| 1 | AA | 977 | A | N1-C6-N6 | -5.09 | 115.54 | 118.60 |
| 26 | DB | 60 | C | C5-C6-N1 | 5.09 | 123.55 | 121.00 |
| 25 | BA | 930 | G | C4-N9-C1' | -5.09 | 119.88 | 126.50 |
| 25 | DA | 461 | C | N3-C4-N4 | 5.09 | 121.56 | 118.00 |
| 25 | DA | 1439 | A | C8-N9-C4 | 5.09 | 107.84 | 105.80 |
| 1 | CA | 1017 | G | N3-C4-C5 | 5.09 | 131.15 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1296 | C | N3-C2-O2 | 5.09 | 125.46 | 121.90 |
| 25 | BA | 816 | G | N9-C4-C5 | -5.09 | 103.36 | 105.40 |
| 1 | CA | 1044 | A | N1-C6-N6 | -5.09 | 115.55 | 118.60 |
| 1 | AA | 167 | G | C6-C5-N7 | -5.09 | 127.35 | 130.40 |
| 1 | AA | 532 | A | P-O3'-C3' | 5.09 | 125.80 | 119.70 |
| 23 | AX | 22 | G | C8-N9-C1' | 5.09 | 133.61 | 127.00 |
| 25 | DA | 783 | A | N3-C4-C5 | -5.09 | 123.24 | 126.80 |
| 25 | DA | 2591 | C | N1-C2-O2 | -5.09 | 115.85 | 118.90 |
| 1 | AA | 220 | G | C4-N9-C1' | 5.08 | 133.11 | 126.50 |
| 1 | AA | 162 | A | N7-C8-N9 | 5.08 | 116.34 | 113.80 |
| 25 | BA | 332 | G | N9-C4-C5 | -5.08 | 103.37 | 105.40 |
| 25 | BA | 2383 | G | N1-C2-N3 | -5.08 | 120.85 | 123.90 |
| 25 | DA | 1614 | A | N1-C6-N6 | -5.08 | 115.55 | 118.60 |
| 25 | DA | 2523 | G | O5'-P-OP1 | 5.08 | 116.80 | 110.70 |
| 25 | BA | 1459 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 25 | DA | 729 | G | C8-N9-C1' | -5.08 | 120.39 | 127.00 |
| 25 | DA | 1588 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 25 | BA | 103 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 25 | DA | 1421 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 1 | AA | 1183 | A | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 25 | BA | 893 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 25 | DA | 116 | C | N3-C2-O2 | -5.08 | 118.34 | 121.90 |
| 25 | DA | 2828 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 25 | DA | 1653 | G | N3-C4-N9 | 5.08 | 129.05 | 126.00 |
| 1 | AA | 1397 | C | C6-N1-C1' | -5.08 | 114.71 | 120.80 |
| 23 | AX | 24 | U | N3-C2-O2 | -5.08 | 118.65 | 122.20 |
| 25 | BA | 1153 | G | O5'-P-OP2 | -5.08 | 101.13 | 105.70 |
| 25 | DA | 1253 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 25 | DA | 1340 | U | C5-C4-O4 | -5.08 | 122.86 | 125.90 |
| 25 | BA | 1417 | G | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 1 | CA | 1034 | G | N9-C4-C5 | 5.07 | 107.43 | 105.40 |
| 1 | CA | 1036 | G | C8-N9-C1' | -5.07 | 120.41 | 127.00 |
| 25 | DA | 148 | C | C5-C6-N1 | -5.07 | 118.46 | 121.00 |
| 25 | BA | 1578 | C | C2-N1-C1' | 5.07 | 124.38 | 118.80 |
| 23 | AX | 14 | A | C4-N9-C1' | 5.07 | 135.42 | 126.30 |
| 25 | BA | 639 | G | C4-C5-N7 | -5.07 | 108.77 | 110.80 |
| 25 | BA | 1076 | G | C2-N3-C4 | -5.07 | 109.37 | 111.90 |
| 25 | BA | 1412 | A | C4-C5-N7 | -5.07 | 108.17 | 110.70 |
| 25 | BA | 1920 | U | C5-C4-O4 | 5.07 | 128.94 | 125.90 |
| 23 | CX | 22 | G | C8-N9-C1' | 5.07 | 133.59 | 127.00 |
| 25 | DA | 2286 | A | C6-C5-N7 | -5.07 | 128.75 | 132.30 |
| 1 | CA | 287 | U | O5'-P-OP2 | -5.06 | 101.14 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | DA | 2347 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 25 | DA | 2519 | U | C5-C6-N1 | -5.06 | 120.17 | 122.70 |
| 1 | CA | 1020 | U | N1-C2-O2 | 5.06 | 126.34 | 122.80 |
| 1 | AA | 460 | G | N7-C8-N9 | 5.06 | 115.63 | 113.10 |
| 25 | BA | 2067 | C | N3-C4-C5 | 5.06 | 123.92 | 121.90 |
| 25 | BA | 179 | A | N1-C6-N6 | 5.06 | 121.64 | 118.60 |
| 25 | BA | 2549 | U | N3-C4-O4 | -5.06 | 115.86 | 119.40 |
| 25 | BA | 2627 | U | C4-C5-C6 | -5.06 | 116.66 | 119.70 |
| 25 | DA | 685 | A | OP1-P-OP2 | 5.06 | 127.19 | 119.60 |
| 25 | DA | 2063 | C | N1-C2-O2 | -5.06 | 115.86 | 118.90 |
| 25 | DA | 2627 | G | N1-C6-O6 | -5.06 | 116.86 | 119.90 |
| 25 | DA | 2042 | A | C2-N3-C4 | -5.06 | 108.07 | 110.60 |
| 25 | BA | 829 | A | C8-N9-C4 | 5.06 | 107.82 | 105.80 |
| 25 | DA | 1123 | C | N3-C2-O2 | 5.06 | 125.44 | 121.90 |
| 25 | BA | 1745 | A | C5-C6-N1 | -5.05 | 115.17 | 117.70 |
| 25 | BA | 2227 | G | N3-C4-C5 | 5.05 | 131.13 | 128.60 |
| 25 | BA | 2697 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 25 | DA | 985 | C | C5-C6-N1 | -5.05 | 118.47 | 121.00 |
| 25 | DA | 1620 | G | O5'-P-OP2 | 5.05 | 116.77 | 110.70 |
| 25 | DA | 2338 | G | C8-N9-C1' | 5.05 | 133.57 | 127.00 |
| 25 | BA | 137 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 25 | BA | 51 | A | C8-N9-C4 | -5.05 | 103.78 | 105.80 |
| 25 | BA | 107 | G | C6-C5-N7 | 5.05 | 133.43 | 130.40 |
| 25 | BA | 2397 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 1 | CA | 1028 | C | C2-N3-C4 | 5.05 | 122.43 | 119.90 |
| 1 | CA | 1224 | G | C8-N9-C4 | -5.05 | 104.38 | 106.40 |
| 23 | AX | 67 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 25 | BA | 1091 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 25 | BA | 1821 | C | P-O3'-C3' | 5.05 | 125.76 | 119.70 |
| 1 | CA | 265 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 25 | DA | 330 | A | N3-C4-C5 | 5.05 | 130.33 | 126.80 |
| 26 | BB | 93 | G | N7-C8-N9 | 5.05 | 115.62 | 113.10 |
| 25 | DA | 729 | G | C6-C5-N7 | -5.05 | 127.37 | 130.40 |
| 25 | BA | 194 | G | N7-C8-N9 | -5.05 | 110.58 | 113.10 |
| 25 | BA | 2265 | G | N9-C4-C5 | -5.05 | 103.38 | 105.40 |
| 1 | CA | 662 | G | N3-C4-N9 | 5.05 | 129.03 | 126.00 |
| 25 | DA | 90 | U | N3-C2-O2 | -5.05 | 118.67 | 122.20 |
| 25 | DA | 315 | G | O5'-P-OP1 | 5.05 | 116.76 | 110.70 |
| 25 | DA | 1189 | A | O5'-P-OP1 | 5.05 | 116.75 | 110.70 |
| 25 | BA | 990 | A | N1-C2-N3 | 5.04 | 131.82 | 129.30 |
| 25 | DA | 1022 | G | N9-C4-C5 | 5.04 | 107.42 | 105.40 |
| 25 | DA | 975 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | DA | 1899 | G | N3-C4-N9 | 5.04 | 129.03 | 126.00 |
| 25 | DA | 2298 | A | C4-C5-N7 | 5.04 | 113.22 | 110.70 |
| 25 | DA | 2440 | C | C2-N1-C1' | -5.04 | 113.25 | 118.80 |
| 1 | AA | 1131 | G | C5-C6-O6 | -5.04 | 125.58 | 128.60 |
| 23 | AX | 14 | A | C8-N9-C1' | -5.04 | 118.63 | 127.70 |
| 25 | BA | 622 | G | C8-N9-C4 | 5.04 | 108.42 | 106.40 |
| 25 | BA | 1823 | G | N3-C4-C5 | 5.04 | 131.12 | 128.60 |
| 1 | CA | 1264 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 25 | DA | 879 | G | N3-C4-C5 | -5.04 | 126.08 | 128.60 |
| 1 | AA | 340 | U | C2-N1-C1' | -5.04 | 111.65 | 117.70 |
| 6 | CF | 75 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |
| 25 | DA | 1251 | C | N3-C2-O2 | 5.04 | 125.43 | 121.90 |
| 25 | DA | 1828 | G | C5-C6-O6 | 5.04 | 131.62 | 128.60 |
| 1 | AA | 1286 | A | O5'-P-OP1 | -5.04 | 101.17 | 105.70 |
| 25 | BA | 1219 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 25 | BA | 2465 | A | N1-C6-N6 | -5.04 | 115.58 | 118.60 |
| 25 | DA | 2024 | G | C5-C6-O6 | -5.04 | 125.58 | 128.60 |
| 1 | AA | 1024 | G | C8-N9-C1' | -5.04 | 120.45 | 127.00 |
| 25 | DA | 1488 | G | N3-C4-C5 | -5.04 | 126.08 | 128.60 |
| 25 | DA | 2321 | G | C4-C5-N7 | 5.04 | 112.81 | 110.80 |
| 25 | BA | 2001 | C | C6-N1-C2 | -5.04 | 118.29 | 120.30 |
| 25 | DA | 374 | A | N1-C6-N6 | 5.04 | 121.62 | 118.60 |
| 25 | DA | 1320 | C | N1-C2-O2 | -5.04 | 115.88 | 118.90 |
| 25 | BA | 418 | G | N9-C4-C5 | -5.03 | 103.39 | 105.40 |
| 25 | DA | 1441 | G | C8-N9-C4 | 5.03 | 108.41 | 106.40 |
| 25 | BA | 666 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 25 | DA | 768 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 1 | AA | 827 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 25 | BA | 512 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 25 | BA | 2610 | A | C8-N9-C4 | 5.03 | 107.81 | 105.80 |
| 39 | BT | 103 | ARG | NE-CZ-NH1 | -5.03 | 117.78 | 120.30 |
| 1 | CA | 266 | G | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 1 | AA | 30 | U | OP2-P-O3' | 5.03 | 116.26 | 105.20 |
| 25 | BA | 1366 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 25 | DA | 1204 | A | C5-C6-N1 | -5.03 | 115.19 | 117.70 |
| 25 | DA | 1339 | G | O5'-P-OP2 | 5.03 | 116.73 | 110.70 |
| 25 | DA | 2292 | C | O5'-P-OP2 | -5.03 | 101.18 | 105.70 |
| 1 | AA | 1395 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 2 | AB | 128 | GLU | N-CA-C | -5.03 | 97.43 | 111.00 |
| 25 | BA | 1687 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 25 | BA | 2899 | C | O5'-P-OP2 | -5.03 | 101.18 | 105.70 |
| 1 | CA | 99 | U | C2-N1-C1' | -5.03 | 111.67 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1169 | A | C8-N9-C4 | -5.03 | 103.79 | 105.80 |
| 1 | AA | 59 | A | C2-N3-C4 | 5.02 | 113.11 | 110.60 |
| 1 | AA | 66 | G | C5-C6-N1 | -5.02 | 108.99 | 111.50 |
| 25 | BA | 1277 | G | N3-C4-C5 | 5.02 | 131.11 | 128.60 |
| 25 | BA | 2527 | C | C5-C4-N4 | -5.02 | 116.69 | 120.20 |
| 25 | BA | 2550 | C | N3-C4-C5 | 5.02 | 123.91 | 121.90 |
| 25 | DA | 1266 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 25 | BA | 1177 | G | N3-C2-N2 | 5.02 | 123.42 | 119.90 |
| 1 | CA | 1206 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 1 | AA | 1007 | C | C6-N1-C1' | -5.02 | 114.78 | 120.80 |
| 1 | AA | 1206 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 25 | BA | 2300 | A | N1-C6-N6 | 5.02 | 121.61 | 118.60 |
| 1 | AA | 975 | A | O4'-C1'-N9 | -5.02 | 104.19 | 108.20 |
| 25 | DA | 1259 | G | OP2-P-O3' | 5.02 | 116.24 | 105.20 |
| 1 | AA | 1502 | A | C5-N7-C8 | -5.02 | 101.39 | 103.90 |
| 25 | BA | 2579 | G | C5-N7-C8 | 5.02 | 106.81 | 104.30 |
| 25 | DA | 1004 | C | N3-C2-O2 | 5.02 | 125.41 | 121.90 |
| 25 | BA | 2843 | G | N3-C4-N9 | 5.01 | 129.01 | 126.00 |
| 1 | AA | 328 | C | O5'-P-OP1 | -5.01 | 101.19 | 105.70 |
| 25 | BA | 1823 | G | N3-C4-N9 | -5.01 | 122.99 | 126.00 |
| 1 | AA | 1335 | C | C6-N1-C2 | 5.01 | 122.30 | 120.30 |
| 25 | BA | 2451 | A | O4'-C1'-N9 | -5.01 | 104.19 | 108.20 |
| 25 | BA | 2906 | U | C2-N1-C1' | 5.01 | 123.72 | 117.70 |
| 23 | CX | 76 | A | C5-C6-N6 | -5.01 | 119.69 | 123.70 |
| 25 | DA | 389 | G | C8-N9-C4 | 5.01 | 108.41 | 106.40 |
| 25 | DA | 2689 | U | OP2-P-O3' | 5.01 | 116.23 | 105.20 |
| 25 | BA | 1417 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 25 | BA | 441 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 25 | DA | 2896 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 1 | AA | 1127 | G | N1-C2-N2 | -5.01 | 111.69 | 116.20 |
| 25 | BA | 120 | G | N1-C6-O6 | 5.01 | 122.90 | 119.90 |
| 25 | BA | 2105 | G | C8-N9-C4 | 5.01 | 108.40 | 106.40 |
| 1 | CA | 46 | G | N1-C6-O6 | 5.00 | 122.90 | 119.90 |
| 25 | DA | 1703 | G | C5-C6-O6 | -5.00 | 125.60 | 128.60 |
| 25 | BA | 26 | G | C6-C5-N7 | -5.00 | 127.40 | 130.40 |
| 25 | DA | 863 | A | OP2-P-O3' | 5.00 | 116.21 | 105.20 |
| 1 | AA | 347 | G | C8-N9-C1' | -5.00 | 120.50 | 127.00 |
| 25 | BA | 2283 | G | C4-N9-C1' | 5.00 | 133.00 | 126.50 |
| 1 | CA | 1132 | C | C5-C6-N1 | 5.00 | 123.50 | 121.00 |
| 25 | DA | 461 | C | N1-C2-O2 | -5.00 | 115.90 | 118.90 |
| 25 | DA | 1432 | C | N3-C2-O2 | 5.00 | 125.40 | 121.90 |
| 25 | DA | 1721 | G | N3-C4-C5 | -5.00 | 126.10 | 128.60 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 23 | CX | 76 | A | C1' |

All (11) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | AB | 231 | GLU | Peptide |
| 2 | AB | 8 | LYS | Peptide |
| 2 | AB | 9 | GLU | Peptide |
| 7 | AG | 79 | ARG | Peptide |
| 24 | AW | 4 | PRO | Peptide |
| 50 | B4 | 59 | PHE | Peptide |
| 38 | BS | 58 | LEU | Peptide |
| 45 | BZ | 136 | PHE | Peptide |
| 4 | CD | 45 | GLN | Peptide |
| 24 | CW | 9 | MVA | Peptide |
| 27 | DD | 274 | ARG | 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 | 32196 | 0 | 16251 | 809 | 0 |
| 1 | CA | 32312 | 0 | 16307 | 915 | 0 |
| 2 | AB | 1846 | 0 | 1867 | 109 | 0 |
| 2 | CB | 1825 | 0 | 1828 | 119 | 0 |
| 3 | AC | 1552 | 0 | 1546 | 59 | 0 |
| 3 | CC | 1542 | 0 | 1517 | 66 | 0 |
| 4 | AD | 1659 | 0 | 1676 | 99 | 0 |
| 4 | CD | 1674 | 0 | 1714 | 78 | 0 |
| 5 | AE | 1129 | 0 | 1185 | 50 | 0 |
| 5 | CE | 1133 | 0 | 1191 | 45 | 0 |
| 6 | AF | 806 | 0 | 793 | 33 | 0 |
| 6 | CF | 816 | 0 | 808 | 27 | 0 |
| 7 | AG | 1231 | 0 | 1238 | 35 | 0 |
| 7 | CG | 1235 | 0 | 1249 | 56 | 0 |
| 8 | AH | 1088 | 0 | 1126 | 48 | 0 |
| 8 | CH | 1088 | 0 | 1126 | 46 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9 | AI | 983 | 0 | 986 | 54 | 0 |
| 9 | CI | 978 | 0 | 966 | 57 | 0 |
| 10 | AJ | 709 | 0 | 650 | 35 | 0 |
| 10 | CJ | 714 | 0 | 672 | 47 | 0 |
| 11 | AK | 829 | 0 | 825 | 19 | 0 |
| 11 | CK | 833 | 0 | 836 | 29 | 0 |
| 12 | AL | 930 | 0 | 980 | 28 | 0 |
| 12 | CL | 930 | 0 | 980 | 34 | 0 |
| 13 | AM | 958 | 0 | 1002 | 25 | 0 |
| 13 | CM | 950 | 0 | 988 | 56 | 0 |
| 14 | AN | 492 | 0 | 529 | 26 | 0 |
| 14 | CN | 492 | 0 | 529 | 29 | 0 |
| 15 | AO | 728 | 0 | 760 | 16 | 0 |
| 15 | CO | 728 | 0 | 760 | 27 | 0 |
| 16 | AP | 681 | 0 | 697 | 29 | 0 |
| 16 | CP | 677 | 0 | 686 | 28 | 0 |
| 17 | AQ | 823 | 0 | 891 | 21 | 0 |
| 17 | CQ | 823 | 0 | 891 | 19 | 0 |
| 18 | AR | 555 | 0 | 618 | 17 | 0 |
| 18 | CR | 555 | 0 | 618 | 27 | 0 |
| 19 | AS | 652 | 0 | 662 | 36 | 0 |
| 19 | CS | 646 | 0 | 644 | 56 | 0 |
| 20 | AT | 728 | 0 | 798 | 30 | 0 |
| 20 | CT | 727 | 0 | 796 | 28 | 0 |
| 21 | AU | 199 | 0 | 208 | 5 | 0 |
| 21 | CU | 199 | 0 | 208 | 7 | 0 |
| 22 | AV | 114 | 0 | 54 | 0 | 0 |
| 22 | CV | 113 | 0 | 54 | 0 | 0 |
| 23 | AX | 1623 | 0 | 823 | 18 | 0 |
| 23 | CX | 1623 | 0 | 824 | 24 | 0 |
| 24 | AW | 93 | 0 | 84 | 9 | 0 |
| 24 | CW | 93 | 0 | 84 | 14 | 0 |
| 25 | BA | 58834 | 0 | 29667 | 785 | 0 |
| 25 | DA | 58458 | 0 | 29482 | 1100 | 0 |
| 26 | BB | 2573 | 0 | 1306 | 38 | 0 |
| 26 | DB | 2573 | 0 | 1306 | 54 | 0 |
| 27 | BD | 2136 | 0 | 2218 | 64 | 0 |
| 27 | DD | 2136 | 0 | 2218 | 74 | 0 |
| 28 | BE | 1559 | 0 | 1618 | 38 | 0 |
| 28 | DE | 1559 | 0 | 1618 | 60 | 0 |
| 29 | BF | 1584 | 0 | 1625 | 46 | 0 |
| 29 | DF | 1580 | 0 | 1619 | 69 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30 | BG | 1425 | 0 | 1443 | 45 | 0 |
| 30 | DG | 1424 | 0 | 1434 | 82 | 0 |
| 31 | BH | 1330 | 0 | 1407 | 33 | 0 |
| 31 | DH | 1330 | 0 | 1407 | 52 | 0 |
| 32 | BI | 1085 | 0 | 1114 | 42 | 0 |
| 32 | DI | 1061 | 0 | 1080 | 31 | 0 |
| 33 | BN | 1117 | 0 | 1183 | 17 | 0 |
| 33 | DN | 1117 | 0 | 1184 | 26 | 0 |
| 34 | BO | 933 | 0 | 996 | 24 | 0 |
| 34 | DO | 933 | 0 | 996 | 36 | 0 |
| 35 | BP | 1135 | 0 | 1212 | 37 | 0 |
| 35 | DP | 1135 | 0 | 1211 | 46 | 0 |
| 36 | BQ | 1122 | 0 | 1179 | 38 | 0 |
| 36 | DQ | 1122 | 0 | 1179 | 47 | 0 |
| 37 | BR | 968 | 0 | 1033 | 24 | 0 |
| 37 | DR | 968 | 0 | 1032 | 30 | 0 |
| 38 | BS | 877 | 0 | 938 | 25 | 0 |
| 38 | DS | 870 | 0 | 923 | 47 | 0 |
| 39 | BT | 1091 | 0 | 1151 | 28 | 0 |
| 39 | DT | 1083 | 0 | 1136 | 36 | 0 |
| 40 | BU | 959 | 0 | 1019 | 26 | 0 |
| 40 | DU | 959 | 0 | 1019 | 37 | 0 |
| 41 | BV | 771 | 0 | 830 | 11 | 0 |
| 41 | DV | 771 | 0 | 830 | 23 | 0 |
| 42 | BW | 886 | 0 | 940 | 9 | 0 |
| 42 | DW | 886 | 0 | 940 | 17 | 0 |
| 43 | BX | 750 | 0 | 814 | 20 | 0 |
| 43 | DX | 750 | 0 | 814 | 25 | 0 |
| 44 | BY | 806 | 0 | 881 | 25 | 0 |
| 44 | DY | 806 | 0 | 881 | 21 | 0 |
| 45 | BZ | 1349 | 0 | 1355 | 47 | 0 |
| 45 | DZ | 1360 | 0 | 1363 | 48 | 0 |
| 46 | B0 | 653 | 0 | 674 | 25 | 0 |
| 46 | D0 | 653 | 0 | 674 | 23 | 0 |
| 47 | B1 | 755 | 0 | 826 | 19 | 0 |
| 47 | D1 | 755 | 0 | 826 | 26 | 0 |
| 48 | B2 | 588 | 0 | 643 | 18 | 0 |
| 48 | D2 | 588 | 0 | 643 | 20 | 0 |
| 49 | B3 | 469 | 0 | 518 | 17 | 0 |
| 49 | D3 | 464 | 0 | 514 | 12 | 0 |
| 50 | B4 | 551 | 0 | 532 | 38 | 0 |
| 50 | D4 | 531 | 0 | 502 | 32 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 51 | B5 | 455 | 0 | 465 | 13 | 0 |
| 51 | D5 | 455 | 0 | 465 | 11 | 0 |
| 52 | B6 | 453 | 0 | 473 | 10 | 0 |
| 52 | D6 | 449 | 0 | 469 | 10 | 0 |
| 53 | B7 | 418 | 0 | 466 | 9 | 0 |
| 53 | D7 | 418 | 0 | 467 | 9 | 0 |
| 54 | B8 | 511 | 0 | 571 | 27 | 0 |
| 54 | D8 | 517 | 0 | 582 | 27 | 0 |
| 55 | B9 | 307 | 0 | 335 | 5 | 0 |
| 55 | D9 | 307 | 0 | 335 | 10 | 0 |
| 56 | AA | 221 | 0 | 0 | 0 | 0 |
| 56 | AD | 1 | 0 | 0 | 0 | 0 |
| 56 | AF | 1 | 0 | 0 | 0 | 0 |
| 56 | AK | 1 | 0 | 0 | 0 | 0 |
| 56 | AM | 1 | 0 | 0 | 0 | 0 |
| 56 | AN | 2 | 0 | 0 | 0 | 0 |
| 56 | AV | 1 | 0 | 0 | 0 | 0 |
| 56 | AX | 9 | 0 | 0 | 0 | 0 |
| 56 | B0 | 4 | 0 | 0 | 0 | 0 |
| 56 | B1 | 1 | 0 | 0 | 0 | 0 |
| 56 | B2 | 1 | 0 | 0 | 0 | 0 |
| 56 | B3 | 3 | 0 | 0 | 0 | 0 |
| 56 | B4 | 1 | 0 | 0 | 0 | 0 |
| 56 | B5 | 1 | 0 | 0 | 0 | 0 |
| 56 | B7 | 4 | 0 | 0 | 0 | 0 |
| 56 | B8 | 3 | 0 | 0 | 0 | 0 |
| 56 | B9 | 1 | 0 | 0 | 0 | 0 |
| 56 | BA | 738 | 0 | 0 | 0 | 0 |
| 56 | BB | 18 | 0 | 0 | 0 | 0 |
| 56 | BD | 12 | 0 | 0 | 0 | 0 |
| 56 | BE | 10 | 0 | 0 | 0 | 0 |
| 56 | BF | 8 | 0 | 0 | 0 | 0 |
| 56 | BG | 4 | 0 | 0 | 0 | 0 |
| 56 | BN | 6 | 0 | 0 | 0 | 0 |
| 56 | BO | 1 | 0 | 0 | 0 | 0 |
| 56 | BP | 4 | 0 | 0 | 0 | 0 |
| 56 | BQ | 5 | 0 | 0 | 0 | 0 |
| 56 | BR | 4 | 0 | 0 | 0 | 0 |
| 56 | BU | 8 | 0 | 0 | 0 | 0 |
| 56 | BV | 4 | 0 | 0 | 0 | 0 |
| 56 | BW | 5 | 0 | 0 | 0 | 0 |
| 56 | BX | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56 | BY | 1 | 0 | 0 | 0 | 0 |
| 56 | BZ | 1 | 0 | 0 | 0 | 0 |
| 56 | CA | 172 | 0 | 0 | 0 | 0 |
| 56 | CE | 2 | 0 | 0 | 0 | 0 |
| 56 | CF | 1 | 0 | 0 | 0 | 0 |
| 56 | CQ | 1 | 0 | 0 | 0 | 0 |
| 56 | CT | 1 | 0 | 0 | 0 | 0 |
| 56 | CX | 3 | 0 | 0 | 0 | 0 |
| 56 | D0 | 1 | 0 | 0 | 0 | 0 |
| 56 | D3 | 1 | 0 | 0 | 0 | 0 |
| 56 | D5 | 2 | 0 | 0 | 0 | 0 |
| 56 | D8 | 1 | 0 | 0 | 0 | 0 |
| 56 | DA | 653 | 0 | 0 | 0 | 0 |
| 56 | DB | 12 | 0 | 0 | 0 | 0 |
| 56 | DD | 8 | 0 | 0 | 0 | 0 |
| 56 | DE | 6 | 0 | 0 | 0 | 0 |
| 56 | DF | 6 | 0 | 0 | 0 | 0 |
| 56 | DG | 1 | 0 | 0 | 0 | 0 |
| 56 | DN | 1 | 0 | 0 | 0 | 0 |
| 56 | DO | 1 | 0 | 0 | 0 | 0 |
| 56 | DQ | 5 | 0 | 0 | 0 | 0 |
| 56 | DR | 2 | 0 | 0 | 0 | 0 |
| 56 | DV | 4 | 0 | 0 | 0 | 0 |
| 56 | DW | 2 | 0 | 0 | 0 | 0 |
| 56 | DY | 1 | 0 | 0 | 0 | 0 |
| 57 | AD | 8 | 0 | 0 | 1 | 0 |
| 57 | CD | 8 | 0 | 0 | 1 | 0 |
| 58 | AN | 1 | 0 | 0 | 0 | 0 |
| 58 | B4 | 1 | 0 | 0 | 0 | 0 |
| 58 | B5 | 1 | 0 | 0 | 0 | 0 |
| 58 | B6 | 1 | 0 | 0 | 0 | 0 |
| 58 | B9 | 1 | 0 | 0 | 0 | 0 |
| 58 | BY | 1 | 0 | 0 | 0 | 0 |
| 58 | CN | 1 | 0 | 0 | 0 | 0 |
| 58 | D4 | 1 | 0 | 0 | 0 | 0 |
| 58 | D5 | 1 | 0 | 0 | 0 | 0 |
| 58 | D6 | 1 | 0 | 0 | 0 | 0 |
| 58 | D9 | 1 | 0 | 0 | 0 | 0 |
| 58 | DY | 1 | 0 | 0 | 0 | 0 |
| 59 | AX | 10 | 0 | 10 | 0 | 0 |
| 59 | CX | 10 | 0 | 10 | 2 | 0 |
| 60 | BA | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 60 | DA | 1 | 0 | 0 | 0 | 0 |
| 61 | AA | 148 | 0 | 0 | 27 | 0 |
| 61 | AD | 1 | 0 | 0 | 0 | 0 |
| 61 | AE | 3 | 0 | 0 | 0 | 0 |
| 61 | AJ | 1 | 0 | 0 | 0 | 0 |
| 61 | AL | 1 | 0 | 0 | 0 | 0 |
| 61 | AP | 1 | 0 | 0 | 0 | 0 |
| 61 | AU | 1 | 0 | 0 | 0 | 0 |
| 61 | AV | 1 | 0 | 0 | 0 | 0 |
| 61 | AX | 1 | 0 | 0 | 0 | 0 |
| 61 | B0 | 4 | 0 | 0 | 0 | 0 |
| 61 | B1 | 2 | 0 | 0 | 0 | 0 |
| 61 | B5 | 3 | 0 | 0 | 1 | 0 |
| 61 | B7 | 1 | 0 | 0 | 1 | 0 |
| 61 | B8 | 8 | 0 | 0 | 1 | 0 |
| 61 | BA | 1092 | 0 | 0 | 113 | 0 |
| 61 | BB | 26 | 0 | 0 | 0 | 0 |
| 61 | BD | 8 | 0 | 0 | 1 | 0 |
| 61 | BE | 9 | 0 | 0 | 4 | 0 |
| 61 | BF | 4 | 0 | 0 | 0 | 0 |
| 61 | BG | 1 | 0 | 0 | 0 | 0 |
| 61 | BN | 3 | 0 | 0 | 0 | 0 |
| 61 | BO | 2 | 0 | 0 | 0 | 0 |
| 61 | BP | 15 | 0 | 0 | 3 | 0 |
| 61 | BQ | 3 | 0 | 0 | 1 | 0 |
| 61 | BR | 1 | 0 | 0 | 0 | 0 |
| 61 | BT | 1 | 0 | 0 | 0 | 0 |
| 61 | BU | 4 | 0 | 0 | 0 | 0 |
| 61 | BV | 2 | 0 | 0 | 0 | 0 |
| 61 | BW | 2 | 0 | 0 | 0 | 0 |
| 61 | BX | 4 | 0 | 0 | 1 | 0 |
| 61 | CA | 187 | 0 | 0 | 24 | 0 |
| 61 | CE | 2 | 0 | 0 | 0 | 0 |
| 61 | CN | 1 | 0 | 0 | 0 | 0 |
| 61 | CT | 1 | 0 | 0 | 0 | 0 |
| 61 | CX | 2 | 0 | 0 | 0 | 0 |
| 61 | D0 | 5 | 0 | 0 | 1 | 0 |
| 61 | D1 | 1 | 0 | 0 | 0 | 0 |
| 61 | D7 | 2 | 0 | 0 | 0 | 0 |
| 61 | D8 | 4 | 0 | 0 | 0 | 0 |
| 61 | DA | 902 | 0 | 0 | 120 | 0 |
| 61 | DB | 7 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61 | DD | 8 | 0 | 0 | 0 | 0 |
| 61 | DE | 13 | 0 | 0 | 1 | 0 |
| 61 | DF | 5 | 0 | 0 | 0 | 0 |
| 61 | DO | 1 | 0 | 0 | 0 | 0 |
| 61 | DP | 14 | 0 | 0 | 0 | 0 |
| 61 | DQ | 3 | 0 | 0 | 1 | 0 |
| 61 | DU | 4 | 0 | 0 | 0 | 0 |
| 61 | DV | 1 | 0 | 0 | 0 | 0 |
| 61 | DX | 2 | 0 | 0 | 0 | 0 |
| 61 | DY | 2 | 0 | 0 | 0 | 0 |
| All | All | 286321 | 0 | 191126 | 6372 | 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 14.

All (6372) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1002:G:H1 | 1:CA:1038:C:N4 | 1.42 | 1.16 |
| 1:AA:348:G:H2' | 1:AA:349:A:H5' | 1.36 | 1.04 |
| 1:AA:1125:U:N3 | 1:AA:1127:G:N7 | 2.06 | 1.03 |
| 39:BT:16:ARG:NH2 | 39:BT:83:ILE:O | 1.92 | 1.02 |
| 2:CB:185:ILE:HG22 | 2:CB:199:TYR:HB2 | 1.40 | 1.02 |
| 2:CB:16:HIS:HB2 | 2:CB:204:ASN:HB3 | 1.41 | 1.01 |
| 1:CA:1162:C:H42 | 1:CA:1174:G:H1 | 1.02 | 1.00 |
| 25:DA:1019:U:HO2' | 25:DA:1021:A:H2 | 1.01 | 1.00 |
| 1:AA:1129:C:N4 | 1:AA:1143:G:H1 | 1.59 | 0.99 |
| 2:AB:16:HIS:HB2 | 2:AB:204:ASN:HB3 | 1.43 | 0.98 |
| 25:DA:2206:G:H3' | 25:DA:2207:G:C8 | 1.98 | 0.98 |
| 1:CA:1007:C:N3 | 1:CA:1022:G:N2 | 2.12 | 0.97 |
| 30:BG:41:GLN:HG3 | 30:BG:60:LEU:HD11 | 1.48 | 0.96 |
| 38:DS:35:ILE:HD11 | 38:DS:101:LEU:HD12 | 1.47 | 0.96 |
| 1:CA:998:G:H1 | 1:CA:1043:C:H42 | 1.14 | 0.95 |
| 25:BA:9:U:H3 | 25:BA:2641:A:H2 | 1.15 | 0.95 |
| 30:BG:66:GLN:HG2 | 50:B4:1:MET:HE3 | 1.44 | 0.95 |
| 10:CJ:8:LEU:HB2 | 10:CJ:70:ARG:HB2 | 1.49 | 0.95 |
| 1:CA:1163:C:H42 | 1:CA:1173:G:H1 | 1.07 | 0.94 |
| 25:DA:1689:A:H62 | 25:DA:1698:A:H2 | 1.15 | 0.93 |
| 25:BA:1065:U:HO2' | 25:BA:1067:A:H2 | 1.05 | 0.93 |
| 25:DA:1798:U:H5' | 27:DD:259:THR:HG22 | 1.50 | 0.92 |
| 35:BP:126:VAL:HG12 | 35:BP:148:LEU:HD22 | 1.49 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1002:G:N2 | 1:CA:1038:C:N3 | 2.16 | 0.92 |
| 1:AA:1129:C:H42 | 1:AA:1143:G:H1 | 0.95 | 0.91 |
| 25:DA:1693:U:O2' | 27:DD:14:ARG:NH2 | 2.02 | 0.91 |
| 25:DA:1648:C:OP1 | 61:DA:4111:HOH:O | 1.88 | 0.91 |
| 1:CA:999:C:N4 | 1:CA:1042:G:N1 | 2.17 | 0.91 |
| 26:DB:22:U:H3 | 26:DB:61:G:H1 | 1.18 | 0.91 |
| 1:CA:1007:C:N4 | 1:CA:1022:G:N1 | 2.19 | 0.91 |
| 1:AA:201:C:H42 | 1:AA:216:G:H1 | 1.11 | 0.90 |
| 25:DA:1204:A:H2 | 25:DA:1241:A:H62 | 1.19 | 0.90 |
| 39:DT:16:ARG:NH2 | 39:DT:83:ILE:O | 2.02 | 0.90 |
| 25:BA:1829:U:H5' | 27:BD:259:THR:HG22 | 1.52 | 0.90 |
| 28:BE:110:GLY:O | 61:BE:406:HOH:O | 1.89 | 0.90 |
| 50:D4:53:GLU:HG2 | 50:D4:55:ARG:H | 1.34 | 0.90 |
| 1:CA:1153:C:H42 | 1:CA:1154:G:H21 | 1.17 | 0.90 |
| 25:DA:526:A:OP1 | 61:DA:4572:HOH:O | 1.89 | 0.90 |
| 25:DA:195:A:N7 | 61:DA:4175:HOH:O | 2.04 | 0.89 |
| 10:AJ:35:SER:HB3 | 10:AJ:73:ASP:HB2 | 1.54 | 0.89 |
| 44:BY:54:LYS:HA | 44:BY:56:PRO:HD3 | 1.52 | 0.89 |
| 25:DA:566:U:H5'' | 35:DP:29:LYS:HE3 | 1.55 | 0.88 |
| 25:DA:2615:U:OP1 | 61:DA:3943:HOH:O | 1.91 | 0.88 |
| 2:AB:69:LEU:HB3 | 2:AB:162:ILE:HG22 | 1.53 | 0.88 |
| 25:DA:740:U:OP2 | 61:DA:4117:HOH:O | 1.92 | 0.88 |
| 11:AK:79:SER:HA | 11:AK:104:GLN:HB2 | 1.55 | 0.88 |
| 1:CA:1163:C:N4 | 1:CA:1173:G:H1 | 1.72 | 0.88 |
| 1:CA:999:C:N4 | 1:CA:1042:G:C6 | 2.42 | 0.88 |
| 1:CA:542:G:OP1 | 4:CD:10:ARG:NH2 | 2.06 | 0.88 |
| 46:D0:11:ARG:O | 46:D0:14:ARG:NH2 | 2.05 | 0.87 |
| 1:CA:563:A:N6 | 61:CA:4065:HOH:O | 2.06 | 0.87 |
| 9:CI:9:ARG:HG2 | 9:CI:14:VAL:HG12 | 1.56 | 0.87 |
| 1:CA:1318:A:H5'' | 19:CS:3:ARG:HH22 | 1.37 | 0.86 |
| 25:DA:981:A:OP1 | 61:DA:4033:HOH:O | 1.92 | 0.86 |
| 16:AP:53:VAL:HG13 | 16:AP:79:VAL:HG13 | 1.57 | 0.86 |
| 25:BA:1395:A:OP1 | 61:BA:4761:HOH:O | 1.93 | 0.86 |
| 25:BA:1686:U:OP1 | 61:BA:4272:HOH:O | 1.93 | 0.86 |
| 25:BA:537:G:N7 | 61:BA:4621:HOH:O | 2.07 | 0.86 |
| 25:DA:2592:G:OP1 | 61:DA:4137:HOH:O | 1.93 | 0.86 |
| 25:DA:323:G:HO2' | 25:DA:1205:U:H3 | 1.23 | 0.86 |
| 25:DA:1268:A:OP1 | 61:DA:3940:HOH:O | 1.93 | 0.86 |
| 25:DA:2807:G:N1 | 25:DA:2893:G:O6 | 2.09 | 0.86 |
| 25:DA:1153:C:OP1 | 40:DU:92:ARG:NH1 | 2.09 | 0.86 |
| 46:B0:11:ARG:O | 46:B0:14:ARG:NH2 | 2.08 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:B3:8:LEU:HD13 | 49:B3:31:LEU:HD23 | 1.58 | 0.85 |
| 29:BF:185:ASP:HA | 29:BF:188:ARG:HD3 | 1.54 | 0.85 |
| 12:AL:36:VAL:HG23 | 24:AW:10:2QY:H89 | 1.57 | 0.85 |
| 13:AM:2:ALA:N | 13:AM:8:GLU:OE1 | 2.09 | 0.85 |
| 1:CA:1493:A:H1' | 25:DA:1913:A:H62 | 1.39 | 0.85 |
| 25:DA:770:G:OP2 | 61:DA:4148:HOH:O | 1.94 | 0.85 |
| 45:DZ:69:THR:HG22 | 45:DZ:90:VAL:HA | 1.57 | 0.85 |
| 25:BA:656:A:OP1 | 35:BP:65:ARG:NH1 | 2.09 | 0.85 |
| 25:BA:303:C:H42 | 25:BA:385:G:H1 | 1.24 | 0.85 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:H1 | 1.24 | 0.85 |
| 4:CD:122:ARG:NH1 | 4:CD:134:ASP:O | 2.09 | 0.85 |
| 25:DA:2879:C:OP2 | 61:DA:4045:HOH:O | 1.95 | 0.85 |
| 25:BA:2720:G:O6 | 61:BA:4017:HOH:O | 1.93 | 0.85 |
| 25:BA:1500:A:OP2 | 61:BA:3907:HOH:O | 1.95 | 0.85 |
| 2:AB:21:ARG:HB3 | 2:AB:39:ILE:HA | 1.57 | 0.84 |
| 13:CM:122:LYS:HD3 | 13:CM:123:ALA:H | 1.41 | 0.84 |
| 25:BA:894:U:O4 | 25:BA:978:A:N6 | 2.10 | 0.84 |
| 1:CA:1162:C:N4 | 1:CA:1174:G:H1 | 1.74 | 0.84 |
| 1:CA:656:C:O2' | 15:CO:28:GLN:NE2 | 2.09 | 0.84 |
| 4:AD:155:LEU:HB3 | 4:AD:158:ILE:HD11 | 1.59 | 0.84 |
| 25:BA:1577:C:O2' | 25:BA:1578:C:O5' | 1.96 | 0.84 |
| 25:DA:1271:G:OP2 | 61:DA:4112:HOH:O | 1.96 | 0.84 |
| 25:DA:1021:A:H62 | 25:DA:1141:U:H3 | 1.22 | 0.84 |
| 8:CH:51:VAL:HG11 | 8:CH:60:ARG:HH12 | 1.40 | 0.84 |
| 25:DA:2632:A:HO2' | 25:DA:2811:G:HO2' | 1.17 | 0.84 |
| 25:DA:301:G:OP2 | 44:DY:84:ARG:NH2 | 2.11 | 0.84 |
| 1:AA:559:A:OP1 | 5:AE:126:ARG:NH2 | 2.11 | 0.83 |
| 25:BA:1736:A:H62 | 25:BA:1745:A:H2 | 1.24 | 0.83 |
| 1:CA:1122:U:O4 | 1:CA:1151:A:N1 | 2.11 | 0.83 |
| 1:AA:1314:C:OP2 | 19:AS:4:SER:OG | 1.94 | 0.83 |
| 4:AD:149:ALA:HB3 | 4:AD:152:SER:HB2 | 1.60 | 0.83 |
| 25:BA:2587:C:OP2 | 61:BA:4081:HOH:O | 1.96 | 0.83 |
| 30:DG:113:ARG:NH1 | 30:DG:139:LEU:O | 2.12 | 0.83 |
| 32:BI:129:THR:HG22 | 32:BI:139:GLN:HE22 | 1.42 | 0.83 |
| 1:CA:999:C:C4 | 1:CA:1042:G:N1 | 2.47 | 0.83 |
| 1:CA:599:C:H2' | 1:CA:600:C:H5'' | 1.61 | 0.83 |
| 15:CO:54:ARG:NH1 | 15:CO:58:MET:SD | 2.51 | 0.83 |
| 1:AA:166:G:H2' | 1:AA:167:G:C8 | 2.14 | 0.83 |
| 30:DG:11:TYR:CZ | 30:DG:16:ARG:HD3 | 2.14 | 0.83 |
| 25:BA:2585:C:OP1 | 61:BA:4081:HOH:O | 1.97 | 0.82 |
| 1:CA:1348:U:H4' | 9:CI:120:ARG:HD2 | 1.61 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DP:96:THR:H | 35:DP:99:LEU:HD21 | 1.44 | 0.82 |
| 25:DA:1030:G:OP2 | 36:DQ:128:LYS:NZ | 2.11 | 0.82 |
| 36:DQ:81:VAL:HB | 46:D0:7:LEU:HD21 | 1.59 | 0.82 |
| 1:CA:64:G:H4' | 1:CA:65:U:H3' | 1.61 | 0.82 |
| 1:CA:972:C:OP1 | 61:CA:4184:HOH:O | 1.95 | 0.82 |
| 25:DA:2748:A:H5' | 31:DH:4:ILE:HD12 | 1.59 | 0.82 |
| 46:D0:53:MET:HG3 | 46:D0:59:LEU:HD23 | 1.61 | 0.82 |
| 16:CP:1:MET:SD | 16:CP:3:LYS:NZ | 2.51 | 0.82 |
| 1:CA:1492:A:N3 | 25:DA:1913:A:N6 | 2.28 | 0.82 |
| 31:DH:98:LEU:HD22 | 31:DH:125:VAL:HG23 | 1.62 | 0.82 |
| 2:CB:178:ARG:HH22 | 8:CH:68:ARG:HH12 | 1.25 | 0.82 |
| 1:AA:1158:C:H5 | 1:AA:1181:G:H1 | 1.26 | 0.82 |
| 1:CA:1125:U:O2' | 1:CA:1126:U:H2' | 1.79 | 0.82 |
| 32:DI:72:LEU:HD21 | 32:DI:107:VAL:HG11 | 1.60 | 0.82 |
| 3:AC:134:ILE:HD11 | 3:AC:153:VAL:HG23 | 1.62 | 0.82 |
| 1:CA:1003:G:N2 | 1:CA:1025:U:O4 | 2.13 | 0.82 |
| 25:BA:237:G:OP1 | 61:BA:4880:HOH:O | 1.96 | 0.81 |
| 1:CA:406:G:H5' | 4:CD:5:ILE:HD11 | 1.59 | 0.81 |
| 23:CX:50:U:H3 | 23:CX:64:G:H1 | 1.28 | 0.81 |
| 1:AA:189(B):C:N4 | 1:AA:189(I):G:O6 | 2.11 | 0.81 |
| 1:CA:664:G:OP1 | 18:CR:64:ARG:NH2 | 2.13 | 0.81 |
| 51:D5:16:ARG:NH1 | 51:D5:17:ASP:OD1 | 2.12 | 0.81 |
| 27:DD:71:ASP:HB2 | 27:DD:103:ARG:HH22 | 1.45 | 0.81 |
| 25:DA:2243:U:OP1 | 61:DA:4350:HOH:O | 1.98 | 0.81 |
| 25:BA:1503:G:OP2 | 61:BA:3908:HOH:O | 1.99 | 0.81 |
| 38:BS:59:LYS:HE3 | 38:BS:60:GLY:H | 1.44 | 0.81 |
| 1:CA:376:G:H5'' | 16:CP:5:ARG:HD3 | 1.63 | 0.81 |
| 1:CA:1007:C:N4 | 1:CA:1022:G:H1 | 1.77 | 0.81 |
| 2:CB:15:VAL:HG21 | 2:CB:213:LEU:HD12 | 1.62 | 0.81 |
| 1:CA:922:G:H4' | 5:CE:20:GLN:HA | 1.61 | 0.81 |
| 25:DA:20:C:OP1 | 40:DU:22:LYS:NZ | 2.12 | 0.81 |
| 19:AS:50:ALA:HB1 | 19:AS:57:HIS:HB3 | 1.63 | 0.81 |
| 25:BA:1683:C:OP2 | 61:BA:4524:HOH:O | 1.99 | 0.81 |
| 25:DA:1782:C:OP1 | 61:DA:4383:HOH:O | 1.99 | 0.81 |
| 25:BA:1462:G:N2 | 25:BA:1629:C:O2 | 2.11 | 0.81 |
| 26:BB:42:C:OP1 | 30:BG:67:LYS:NZ | 2.13 | 0.81 |
| 25:BA:1036:A:OP2 | 61:BA:4503:HOH:O | 1.99 | 0.80 |
| 2:CB:16:HIS:HB3 | 2:CB:210:SER:HB3 | 1.62 | 0.80 |
| 1:AA:1124:G:O2' | 1:AA:1145:C:N4 | 2.14 | 0.80 |
| 1:AA:1414:U:H3 | 1:AA:1486:G:H1 | 1.28 | 0.80 |
| 23:CX:4:G:H1 | 23:CX:69:C:H42 | 1.28 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:570:G:O6 | 61:DA:4475:HOH:O | 1.99 | 0.80 |
| 1:CA:608:A:OP2 | 61:CA:4182:HOH:O | 1.99 | 0.80 |
| 1:CA:768:A:OP2 | 61:CA:4023:HOH:O | 1.98 | 0.80 |
| 1:CA:953:G:H5' | 1:CA:965:A:H61 | 1.47 | 0.80 |
| 1:CA:975:A:H4' | 1:CA:976:G:H5'' | 1.63 | 0.80 |
| 25:DA:2022:U:OP1 | 61:DA:4084:HOH:O | 1.99 | 0.80 |
| 1:AA:1304:G:OP2 | 61:AA:4087:HOH:O | 1.97 | 0.80 |
| 1:CA:1318:A:OP1 | 19:CS:3:ARG:NH1 | 2.15 | 0.80 |
| 25:DA:198:C:OP2 | 61:DA:4175:HOH:O | 1.99 | 0.80 |
| 1:AA:1183:A:O2' | 1:AA:1184:G:OP1 | 2.00 | 0.80 |
| 2:CB:80:ILE:HD11 | 2:CB:212:GLN:HA | 1.62 | 0.80 |
| 1:AA:421:U:O2' | 1:AA:423:G:N7 | 2.14 | 0.80 |
| 25:BA:238:C:O2 | 54:B8:12:LYS:NZ | 2.14 | 0.80 |
| 25:DA:1352:U:OP1 | 61:DA:3785:HOH:O | 1.98 | 0.80 |
| 25:DA:2052:G:O2' | 61:DA:3729:HOH:O | 1.99 | 0.80 |
| 9:AI:64:THR:HG23 | 9:AI:66:ARG:HH21 | 1.47 | 0.80 |
| 25:BA:1694:G:OP1 | 61:BA:4516:HOH:O | 1.99 | 0.80 |
| 1:CA:1030(A):G:N1 | 1:CA:1030(D):A:OP2 | 2.13 | 0.80 |
| 1:CA:444:C:H2' | 1:CA:445:G:H8 | 1.48 | 0.80 |
| 25:DA:2037:G:O6 | 61:DA:4103:HOH:O | 2.00 | 0.80 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:H1 | 1.25 | 0.79 |
| 1:AA:166:G:H2' | 1:AA:167:G:H8 | 1.47 | 0.79 |
| 25:BA:2297:C:OP2 | 52:B6:6:ARG:NH1 | 2.16 | 0.79 |
| 29:BF:18:ARG:NH2 | 29:BF:127:GLU:OE1 | 2.14 | 0.79 |
| 2:AB:16:HIS:HB3 | 2:AB:210:SER:HB2 | 1.64 | 0.79 |
| 1:AA:509:A:OP2 | 61:AA:4088:HOH:O | 2.01 | 0.79 |
| 35:BP:50:ARG:HH21 | 54:B8:7:HIS:HD2 | 1.28 | 0.79 |
| 1:CA:673:G:H2' | 1:CA:674:G:C8 | 2.16 | 0.79 |
| 28:DE:47:VAL:HG11 | 28:DE:86:PRO:HD2 | 1.65 | 0.79 |
| 29:BF:53:THR:HG23 | 29:BF:55:GLY:H | 1.48 | 0.79 |
| 20:CT:57:ARG:HH22 | 20:CT:100:ILE:HD12 | 1.46 | 0.79 |
| 1:AA:1145:C:H4' | 1:AA:1146:A:H5' | 1.65 | 0.79 |
| 25:BA:831:A:OP2 | 61:BA:4454:HOH:O | 1.99 | 0.79 |
| 35:BP:36:LYS:O | 61:BP:304:HOH:O | 1.99 | 0.79 |
| 30:DG:161:THR:HG22 | 30:DG:163:ALA:H | 1.45 | 0.79 |
| 1:AA:656:C:O2' | 15:AO:28:GLN:NE2 | 2.15 | 0.79 |
| 1:AA:1492:A:N3 | 25:BA:1935:A:N6 | 2.31 | 0.79 |
| 2:AB:16:HIS:CG | 2:AB:17:PHE:H | 2.01 | 0.79 |
| 25:BA:2299:A:H62 | 25:BA:2356:U:H3 | 1.28 | 0.79 |
| 25:BA:2804:C:H2' | 25:BA:2805:G:H8 | 1.47 | 0.79 |
| 1:AA:165:C:H2' | 1:AA:166:G:C8 | 2.18 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:BA:241:G:OP1 | 35:BP:50:ARG:NH1 | 2.16 | 0.79 |
| 30:BG:161:THR:HG22 | 30:BG:163:ALA:H | 1.48 | 0.79 |
| 1:CA:939:G:H1 | 1:CA:1344:C:H42 | 1.27 | 0.79 |
| 2:CB:15:VAL:HG13 | 2:CB:209:ARG:HB3 | 1.65 | 0.79 |
| 3:AC:15:THR:HG21 | 3:AC:181:ASN:HA | 1.64 | 0.79 |
| 25:BA:1001:G:O6 | 61:BA:3865:HOH:O | 2.00 | 0.78 |
| 28:BE:105:THR:OG1 | 28:BE:199:ARG:NH2 | 2.16 | 0.78 |
| 1:AA:97:G:O2' | 1:AA:98:G:O4' | 2.00 | 0.78 |
| 25:BA:2614:A:OP1 | 61:BA:4815:HOH:O | 2.01 | 0.78 |
| 25:DA:1250:G:OP1 | 61:DA:4455:HOH:O | 2.00 | 0.78 |
| 25:DA:1159:U:H2' | 25:DA:1160:G:H8 | 1.48 | 0.78 |
| 25:BA:988:U:OP2 | 61:BA:4601:HOH:O | 2.01 | 0.78 |
| 39:BT:95:ARG:HH11 | 39:BT:95:ARG:HG2 | 1.47 | 0.78 |
| 1:CA:1005:A:H1' | 1:CA:1036:G:H1 | 1.49 | 0.78 |
| 1:CA:289:G:OP2 | 61:CA:4053:HOH:O | 2.01 | 0.78 |
| 25:DA:2005:A:OP1 | 61:DA:4386:HOH:O | 2.01 | 0.78 |
| 25:BA:455:A:OP1 | 61:BA:3961:HOH:O | 2.00 | 0.78 |
| 1:CA:1142:G:H3' | 1:CA:1143:G:H8 | 1.47 | 0.78 |
| 25:DA:1019:U:H3 | 25:DA:1142(A):A:H62 | 1.28 | 0.78 |
| 1:AA:1124:G:HO2' | 1:AA:1145:C:N4 | 1.82 | 0.78 |
| 25:DA:1997:G:OP2 | 61:DA:4560:HOH:O | 2.01 | 0.78 |
| 25:BA:611:U:OP2 | 61:BA:4160:HOH:O | 2.01 | 0.78 |
| 25:BA:1018:A:OP2 | 61:BA:4046:HOH:O | 2.01 | 0.78 |
| 25:BA:1404:G:OP2 | 61:BA:4219:HOH:O | 2.02 | 0.77 |
| 25:BA:535:C:OP1 | 61:BA:4621:HOH:O | 2.00 | 0.77 |
| 25:DA:271(A):A:N7 | 25:DA:271(W):G:N2 | 2.32 | 0.77 |
| 29:DF:53:THR:HG23 | 29:DF:55:GLY:H | 1.50 | 0.77 |
| 1:AA:289:G:OP2 | 61:AA:4071:HOH:O | 2.02 | 0.77 |
| 4:CD:13:ARG:HB2 | 4:CD:40:PRO:HD3 | 1.66 | 0.77 |
| 12:AL:49:ASN:ND2 | 12:AL:92:ASP:OD2 | 2.16 | 0.77 |
| 28:BE:93:VAL:HG21 | 28:BE:180:ASN:HA | 1.67 | 0.77 |
| 39:BT:65:LYS:HE2 | 39:BT:67:SER:HB2 | 1.66 | 0.77 |
| 13:CM:3:ARG:HA | 50:D4:34:GLU:HG2 | 1.66 | 0.77 |
| 34:BO:35:VAL:HG11 | 34:BO:103:ALA:HB3 | 1.66 | 0.77 |
| 25:DA:1604:C:OP1 | 61:DA:3956:HOH:O | 2.03 | 0.77 |
| 25:DA:1800:C:OP2 | 27:DD:183:ARG:NH2 | 2.18 | 0.77 |
| 30:DG:5:VAL:HG22 | 30:DG:8:LYS:H | 1.50 | 0.77 |
| 25:BA:808:A:OP1 | 61:BA:4592:HOH:O | 2.01 | 0.77 |
| 10:CJ:49:VAL:HG23 | 14:CN:41:ARG:HB2 | 1.67 | 0.77 |
| 25:DA:2032:G:N7 | 61:DA:3886:HOH:O | 2.16 | 0.77 |
| 32:DI:110:ASP:N | 32:DI:130:TYR:OH | 2.16 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1133:G:H1 | 1:CA:1141:C:H42 | 1.33 | 0.77 |
| 25:BA:1717:C:OP1 | 61:BA:3893:HOH:O | 2.02 | 0.77 |
| 25:BA:2227:G:H3' | 25:BA:2228:G:C8 | 2.19 | 0.77 |
| 1:CA:1048:G:OP1 | 14:CN:3:ARG:NH2 | 2.18 | 0.77 |
| 1:AA:1128:C:O2 | 1:AA:1147:C:N4 | 2.17 | 0.77 |
| 1:AA:1075:C:OP1 | 2:AB:179:LYS:NZ | 2.18 | 0.77 |
| 25:BA:11:G:H2' | 25:BA:12:U:H5' | 1.65 | 0.77 |
| 25:DA:2296:U:OP2 | 38:DS:9:ARG:NH2 | 2.18 | 0.77 |
| 8:AH:10:LEU:HD22 | 8:AH:83:ILE:HD11 | 1.67 | 0.76 |
| 1:AA:1126:U:H5 | 10:AJ:71:LEU:HD22 | 1.49 | 0.76 |
| 25:BA:1016:C:OP2 | 61:BA:4637:HOH:O | 2.04 | 0.76 |
| 1:CA:677:U:H3 | 1:CA:713:G:H22 | 1.33 | 0.76 |
| 25:DA:1488:G:C6 | 25:DA:1489:U:H5 | 2.03 | 0.76 |
| 1:AA:642:A:N3 | 8:AH:113:SER:OG | 2.17 | 0.76 |
| 1:AA:1492:A:O2' | 25:BA:1935:A:N1 | 2.18 | 0.76 |
| 1:CA:352:C:OP2 | 61:CA:4051:HOH:O | 2.02 | 0.76 |
| 4:AD:13:ARG:NH1 | 4:AD:38:TYR:O | 2.18 | 0.76 |
| 25:DA:120:U:OP2 | 61:DA:3744:HOH:O | 2.03 | 0.76 |
| 4:AD:108:LEU:HD13 | 4:AD:174:LEU:HD13 | 1.65 | 0.76 |
| 4:CD:100:ARG:NH1 | 4:CD:137:SER:OG | 2.19 | 0.76 |
| 26:DB:44:G:OP1 | 30:DG:98:ARG:NH2 | 2.19 | 0.76 |
| 1:AA:167:G:H2' | 1:AA:168:G:H8 | 1.49 | 0.76 |
| 25:BA:2604:G:O2' | 61:BA:4655:HOH:O | 1.99 | 0.76 |
| 25:DA:2805:G:H2' | 25:DA:2807:G:H8 | 1.51 | 0.76 |
| 25:BA:667:G:H21 | 25:BA:671:A:H2 | 1.34 | 0.76 |
| 1:CA:1132:C:H2' | 1:CA:1133:G:H8 | 1.49 | 0.76 |
| 19:CS:30:LEU:HD11 | 19:CS:32:LYS:HG3 | 1.67 | 0.76 |
| 25:DA:1253:A:N7 | 61:DA:3854:HOH:O | 2.18 | 0.76 |
| 1:CA:1015:A:N3 | 1:CA:1218:C:O2' | 2.18 | 0.76 |
| 1:CA:610:G:O6 | 61:CA:4180:HOH:O | 2.04 | 0.76 |
| 25:DA:801:G:OP2 | 61:DA:3762:HOH:O | 2.02 | 0.76 |
| 1:AA:803:G:OP1 | 61:AA:4050:HOH:O | 2.03 | 0.76 |
| 25:BA:1431:G:O2' | 25:BA:1442:U:O2 | 2.03 | 0.76 |
| 25:BA:934:A:H4' | 25:BA:935:C:H5 | 1.51 | 0.76 |
| 25:DA:1022:G:H22 | 25:DA:1142(A):A:H2 | 1.32 | 0.76 |
| 27:BD:17:THR:O | 27:BD:211:ARG:NH2 | 2.19 | 0.76 |
| 43:BX:31:HIS:HD2 | 43:BX:33:LYS:H | 1.29 | 0.76 |
| 43:DX:11:PRO:HB3 | 43:DX:92:LEU:HD11 | 1.66 | 0.76 |
| 1:AA:975:A:H4' | 1:AA:976:G:H5'' | 1.67 | 0.76 |
| 7:AG:50:ILE:HD11 | 7:AG:58:PRO:HA | 1.66 | 0.76 |
| 26:BB:31:C:O2 | 26:BB:53:A:N6 | 2.19 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1494:G:HO2' | 25:BA:1934:A:HO2' | 1.32 | 0.75 |
| 25:BA:2331:G:H22 | 38:BS:3:ARG:HE | 1.34 | 0.75 |
| 1:CA:323:U:OP1 | 20:CT:26:ASN:ND2 | 2.18 | 0.75 |
| 4:CD:25:ARG:NH1 | 4:CD:30:LYS:O | 2.20 | 0.75 |
| 1:CA:999:C:N3 | 1:CA:1042:G:N2 | 2.34 | 0.75 |
| 10:CJ:38:ILE:HD11 | 10:CJ:71:LEU:HD23 | 1.68 | 0.75 |
| 2:AB:87:ARG:HH21 | 2:AB:219:VAL:HG12 | 1.51 | 0.75 |
| 20:AT:9:ASN:HB3 | 20:AT:10:LEU:HD12 | 1.69 | 0.75 |
| 25:DA:2371:G:O6 | 61:DA:3975:HOH:O | 2.03 | 0.75 |
| 1:AA:348:G:H2' | 1:AA:349:A:C5' | 2.16 | 0.75 |
| 13:AM:58:GLU:O | 13:AM:62:ASN:ND2 | 2.19 | 0.75 |
| 29:BF:13:SER:HA | 29:BF:127:GLU:HG3 | 1.66 | 0.75 |
| 25:BA:2331:G:H22 | 38:BS:3:ARG:NE | 1.85 | 0.75 |
| 15:CO:14:GLU:OE2 | 15:CO:84:LYS:NZ | 2.20 | 0.75 |
| 25:BA:2732:G:OP2 | 61:BA:4645:HOH:O | 2.03 | 0.75 |
| 25:DA:1412:A:H2' | 25:DA:1413:G:C8 | 2.21 | 0.75 |
| 25:DA:1762:A:N1 | 61:DA:4178:HOH:O | 2.18 | 0.75 |
| 1:AA:954:G:H21 | 1:AA:1227:A:H62 | 1.30 | 0.75 |
| 1:AA:165:C:H2' | 1:AA:166:G:H8 | 1.52 | 0.75 |
| 1:AA:180:U:O2 | 1:AA:196:A:N6 | 2.19 | 0.75 |
| 1:AA:474:G:H2' | 1:AA:475:G:H8 | 1.51 | 0.75 |
| 25:BA:2510:C:OP2 | 61:BA:4510:HOH:O | 2.05 | 0.75 |
| 25:BA:880:U:O2 | 35:BP:55:ARG:NH2 | 2.20 | 0.75 |
| 44:BY:92:ASN:HB3 | 44:BY:94:LYS:H | 1.52 | 0.75 |
| 25:DA:1376:C:OP2 | 61:DA:3757:HOH:O | 2.05 | 0.75 |
| 25:DA:2683:C:OP1 | 39:DT:53:ARG:NH2 | 2.20 | 0.75 |
| 1:AA:406:G:H5' | 4:AD:5:ILE:HD11 | 1.67 | 0.74 |
| 25:BA:945:A:O2' | 25:BA:946:A:O5' | 2.05 | 0.74 |
| 3:CC:58:GLU:HB3 | 10:CJ:92:THR:HG21 | 1.67 | 0.74 |
| 25:BA:1065:U:H3 | 25:BA:1188:A:H62 | 1.36 | 0.74 |
| 25:BA:2059:G:N7 | 61:BA:4504:HOH:O | 2.20 | 0.74 |
| 32:BI:77:LEU:HB3 | 32:BI:142:VAL:HG12 | 1.68 | 0.74 |
| 25:DA:2049:G:OP2 | 61:DA:3941:HOH:O | 2.05 | 0.74 |
| 25:DA:452:G:OP2 | 61:DA:4105:HOH:O | 2.04 | 0.74 |
| 25:DA:631:A:OP1 | 35:DP:65:ARG:NH1 | 2.19 | 0.74 |
| 7:AG:62:PHE:HA | 7:AG:124:LEU:HD22 | 1.70 | 0.74 |
| 25:BA:139:A:H8 | 25:BA:1454:C:HO2' | 1.35 | 0.74 |
| 1:CA:522:C:H41 | 12:CL:53:ARG:HH22 | 1.32 | 0.74 |
| 25:DA:1315:C:OP2 | 61:DA:4076:HOH:O | 2.05 | 0.74 |
| 25:BA:1356:G:OP2 | 53:B7:9:ARG:NH1 | 2.20 | 0.74 |
| 25:BA:2695:C:O2 | 34:BO:70:LYS:NZ | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:BE:47:VAL:HG21 | 28:BE:86:PRO:HD2 | 1.69 | 0.74 |
| 39:DT:26:ASP:OD1 | 39:DT:120:ARG:NH2 | 2.21 | 0.74 |
| 25:BA:2365:G:N7 | 61:BA:4327:HOH:O | 2.19 | 0.74 |
| 1:CA:1223:C:H5' | 1:CA:1224:G:H5' | 1.68 | 0.74 |
| 15:CO:39:LEU:HD13 | 15:CO:56:LEU:HB2 | 1.68 | 0.74 |
| 26:DB:105:A:OP1 | 45:DZ:72:ARG:NH1 | 2.20 | 0.74 |
| 1:AA:574:A:OP2 | 61:AA:4004:HOH:O | 2.04 | 0.74 |
| 25:BA:591:U:O4 | 61:BA:4046:HOH:O | 2.05 | 0.74 |
| 3:CC:32:LEU:HD12 | 3:CC:59:ARG:HH12 | 1.53 | 0.74 |
| 7:CG:111:ARG:NH1 | 7:CG:113:GLU:OE2 | 2.21 | 0.74 |
| 25:DA:2287:A:H62 | 25:DA:2344:U:H3 | 1.31 | 0.74 |
| 25:BA:130:G:O6 | 61:BA:4550:HOH:O | 2.04 | 0.74 |
| 8:AH:49:GLU:HG2 | 8:AH:62:TYR:HE2 | 1.53 | 0.74 |
| 1:CA:1153:C:H42 | 1:CA:1154:G:N2 | 1.86 | 0.74 |
| 25:DA:832:G:OP1 | 61:DA:4165:HOH:O | 2.06 | 0.74 |
| 25:DA:848:G:H2' | 25:DA:849:A:C8 | 2.22 | 0.74 |
| 1:AA:1054:C:OP1 | 61:AA:4053:HOH:O | 2.04 | 0.73 |
| 1:AA:1162:C:H42 | 1:AA:1174:G:H1 | 1.35 | 0.73 |
| 25:BA:874:U:OP1 | 61:BA:4633:HOH:O | 2.05 | 0.73 |
| 1:CA:504:C:OP1 | 61:CA:4009:HOH:O | 2.05 | 0.73 |
| 1:CA:804:U:OP1 | 61:CA:4020:HOH:O | 2.06 | 0.73 |
| 1:CA:998:G:H1 | 1:CA:1043:C:N4 | 1.83 | 0.73 |
| 4:CD:187:ARG:NH2 | 4:CD:193:ASP:OD2 | 2.21 | 0.73 |
| 25:BA:1809:U:O2 | 61:BA:4722:HOH:O | 2.05 | 0.73 |
| 1:CA:1251:A:H2' | 1:CA:1252:A:C8 | 2.24 | 0.73 |
| 25:DA:2248:C:OP2 | 61:DA:3945:HOH:O | 2.06 | 0.73 |
| 2:CB:163:PHE:HD1 | 2:CB:185:ILE:HG13 | 1.53 | 0.73 |
| 25:DA:919:G:N2 | 25:DA:2269:A:OP2 | 2.21 | 0.73 |
| 1:AA:184:G:H2' | 1:AA:185:A:H8 | 1.54 | 0.73 |
| 1:CA:316:G:OP2 | 1:CA:351:G:O2' | 2.06 | 0.73 |
| 8:CH:51:VAL:HG12 | 8:CH:52:ASP:H | 1.53 | 0.73 |
| 25:DA:963:U:OP2 | 61:DA:4173:HOH:O | 2.04 | 0.73 |
| 1:AA:976:G:H5' | 1:AA:1358:U:O2' | 1.89 | 0.73 |
| 1:AA:812:C:N3 | 61:AA:4028:HOH:O | 2.22 | 0.73 |
| 25:BA:2227:G:H5' | 25:BA:2228:G:N7 | 2.03 | 0.73 |
| 37:BR:67:LEU:HD13 | 37:BR:76:VAL:HG21 | 1.71 | 0.73 |
| 43:BX:31:HIS:CD2 | 43:BX:33:LYS:H | 2.07 | 0.73 |
| 1:CA:1347:G:N2 | 1:CA:1373:G:H2' | 2.02 | 0.73 |
| 3:AC:35:GLU:OE2 | 3:AC:59:ARG:NH2 | 2.21 | 0.73 |
| 25:BA:1513:G:HO2' | 25:BA:1593:C:HO2' | 1.34 | 0.73 |
| 25:BA:985:G:OP1 | 61:BA:4728:HOH:O | 2.07 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:959:A:HO2' | 1:CA:984:C:HO2' | 1.37 | 0.73 |
| 2:CB:91:PRO:HG2 | 2:CB:155:LEU:HD23 | 1.71 | 0.73 |
| 1:AA:262:A:H2' | 1:AA:263:A:C8 | 2.24 | 0.73 |
| 1:CA:664:G:P | 18:CR:64:ARG:HH22 | 2.10 | 0.73 |
| 1:CA:976:G:H5' | 1:CA:1358:U:O2' | 1.87 | 0.73 |
| 13:CM:27:LYS:HE2 | 13:CM:27:LYS:HA | 1.69 | 0.73 |
| 50:D4:38:LYS:O | 50:D4:40:HIS:N | 2.21 | 0.73 |
| 25:DA:900:A:H2' | 25:DA:901:A:C8 | 2.24 | 0.73 |
| 25:DA:1817:G:OP1 | 27:DD:88:ARG:NH2 | 2.21 | 0.73 |
| 1:AA:742:G:OP2 | 15:AO:35:ARG:NH2 | 2.20 | 0.73 |
| 27:BD:69:ARG:NH2 | 27:BD:128:GLY:O | 2.20 | 0.73 |
| 25:BA:1398:U:OP2 | 61:BA:3932:HOH:O | 2.05 | 0.73 |
| 1:CA:989:C:N4 | 1:CA:1216:G:O6 | 2.17 | 0.73 |
| 25:DA:2445:G:OP1 | 29:DF:74:ARG:NH2 | 2.22 | 0.73 |
| 1:AA:266:G:H5'' | 1:AA:268:C:H41 | 1.53 | 0.73 |
| 1:AA:558:G:OP1 | 61:AA:4042:HOH:O | 2.07 | 0.73 |
| 13:AM:34:LEU:HD13 | 13:AM:41:PRO:HA | 1.70 | 0.73 |
| 30:DG:80:PHE:O | 30:DG:82:LEU:N | 2.20 | 0.73 |
| 30:BG:48:GLU:HA | 30:BG:51:ARG:HE | 1.53 | 0.72 |
| 40:DU:83:LEU:HD12 | 40:DU:88:ILE:HD12 | 1.70 | 0.72 |
| 1:AA:601:C:H2' | 1:AA:602:A:C8 | 2.24 | 0.72 |
| 1:CA:1251:A:HO2' | 1:CA:1369:C:HO2' | 1.32 | 0.72 |
| 25:DA:2749:A:H1' | 31:DH:63:SER:HB3 | 1.71 | 0.72 |
| 25:BA:2745:G:OP1 | 28:BE:203:LYS:NZ | 2.17 | 0.72 |
| 2:CB:52:GLU:HG2 | 2:CB:56:ARG:HH22 | 1.54 | 0.72 |
| 46:D0:27:GLU:HG3 | 46:D0:68:GLU:HA | 1.71 | 0.72 |
| 1:AA:1028:C:H42 | 1:AA:1033:G:H1 | 1.36 | 0.72 |
| 11:AK:15:ALA:HB1 | 11:AK:78:GLN:HB2 | 1.69 | 0.72 |
| 1:AA:864:A:OP1 | 61:AA:4127:HOH:O | 2.08 | 0.72 |
| 10:AJ:38:ILE:HD11 | 10:AJ:71:LEU:HD23 | 1.71 | 0.72 |
| 15:AO:56:LEU:O | 15:AO:60:VAL:HG23 | 1.88 | 0.72 |
| 1:CA:1003:G:H1 | 1:CA:1035:A:H61 | 1.37 | 0.72 |
| 1:CA:1277:C:HO2' | 1:CA:1279:A:H8 | 1.35 | 0.72 |
| 25:DA:963:U:OP1 | 61:DA:3740:HOH:O | 2.08 | 0.72 |
| 1:AA:972:C:OP1 | 61:AA:4123:HOH:O | 2.08 | 0.72 |
| 1:AA:881:G:P | 12:AL:12:ARG:HH22 | 2.12 | 0.72 |
| 25:BA:2019:G:OP2 | 61:BA:4565:HOH:O | 2.07 | 0.72 |
| 38:BS:15:ARG:O | 38:BS:19:LYS:HG2 | 1.89 | 0.72 |
| 17:CQ:57:VAL:HG12 | 17:CQ:76:LEU:HA | 1.72 | 0.72 |
| 25:DA:1876:A:H2' | 25:DA:1877:A:C8 | 2.24 | 0.72 |
| 25:DA:574:C:OP1 | 61:DA:3788:HOH:O | 2.08 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1695:C:OP1 | 61:BA:4516:HOH:O | 2.07 | 0.72 |
| 4:CD:18:LYS:NZ | 4:CD:31:CYS:SG | 2.63 | 0.72 |
| 34:DO:115:VAL:HG13 | 34:DO:121:VAL:HG21 | 1.72 | 0.72 |
| 25:DA:1670:C:OP1 | 61:DA:3750:HOH:O | 2.07 | 0.72 |
| 25:DA:400:G:O6 | 61:DA:4274:HOH:O | 2.06 | 0.72 |
| 1:AA:346:G:O6 | 1:AA:348:G:N2 | 2.23 | 0.72 |
| 50:B4:57:GLU:HB3 | 50:B4:58:ARG:HA | 1.71 | 0.72 |
| 1:CA:1135:U:O2' | 1:CA:1137:C:O2 | 2.05 | 0.72 |
| 13:CM:16:ASP:HB3 | 13:CM:34:LEU:HD11 | 1.72 | 0.72 |
| 27:DD:71:ASP:CB | 27:DD:103:ARG:HH22 | 2.03 | 0.72 |
| 2:CB:88:ALA:HB2 | 2:CB:219:VAL:HG13 | 1.72 | 0.72 |
| 1:CA:559:A:OP1 | 5:CE:126:ARG:NH2 | 2.22 | 0.72 |
| 7:CG:68:ASN:ND2 | 7:CG:127:ALA:O | 2.19 | 0.72 |
| 30:DG:136:ARG:HH11 | 30:DG:137:GLU:H | 1.37 | 0.72 |
| 51:B5:17:ASP:OD2 | 61:B5:602:HOH:O | 2.07 | 0.71 |
| 32:BI:48:GLU:HG2 | 32:BI:52:ARG:HH22 | 1.55 | 0.71 |
| 25:DA:731:C:OP1 | 61:DA:4224:HOH:O | 2.08 | 0.71 |
| 5:AE:100:VAL:O | 5:AE:107:ARG:NH2 | 2.22 | 0.71 |
| 30:BG:16:ARG:NE | 30:BG:31:VAL:HG11 | 2.05 | 0.71 |
| 35:BP:100:LEU:HD12 | 35:BP:112:LEU:HD11 | 1.70 | 0.71 |
| 1:CA:693:G:H2' | 1:CA:694:A:C8 | 2.25 | 0.71 |
| 1:AA:1027:C:O2' | 1:AA:1034:G:N2 | 2.23 | 0.71 |
| 35:BP:50:ARG:HH21 | 54:B8:7:HIS:CD2 | 2.09 | 0.71 |
| 25:BA:1679:A:OP2 | 61:BA:4622:HOH:O | 2.07 | 0.71 |
| 26:BB:48:A:H4' | 38:BS:95:HIS:HD2 | 1.53 | 0.71 |
| 1:CA:1376:U:OP1 | 7:CG:98:SER:OG | 2.08 | 0.71 |
| 25:DA:89:G:H3' | 25:DA:90:U:H5'' | 1.71 | 0.71 |
| 10:AJ:7:LYS:HE2 | 10:AJ:9:ARG:HH12 | 1.55 | 0.71 |
| 1:AA:974:A:OP2 | 14:AN:41:ARG:NH1 | 2.24 | 0.71 |
| 25:BA:1379:C:OP2 | 61:BA:4121:HOH:O | 2.07 | 0.71 |
| 25:BA:2804:C:H2' | 25:BA:2805:G:C8 | 2.24 | 0.71 |
| 2:CB:96:ARG:HD2 | 2:CB:98:LEU:HD22 | 1.72 | 0.71 |
| 1:CA:1457:G:OP1 | 20:CT:39:LYS:NZ | 2.22 | 0.71 |
| 25:DA:11:G:H2' | 25:DA:12:U:H5' | 1.71 | 0.71 |
| 25:DA:600:G:N3 | 61:DA:3733:HOH:O | 2.23 | 0.71 |
| 1:AA:1036:G:H5' | 1:AA:1037:C:H5 | 1.55 | 0.71 |
| 46:B0:40:GLN:HE21 | 46:B0:57:PHE:HB3 | 1.55 | 0.71 |
| 25:DA:2267:A:H5'' | 25:DA:2268:A:H5' | 1.71 | 0.71 |
| 25:DA:819:A:OP2 | 25:DA:1187:G:N2 | 2.19 | 0.71 |
| 25:DA:1140:C:O3' | 33:DN:25:ARG:NH1 | 2.23 | 0.71 |
| 1:CA:21:G:OP1 | 61:CA:4062:HOH:O | 2.07 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:2228:G:O2' | 25:BA:2229:A:OP1 | 2.07 | 0.71 |
| 1:CA:148:G:H2' | 1:CA:149:A:H8 | 1.54 | 0.71 |
| 49:D3:8:LEU:HD13 | 49:D3:31:LEU:HD23 | 1.73 | 0.71 |
| 25:DA:1665:A:OP2 | 61:DA:4385:HOH:O | 2.08 | 0.71 |
| 49:B3:3:ARG:NH1 | 49:B3:60:GLU:OE2 | 2.19 | 0.71 |
| 25:BA:1094:A:OP2 | 25:BA:1155:C:N4 | 2.23 | 0.71 |
| 1:AA:1223:C:H5'' | 1:AA:1224:G:H5' | 1.72 | 0.71 |
| 4:AD:15:GLU:HG3 | 4:AD:63:LYS:HE2 | 1.72 | 0.71 |
| 25:BA:597:C:OP1 | 61:BA:3998:HOH:O | 2.09 | 0.71 |
| 1:CA:1189:C:O2 | 61:CA:4087:HOH:O | 2.08 | 0.71 |
| 31:DH:159:GLU:HG3 | 31:DH:169:VAL:HG11 | 1.72 | 0.71 |
| 36:DQ:34:LEU:HD11 | 36:DQ:129:THR:HB | 1.73 | 0.71 |
| 1:CA:954:G:H21 | 1:CA:1227:A:H62 | 1.39 | 0.70 |
| 3:CC:73:PRO:HB3 | 3:CC:103:VAL:HG11 | 1.70 | 0.70 |
| 4:CD:13:ARG:NH1 | 4:CD:38:TYR:O | 2.23 | 0.70 |
| 46:D0:14:ARG:NH1 | 61:D0:202:HOH:O | 2.23 | 0.70 |
| 25:DA:1593:G:H2' | 25:DA:1594:G:C8 | 2.26 | 0.70 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.26 | 0.70 |
| 1:AA:411:A:OP1 | 4:AD:30:LYS:NZ | 2.19 | 0.70 |
| 25:BA:1039:G:OP1 | 40:BU:50:ARG:NH2 | 2.25 | 0.70 |
| 30:BG:102:PHE:HE1 | 30:BG:141:PHE:HE2 | 1.37 | 0.70 |
| 25:DA:1488:G:C6 | 25:DA:1489:U:C5 | 2.78 | 0.70 |
| 25:DA:2819:G:N7 | 61:DA:4006:HOH:O | 2.24 | 0.70 |
| 25:DA:287:C:H2' | 25:DA:288:C:H6 | 1.56 | 0.70 |
| 1:AA:167:G:H2' | 1:AA:168:G:C8 | 2.26 | 0.70 |
| 9:AI:53:VAL:O | 9:AI:55:ALA:N | 2.21 | 0.70 |
| 25:BA:1189:A:OP1 | 33:BN:25:ARG:NH2 | 2.24 | 0.70 |
| 25:BA:322:G:N7 | 61:BA:3883:HOH:O | 2.23 | 0.70 |
| 25:BA:932:C:H3' | 25:BA:933:C:H5'' | 1.73 | 0.70 |
| 1:CA:1142:G:H3' | 1:CA:1143:G:C8 | 2.26 | 0.70 |
| 2:CB:54:THR:HG23 | 2:CB:199:TYR:HB3 | 1.72 | 0.70 |
| 25:DA:1310:G:OP2 | 53:D7:9:ARG:NH1 | 2.21 | 0.70 |
| 2:AB:16:HIS:CD2 | 2:AB:17:PHE:H | 2.09 | 0.70 |
| 8:AH:51:VAL:HG12 | 8:AH:52:ASP:H | 1.56 | 0.70 |
| 10:AJ:78:ASN:O | 10:AJ:80:LYS:N | 2.25 | 0.70 |
| 25:BA:2862:G:OP1 | 61:BA:4875:HOH:O | 2.10 | 0.70 |
| 35:BP:33:ARG:O | 61:BP:301:HOH:O | 2.07 | 0.70 |
| 1:CA:572:A:OP1 | 61:CA:4046:HOH:O | 2.10 | 0.70 |
| 25:DA:2805:G:H2' | 25:DA:2807:G:C8 | 2.25 | 0.70 |
| 1:AA:221:C:H2' | 1:AA:222:U:H6 | 1.54 | 0.70 |
| 25:BA:1055:A:OP2 | 33:BN:37:LYS:NZ | 2.19 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CJ:17:ASP:OD1 | 10:CJ:70:ARG:NH1 | 2.24 | 0.70 |
| 25:DA:1235:G:OP1 | 61:DA:4361:HOH:O | 2.08 | 0.70 |
| 25:DA:2849:U:OP2 | 39:DT:95:ARG:NH1 | 2.24 | 0.70 |
| 25:DA:827:U:OP1 | 61:DA:4180:HOH:O | 2.08 | 0.70 |
| 27:DD:148:GLU:HB2 | 27:DD:151:LYS:HD2 | 1.73 | 0.70 |
| 1:AA:1129:C:N3 | 1:AA:1143:G:N2 | 2.37 | 0.70 |
| 4:AD:173:TRP:CZ3 | 4:AD:174:LEU:HG | 2.27 | 0.70 |
| 1:CA:811:C:N4 | 61:CA:4026:HOH:O | 2.25 | 0.70 |
| 25:BA:147:U:O4 | 61:BA:4550:HOH:O | 2.06 | 0.70 |
| 25:BA:2101:U:O4 | 61:BA:4300:HOH:O | 2.09 | 0.70 |
| 50:D4:68:ARG:HH21 | 50:D4:68:ARG:HG3 | 1.54 | 0.70 |
| 42:DW:14:PRO:HG2 | 42:DW:78:GLU:HG2 | 1.73 | 0.70 |
| 45:DZ:93:ASP:O | 45:DZ:131:ARG:NH1 | 2.23 | 0.70 |
| 25:DA:2705:A:OP2 | 61:DA:4123:HOH:O | 2.08 | 0.70 |
| 36:DQ:85:LYS:HG2 | 46:D0:7:LEU:HB3 | 1.74 | 0.70 |
| 1:AA:148:G:HO2' | 1:AA:149:A:H8 | 1.40 | 0.70 |
| 36:BQ:10:ARG:NH1 | 61:BQ:302:HOH:O | 2.25 | 0.70 |
| 2:CB:178:ARG:NH2 | 8:CH:68:ARG:HH12 | 1.90 | 0.70 |
| 24:CW:9:MVA:O | 24:CW:10:2QY:H86 | 1.91 | 0.70 |
| 25:DA:2206:G:H3' | 25:DA:2207:G:H8 | 1.56 | 0.70 |
| 36:DQ:48:GLU:OE1 | 36:DQ:51:ARG:NH2 | 2.24 | 0.70 |
| 25:BA:70:A:N7 | 43:BX:31:HIS:HE1 | 1.90 | 0.69 |
| 1:CA:1269:A:N1 | 1:CA:1312:G:O2' | 2.24 | 0.69 |
| 25:BA:1249:A:H2 | 25:BA:1287:A:H62 | 1.40 | 0.69 |
| 25:BA:284:G:O6 | 61:BA:4714:HOH:O | 2.09 | 0.69 |
| 2:CB:18:GLY:HA2 | 2:CB:42:ILE:HG13 | 1.73 | 0.69 |
| 12:CL:24:VAL:HG11 | 12:CL:27:LEU:HD22 | 1.74 | 0.69 |
| 1:AA:1292:U:OP2 | 7:AG:41:ARG:NH2 | 2.24 | 0.69 |
| 25:BA:9:U:N3 | 25:BA:2641:A:H2 | 1.89 | 0.69 |
| 2:CB:77:ALA:HB2 | 2:CB:211:ILE:HD13 | 1.73 | 0.69 |
| 4:CD:119:GLN:HG2 | 4:CD:123:HIS:CD2 | 2.27 | 0.69 |
| 20:CT:49:ALA:HB3 | 20:CT:99:LEU:HD22 | 1.74 | 0.69 |
| 25:BA:2339:A:H2' | 25:BA:2340:A:C8 | 2.27 | 0.69 |
| 25:BA:388:A:H2' | 25:BA:389:G:C8 | 2.27 | 0.69 |
| 1:CA:1002:G:H2' | 1:CA:1003:G:C8 | 2.27 | 0.69 |
| 25:DA:1671:U:HO2' | 25:DA:1673:U:H5 | 1.40 | 0.69 |
| 25:DA:993:G:OP1 | 40:DU:50:ARG:NH2 | 2.25 | 0.69 |
| 5:AE:100:VAL:HG22 | 5:AE:118:ILE:HG22 | 1.74 | 0.69 |
| 52:D6:13:CYS:SG | 52:D6:47:THR:HG21 | 2.33 | 0.69 |
| 25:DA:1803:A:O2' | 27:DD:259:THR:HG21 | 1.92 | 0.69 |
| 13:AM:122:LYS:HD3 | 13:AM:123:ALA:H | 1.58 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:BH:56:SER:OG | 31:BH:57:ASP:N | 2.26 | 0.69 |
| 2:CB:178:ARG:HH22 | 8:CH:68:ARG:NH1 | 1.91 | 0.69 |
| 25:DA:1017:G:N7 | 61:DA:4208:HOH:O | 2.25 | 0.69 |
| 25:BA:1480:A:H61 | 25:BA:1605:A:H62 | 1.40 | 0.69 |
| 25:BA:1831:C:OP1 | 27:BD:264:LYS:NZ | 2.24 | 0.69 |
| 25:BA:2457:G:OP1 | 29:BF:74:ARG:NH2 | 2.26 | 0.69 |
| 1:CA:503:C:OP2 | 12:CL:116:SER:HB3 | 1.93 | 0.69 |
| 25:DA:1637:A:OP2 | 61:DA:4412:HOH:O | 2.10 | 0.69 |
| 25:BA:956:A:H62 | 36:BQ:12:GLN:HA | 1.58 | 0.69 |
| 1:CA:652:U:O4 | 1:CA:752:G:O2' | 2.10 | 0.69 |
| 1:CA:427:U:OP1 | 4:CD:13:ARG:NH2 | 2.26 | 0.69 |
| 25:DA:1509(B):A:H2' | 25:DA:1510:G:C8 | 2.28 | 0.69 |
| 25:DA:2682:U:OP2 | 61:DA:3802:HOH:O | 2.09 | 0.69 |
| 1:AA:1025:U:O2 | 1:AA:1036:G:O6 | 2.11 | 0.69 |
| 12:AL:24:VAL:HG11 | 12:AL:27:LEU:HD22 | 1.74 | 0.69 |
| 19:AS:3:ARG:NH1 | 19:AS:8:GLY:O | 2.25 | 0.69 |
| 4:CD:15:GLU:HG2 | 4:CD:63:LYS:HB3 | 1.75 | 0.69 |
| 25:DA:1430:C:H2' | 25:DA:1431:U:H6 | 1.57 | 0.69 |
| 25:BA:2101:U:O3' | 47:B1:35:THR:OG1 | 2.11 | 0.69 |
| 19:AS:9:VAL:HG21 | 50:B4:61:ARG:HH22 | 1.57 | 0.69 |
| 25:BA:1648:U:O4 | 61:BA:4117:HOH:O | 2.08 | 0.69 |
| 44:BY:102:CYS:SG | 44:BY:103:GLY:N | 2.66 | 0.69 |
| 1:CA:532:A:O2' | 1:CA:533:A:OP1 | 2.11 | 0.69 |
| 25:DA:649:G:H4' | 54:D8:46:ARG:HH22 | 1.57 | 0.69 |
| 25:DA:1143:A:OP1 | 33:DN:25:ARG:NH2 | 2.26 | 0.69 |
| 29:DF:185:ASP:HA | 29:DF:188:ARG:HD3 | 1.75 | 0.69 |
| 1:AA:596:C:OP2 | 61:AA:4043:HOH:O | 2.11 | 0.69 |
| 4:AD:120:LEU:HB3 | 4:AD:126:ILE:HD11 | 1.73 | 0.69 |
| 25:BA:1613:A:OP1 | 27:BD:211:ARG:NH1 | 2.26 | 0.69 |
| 25:BA:2619:G:O3' | 61:BA:4188:HOH:O | 2.11 | 0.69 |
| 25:BA:551:A:OP1 | 61:BA:4499:HOH:O | 2.11 | 0.69 |
| 1:CA:837:G:H1 | 1:CA:849:C:H42 | 1.41 | 0.69 |
| 18:CR:54:ARG:HH11 | 18:CR:54:ARG:HB2 | 1.58 | 0.69 |
| 20:CT:60:GLU:HG3 | 20:CT:81:LYS:HD2 | 1.75 | 0.69 |
| 28:DE:72:VAL:HG22 | 28:DE:73:GLU:HG2 | 1.75 | 0.69 |
| 1:AA:1003:G:N2 | 1:AA:1038:C:N3 | 2.41 | 0.68 |
| 6:AF:69:GLU:O | 6:AF:72:VAL:HG12 | 1.93 | 0.68 |
| 27:BD:71:ASP:HB3 | 27:BD:103:ARG:HH22 | 1.58 | 0.68 |
| 1:CA:891:U:OP2 | 61:CA:4083:HOH:O | 2.11 | 0.68 |
| 5:CE:12:LEU:HB3 | 5:CE:31:LEU:HB2 | 1.74 | 0.68 |
| 9:CI:24:GLY:HA2 | 9:CI:59:PHE:O | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:1963:U:O2' | 61:DA:4441:HOH:O | 2.11 | 0.68 |
| 25:DA:2016:U:H2' | 25:DA:2017:U:C6 | 2.29 | 0.68 |
| 28:DE:72:VAL:HG13 | 28:DE:73:GLU:O | 1.93 | 0.68 |
| 29:DF:195:ASP:OD1 | 29:DF:196:LEU:N | 2.26 | 0.68 |
| 1:AA:21:G:OP1 | 61:AA:4080:HOH:O | 2.10 | 0.68 |
| 1:AA:839:U:O2' | 1:AA:840:C:OP1 | 2.11 | 0.68 |
| 1:AA:35:G:O2' | 12:AL:118:SER:O | 2.12 | 0.68 |
| 25:BA:1315:A:N7 | 61:BA:4265:HOH:O | 2.25 | 0.68 |
| 25:BA:272:U:H4' | 32:BI:50:ARG:HH12 | 1.58 | 0.68 |
| 32:BI:92:VAL:HG13 | 32:BI:120:ILE:HB | 1.75 | 0.68 |
| 7:CG:108:ALA:HA | 7:CG:111:ARG:HD2 | 1.73 | 0.68 |
| 25:DA:1593:G:H2' | 25:DA:1594:G:H8 | 1.56 | 0.68 |
| 1:AA:1025:U:O2' | 1:AA:1026:G:O4' | 2.12 | 0.68 |
| 1:AA:1125:U:O2' | 1:AA:1126:U:OP2 | 2.10 | 0.68 |
| 10:AJ:5:ARG:NE | 10:AJ:73:ASP:OD1 | 2.25 | 0.68 |
| 25:BA:2460:A:OP2 | 61:BA:4510:HOH:O | 2.11 | 0.68 |
| 42:BW:14:PRO:HG2 | 42:BW:78:GLU:HG2 | 1.76 | 0.68 |
| 61:DA:4599:HOH:O | 46:D0:4:LYS:NZ | 2.24 | 0.68 |
| 25:DA:2552:U:H2' | 25:DA:2554:U:OP2 | 1.93 | 0.68 |
| 6:AF:18:GLN:HA | 6:AF:21:LEU:HD12 | 1.76 | 0.68 |
| 25:BA:1576:G:C6 | 25:BA:1577:C:N4 | 2.61 | 0.68 |
| 25:BA:1815:A:OP2 | 61:BA:4519:HOH:O | 2.10 | 0.68 |
| 1:CA:1003:G:H1 | 1:CA:1035:A:N6 | 1.91 | 0.68 |
| 44:DY:102:CYS:SG | 44:DY:103:GLY:N | 2.67 | 0.68 |
| 25:BA:1463:C:O2' | 25:BA:1633:A:N3 | 2.27 | 0.68 |
| 39:BT:24:PRO:HA | 39:BT:49:VAL:HG22 | 1.74 | 0.68 |
| 2:CB:144:ARG:NH1 | 2:CB:148:TYR:OH | 2.26 | 0.68 |
| 47:D1:50:ARG:HG2 | 47:D1:59:THR:HB | 1.76 | 0.68 |
| 50:D4:44:THR:O | 50:D4:46:GLN:N | 2.27 | 0.68 |
| 19:CS:42:PRO:HG3 | 50:D4:61:ARG:HG2 | 1.75 | 0.68 |
| 27:DD:132:PRO:HD3 | 27:DD:190:TYR:CZ | 2.28 | 0.68 |
| 2:AB:17:PHE:HB2 | 2:AB:44:LEU:HD21 | 1.74 | 0.68 |
| 25:BA:927:G:N2 | 25:BA:944:C:N3 | 2.41 | 0.68 |
| 1:CA:1193:G:O2' | 5:CE:25:ARG:NH2 | 2.27 | 0.68 |
| 12:CL:57:LYS:HG2 | 12:CL:67:THR:HG22 | 1.73 | 0.68 |
| 13:CM:3:ARG:HE | 13:CM:4:ILE:HG22 | 1.58 | 0.68 |
| 50:D4:24:THR:OG1 | 50:D4:25:TYR:N | 2.27 | 0.68 |
| 25:DA:639:U:H2' | 25:DA:640:C:C6 | 2.29 | 0.68 |
| 1:AA:836:G:OP2 | 18:AR:61:LYS:NZ | 2.27 | 0.68 |
| 31:BH:149:ARG:NH1 | 31:BH:167:GLU:OE2 | 2.27 | 0.68 |
| 1:CA:419:C:OP1 | 1:CA:513:C:O2' | 2.10 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:735:C:H2' | 1:CA:736:C:H6 | 1.58 | 0.68 |
| 3:CC:152:ILE:HG23 | 3:CC:199:LYS:HB2 | 1.76 | 0.68 |
| 25:DA:1200:C:H5' | 61:DA:3770:HOH:O | 1.94 | 0.68 |
| 27:DD:132:PRO:HG2 | 27:DD:135:PHE:HD2 | 1.57 | 0.68 |
| 1:AA:661:G:H1 | 1:AA:744:C:H42 | 1.39 | 0.68 |
| 2:AB:185:ILE:HG22 | 2:AB:199:TYR:HB2 | 1.74 | 0.68 |
| 25:BA:1047:A:OP2 | 61:BA:3917:HOH:O | 2.11 | 0.68 |
| 29:BF:8:GLN:NE2 | 29:BF:21:ALA:HB2 | 2.09 | 0.68 |
| 1:CA:646:U:H2' | 1:CA:647:C:C6 | 2.29 | 0.68 |
| 25:DA:2394:C:OP2 | 54:D8:30:ARG:NH1 | 2.27 | 0.68 |
| 25:DA:2393:A:H5'' | 35:DP:63:PRO:HB3 | 1.76 | 0.68 |
| 1:AA:1086:U:H3 | 1:AA:1099:G:H22 | 1.42 | 0.68 |
| 1:AA:278:G:OP2 | 17:AQ:92:ARG:NH2 | 2.27 | 0.68 |
| 1:AA:664:G:H22 | 1:AA:741:G:H1 | 1.39 | 0.68 |
| 3:AC:3:ASN:OD1 | 3:AC:3:ASN:N | 2.26 | 0.68 |
| 25:BA:2734:A:N7 | 61:BA:4015:HOH:O | 2.27 | 0.68 |
| 1:CA:460:G:O6 | 1:CA:470:C:H5'' | 1.93 | 0.68 |
| 2:CB:210:SER:O | 2:CB:214:ILE:HG12 | 1.94 | 0.68 |
| 25:BA:2212:G:H2' | 25:BA:2213:G:O4' | 1.93 | 0.68 |
| 40:BU:76:TYR:OH | 40:BU:92:ARG:NH1 | 2.26 | 0.68 |
| 1:CA:474:G:H2' | 1:CA:475:G:H8 | 1.58 | 0.68 |
| 25:DA:2287:A:N6 | 25:DA:2344:U:H3 | 1.92 | 0.68 |
| 25:DA:2427:C:OP1 | 61:DA:4257:HOH:O | 2.11 | 0.68 |
| 1:AA:342:C:N3 | 1:AA:343:U:H5 | 1.92 | 0.67 |
| 25:BA:335:A:OP2 | 61:BA:4497:HOH:O | 2.11 | 0.67 |
| 61:BE:406:HOH:O | 37:BR:3:HIS:NE2 | 2.27 | 0.67 |
| 5:CE:9:LYS:HB2 | 5:CE:112:LEU:HD11 | 1.76 | 0.67 |
| 25:DA:652(D):C:H42 | 25:DA:652(U):G:H1 | 1.42 | 0.67 |
| 1:AA:59:A:H3' | 1:AA:331:G:H22 | 1.59 | 0.67 |
| 25:BA:1361:C:OP2 | 61:BA:4471:HOH:O | 2.12 | 0.67 |
| 46:D0:24:LYS:HA | 46:D0:24:LYS:HE2 | 1.76 | 0.67 |
| 47:D1:65:SER:HG | 47:D1:66:HIS:HD1 | 1.39 | 0.67 |
| 25:DA:1607:C:N4 | 25:DA:1622:G:OP2 | 2.27 | 0.67 |
| 1:AA:946:A:H2' | 1:AA:947:G:C8 | 2.28 | 0.67 |
| 1:CA:1042:G:O2' | 1:CA:1043:C:O4' | 2.12 | 0.67 |
| 1:CA:382:A:H2' | 1:CA:383:A:C8 | 2.28 | 0.67 |
| 9:AI:4:TYR:HB2 | 9:AI:19:LEU:HB2 | 1.77 | 0.67 |
| 25:BA:2081:A:OP2 | 61:BA:4212:HOH:O | 2.12 | 0.67 |
| 25:BA:2361:G:OP1 | 61:BA:3947:HOH:O | 2.12 | 0.67 |
| 1:CA:565:U:OP2 | 61:CA:4054:HOH:O | 2.13 | 0.67 |
| 2:CB:84:GLU:HB3 | 2:CB:219:VAL:HG21 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 47:D1:77:ALA:HA | 47:D1:80:LEU:HD13 | 1.77 | 0.67 |
| 25:DA:2006:C:OP2 | 61:DA:4388:HOH:O | 2.12 | 0.67 |
| 25:DA:588:U:OP2 | 61:DA:3873:HOH:O | 2.11 | 0.67 |
| 25:DA:962:G:OP1 | 61:DA:4173:HOH:O | 2.12 | 0.67 |
| 34:DO:68:GLU:HB3 | 34:DO:78:ARG:HB2 | 1.74 | 0.67 |
| 31:BH:56:SER:HB3 | 31:BH:61:HIS:ND1 | 2.10 | 0.67 |
| 1:CA:1251:A:O2' | 1:CA:1369:C:O2' | 2.08 | 0.67 |
| 50:D4:62:ARG:O | 50:D4:64:GLY:N | 2.28 | 0.67 |
| 25:DA:2431:U:OP2 | 61:DA:3860:HOH:O | 2.12 | 0.67 |
| 25:DA:272:G:H4' | 25:DA:272(A):U:H5'' | 1.74 | 0.67 |
| 25:DA:994:C:OP2 | 40:DU:54:LYS:NZ | 2.28 | 0.67 |
| 1:AA:1030(D):A:H62 | 1:AA:1031:G:H21 | 1.43 | 0.67 |
| 51:B5:16:ARG:NH1 | 51:B5:17:ASP:OD1 | 2.28 | 0.67 |
| 25:BA:1391:C:OP2 | 61:BA:3931:HOH:O | 2.10 | 0.67 |
| 23:CX:73:A:H5'' | 23:CX:74:C:H5' | 1.77 | 0.67 |
| 1:AA:1063:C:OP2 | 1:AA:1064:G:O2' | 2.10 | 0.67 |
| 1:AA:1108:G:O6 | 61:AA:4120:HOH:O | 2.10 | 0.67 |
| 1:AA:933:G:O6 | 7:AG:3:ARG:NH2 | 2.28 | 0.67 |
| 25:BA:2460:A:OP1 | 61:BA:4034:HOH:O | 2.11 | 0.67 |
| 25:BA:324:A:OP2 | 44:BY:86:ARG:NH2 | 2.28 | 0.67 |
| 25:DA:1971:A:OP1 | 61:DA:3909:HOH:O | 2.13 | 0.67 |
| 25:DA:2291:U:H2' | 25:DA:2292:C:C6 | 2.29 | 0.67 |
| 25:DA:754:C:H2' | 25:DA:755:C:H6 | 1.60 | 0.67 |
| 25:BA:2420:U:OP2 | 61:BA:4137:HOH:O | 2.13 | 0.67 |
| 1:CA:117:G:OP2 | 61:CA:4053:HOH:O | 2.13 | 0.67 |
| 1:CA:1226:C:N4 | 13:CM:104:ARG:HG3 | 2.10 | 0.67 |
| 1:CA:1075:C:OP1 | 2:CB:179:LYS:NZ | 2.28 | 0.67 |
| 9:CI:33:PHE:HE1 | 9:CI:43:ALA:HB1 | 1.59 | 0.67 |
| 25:DA:2430:A:OP2 | 61:DA:4180:HOH:O | 2.12 | 0.67 |
| 6:AF:68:PRO:HB2 | 6:AF:71:ARG:HG3 | 1.77 | 0.67 |
| 38:BS:25:ARG:NH1 | 38:BS:42:ASP:OD1 | 2.27 | 0.67 |
| 25:DA:1359:A:H2' | 25:DA:1360:A:H5' | 1.77 | 0.67 |
| 30:DG:16:ARG:O | 30:DG:20:ILE:HG13 | 1.95 | 0.67 |
| 32:DI:104:GLN:O | 32:DI:105:HIS:ND1 | 2.28 | 0.67 |
| 14:AN:37:PHE:HB3 | 14:AN:39:LEU:HD12 | 1.76 | 0.67 |
| 1:CA:1352:C:H2' | 1:CA:1353:G:C8 | 2.30 | 0.67 |
| 1:CA:619:U:N3 | 4:CD:134:ASP:OD1 | 2.20 | 0.67 |
| 25:BA:2897:U:H2' | 25:BA:2898:C:C6 | 2.30 | 0.66 |
| 27:BD:132:PRO:HG2 | 27:BD:135:PHE:HD2 | 1.60 | 0.66 |
| 45:BZ:69:THR:HG22 | 45:BZ:90:VAL:HA | 1.77 | 0.66 |
| 1:CA:1004:A:C6 | 1:CA:1037:C:C2 | 2.82 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1133:G:H2' | 1:CA:1134:G:C8 | 2.31 | 0.66 |
| 1:CA:1170:A:O2' | 1:CA:1171:G:O4' | 2.12 | 0.66 |
| 23:CX:64:G:H4' | 36:DQ:10:ARG:HH21 | 1.59 | 0.66 |
| 25:DA:602:G:O2' | 25:DA:655:A:N6 | 2.28 | 0.66 |
| 1:AA:1286:A:C8 | 1:AA:1287:A:H4' | 2.30 | 0.66 |
| 1:AA:1422:G:H5'' | 34:BO:48:PRO:HB3 | 1.77 | 0.66 |
| 9:AI:3:GLN:OE1 | 9:AI:20:ARG:NH2 | 2.27 | 0.66 |
| 25:BA:1007:G:OP1 | 61:BA:4616:HOH:O | 2.12 | 0.66 |
| 25:BA:449:A:OP2 | 61:BA:3954:HOH:O | 2.13 | 0.66 |
| 1:CA:947:G:O3' | 13:CM:109:THR:OG1 | 2.14 | 0.66 |
| 1:AA:1321:C:H5'' | 1:AA:1322:C:H2' | 1.77 | 0.66 |
| 25:DA:1652:A:OP1 | 37:DR:8:ARG:NH1 | 2.28 | 0.66 |
| 45:DZ:108:PRO:HG3 | 45:DZ:141:VAL:HB | 1.77 | 0.66 |
| 48:B2:16:LEU:O | 48:B2:67:LYS:NZ | 2.27 | 0.66 |
| 25:BA:2600:G:OP2 | 61:BA:4789:HOH:O | 2.14 | 0.66 |
| 25:DA:1606:G:OP1 | 61:DA:4577:HOH:O | 2.13 | 0.66 |
| 25:DA:2685:G:O6 | 61:DA:3896:HOH:O | 2.09 | 0.66 |
| 25:DA:773:U:OP1 | 61:DA:4405:HOH:O | 2.12 | 0.66 |
| 33:DN:42:TRP:HA | 33:DN:48:MET:HE1 | 1.78 | 0.66 |
| 33:DN:20:GLY:HA2 | 33:DN:61:ARG:HE | 1.58 | 0.66 |
| 1:AA:1189:C:OP1 | 10:AJ:51:ARG:NH2 | 2.28 | 0.66 |
| 23:CX:23:C:H2' | 23:CX:24:U:C6 | 2.30 | 0.66 |
| 27:DD:206:LEU:HD22 | 27:DD:211:ARG:HG2 | 1.76 | 0.66 |
| 1:AA:243:A:H4' | 1:AA:244:U:H5'' | 1.77 | 0.66 |
| 1:CA:1256:A:N6 | 1:CA:1278:U:H1' | 2.10 | 0.66 |
| 25:DA:1301:A:OP1 | 61:DA:4411:HOH:O | 2.13 | 0.66 |
| 25:DA:271(E):U:H2' | 25:DA:271(F):C:C6 | 2.30 | 0.66 |
| 29:DF:18:ARG:NH2 | 29:DF:127:GLU:OE1 | 2.28 | 0.66 |
| 45:DZ:72:ARG:NH2 | 45:DZ:97:GLU:O | 2.29 | 0.66 |
| 25:BA:2817:G:N1 | 25:BA:2902:G:O6 | 2.19 | 0.66 |
| 7:CG:113:GLU:HG2 | 7:CG:119:ARG:HG2 | 1.78 | 0.66 |
| 25:DA:1774:C:OP1 | 61:DA:3936:HOH:O | 2.13 | 0.66 |
| 29:DF:13:SER:HA | 29:DF:127:GLU:HG3 | 1.77 | 0.66 |
| 1:AA:407:G:H5'' | 4:AD:115:ARG:HB3 | 1.78 | 0.66 |
| 1:AA:452:A:H4' | 16:AP:72:ARG:NH1 | 2.11 | 0.66 |
| 2:AB:166:ASP:HB3 | 2:AB:169:LYS:HB2 | 1.78 | 0.66 |
| 25:BA:1218:G:O2' | 25:BA:1219:A:O4' | 2.13 | 0.66 |
| 25:BA:2324:U:H5' | 30:BG:88:ILE:HD11 | 1.78 | 0.66 |
| 42:BW:12:ILE:HD13 | 42:BW:17:VAL:HG13 | 1.77 | 0.66 |
| 3:CC:78:GLY:HA3 | 3:CC:83:ARG:H | 1.60 | 0.66 |
| 5:CE:137:GLU:HG2 | 5:CE:140:ARG:HH11 | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:117:G:OP2 | 61:AA:4071:HOH:O | 2.14 | 0.66 |
| 27:BD:108:PRO:HD2 | 27:BD:111:LEU:HG | 1.78 | 0.66 |
| 1:CA:1120:G:O6 | 1:CA:1154:G:N2 | 2.29 | 0.66 |
| 4:CD:43:HIS:HA | 4:CD:46:LYS:HG3 | 1.77 | 0.66 |
| 50:D4:61:ARG:O | 50:D4:61:ARG:NH1 | 2.28 | 0.66 |
| 25:DA:2070:G:OP2 | 61:DA:4339:HOH:O | 2.13 | 0.66 |
| 25:DA:818:G:OP2 | 61:DA:3837:HOH:O | 2.13 | 0.66 |
| 25:BA:1091:A:OP1 | 25:BA:1091:A:H4' | 1.94 | 0.65 |
| 1:CA:1236:A:O2' | 1:CA:1304:G:H4' | 1.96 | 0.65 |
| 1:CA:539:A:H2' | 1:CA:540:G:C8 | 2.31 | 0.65 |
| 5:CE:122:GLU:O | 5:CE:126:ARG:NH1 | 2.30 | 0.65 |
| 10:CJ:29:ARG:HB2 | 10:CJ:84:GLN:HE22 | 1.60 | 0.65 |
| 25:DA:1313:U:OP1 | 61:DA:3981:HOH:O | 2.15 | 0.65 |
| 25:DA:900:A:H2' | 25:DA:901:A:H8 | 1.61 | 0.65 |
| 25:DA:2867:G:OP2 | 39:DT:119:LYS:NZ | 2.28 | 0.65 |
| 26:DB:75:G:N2 | 45:DZ:87:ASP:OD1 | 2.28 | 0.65 |
| 9:AI:46:ALA:HB2 | 9:AI:74:ILE:HG23 | 1.78 | 0.65 |
| 25:BA:839:G:OP2 | 61:BA:4064:HOH:O | 2.13 | 0.65 |
| 35:BP:59:LEU:HD11 | 54:B8:10:ALA:HB2 | 1.78 | 0.65 |
| 1:CA:56:U:H2' | 1:CA:57:G:C8 | 2.31 | 0.65 |
| 2:CB:47:THR:O | 2:CB:51:LEU:N | 2.27 | 0.65 |
| 9:CI:85:LEU:HB3 | 9:CI:92:TYR:CD2 | 2.31 | 0.65 |
| 10:CJ:42:THR:HG21 | 10:CJ:68:HIS:HD2 | 1.61 | 0.65 |
| 19:CS:15:LEU:HD12 | 19:CS:18:LYS:HD2 | 1.79 | 0.65 |
| 1:AA:1182:G:H4' | 1:AA:1183:A:H5' | 1.78 | 0.65 |
| 2:AB:15:VAL:HB | 2:AB:209:ARG:HG2 | 1.79 | 0.65 |
| 25:BA:601:A:OP2 | 61:BA:4002:HOH:O | 2.14 | 0.65 |
| 1:CA:333:G:H4' | 20:CT:16:HIS:CE1 | 2.30 | 0.65 |
| 25:DA:411:G:OP1 | 61:DA:3857:HOH:O | 2.14 | 0.65 |
| 28:DE:14:ILE:HD11 | 28:DE:173:VAL:HG11 | 1.76 | 0.65 |
| 30:DG:25:TYR:HB3 | 30:DG:30:GLU:HB2 | 1.79 | 0.65 |
| 26:DB:55:U:O3' | 30:DG:27:ASN:ND2 | 2.30 | 0.65 |
| 33:DN:15:LEU:HB2 | 33:DN:135:PRO:HB2 | 1.77 | 0.65 |
| 1:AA:1198:G:OP2 | 61:AA:4053:HOH:O | 2.14 | 0.65 |
| 4:AD:31:CYS:SG | 4:AD:32:ALA:N | 2.69 | 0.65 |
| 25:BA:2832:G:OP2 | 61:BE:406:HOH:O | 2.13 | 0.65 |
| 44:BY:98:VAL:HG12 | 44:BY:105:ALA:HA | 1.78 | 0.65 |
| 8:CH:12:ARG:HD2 | 8:CH:26:VAL:HG12 | 1.79 | 0.65 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C6 | 2.32 | 0.65 |
| 1:AA:159:G:H2' | 1:AA:161:A:OP2 | 1.97 | 0.65 |
| 25:BA:950:C:H2' | 25:BA:951:U:C6 | 2.32 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:31:C:OP1 | 61:DA:4153:HOH:O | 2.14 | 0.65 |
| 1:AA:1095:U:OP1 | 1:AA:1108:G:N2 | 2.30 | 0.65 |
| 1:AA:1320:C:H5' | 19:AS:70:LYS:HG3 | 1.78 | 0.65 |
| 2:AB:87:ARG:NH1 | 2:AB:233:SER:OG | 2.30 | 0.65 |
| 9:AI:16:ARG:HB2 | 9:AI:64:THR:HB | 1.77 | 0.65 |
| 25:BA:2349:G:OP1 | 61:BA:4028:HOH:O | 2.13 | 0.65 |
| 25:BA:849:A:OP1 | 61:BA:4293:HOH:O | 2.13 | 0.65 |
| 35:BP:44:GLY:O | 61:BP:302:HOH:O | 2.14 | 0.65 |
| 1:CA:1305:G:N2 | 1:CA:1331:G:H1' | 2.12 | 0.65 |
| 8:CH:49:GLU:HG2 | 8:CH:62:TYR:HE2 | 1.62 | 0.65 |
| 23:CX:40:C:H2' | 23:CX:41:C:H6 | 1.62 | 0.65 |
| 53:B7:33:ARG:NH2 | 61:B7:4001:HOH:O | 2.30 | 0.65 |
| 1:CA:1133:G:H2' | 1:CA:1134:G:H8 | 1.62 | 0.65 |
| 1:CA:558:G:OP1 | 61:CA:4171:HOH:O | 2.14 | 0.65 |
| 25:DA:1557:C:OP2 | 25:DA:1558:A:O2' | 2.14 | 0.65 |
| 32:DI:77:LEU:HB3 | 32:DI:142:VAL:HG12 | 1.79 | 0.65 |
| 1:AA:659:U:H2' | 1:AA:660:G:H8 | 1.62 | 0.65 |
| 1:AA:673:G:H2' | 1:AA:674:G:C8 | 2.32 | 0.65 |
| 24:AW:1:2QZ:H11 | 24:AW:9:MVA:HG23 | 1.77 | 0.65 |
| 25:BA:2442:A:OP2 | 61:BA:4633:HOH:O | 2.14 | 0.65 |
| 2:CB:19:HIS:CE1 | 2:CB:206:ASP:HB2 | 2.32 | 0.65 |
| 25:DA:370:G:OP1 | 25:DA:403:U:N3 | 2.24 | 0.65 |
| 2:AB:16:HIS:HB3 | 2:AB:210:SER:CB | 2.26 | 0.64 |
| 4:AD:173:TRP:NE1 | 4:AD:193:ASP:OD1 | 2.29 | 0.64 |
| 25:BA:1398:U:OP1 | 61:BA:3990:HOH:O | 2.15 | 0.64 |
| 43:BX:92:LEU:C | 43:BX:94:GLY:H | 2.00 | 0.64 |
| 1:CA:353:A:H8 | 1:CA:353:A:H5' | 1.62 | 0.64 |
| 2:CB:201:ILE:HG21 | 2:CB:214:ILE:HG21 | 1.77 | 0.64 |
| 17:CQ:22:LEU:HD13 | 17:CQ:41:LYS:HG3 | 1.79 | 0.64 |
| 25:DA:1430:C:H2' | 25:DA:1431:U:C6 | 2.32 | 0.64 |
| 25:DA:2680:C:H1' | 28:DE:187:ALA:HB1 | 1.78 | 0.64 |
| 39:DT:65:LYS:HE2 | 39:DT:67:SER:HB2 | 1.79 | 0.64 |
| 5:AE:137:GLU:HG2 | 5:AE:140:ARG:HH11 | 1.63 | 0.64 |
| 54:B8:6:THR:HG22 | 54:B8:63:PRO:HD2 | 1.79 | 0.64 |
| 25:BA:589:U:H5'' | 35:BP:29:LYS:HE3 | 1.79 | 0.64 |
| 1:CA:662:G:O2' | 1:CA:836:G:OP1 | 2.14 | 0.64 |
| 25:DA:2708:G:H1' | 37:DR:71:GLN:HE22 | 1.62 | 0.64 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C6 | 2.32 | 0.64 |
| 2:AB:210:SER:O | 2:AB:214:ILE:HG12 | 1.97 | 0.64 |
| 5:AE:12:LEU:HB3 | 5:AE:31:LEU:HB2 | 1.78 | 0.64 |
| 25:BA:1848:G:OP1 | 27:BD:88:ARG:NH2 | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:BR:28:LEU:HD12 | 37:BR:48:VAL:HG21 | 1.79 | 0.64 |
| 1:CA:69:G:H2' | 1:CA:70:G:H8 | 1.62 | 0.64 |
| 25:DA:143:G:H2' | 25:DA:143(A):C:C6 | 2.32 | 0.64 |
| 25:DA:455:C:N3 | 25:DA:472:A:H2' | 2.12 | 0.64 |
| 30:DG:129:GLY:O | 30:DG:161:THR:HB | 1.97 | 0.64 |
| 25:BA:1093:G:H2' | 25:BA:1156:G:H22 | 1.61 | 0.64 |
| 1:CA:1154:G:N7 | 1:CA:1155:G:C4 | 2.66 | 0.64 |
| 1:CA:1273:G:H3' | 1:CA:1274:G:H8 | 1.62 | 0.64 |
| 1:CA:1305:G:H5' | 21:CU:4:GLY:HA3 | 1.79 | 0.64 |
| 45:DZ:153:SER:OG | 45:DZ:154:ASP:OD1 | 2.14 | 0.64 |
| 2:AB:231:GLU:HB3 | 2:AB:232:PRO:CD | 2.28 | 0.64 |
| 19:AS:27:GLU:HB3 | 19:AS:28:LYS:HB3 | 1.77 | 0.64 |
| 25:DA:2062:A:OP1 | 61:DA:3798:HOH:O | 2.14 | 0.64 |
| 25:DA:524:U:H2' | 25:DA:525:U:C6 | 2.33 | 0.64 |
| 33:DN:38:HIS:CE1 | 33:DN:39:ARG:HG3 | 2.32 | 0.64 |
| 1:AA:123:C:OP1 | 1:AA:311:C:O2' | 2.13 | 0.64 |
| 1:AA:1346:A:N1 | 1:AA:1374:A:H5'' | 2.12 | 0.64 |
| 1:AA:457:C:H2' | 1:AA:458:C:C6 | 2.33 | 0.64 |
| 1:AA:476:G:H2' | 1:AA:477:A:O4' | 1.98 | 0.64 |
| 1:AA:56:U:H2' | 1:AA:57:G:C8 | 2.33 | 0.64 |
| 23:AX:6:G:H1 | 23:AX:67:C:H42 | 1.45 | 0.64 |
| 19:CS:37:ARG:O | 19:CS:70:LYS:NZ | 2.28 | 0.64 |
| 20:CT:86:ARG:O | 20:CT:90:GLN:HB2 | 1.98 | 0.64 |
| 25:BA:2405:A:H5' | 35:BP:63:PRO:HB3 | 1.79 | 0.64 |
| 4:CD:92:VAL:O | 4:CD:96:LEU:HD22 | 1.97 | 0.64 |
| 10:CJ:16:LEU:HD13 | 10:CJ:70:ARG:HG2 | 1.78 | 0.64 |
| 1:CA:254:G:OP1 | 17:CQ:66:SER:OG | 2.16 | 0.64 |
| 59:CX:101:FME:HCN | 25:DA:2451:A:H2 | 1.62 | 0.64 |
| 50:D4:64:GLY:C | 50:D4:66:SER:H | 2.01 | 0.64 |
| 25:DA:1776:G:OP2 | 61:DA:3756:HOH:O | 2.14 | 0.64 |
| 28:DE:150:VAL:HG13 | 28:DE:154:LYS:HG3 | 1.79 | 0.64 |
| 1:AA:1042:G:O2' | 1:AA:1043:C:O4' | 2.14 | 0.64 |
| 1:AA:1530:G:H2' | 1:AA:1531:A:O4' | 1.97 | 0.64 |
| 1:AA:161:A:H2' | 1:AA:162:A:C8 | 2.32 | 0.64 |
| 1:AA:193:C:H2' | 1:AA:194:C:H6 | 1.61 | 0.64 |
| 3:AC:12:LEU:HD23 | 3:AC:16:ARG:HB3 | 1.78 | 0.64 |
| 25:BA:1997:G:OP2 | 61:BA:4529:HOH:O | 2.15 | 0.64 |
| 25:BA:325:G:OP2 | 44:BY:84:ARG:NH2 | 2.31 | 0.64 |
| 1:CA:1015:A:H2' | 1:CA:1016:A:C8 | 2.33 | 0.64 |
| 1:CA:1133:G:H1 | 1:CA:1141:C:N4 | 1.95 | 0.64 |
| 1:CA:1312:G:N7 | 19:CS:2:PRO:HG2 | 2.12 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:814:A:H2' | 1:CA:816:A:H5'' | 1.78 | 0.64 |
| 13:CM:37:THR:O | 13:CM:55:ARG:NH1 | 2.31 | 0.64 |
| 25:DA:1973:G:OP1 | 61:DA:4138:HOH:O | 2.15 | 0.64 |
| 25:DA:586:A:N1 | 25:DA:809:G:O2' | 2.25 | 0.64 |
| 25:DA:594:U:H3 | 25:DA:663:G:H1 | 1.44 | 0.64 |
| 36:DQ:26:TYR:O | 36:DQ:67:ARG:NH1 | 2.28 | 0.64 |
| 37:DR:97:VAL:HG22 | 37:DR:114:VAL:HG22 | 1.79 | 0.64 |
| 1:AA:630:G:H2' | 1:AA:631:G:H8 | 1.62 | 0.64 |
| 12:AL:70:ILE:HG12 | 12:AL:100:ILE:HD12 | 1.80 | 0.64 |
| 16:AP:19:ILE:HD13 | 16:AP:36:ILE:HG13 | 1.78 | 0.64 |
| 37:BR:53:HIS:ND1 | 37:BR:94:TYR:OH | 2.30 | 0.64 |
| 25:DA:1604:C:OP2 | 61:DA:4392:HOH:O | 2.15 | 0.64 |
| 25:DA:2781:A:H5'' | 25:DA:2782:G:H5' | 1.79 | 0.64 |
| 26:DB:11:C:OP2 | 26:DB:12:C:N4 | 2.27 | 0.64 |
| 3:AC:36:ASP:O | 3:AC:40:ARG:HG3 | 1.98 | 0.64 |
| 25:BA:778:C:OP2 | 61:BA:4592:HOH:O | 2.15 | 0.64 |
| 2:CB:16:HIS:CB | 2:CB:204:ASN:HB3 | 2.24 | 0.64 |
| 19:CS:64:GLU:HB2 | 50:D4:59:PHE:HE1 | 1.62 | 0.64 |
| 25:DA:1266:G:O5' | 42:DW:15:ARG:NH2 | 2.30 | 0.64 |
| 25:DA:2298:A:C6 | 25:DA:2321:G:N1 | 2.66 | 0.64 |
| 28:DE:73:GLU:HG3 | 28:DE:73:GLU:O | 1.96 | 0.64 |
| 42:DW:71:VAL:HA | 42:DW:107:LEU:HD12 | 1.79 | 0.64 |
| 1:AA:1015:A:H2' | 1:AA:1016:A:C8 | 2.31 | 0.63 |
| 1:AA:518:C:O2' | 1:AA:530:G:N2 | 2.31 | 0.63 |
| 1:AA:598:U:H4' | 8:AH:94:TYR:CD2 | 2.33 | 0.63 |
| 25:BA:1091:A:H1' | 25:BA:1093:G:N3 | 2.13 | 0.63 |
| 25:BA:641:G:OP1 | 29:BF:40:GLN:NE2 | 2.24 | 0.63 |
| 13:CM:22:ILE:HB | 13:CM:25:ILE:HD13 | 1.79 | 0.63 |
| 19:CS:50:ALA:HB1 | 19:CS:57:HIS:HB3 | 1.80 | 0.63 |
| 20:CT:64:ASP:OD2 | 20:CT:81:LYS:NZ | 2.28 | 0.63 |
| 25:DA:365:C:OP2 | 61:DA:4447:HOH:O | 2.15 | 0.63 |
| 36:DQ:59:ARG:O | 36:DQ:61:GLY:N | 2.23 | 0.63 |
| 1:AA:945:G:OP2 | 61:AA:4057:HOH:O | 2.15 | 0.63 |
| 25:BA:2331:G:N2 | 38:BS:3:ARG:HA | 2.14 | 0.63 |
| 25:BA:2369:U:OP1 | 46:B0:20:ARG:NH1 | 2.31 | 0.63 |
| 1:CA:404:U:H5' | 4:CD:122:ARG:HD3 | 1.80 | 0.63 |
| 1:CA:59:A:H3' | 1:CA:331:G:H22 | 1.62 | 0.63 |
| 1:CA:953:G:H5' | 1:CA:965:A:N6 | 2.13 | 0.63 |
| 5:CE:78:HIS:HE1 | 5:CE:143:ARG:H | 1.45 | 0.63 |
| 6:AF:97:PHE:N | 18:AR:30:ASP:OD1 | 2.29 | 0.63 |
| 25:BA:53:G:O2' | 53:B7:35:ARG:HD3 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 25:BA:1466:U:O2' | 25:BA:1467:G:OP1 | 2.13 | 0.63 |
| 25:BA:2701:U:H4' | 25:BA:2702:C:O5' | 1.97 | 0.63 |
| 1:CA:1129:C:H2' | 1:CA:1139:G:N7 | 2.13 | 0.63 |
| 1:CA:1362:C:H2' | 1:CA:1363:C:H5'' | 1.81 | 0.63 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C6 | 2.34 | 0.63 |
| 1:CA:405:U:O4 | 4:CD:2:GLY:N | 2.32 | 0.63 |
| 2:CB:187:LEU:HA | 2:CB:201:ILE:HB | 1.80 | 0.63 |
| 25:DA:910:A:H62 | 36:DQ:12:GLN:HA | 1.63 | 0.63 |
| 50:B4:24:THR:OG1 | 50:B4:25:TYR:N | 2.31 | 0.63 |
| 25:DA:1766:U:H2' | 25:DA:1767:C:H6 | 1.63 | 0.63 |
| 25:DA:1667:G:O2' | 25:DA:1991:U:O4 | 2.13 | 0.63 |
| 25:DA:2816:C:O3' | 37:DR:99:LYS:NZ | 2.32 | 0.63 |
| 1:AA:333:G:H4' | 20:AT:16:HIS:CE1 | 2.33 | 0.63 |
| 25:BA:1639:G:H2' | 25:BA:1640:G:C8 | 2.33 | 0.63 |
| 25:BA:560:C:O3' | 40:BU:53:ARG:NH1 | 2.31 | 0.63 |
| 1:CA:1320:C:H5' | 19:CS:70:LYS:HG3 | 1.80 | 0.63 |
| 2:CB:87:ARG:HE | 2:CB:233:SER:HB3 | 1.63 | 0.63 |
| 2:CB:56:ARG:HB3 | 2:CB:56:ARG:HH11 | 1.63 | 0.63 |
| 25:DA:298:G:H5'' | 25:DA:299:A:OP1 | 1.98 | 0.63 |
| 26:DB:14:U:OP2 | 26:DB:70:C:O2' | 2.14 | 0.63 |
| 31:DH:28:GLY:HA3 | 31:DH:79:VAL:HB | 1.80 | 0.63 |
| 12:AL:79:GLU:HB3 | 12:AL:80:HIS:HD2 | 1.64 | 0.63 |
| 25:BA:1701:A:OP2 | 61:BA:4089:HOH:O | 2.15 | 0.63 |
| 1:CA:1145:C:H4' | 1:CA:1146:A:H5' | 1.81 | 0.63 |
| 4:CD:31:CYS:SG | 4:CD:33:MET:N | 2.71 | 0.63 |
| 25:DA:568:U:H5' | 25:DA:945:A:N1 | 2.14 | 0.63 |
| 1:AA:922:G:H4' | 5:AE:20:GLN:HA | 1.80 | 0.63 |
| 2:AB:62:ALA:HB2 | 2:AB:222:ILE:HG22 | 1.80 | 0.63 |
| 4:AD:177:ASP:HB3 | 4:AD:182:LYS:HD3 | 1.81 | 0.63 |
| 2:AB:195:ASP:O | 8:AH:68:ARG:NH2 | 2.31 | 0.63 |
| 25:BA:1020:C:OP1 | 61:BA:4060:HOH:O | 2.16 | 0.63 |
| 25:BA:1044:C:OP1 | 61:BA:4480:HOH:O | 2.15 | 0.63 |
| 11:CK:98:LEU:O | 11:CK:101:SER:OG | 2.13 | 0.63 |
| 23:CX:48:C:C2 | 23:CX:59:A:H1' | 2.34 | 0.63 |
| 25:DA:144:C:H2' | 25:DA:145:G:H8 | 1.62 | 0.63 |
| 40:DU:92:ARG:HA | 40:DU:95:LEU:HB2 | 1.81 | 0.63 |
| 1:AA:1346:A:OP1 | 9:AI:120:ARG:NH1 | 2.28 | 0.63 |
| 1:AA:503:C:OP2 | 12:AL:116:SER:HB3 | 1.99 | 0.63 |
| 1:AA:427:U:OP1 | 4:AD:13:ARG:NH2 | 2.32 | 0.63 |
| 15:AO:5:LYS:HD2 | 15:AO:5:LYS:H | 1.63 | 0.63 |
| 25:BA:599:U:OP1 | 61:BA:4467:HOH:O | 2.15 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DF:21:ALA:CB | 29:DF:22:ALA:HA | 2.28 | 0.63 |
| 2:AB:78:GLN:O | 2:AB:81:VAL:HG23 | 1.98 | 0.63 |
| 5:AE:78:HIS:CD2 | 5:AE:142:LEU:HD23 | 2.34 | 0.63 |
| 38:BS:27:SER:HA | 38:BS:88:ASP:HB3 | 1.80 | 0.63 |
| 25:DA:1653:G:H3' | 37:DR:2:ARG:HD3 | 1.81 | 0.63 |
| 25:DA:1688:U:O2 | 25:DA:1700:A:H5' | 1.99 | 0.63 |
| 25:DA:1721:G:H8 | 25:DA:1741:A:H62 | 1.46 | 0.63 |
| 25:DA:1889:A:H2' | 25:DA:1890:A:C8 | 2.33 | 0.63 |
| 25:DA:2803:C:H2' | 25:DA:2804:C:H6 | 1.63 | 0.63 |
| 27:DD:183:ARG:HG3 | 27:DD:270:ILE:HG12 | 1.81 | 0.63 |
| 1:AA:200:G:H5' | 1:AA:201:C:OP2 | 1.99 | 0.62 |
| 1:AA:400:C:H5'' | 4:AD:73:ARG:HH22 | 1.63 | 0.62 |
| 1:AA:445:G:H2' | 1:AA:446:G:C8 | 2.33 | 0.62 |
| 4:AD:173:TRP:CE3 | 4:AD:174:LEU:HG | 2.34 | 0.62 |
| 1:CA:45:U:H2' | 1:CA:46:G:C8 | 2.34 | 0.62 |
| 1:CA:585:G:OP1 | 17:CQ:37:LYS:NZ | 2.24 | 0.62 |
| 50:D4:59:PHE:HA | 50:D4:61:ARG:N | 2.14 | 0.62 |
| 25:DA:1159:U:H2' | 25:DA:1160:G:C8 | 2.32 | 0.62 |
| 25:DA:2016:U:H2' | 25:DA:2017:U:H6 | 1.64 | 0.62 |
| 25:DA:2098:U:H2' | 25:DA:2099:U:O4' | 1.99 | 0.62 |
| 25:DA:2469:A:H4' | 36:DQ:56:ARG:HD2 | 1.79 | 0.62 |
| 29:DF:165:ARG:HG2 | 29:DF:168:ARG:NH2 | 2.14 | 0.62 |
| 1:AA:404:U:H5' | 4:AD:122:ARG:HD2 | 1.81 | 0.62 |
| 10:AJ:37:PRO:HA | 10:AJ:72:VAL:HG12 | 1.81 | 0.62 |
| 10:AJ:49:VAL:HG23 | 14:AN:41:ARG:HB2 | 1.81 | 0.62 |
| 25:BA:2367:C:H1' | 46:B0:39:ARG:HH21 | 1.63 | 0.62 |
| 44:BY:6:HIS:H | 44:BY:6:HIS:CD2 | 2.15 | 0.62 |
| 1:CA:1163:C:N3 | 1:CA:1173:G:N2 | 2.47 | 0.62 |
| 13:CM:13:LYS:HA | 13:CM:44:ARG:HH11 | 1.63 | 0.62 |
| 28:DE:72:VAL:HA | 28:DE:73:GLU:HB3 | 1.81 | 0.62 |
| 1:AA:187:C:H2' | 1:AA:188:C:H6 | 1.65 | 0.62 |
| 45:BZ:151:HIS:O | 45:BZ:153:SER:N | 2.31 | 0.62 |
| 25:DA:2079:U:OP1 | 47:D1:21:ARG:NH2 | 2.32 | 0.62 |
| 25:DA:2206:G:H3' | 25:DA:2207:G:N7 | 2.14 | 0.62 |
| 25:DA:854:G:H2' | 25:DA:855:G:H8 | 1.64 | 0.62 |
| 1:AA:486:U:H2' | 1:AA:487:A:C8 | 2.35 | 0.62 |
| 1:AA:552:U:C2' | 1:AA:553:A:H5' | 2.29 | 0.62 |
| 1:AA:937:A:OP2 | 61:AA:4095:HOH:O | 2.16 | 0.62 |
| 8:AH:14:ARG:NH2 | 8:AH:83:ILE:O | 2.33 | 0.62 |
| 16:AP:43:LYS:HG2 | 16:AP:48:TRP:CD2 | 2.34 | 0.62 |
| 32:BI:40:THR:O | 32:BI:44:LEU:HB2 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:62:C:H42 | 25:DA:93:G:H1 | 1.46 | 0.62 |
| 25:DA:994:C:OP1 | 40:DU:53:ARG:NH2 | 2.32 | 0.62 |
| 1:AA:1305:G:N2 | 1:AA:1331:G:H1' | 2.15 | 0.62 |
| 1:AA:560:U:O2' | 1:AA:561:U:OP2 | 2.16 | 0.62 |
| 3:AC:114:PRO:O | 3:AC:118:GLN:NE2 | 2.32 | 0.62 |
| 18:AR:32:ARG:HA | 18:AR:69:THR:HG21 | 1.81 | 0.62 |
| 25:DA:2079:U:O3' | 47:D1:35:THR:OG1 | 2.17 | 0.62 |
| 43:DX:53:LYS:HB3 | 43:DX:82:GLN:HB3 | 1.80 | 0.62 |
| 2:AB:74:LYS:NZ | 2:AB:205:ASP:OD2 | 2.32 | 0.62 |
| 52:B6:13:CYS:SG | 52:B6:47:THR:HG21 | 2.39 | 0.62 |
| 2:CB:163:PHE:CD1 | 2:CB:185:ILE:HG13 | 2.34 | 0.62 |
| 12:CL:49:ASN:ND2 | 12:CL:92:ASP:OD2 | 2.31 | 0.62 |
| 25:DA:1036:G:H1 | 25:DA:1119:C:H42 | 1.45 | 0.62 |
| 25:DA:333:G:H5'' | 25:DA:334:C:OP2 | 1.99 | 0.62 |
| 28:DE:3:GLY:HA3 | 28:DE:81:ILE:HD12 | 1.80 | 0.62 |
| 30:DG:179:PRO:HB2 | 50:D4:42:PHE:HE1 | 1.64 | 0.62 |
| 1:AA:96:U:H2' | 1:AA:97:G:C8 | 2.35 | 0.62 |
| 1:AA:406:G:N3 | 4:AD:119:GLN:NE2 | 2.46 | 0.62 |
| 16:AP:53:VAL:HG22 | 16:AP:79:VAL:HG22 | 1.80 | 0.62 |
| 19:AS:36:ARG:HB3 | 19:AS:72:GLY:HA3 | 1.79 | 0.62 |
| 1:CA:1108:G:O6 | 61:CA:4092:HOH:O | 2.14 | 0.62 |
| 3:CC:6:HIS:HB3 | 14:CN:49:HIS:ND1 | 2.14 | 0.62 |
| 1:AA:983:A:H1' | 1:AA:1049:U:O2 | 2.00 | 0.62 |
| 16:AP:43:LYS:HG2 | 16:AP:48:TRP:CE2 | 2.35 | 0.62 |
| 25:BA:2348:A:H61 | 46:B0:43:THR:CG2 | 2.12 | 0.62 |
| 1:CA:1036:G:H5' | 1:CA:1037:C:C6 | 2.35 | 0.62 |
| 1:CA:586:C:O2' | 1:CA:878:G:H4' | 1.98 | 0.62 |
| 2:CB:69:LEU:HB3 | 2:CB:162:ILE:HG22 | 1.81 | 0.62 |
| 3:CC:179:ARG:NH1 | 3:CC:206:GLU:OE1 | 2.33 | 0.62 |
| 23:CX:9:G:O2' | 23:CX:10:G:N7 | 2.23 | 0.62 |
| 25:DA:1495:A:H2' | 25:DA:1496:A:C8 | 2.35 | 0.62 |
| 25:DA:2584:U:O4 | 61:DA:3959:HOH:O | 2.13 | 0.62 |
| 34:DO:35:VAL:HG11 | 34:DO:103:ALA:HB3 | 1.80 | 0.62 |
| 1:AA:863:U:OP1 | 61:AA:4128:HOH:O | 2.16 | 0.62 |
| 25:DA:1005:C:H2' | 25:DA:1006:C:C6 | 2.35 | 0.62 |
| 25:DA:658:C:H2' | 25:DA:659:C:C6 | 2.35 | 0.62 |
| 1:AA:1125:U:C2 | 1:AA:1127:G:N7 | 2.68 | 0.62 |
| 9:AI:29:ASN:ND2 | 9:AI:65:VAL:O | 2.33 | 0.62 |
| 50:B4:15:ILE:HD12 | 50:B4:21:VAL:HG22 | 1.82 | 0.62 |
| 32:BI:72:LEU:O | 32:BI:74:ASN:N | 2.31 | 0.62 |
| 45:BZ:102:LEU:HD13 | 45:BZ:123:ASP:HA | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CI:85:LEU:HB3 | 9:CI:92:TYR:HD2 | 1.64 | 0.62 |
| 11:CK:110:ASP:HB3 | 18:CR:85:LEU:HB3 | 1.81 | 0.62 |
| 30:DG:11:TYR:CE2 | 30:DG:16:ARG:HD3 | 2.35 | 0.62 |
| 45:DZ:45:ASP:OD1 | 45:DZ:49:ARG:NH1 | 2.32 | 0.62 |
| 1:AA:175:C:H2' | 1:AA:176:C:H6 | 1.64 | 0.61 |
| 1:AA:460:G:O6 | 1:AA:470:C:H5'' | 2.00 | 0.61 |
| 20:AT:14:LYS:HG3 | 20:AT:17:ARG:NH2 | 2.15 | 0.61 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:N1 | 1.95 | 0.61 |
| 1:CA:447:G:O6 | 61:CA:4157:HOH:O | 2.16 | 0.61 |
| 19:CS:41:VAL:HG12 | 19:CS:43:GLU:H | 1.63 | 0.61 |
| 25:DA:2285:C:OP2 | 52:D6:6:ARG:NH1 | 2.33 | 0.61 |
| 25:DA:579:G:H2' | 25:DA:580:C:C6 | 2.35 | 0.61 |
| 29:DF:183:VAL:O | 29:DF:187:VAL:HG23 | 2.00 | 0.61 |
| 1:AA:993:G:H1 | 1:AA:1045:C:H42 | 1.48 | 0.61 |
| 1:AA:1305:G:H22 | 1:AA:1331:G:H1' | 1.64 | 0.61 |
| 1:AA:1442(A):G:C8 | 39:BT:118:ARG:HG2 | 2.35 | 0.61 |
| 8:AH:51:VAL:HG11 | 8:AH:60:ARG:HH12 | 1.65 | 0.61 |
| 11:AK:99:GLN:HG2 | 11:AK:105:VAL:HG21 | 1.82 | 0.61 |
| 1:CA:1239:A:H62 | 1:CA:1299:A:H62 | 1.47 | 0.61 |
| 25:DA:2218:U:O2 | 47:D1:52:ARG:NH2 | 2.33 | 0.61 |
| 30:DG:18:GLU:OE2 | 30:DG:21:ARG:NH1 | 2.32 | 0.61 |
| 1:AA:1241:G:H1 | 1:AA:1296:C:H42 | 1.49 | 0.61 |
| 19:AS:64:GLU:HB2 | 50:B4:59:PHE:HE1 | 1.65 | 0.61 |
| 25:BA:2713:C:H2' | 25:BA:2714:U:H2' | 1.81 | 0.61 |
| 1:CA:202:U:H3' | 1:CA:203:U:H6 | 1.63 | 0.61 |
| 3:CC:47:LEU:HD12 | 3:CC:68:VAL:HG11 | 1.81 | 0.61 |
| 34:DO:119:PRO:HB2 | 39:DT:68:TYR:CE2 | 2.35 | 0.61 |
| 35:DP:50:ARG:HH21 | 35:DP:50:ARG:HG3 | 1.66 | 0.61 |
| 39:DT:85:LYS:NZ | 39:DT:87:ASP:OD2 | 2.33 | 0.61 |
| 25:BA:2412:G:O6 | 61:BA:4067:HOH:O | 2.14 | 0.61 |
| 1:CA:1041:A:N6 | 1:CA:1042:G:O6 | 2.33 | 0.61 |
| 25:DA:1496:A:N3 | 25:DA:1577:C:O2' | 2.32 | 0.61 |
| 25:DA:2640:G:N7 | 61:DA:3808:HOH:O | 2.31 | 0.61 |
| 25:DA:867:C:H2' | 25:DA:868:U:C6 | 2.35 | 0.61 |
| 1:AA:1158:C:H5 | 1:AA:1181:G:N1 | 1.98 | 0.61 |
| 1:AA:1356:G:H2' | 1:AA:1357:A:C8 | 2.35 | 0.61 |
| 6:AF:38:GLU:HB2 | 6:AF:64:GLN:HG2 | 1.83 | 0.61 |
| 27:BD:71:ASP:CB | 27:BD:103:ARG:HH22 | 2.13 | 0.61 |
| 1:CA:1004:A:H8 | 1:CA:1005:A:H4' | 1.66 | 0.61 |
| 2:CB:48:MET:HA | 2:CB:51:LEU:HB2 | 1.83 | 0.61 |
| 11:CK:58:PRO:HG3 | 11:CK:89:ALA:O | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:CN:37:PHE:HB3 | 14:CN:39:LEU:HD12 | 1.81 | 0.61 |
| 25:DA:1773:A:H5'' | 61:DA:4248:HOH:O | 1.99 | 0.61 |
| 25:DA:2303:G:O2' | 30:DG:132:ASN:HB2 | 2.01 | 0.61 |
| 25:DA:2748:A:O2' | 31:DH:63:SER:O | 2.19 | 0.61 |
| 39:DT:24:PRO:HA | 39:DT:49:VAL:HG22 | 1.82 | 0.61 |
| 9:AI:50:LEU:HD13 | 9:AI:56:LEU:HA | 1.82 | 0.61 |
| 28:BE:175:VAL:HG22 | 28:BE:177:PRO:HD3 | 1.82 | 0.61 |
| 15:CO:88:ARG:HB3 | 15:CO:88:ARG:HH21 | 1.63 | 0.61 |
| 25:DA:2404:C:O3' | 35:DP:77:ARG:NH2 | 2.33 | 0.61 |
| 25:DA:2557:G:H2' | 25:DA:2558:C:H6 | 1.66 | 0.61 |
| 1:CA:1422:G:O3' | 34:DO:49:ARG:NH1 | 2.34 | 0.61 |
| 1:AA:1260:C:O5' | 1:AA:1284:C:H4' | 2.01 | 0.61 |
| 1:AA:154:C:N4 | 1:AA:168:G:O6 | 2.34 | 0.61 |
| 1:AA:601:C:H2' | 1:AA:602:A:H8 | 1.63 | 0.61 |
| 28:BE:24:THR:HG22 | 28:BE:186:GLY:O | 2.01 | 0.61 |
| 1:CA:192:U:O2' | 1:CA:193:C:H5' | 2.00 | 0.61 |
| 6:CF:24:GLU:HG3 | 6:CF:28:ARG:HH11 | 1.65 | 0.61 |
| 15:CO:5:LYS:HD2 | 15:CO:5:LYS:H | 1.64 | 0.61 |
| 23:CX:4:G:H1 | 23:CX:69:C:N4 | 1.97 | 0.61 |
| 25:DA:2273:A:H2' | 25:DA:2274:A:C8 | 2.36 | 0.61 |
| 25:DA:307:G:N1 | 25:DA:310:A:OP2 | 2.33 | 0.61 |
| 25:DA:958:U:OP2 | 36:DQ:14:ARG:NH1 | 2.34 | 0.61 |
| 4:AD:184:LYS:HB3 | 4:AD:184:LYS:NZ | 2.16 | 0.61 |
| 4:CD:17:VAL:HG11 | 4:CD:197:PRO:HG3 | 1.82 | 0.61 |
| 6:CF:25:ILE:HD13 | 6:CF:82:ARG:HE | 1.65 | 0.61 |
| 25:DA:2589:A:OP1 | 61:DA:4063:HOH:O | 2.15 | 0.61 |
| 41:DV:5:VAL:HG11 | 41:DV:57:VAL:HG21 | 1.83 | 0.61 |
| 1:AA:923:A:O2' | 1:AA:1399:C:OP2 | 2.18 | 0.61 |
| 1:CA:1150:U:O4 | 1:CA:1151:A:N6 | 2.34 | 0.61 |
| 1:CA:9:G:H2' | 1:CA:10:A:H8 | 1.65 | 0.61 |
| 20:CT:57:ARG:HH12 | 20:CT:100:ILE:HG13 | 1.65 | 0.61 |
| 25:DA:867:C:H2' | 25:DA:868:U:H6 | 1.66 | 0.61 |
| 25:DA:887:A:O2' | 25:DA:889:C:OP2 | 2.18 | 0.61 |
| 25:DA:948:G:OP1 | 61:DA:4173:HOH:O | 2.16 | 0.61 |
| 29:DF:103:LYS:HA | 29:DF:106:ARG:HG3 | 1.82 | 0.61 |
| 37:DR:36:THR:HG22 | 37:DR:37:THR:H | 1.66 | 0.61 |
| 39:DT:95:ARG:HG2 | 39:DT:95:ARG:HH11 | 1.64 | 0.61 |
| 1:AA:1104:G:H4' | 2:AB:111:ARG:NH1 | 2.16 | 0.61 |
| 5:AE:92:LYS:HB3 | 5:AE:119:LEU:HB2 | 1.83 | 0.61 |
| 25:BA:1405:A:H61 | 25:BA:1418:U:H3 | 1.49 | 0.61 |
| 25:BA:1577:C:HO2' | 25:BA:1578:C:P | 2.23 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:2460:A:N1 | 61:BA:4605:HOH:O | 2.31 | 0.61 |
| 25:BA:787:U:OP2 | 61:BA:4519:HOH:O | 2.16 | 0.61 |
| 29:BF:65:TRP:CZ2 | 29:BF:75:HIS:HD2 | 2.19 | 0.61 |
| 25:BA:1199:C:OP1 | 40:BU:92:ARG:NH1 | 2.30 | 0.61 |
| 10:CJ:32:ALA:HB1 | 10:CJ:33:GLN:HA | 1.82 | 0.61 |
| 25:DA:1900:A:OP2 | 61:DA:3902:HOH:O | 2.16 | 0.61 |
| 25:DA:2845:G:H2' | 25:DA:2846:G:C8 | 2.36 | 0.61 |
| 29:DF:11:VAL:HG22 | 29:DF:125:LEU:HB2 | 1.83 | 0.61 |
| 1:AA:552:U:H2' | 1:AA:553:A:H5' | 1.83 | 0.60 |
| 25:BA:1219:A:H4' | 25:BA:1220:U:OP1 | 2.01 | 0.60 |
| 25:BA:1231:G:H2' | 25:BA:1232:G:O4' | 2.01 | 0.60 |
| 25:BA:1701:A:OP1 | 37:BR:1:MET:HA | 2.00 | 0.60 |
| 1:CA:1053:G:N7 | 1:CA:1200:C:H5'' | 2.16 | 0.60 |
| 1:CA:1062:U:H2' | 1:CA:1063:C:C6 | 2.36 | 0.60 |
| 1:CA:346:G:OP1 | 39:DT:41:ARG:NH2 | 2.32 | 0.60 |
| 3:CC:150:LYS:HG3 | 3:CC:169:ALA:HB2 | 1.83 | 0.60 |
| 6:CF:61:LEU:HB3 | 6:CF:63:TYR:HE1 | 1.65 | 0.60 |
| 25:DA:289:A:N6 | 25:DA:351:G:O2' | 2.34 | 0.60 |
| 25:DA:973:A:OP2 | 61:DA:3814:HOH:O | 2.17 | 0.60 |
| 26:DB:41:U:H5 | 30:DG:70:VAL:H | 1.48 | 0.60 |
| 39:DT:16:ARG:NH1 | 39:DT:18:ASP:OD2 | 2.35 | 0.60 |
| 1:AA:1026:G:H5' | 1:AA:1027:C:H5'' | 1.83 | 0.60 |
| 3:AC:40:ARG:NH2 | 3:AC:55:VAL:O | 2.35 | 0.60 |
| 1:CA:1256:A:H61 | 1:CA:1278:U:H1' | 1.65 | 0.60 |
| 11:CK:62:GLN:HG3 | 11:CK:97:ALA:HB2 | 1.82 | 0.60 |
| 16:CP:52:ASP:O | 16:CP:54:GLU:N | 2.32 | 0.60 |
| 25:DA:667:U:O2 | 54:D8:2:PRO:HD2 | 2.01 | 0.60 |
| 25:DA:585:G:O2' | 25:DA:1254:A:N6 | 2.31 | 0.60 |
| 25:DA:1531:C:H42 | 25:DA:1538:G:H1 | 1.49 | 0.60 |
| 1:AA:1271:G:H5'' | 1:AA:1314:C:OP1 | 2.02 | 0.60 |
| 1:AA:201:C:N4 | 1:AA:216:G:H1 | 1.91 | 0.60 |
| 1:AA:827:U:H5'' | 1:AA:828:A:OP2 | 2.02 | 0.60 |
| 1:AA:881:G:OP2 | 12:AL:12:ARG:NH2 | 2.34 | 0.60 |
| 25:BA:2340:A:H2' | 25:BA:2341:G:C8 | 2.36 | 0.60 |
| 25:BA:649:C:O2' | 25:BA:704:U:OP1 | 2.19 | 0.60 |
| 25:BA:272:U:H4' | 32:BI:50:ARG:NH1 | 2.16 | 0.60 |
| 45:BZ:109:ALA:HB3 | 45:BZ:145:GLU:HG3 | 1.83 | 0.60 |
| 1:CA:826:C:H2' | 1:CA:827:U:C6 | 2.35 | 0.60 |
| 3:CC:18:TRP:CD1 | 14:CN:54:PRO:HA | 2.36 | 0.60 |
| 25:DA:390:A:N6 | 61:DA:4490:HOH:O | 2.33 | 0.60 |
| 1:AA:677:U:H3 | 1:AA:713:G:H22 | 1.47 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:1829:U:H5' | 27:BD:259:THR:CG2 | 2.28 | 0.60 |
| 1:CA:67:C:H2' | 1:CA:68:G:C8 | 2.35 | 0.60 |
| 25:DA:1125:G:H5' | 55:D9:37:GLY:HA2 | 1.81 | 0.60 |
| 25:DA:2570:G:O6 | 61:DA:4417:HOH:O | 2.12 | 0.60 |
| 25:DA:2870:C:H2' | 25:DA:2871:C:O4' | 2.00 | 0.60 |
| 1:AA:953:G:H5' | 1:AA:965:A:H61 | 1.66 | 0.60 |
| 5:AE:11:ILE:HB | 5:AE:31:LEU:HB3 | 1.83 | 0.60 |
| 10:AJ:11:PHE:HE1 | 10:AJ:67:THR:HG22 | 1.66 | 0.60 |
| 25:BA:594:A:O2' | 41:BV:78:LYS:NZ | 2.32 | 0.60 |
| 25:DA:2785:C:OP1 | 28:DE:41:LYS:NZ | 2.17 | 0.60 |
| 1:AA:1007:C:N3 | 1:AA:1022:G:O6 | 2.35 | 0.60 |
| 1:AA:486:U:H2' | 1:AA:487:A:H8 | 1.65 | 0.60 |
| 1:AA:691:G:H2' | 1:AA:692:U:C6 | 2.36 | 0.60 |
| 9:AI:86:VAL:HG13 | 9:AI:96:LEU:HD12 | 1.83 | 0.60 |
| 1:CA:235:C:H5' | 17:CQ:70:ARG:HG2 | 1.82 | 0.60 |
| 6:CF:82:ARG:HB2 | 6:CF:85:VAL:HG23 | 1.82 | 0.60 |
| 1:CA:390:C:O3' | 16:CP:28:ARG:NH2 | 2.34 | 0.60 |
| 25:DA:898:C:H2' | 25:DA:899:A:O4' | 2.02 | 0.60 |
| 28:DE:52:LEU:O | 28:DE:76:ARG:N | 2.24 | 0.60 |
| 33:DN:34:LEU:O | 33:DN:49:GLY:HA3 | 2.01 | 0.60 |
| 43:DX:59:VAL:HG21 | 43:DX:78:LYS:HE3 | 1.84 | 0.60 |
| 44:DY:38:ILE:HD13 | 44:DY:66:PRO:HA | 1.83 | 0.60 |
| 1:AA:383:A:C2 | 1:AA:384:G:H1' | 2.36 | 0.60 |
| 12:AL:59:ARG:HD3 | 24:AW:1:2QZ:OG1 | 2.02 | 0.60 |
| 25:BA:1739:U:H2' | 25:BA:1741:C:C5 | 2.37 | 0.60 |
| 25:BA:2227:G:H3' | 25:BA:2228:G:N7 | 2.15 | 0.60 |
| 31:BH:3:ARG:HG2 | 31:BH:6:ARG:HG2 | 1.84 | 0.60 |
| 1:CA:491:G:O6 | 61:CA:4132:HOH:O | 2.11 | 0.60 |
| 1:CA:749:C:OP2 | 61:CA:4142:HOH:O | 2.16 | 0.60 |
| 25:DA:2397:G:N2 | 25:DA:2420:C:H1' | 2.16 | 0.60 |
| 30:DG:39:ILE:HG23 | 30:DG:157:ILE:HG12 | 1.83 | 0.60 |
| 35:DP:89:ALA:O | 35:DP:121:LYS:NZ | 2.29 | 0.60 |
| 1:AA:232:G:H1' | 1:AA:262:A:N1 | 2.17 | 0.60 |
| 1:AA:322:C:O2' | 20:AT:23:ARG:HD2 | 2.02 | 0.60 |
| 25:BA:1668:G:OP2 | 61:BA:4215:HOH:O | 2.17 | 0.60 |
| 28:BE:120:TRP:CE3 | 28:BE:155:LYS:HD3 | 2.37 | 0.60 |
| 30:BG:170:ARG:NH2 | 30:BG:182:LYS:O | 2.35 | 0.60 |
| 31:BH:40:GLU:OE1 | 31:BH:61:HIS:NE2 | 2.31 | 0.60 |
| 31:BH:92:ILE:H | 31:BH:92:ILE:HD12 | 1.67 | 0.60 |
| 1:CA:1286:A:H2 | 21:CU:18:TYR:HH | 1.50 | 0.60 |
| 1:CA:69:G:H2' | 1:CA:70:G:C8 | 2.37 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:D4:15:ILE:HB | 50:D4:32:TYR:HD1 | 1.66 | 0.60 |
| 25:DA:1266:G:O2' | 25:DA:2012:G:O6 | 2.13 | 0.60 |
| 30:DG:16:ARG:HE | 30:DG:31:VAL:HG11 | 1.65 | 0.60 |
| 1:AA:961:U:OP2 | 1:AA:1223:C:O2' | 2.16 | 0.60 |
| 29:BF:183:VAL:O | 29:BF:187:VAL:HG23 | 2.01 | 0.60 |
| 1:CA:1442:G:O2' | 1:CA:1442(A):G:OP1 | 2.18 | 0.60 |
| 1:CA:735:C:H2' | 1:CA:736:C:C6 | 2.35 | 0.60 |
| 1:CA:939:G:H1 | 1:CA:1344:C:N4 | 1.98 | 0.60 |
| 36:DQ:66:ILE:HG12 | 36:DQ:104:PHE:CE2 | 2.37 | 0.60 |
| 38:DS:14:VAL:O | 38:DS:18:ILE:HG12 | 2.02 | 0.60 |
| 1:AA:454:C:P | 16:AP:75:ARG:HH22 | 2.24 | 0.60 |
| 6:AF:61:LEU:HB3 | 6:AF:63:TYR:HE1 | 1.65 | 0.60 |
| 50:B4:62:ARG:HB2 | 50:B4:63:TYR:HD1 | 1.67 | 0.60 |
| 25:BA:1889:G:N2 | 25:BA:1905:G:H2' | 2.17 | 0.60 |
| 25:BA:278:G:H2' | 25:BA:279:G:H5'' | 1.82 | 0.60 |
| 1:CA:426:G:OP1 | 4:CD:36:ARG:NH1 | 2.33 | 0.60 |
| 16:CP:14:ASN:OD1 | 16:CP:16:HIS:HE1 | 1.85 | 0.60 |
| 20:CT:58:LYS:HE3 | 20:CT:62:LEU:HD12 | 1.84 | 0.60 |
| 25:DA:981:A:N1 | 25:DA:2027:G:O2' | 2.28 | 0.60 |
| 35:DP:47:ASP:OD2 | 35:DP:50:ARG:NH2 | 2.34 | 0.60 |
| 36:DQ:34:LEU:HB2 | 36:DQ:118:LEU:HD22 | 1.83 | 0.60 |
| 2:AB:163:PHE:HD1 | 2:AB:185:ILE:HD12 | 1.67 | 0.59 |
| 20:AT:44:ALA:HB2 | 20:AT:52:ALA:HB1 | 1.83 | 0.59 |
| 25:BA:599:U:H2' | 25:BA:600:G:C8 | 2.36 | 0.59 |
| 25:BA:830:A:OP2 | 61:BA:4454:HOH:O | 2.17 | 0.59 |
| 25:BA:922:G:H1 | 25:BA:948:C:H42 | 1.49 | 0.59 |
| 25:BA:98:U:OP1 | 25:BA:99:G:O2' | 2.14 | 0.59 |
| 34:BO:98:VAL:HG11 | 34:BO:114:ILE:HG23 | 1.84 | 0.59 |
| 1:CA:1151:A:C5' | 10:CJ:41:PRO:HA | 2.32 | 0.59 |
| 2:CB:100:GLY:O | 2:CB:104:ASN:N | 2.34 | 0.59 |
| 3:CC:157:ILE:HD12 | 3:CC:164:ARG:HB3 | 1.84 | 0.59 |
| 3:CC:189:ALA:HB3 | 3:CC:196:LEU:HB2 | 1.84 | 0.59 |
| 11:CK:48:ILE:O | 11:CK:50:TYR:N | 2.33 | 0.59 |
| 25:DA:82:G:N1 | 25:DA:103:A:OP2 | 2.28 | 0.59 |
| 25:DA:443:A:H5'' | 25:DA:444:C:OP1 | 2.02 | 0.59 |
| 25:DA:704:G:H1' | 25:DA:726:G:N2 | 2.17 | 0.59 |
| 34:DO:98:VAL:HG13 | 34:DO:117:LEU:HB3 | 1.84 | 0.59 |
| 1:AA:128:G:O2' | 17:AQ:3:LYS:NZ | 2.34 | 0.59 |
| 25:BA:2406:C:OP2 | 54:B8:30:ARG:NH1 | 2.35 | 0.59 |
| 25:BA:542:C:OP1 | 51:B5:16:ARG:NH2 | 2.35 | 0.59 |
| 19:CS:48:THR:HG22 | 19:CS:61:TYR:HA | 1.82 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:D4:15:ILE:HB | 50:D4:32:TYR:CD1 | 2.36 | 0.59 |
| 54:D8:33:ASN:HA | 54:D8:36:LYS:HD2 | 1.84 | 0.59 |
| 27:DD:108:PRO:HG2 | 27:DD:111:LEU:HB2 | 1.84 | 0.59 |
| 1:AA:1277:C:O2' | 1:AA:1279:A:H1' | 2.02 | 0.59 |
| 46:B0:53:MET:HG3 | 46:B0:59:LEU:HD23 | 1.83 | 0.59 |
| 1:CA:1016:A:H2' | 1:CA:1017:G:O4' | 2.02 | 0.59 |
| 6:CF:33:TYR:HB2 | 6:CF:75:LEU:HD23 | 1.83 | 0.59 |
| 48:D2:29:LYS:HG2 | 48:D2:57:ILE:HD13 | 1.84 | 0.59 |
| 29:DF:21:ALA:HB3 | 29:DF:22:ALA:HA | 1.84 | 0.59 |
| 1:AA:501:C:H1' | 1:AA:549:C:H1' | 1.84 | 0.59 |
| 2:AB:51:LEU:HD23 | 2:AB:201:ILE:HD12 | 1.85 | 0.59 |
| 10:AJ:7:LYS:HB3 | 10:AJ:97:GLU:HB2 | 1.83 | 0.59 |
| 18:AR:42:ARG:HH21 | 18:AR:42:ARG:HA | 1.67 | 0.59 |
| 25:BA:139:A:H8 | 25:BA:1454:C:O2' | 1.86 | 0.59 |
| 25:BA:2092:G:N3 | 61:BA:3834:HOH:O | 2.31 | 0.59 |
| 25:BA:2274:U:OP2 | 46:B0:19:LYS:NZ | 2.34 | 0.59 |
| 35:BP:89:ALA:O | 35:BP:121:LYS:NZ | 2.29 | 0.59 |
| 39:BT:53:ARG:HH11 | 39:BT:53:ARG:HB3 | 1.67 | 0.59 |
| 12:CL:36:VAL:HG23 | 24:CW:10:2QY:H89 | 1.85 | 0.59 |
| 15:CO:3:ILE:HG21 | 15:CO:34:LEU:HD21 | 1.83 | 0.59 |
| 19:CS:51:VAL:O | 19:CS:58:VAL:N | 2.30 | 0.59 |
| 25:DA:1405:U:H2' | 25:DA:1406:U:C6 | 2.37 | 0.59 |
| 25:DA:226:G:H21 | 25:DA:228:A:H62 | 1.50 | 0.59 |
| 25:DA:885:C:H2' | 25:DA:886:C:H4' | 1.84 | 0.59 |
| 25:DA:1903:G:OP1 | 27:DD:241:PRO:HB2 | 2.02 | 0.59 |
| 29:DF:184:TYR:CE2 | 29:DF:188:ARG:HD2 | 2.37 | 0.59 |
| 1:AA:1009:G:O6 | 1:AA:1020:U:O2 | 2.20 | 0.59 |
| 1:AA:1342:C:H4' | 9:AI:125:TYR:HB3 | 1.84 | 0.59 |
| 9:AI:24:GLY:HA2 | 9:AI:59:PHE:O | 2.02 | 0.59 |
| 25:BA:1229:G:H5' | 49:B3:29:ARG:NH1 | 2.17 | 0.59 |
| 25:BA:1501:U:O2' | 25:BA:1502:G:N7 | 2.33 | 0.59 |
| 25:BA:2213:G:H5' | 25:BA:2214:G:OP2 | 2.03 | 0.59 |
| 1:CA:827:U:H5'' | 1:CA:828:A:OP2 | 2.02 | 0.59 |
| 2:CB:68:ILE:HG12 | 2:CB:161:ALA:HB3 | 1.84 | 0.59 |
| 5:CE:50:GLU:HB2 | 5:CE:53:LEU:HD13 | 1.84 | 0.59 |
| 47:D1:3:LYS:HB2 | 47:D1:61:ARG:NH1 | 2.18 | 0.59 |
| 25:DA:1632:A:OP2 | 61:DA:4177:HOH:O | 2.17 | 0.59 |
| 25:DA:212:G:H2' | 25:DA:213:A:O4' | 2.02 | 0.59 |
| 25:DA:799:G:O6 | 61:DA:4430:HOH:O | 2.15 | 0.59 |
| 26:DB:48:A:H4' | 38:DS:95:HIS:HD2 | 1.68 | 0.59 |
| 1:AA:623:C:H2' | 1:AA:624:C:H6 | 1.68 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:78:G:H1 | 1:AA:92:C:N4 | 2.01 | 0.59 |
| 2:AB:95:GLN:HG3 | 2:AB:147:LYS:HD3 | 1.84 | 0.59 |
| 4:AD:182:LYS:HG2 | 4:AD:183:GLY:N | 2.16 | 0.59 |
| 25:BA:1385:G:H5'' | 43:BX:16:LYS:HD3 | 1.83 | 0.59 |
| 25:BA:1897:C:H2' | 25:BA:1898:A:O4' | 2.02 | 0.59 |
| 25:BA:479:C:OP1 | 61:BA:4179:HOH:O | 2.17 | 0.59 |
| 1:CA:1104:G:H4' | 2:CB:111:ARG:NH1 | 2.17 | 0.59 |
| 2:CB:7:VAL:HB | 2:CB:9:GLU:HG3 | 1.85 | 0.59 |
| 4:CD:8:VAL:HB | 4:CD:115:ARG:HH12 | 1.67 | 0.59 |
| 10:CJ:8:LEU:HD12 | 10:CJ:20:ALA:HB2 | 1.85 | 0.59 |
| 3:AC:70:VAL:HG12 | 3:AC:72:LYS:H | 1.66 | 0.59 |
| 1:CA:776:G:N2 | 1:CA:802:A:OP2 | 2.29 | 0.59 |
| 47:D1:3:LYS:HB2 | 47:D1:61:ARG:HH11 | 1.66 | 0.59 |
| 1:AA:1442:G:O2' | 1:AA:1442(A):G:OP1 | 2.18 | 0.59 |
| 16:AP:50:LYS:HA | 16:AP:50:LYS:HE2 | 1.85 | 0.59 |
| 25:BA:1410:G:P | 47:B1:3:LYS:HG3 | 2.43 | 0.59 |
| 27:BD:183:ARG:HG3 | 27:BD:270:ILE:HG12 | 1.85 | 0.59 |
| 30:BG:12:TYR:HA | 30:BG:16:ARG:HG2 | 1.84 | 0.59 |
| 1:CA:427:U:H3' | 1:CA:428:G:H2' | 1.85 | 0.59 |
| 1:CA:457:C:H2' | 1:CA:458:C:H6 | 1.68 | 0.59 |
| 3:CC:114:PRO:O | 3:CC:118:GLN:HG2 | 2.03 | 0.59 |
| 55:D9:25:VAL:HB | 55:D9:34:GLN:HB2 | 1.83 | 0.59 |
| 25:DA:2074:U:OP1 | 61:DA:3911:HOH:O | 2.17 | 0.59 |
| 25:DA:2802:G:H2' | 25:DA:2803:C:O4' | 2.01 | 0.59 |
| 30:DG:50:ALA:O | 30:DG:52:ILE:N | 2.35 | 0.59 |
| 34:DO:77:ILE:HG13 | 39:DT:74:ARG:HG2 | 1.83 | 0.59 |
| 1:AA:1221:G:OP1 | 1:AA:1320:C:N4 | 2.34 | 0.59 |
| 1:AA:433:C:H2' | 1:AA:434:U:H6 | 1.67 | 0.59 |
| 1:AA:1126:U:C5 | 10:AJ:71:LEU:HD22 | 2.36 | 0.59 |
| 25:BA:1077:G:H21 | 55:B9:36:GLN:HE22 | 1.50 | 0.59 |
| 1:CA:1084:G:H5' | 1:CA:1102:A:OP2 | 2.02 | 0.59 |
| 1:CA:1172:C:H2' | 1:CA:1173:G:C8 | 2.38 | 0.59 |
| 1:CA:1493:A:H1' | 25:DA:1913:A:N6 | 2.13 | 0.59 |
| 1:CA:693:G:H2' | 1:CA:694:A:H8 | 1.68 | 0.59 |
| 3:CC:36:ASP:HA | 3:CC:39:ILE:HD12 | 1.85 | 0.59 |
| 3:CC:6:HIS:HD2 | 3:CC:8:ILE:H | 1.51 | 0.59 |
| 5:CE:36:ASP:O | 5:CE:38:GLN:N | 2.36 | 0.59 |
| 25:DA:1314:C:OP1 | 61:DA:4076:HOH:O | 2.17 | 0.59 |
| 25:DA:1359:A:N1 | 25:DA:1372:U:O4 | 2.35 | 0.59 |
| 31:DH:30:LYS:HG3 | 31:DH:80:SER:O | 2.02 | 0.59 |
| 1:AA:174:C:H2' | 1:AA:175:C:C6 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:323:U:H2' | 1:AA:324:G:O4' | 2.02 | 0.59 |
| 1:AA:382:A:C2 | 1:AA:383:A:N7 | 2.70 | 0.59 |
| 1:AA:501:C:O2' | 1:AA:549:C:O2 | 2.21 | 0.59 |
| 1:AA:659:U:H2' | 1:AA:660:G:C8 | 2.38 | 0.59 |
| 1:AA:711:G:OP1 | 6:AF:54:LYS:NZ | 2.35 | 0.59 |
| 1:AA:715:A:H2' | 1:AA:716:A:C8 | 2.38 | 0.59 |
| 1:AA:913:A:OP1 | 12:AL:46:LYS:NZ | 2.36 | 0.59 |
| 52:B6:14:THR:HB | 52:B6:48:VAL:O | 2.03 | 0.59 |
| 25:BA:129:G:OP1 | 61:BA:3963:HOH:O | 2.17 | 0.59 |
| 45:BZ:111:VAL:C | 45:BZ:113:ALA:H | 2.06 | 0.59 |
| 1:CA:1287:A:N3 | 1:CA:1353:G:O2' | 2.32 | 0.59 |
| 1:CA:826:C:H2' | 1:CA:827:U:H6 | 1.68 | 0.59 |
| 11:CK:22:HIS:HB3 | 11:CK:29:ILE:HB | 1.84 | 0.59 |
| 16:CP:51:VAL:HG12 | 16:CP:53:VAL:H | 1.68 | 0.59 |
| 25:DA:1359:A:H61 | 25:DA:1372:U:H3 | 1.50 | 0.59 |
| 25:DA:1840:G:OP2 | 61:DA:4306:HOH:O | 2.16 | 0.59 |
| 25:DA:2298:A:N1 | 25:DA:2321:G:C6 | 2.71 | 0.59 |
| 1:AA:692:U:O2' | 1:AA:694:A:N7 | 2.28 | 0.58 |
| 1:AA:833:U:H2' | 1:AA:834:C:C6 | 2.38 | 0.58 |
| 25:BA:2579:G:H2' | 25:BA:2580:C:C6 | 2.38 | 0.58 |
| 43:BX:31:HIS:CD2 | 43:BX:33:LYS:HB2 | 2.37 | 0.58 |
| 1:CA:1005:A:H1' | 1:CA:1036:G:N1 | 2.16 | 0.58 |
| 7:CG:76:ARG:O | 7:CG:87:VAL:N | 2.36 | 0.58 |
| 25:DA:143:G:H2' | 25:DA:143(A):C:H6 | 1.66 | 0.58 |
| 25:DA:2299:G:N1 | 25:DA:2318:G:C8 | 2.71 | 0.58 |
| 25:DA:2472:G:N1 | 25:DA:2477:C:OP1 | 2.25 | 0.58 |
| 4:AD:31:CYS:SG | 4:AD:33:MET:N | 2.74 | 0.58 |
| 5:AE:143:ARG:NH1 | 8:AH:77:GLU:OE1 | 2.36 | 0.58 |
| 25:BA:2745:G:P | 28:BE:203:LYS:HZ1 | 2.26 | 0.58 |
| 39:BT:51:ARG:HG3 | 39:BT:98:LYS:HD2 | 1.86 | 0.58 |
| 1:CA:1005:A:O2' | 1:CA:1006:C:OP1 | 2.20 | 0.58 |
| 1:CA:1286:A:C8 | 1:CA:1287:A:H4' | 2.38 | 0.58 |
| 1:CA:552:U:C2' | 1:CA:553:A:H5' | 2.33 | 0.58 |
| 1:CA:999:C:N4 | 1:CA:1043:C:N3 | 2.51 | 0.58 |
| 5:CE:9:LYS:HD2 | 5:CE:112:LEU:HD21 | 1.86 | 0.58 |
| 7:CG:113:GLU:CG | 7:CG:119:ARG:HG2 | 2.32 | 0.58 |
| 7:CG:75:VAL:HG13 | 7:CG:145:ALA:HA | 1.85 | 0.58 |
| 48:D2:22:GLU:OE2 | 48:D2:68:ARG:NH2 | 2.36 | 0.58 |
| 28:DE:28:ALA:HB3 | 28:DE:93:VAL:HG12 | 1.84 | 0.58 |
| 42:DW:60:ASN:HD22 | 42:DW:60:ASN:N | 2.02 | 0.58 |
| 43:DX:31:HIS:CD2 | 43:DX:33:LYS:H | 2.21 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:600:C:H2' | 1:AA:601:C:C6 | 2.38 | 0.58 |
| 1:AA:713:G:H2' | 1:AA:714:G:C8 | 2.38 | 0.58 |
| 1:AA:737:A:H2' | 1:AA:738:C:C6 | 2.37 | 0.58 |
| 3:AC:157:ILE:HD12 | 3:AC:164:ARG:HB3 | 1.84 | 0.58 |
| 5:AE:110:LEU:HD13 | 5:AE:118:ILE:HG21 | 1.86 | 0.58 |
| 32:BI:4:ILE:HG12 | 32:BI:18:VAL:HG22 | 1.84 | 0.58 |
| 25:BA:1233:U:H4' | 41:BV:79:VAL:HG22 | 1.84 | 0.58 |
| 45:BZ:151:HIS:C | 45:BZ:153:SER:H | 2.06 | 0.58 |
| 1:CA:1047:G:H1 | 1:CA:1210:C:H42 | 1.51 | 0.58 |
| 1:CA:1121:U:H2' | 1:CA:1122:U:O4' | 2.03 | 0.58 |
| 1:CA:1271:G:H5'' | 1:CA:1314:C:OP1 | 2.04 | 0.58 |
| 1:CA:202:U:H3' | 1:CA:203:U:C6 | 2.38 | 0.58 |
| 1:CA:9:G:H2' | 1:CA:10:A:C8 | 2.38 | 0.58 |
| 2:CB:40:HIS:HB3 | 2:CB:190:THR:HG21 | 1.85 | 0.58 |
| 53:D7:5:TRP:CD1 | 53:D7:7:PRO:HD3 | 2.38 | 0.58 |
| 25:DA:2314:C:H2' | 25:DA:2315:G:C8 | 2.38 | 0.58 |
| 25:DA:2502:G:N7 | 61:DA:4548:HOH:O | 2.31 | 0.58 |
| 29:DF:137:LYS:HA | 29:DF:140:LEU:HD23 | 1.85 | 0.58 |
| 1:AA:1030(C):G:H2' | 1:AA:1030(D):A:C8 | 2.39 | 0.58 |
| 20:AT:45:GLN:HA | 20:AT:91:LEU:HB3 | 1.84 | 0.58 |
| 1:CA:1086:U:H3 | 1:CA:1099:G:H22 | 1.51 | 0.58 |
| 3:CC:180:ALA:HB1 | 3:CC:203:PHE:HE1 | 1.69 | 0.58 |
| 1:AA:1392:G:N2 | 1:AA:1502:A:H8 | 2.02 | 0.58 |
| 1:AA:269:C:H2' | 1:AA:270:A:C8 | 2.37 | 0.58 |
| 11:AK:15:ALA:HA | 11:AK:77:MET:HA | 1.84 | 0.58 |
| 25:BA:1185:C:O3' | 33:BN:25:ARG:NH1 | 2.36 | 0.58 |
| 25:BA:2853:G:O6 | 61:BA:4561:HOH:O | 2.17 | 0.58 |
| 31:BH:33:LEU:HD21 | 31:BH:136:ILE:HG13 | 1.85 | 0.58 |
| 31:BH:40:GLU:OE2 | 31:BH:60:ARG:NH1 | 2.37 | 0.58 |
| 1:CA:1138:G:C6 | 1:CA:1140:C:H1' | 2.38 | 0.58 |
| 1:CA:769:G:H4' | 1:CA:1513:A:H4' | 1.85 | 0.58 |
| 6:CF:81:ILE:HD11 | 27:DD:125:ILE:HB | 1.86 | 0.58 |
| 34:DO:80:ASP:OD1 | 39:DT:64:ARG:NH2 | 2.36 | 0.58 |
| 25:DA:1188:U:H4' | 41:DV:79:VAL:HG22 | 1.84 | 0.58 |
| 45:DZ:130:PRO:O | 45:DZ:133:ILE:HG13 | 2.03 | 0.58 |
| 7:AG:46:ALA:O | 7:AG:50:ILE:HG23 | 2.04 | 0.58 |
| 19:AS:41:VAL:HG12 | 19:AS:43:GLU:H | 1.68 | 0.58 |
| 25:BA:2080:A:N7 | 61:BA:4112:HOH:O | 2.32 | 0.58 |
| 1:CA:222:U:H2' | 1:CA:223:U:C6 | 2.38 | 0.58 |
| 1:CA:1123:A:H4' | 10:CJ:37:PRO:HD2 | 1.86 | 0.58 |
| 25:DA:83:G:O2' | 25:DA:102:G:N2 | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:DE:9:VAL:HB | 39:DT:3:ARG:HG2 | 1.85 | 0.58 |
| 40:DU:65:ILE:HD11 | 40:DU:95:LEU:HB3 | 1.86 | 0.58 |
| 44:DY:23:ARG:HG2 | 44:DY:42:VAL:HG22 | 1.84 | 0.58 |
| 1:AA:924:C:O2' | 1:AA:1502:A:N6 | 2.35 | 0.58 |
| 5:AE:94:ALA:HB2 | 5:AE:119:LEU:HG | 1.85 | 0.58 |
| 12:AL:36:VAL:HG22 | 12:AL:82:VAL:HG22 | 1.86 | 0.58 |
| 53:B7:47:ARG:HH11 | 53:B7:47:ARG:HB3 | 1.67 | 0.58 |
| 25:BA:1779:G:H5'' | 25:BA:1779:G:H8 | 1.68 | 0.58 |
| 26:BB:6:C:H2' | 26:BB:7:G:H5'' | 1.85 | 0.58 |
| 34:BO:35:VAL:HG21 | 34:BO:69:ILE:HD13 | 1.85 | 0.58 |
| 43:BX:41:ASN:O | 43:BX:45:THR:HG23 | 2.04 | 0.58 |
| 1:CA:130:A:O2' | 1:CA:131:C:O5' | 2.19 | 0.58 |
| 1:CA:975:A:N1 | 10:CJ:48:THR:HB | 2.19 | 0.58 |
| 31:DH:124:GLU:HB2 | 31:DH:132:ARG:HB3 | 1.86 | 0.58 |
| 7:AG:42:ILE:HG23 | 7:AG:117:ALA:HA | 1.84 | 0.58 |
| 9:AI:16:ARG:HD3 | 9:AI:64:THR:HG21 | 1.85 | 0.58 |
| 25:BA:2022:G:OP1 | 37:BR:5:LYS:NZ | 2.37 | 0.58 |
| 25:BA:2251:G:OP2 | 61:BA:4210:HOH:O | 2.17 | 0.58 |
| 39:BT:53:ARG:NH1 | 39:BT:53:ARG:HB3 | 2.18 | 0.58 |
| 1:CA:1026:G:H5' | 1:CA:1027:C:H5'' | 1.85 | 0.58 |
| 1:CA:426:G:H2' | 1:CA:427:U:C6 | 2.39 | 0.58 |
| 5:CE:78:HIS:CE1 | 5:CE:143:ARG:H | 2.22 | 0.58 |
| 1:CA:913:A:OP1 | 12:CL:46:LYS:NZ | 2.36 | 0.58 |
| 25:DA:171:G:H2' | 25:DA:172:C:C6 | 2.39 | 0.58 |
| 25:DA:7:G:H2' | 25:DA:8:A:C8 | 2.38 | 0.58 |
| 30:DG:38:VAL:HG22 | 30:DG:93:THR:HG23 | 1.84 | 0.58 |
| 32:BI:104:GLN:HG3 | 32:BI:105:HIS:CD2 | 2.38 | 0.58 |
| 36:BQ:110:THR:HG23 | 36:BQ:113:GLN:OE1 | 2.04 | 0.58 |
| 1:CA:1316:G:H2' | 1:CA:1318:A:OP2 | 2.04 | 0.58 |
| 2:CB:30:ARG:HH21 | 2:CB:194:PRO:HB2 | 1.68 | 0.58 |
| 1:CA:437:U:H5' | 4:CD:155:LEU:HD21 | 1.85 | 0.58 |
| 1:CA:642:A:N3 | 8:CH:113:SER:OG | 2.35 | 0.58 |
| 25:DA:2680:C:OP2 | 28:DE:111:ARG:NH2 | 2.37 | 0.58 |
| 6:AF:10:LEU:HD23 | 6:AF:61:LEU:HD13 | 1.86 | 0.58 |
| 8:AH:83:ILE:HB | 8:AH:137:VAL:HG13 | 1.86 | 0.58 |
| 25:BA:945:A:O2' | 25:BA:946:A:H8 | 1.87 | 0.58 |
| 1:CA:582:U:OP1 | 15:CO:68:ARG:NH2 | 2.25 | 0.58 |
| 3:CC:39:ILE:O | 3:CC:43:LEU:HG | 2.04 | 0.58 |
| 25:DA:1618:A:H5' | 61:DA:3986:HOH:O | 2.04 | 0.58 |
| 1:AA:997:U:H3 | 1:AA:1044:A:H61 | 1.52 | 0.57 |
| 1:AA:1521:G:N3 | 61:AA:4036:HOH:O | 2.32 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:147:ASP:O | 5:AE:151:LEU:HG | 2.03 | 0.57 |
| 2:CB:87:ARG:NE | 2:CB:233:SER:HB3 | 2.18 | 0.57 |
| 4:CD:150:GLU:OE2 | 4:CD:151:LYS:N | 2.37 | 0.57 |
| 7:CG:14:PRO:HG3 | 7:CG:21:VAL:HG13 | 1.86 | 0.57 |
| 25:DA:1169:G:H1 | 25:DA:1180:C:H42 | 1.52 | 0.57 |
| 25:DA:1327:C:OP2 | 61:DA:3851:HOH:O | 2.17 | 0.57 |
| 1:AA:1189:C:O2 | 61:AA:4114:HOH:O | 2.16 | 0.57 |
| 3:AC:56:ASP:HB2 | 3:AC:67:THR:HB | 1.86 | 0.57 |
| 19:AS:31:ILE:HB | 19:AS:49:ILE:HG12 | 1.85 | 0.57 |
| 25:BA:1425:A:H4' | 25:BA:1426:G:OP2 | 2.04 | 0.57 |
| 29:BF:53:THR:HG22 | 29:BF:56:GLU:HG3 | 1.85 | 0.57 |
| 31:BH:98:LEU:HD22 | 31:BH:125:VAL:HG23 | 1.85 | 0.57 |
| 1:CA:1422:G:H5'' | 34:DO:48:PRO:HB3 | 1.86 | 0.57 |
| 1:CA:17:U:H2' | 1:CA:18:C:C6 | 2.39 | 0.57 |
| 1:CA:392:G:H2' | 1:CA:393:A:C8 | 2.39 | 0.57 |
| 1:CA:689:C:OP2 | 11:CK:55:LYS:NZ | 2.35 | 0.57 |
| 2:CB:162:ILE:HD11 | 2:CB:184:VAL:HG22 | 1.84 | 0.57 |
| 7:CG:26:PHE:O | 7:CG:30:ILE:HG13 | 2.04 | 0.57 |
| 23:CX:23:C:H2' | 23:CX:24:U:H6 | 1.69 | 0.57 |
| 25:DA:2591:C:OP1 | 27:DD:239:ARG:HD2 | 2.03 | 0.57 |
| 28:DE:116:VAL:HG13 | 28:DE:122:PHE:HB2 | 1.85 | 0.57 |
| 43:DX:31:HIS:HD2 | 43:DX:33:LYS:H | 1.51 | 0.57 |
| 44:BY:54:LYS:HA | 44:BY:56:PRO:CD | 2.31 | 0.57 |
| 1:CA:1269:A:C8 | 1:CA:1270:C:H1' | 2.38 | 0.57 |
| 1:CA:1309:G:O2' | 13:CM:77:ASN:ND2 | 2.38 | 0.57 |
| 1:CA:839:U:O2' | 1:CA:840:C:OP1 | 2.20 | 0.57 |
| 9:CI:51:ARG:HG2 | 9:CI:56:LEU:HD21 | 1.85 | 0.57 |
| 15:CO:54:ARG:O | 15:CO:58:MET:HG3 | 2.04 | 0.57 |
| 25:DA:286:C:H2' | 25:DA:287:C:C6 | 2.38 | 0.57 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.39 | 0.57 |
| 1:AA:444:C:H2' | 1:AA:445:G:H8 | 1.69 | 0.57 |
| 2:AB:60:ASP:OD1 | 2:AB:64:ARG:NE | 2.35 | 0.57 |
| 7:AG:27:ILE:HD12 | 7:AG:40:ALA:HA | 1.85 | 0.57 |
| 24:AW:4:PRO:O | 24:AW:6:2R1:N | 2.37 | 0.57 |
| 25:BA:1890:A:N6 | 25:BA:1905:G:O2' | 2.38 | 0.57 |
| 25:BA:2045:G:H5' | 25:BA:2629:C:H4' | 1.86 | 0.57 |
| 28:BE:12:THR:HG22 | 28:BE:13:ARG:H | 1.68 | 0.57 |
| 29:BF:197:ASP:OD1 | 29:BF:197:ASP:N | 2.37 | 0.57 |
| 1:CA:148:G:H2' | 1:CA:149:A:C8 | 2.37 | 0.57 |
| 7:CG:76:ARG:CZ | 7:CG:89:MET:HB2 | 2.34 | 0.57 |
| 19:CS:64:GLU:HB2 | 50:D4:59:PHE:CE1 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:DR:83:ILE:O | 37:DR:86:ARG:HG2 | 2.04 | 0.57 |
| 1:AA:1270:C:C2' | 1:AA:1271:G:H5' | 2.34 | 0.57 |
| 25:BA:303:C:N4 | 25:BA:385:G:H1 | 1.98 | 0.57 |
| 1:CA:1160:G:H22 | 1:CA:1176:A:H2 | 1.52 | 0.57 |
| 1:CA:785:G:C2' | 1:CA:786:G:H5' | 2.34 | 0.57 |
| 11:CK:20:TYR:CZ | 11:CK:83:ILE:HD12 | 2.38 | 0.57 |
| 18:CR:47:THR:HG23 | 18:CR:49:LYS:HG3 | 1.87 | 0.57 |
| 25:DA:1031:G:H21 | 55:D9:36:GLN:HE22 | 1.52 | 0.57 |
| 25:DA:2023:G:H5' | 25:DA:2617:C:H4' | 1.87 | 0.57 |
| 25:DA:956:G:H5' | 25:DA:957:A:OP2 | 2.04 | 0.57 |
| 25:DA:674:G:H1' | 29:DF:74:ARG:HD3 | 1.87 | 0.57 |
| 34:DO:87:ILE:HD12 | 34:DO:91:LEU:HA | 1.86 | 0.57 |
| 25:DA:2839:G:H5' | 37:DR:46:GLY:HA2 | 1.87 | 0.57 |
| 45:DZ:39:VAL:HG21 | 45:DZ:44:PHE:HB2 | 1.85 | 0.57 |
| 1:AA:347:G:H21 | 1:AA:348:G:H3' | 1.69 | 0.57 |
| 1:AA:96:U:O2' | 1:AA:97:G:H5' | 2.04 | 0.57 |
| 3:AC:15:THR:CG2 | 3:AC:181:ASN:HA | 2.34 | 0.57 |
| 5:AE:50:GLU:HB2 | 5:AE:53:LEU:HD13 | 1.85 | 0.57 |
| 6:AF:44:GLY:HA2 | 6:AF:59:TYR:CZ | 2.40 | 0.57 |
| 1:CA:1318:A:H5'' | 19:CS:3:ARG:NH2 | 2.15 | 0.57 |
| 1:CA:243:A:H4' | 1:CA:244:U:H5'' | 1.85 | 0.57 |
| 2:CB:102:LEU:HD23 | 2:CB:182:ILE:HD12 | 1.86 | 0.57 |
| 2:CB:166:ASP:HB3 | 2:CB:169:LYS:HB2 | 1.86 | 0.57 |
| 3:CC:58:GLU:HB2 | 3:CC:65:ALA:HB3 | 1.86 | 0.57 |
| 10:CJ:8:LEU:HB3 | 10:CJ:16:LEU:HD22 | 1.86 | 0.57 |
| 11:CK:48:ILE:HD11 | 11:CK:64:ALA:HA | 1.87 | 0.57 |
| 1:CA:974:A:OP2 | 14:CN:41:ARG:NH1 | 2.38 | 0.57 |
| 25:DA:195:A:H5'' | 25:DA:196:A:O5' | 2.03 | 0.57 |
| 33:DN:58:ASP:OD1 | 33:DN:58:ASP:N | 2.34 | 0.57 |
| 25:BA:1068:G:H22 | 25:BA:1188:A:H2 | 1.47 | 0.57 |
| 25:BA:625:G:O2' | 25:BA:702:A:N6 | 2.38 | 0.57 |
| 1:CA:706:A:H5'' | 11:CK:22:HIS:CE1 | 2.39 | 0.57 |
| 2:CB:179:LYS:HA | 8:CH:72:PRO:HG3 | 1.85 | 0.57 |
| 35:DP:86:LYS:HB3 | 35:DP:118:GLY:HA3 | 1.86 | 0.57 |
| 40:DU:76:TYR:HH | 40:DU:92:ARG:HH11 | 1.52 | 0.57 |
| 1:AA:1162:C:N4 | 1:AA:1174:G:H1 | 2.01 | 0.57 |
| 1:AA:1392:G:H21 | 1:AA:1502:A:H8 | 1.53 | 0.57 |
| 1:AA:828:A:H2' | 1:AA:829:G:O4' | 2.05 | 0.57 |
| 25:BA:181:C:OP1 | 61:BA:3915:HOH:O | 2.17 | 0.57 |
| 25:BA:2786:C:H2' | 25:BA:2787:C:H6 | 1.68 | 0.57 |
| 25:BA:572:A:O2' | 25:BA:573:G:OP1 | 2.21 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1125:U:HO2' | 1:CA:1126:U:H2' | 1.69 | 0.57 |
| 14:CN:4:LYS:HA | 14:CN:7:ILE:HD13 | 1.87 | 0.57 |
| 15:CO:4:THR:HB | 15:CO:5:LYS:HD2 | 1.87 | 0.57 |
| 25:DA:10:G:H2' | 25:DA:11:G:H8 | 1.70 | 0.57 |
| 25:DA:1778:U:H2' | 25:DA:1784:A:N6 | 2.19 | 0.57 |
| 1:AA:216:G:H2' | 1:AA:217:C:C6 | 2.40 | 0.57 |
| 14:AN:48:ALA:HB2 | 14:AN:53:LEU:HD12 | 1.87 | 0.57 |
| 48:B2:1:MET:HE2 | 48:B2:6:VAL:HG22 | 1.86 | 0.57 |
| 25:BA:2308:U:OP2 | 38:BS:9:ARG:NH2 | 2.37 | 0.57 |
| 25:BA:2299:A:N6 | 25:BA:2356:U:H3 | 2.01 | 0.57 |
| 25:BA:676:G:OP1 | 54:B8:19:SER:OG | 2.21 | 0.57 |
| 28:BE:174:ASP:OD1 | 28:BE:175:VAL:N | 2.38 | 0.57 |
| 30:BG:47:LYS:HG3 | 30:BG:48:GLU:H | 1.69 | 0.57 |
| 10:CJ:55:LYS:HG3 | 10:CJ:56:HIS:CD2 | 2.40 | 0.57 |
| 25:DA:2189:U:H2' | 25:DA:2190:G:C8 | 2.40 | 0.57 |
| 25:DA:2312:U:C5 | 25:DA:2313:C:H5 | 2.23 | 0.57 |
| 25:DA:2689:U:OP2 | 25:DA:2719:G:N2 | 2.36 | 0.57 |
| 25:DA:30:G:H2' | 25:DA:31:C:C6 | 2.40 | 0.57 |
| 25:DA:38:A:H2' | 25:DA:39:C:C6 | 2.40 | 0.57 |
| 27:DD:182:LEU:HB2 | 27:DD:272:ALA:HB3 | 1.86 | 0.57 |
| 28:DE:101:ARG:NH2 | 28:DE:171:GLU:HB2 | 2.19 | 0.57 |
| 25:DA:660:G:H5' | 29:DF:99:TYR:CE2 | 2.40 | 0.57 |
| 30:DG:103:LEU:HD23 | 30:DG:106:LEU:HD23 | 1.86 | 0.57 |
| 30:DG:114:ILE:HB | 30:DG:117:PHE:HB2 | 1.87 | 0.57 |
| 25:DA:2562:U:H1' | 34:DO:23:ARG:HH11 | 1.70 | 0.57 |
| 1:AA:1028:C:N4 | 1:AA:1033:G:H1 | 2.00 | 0.57 |
| 25:BA:311:C:H2' | 25:BA:312:C:H6 | 1.69 | 0.57 |
| 25:BA:1836:U:O2 | 27:BD:50:THR:HB | 2.04 | 0.57 |
| 35:BP:2:LYS:NZ | 35:BP:4:SER:HB3 | 2.20 | 0.57 |
| 1:CA:1513:A:H2' | 1:CA:1514:C:C6 | 2.40 | 0.57 |
| 2:CB:44:LEU:H | 2:CB:44:LEU:HD22 | 1.70 | 0.57 |
| 25:DA:2074:U:H2' | 25:DA:2075:U:C6 | 2.39 | 0.57 |
| 25:DA:82:G:O6 | 61:DA:4494:HOH:O | 2.17 | 0.57 |
| 28:DE:174:ASP:OD1 | 28:DE:175:VAL:N | 2.37 | 0.57 |
| 45:DZ:48:PHE:CE1 | 45:DZ:52:SER:HA | 2.40 | 0.57 |
| 1:AA:1002:G:H3' | 1:AA:1003:G:H8 | 1.70 | 0.56 |
| 1:AA:994:A:N1 | 1:AA:1047:G:H4' | 2.20 | 0.56 |
| 1:AA:175:C:H2' | 1:AA:176:C:C6 | 2.39 | 0.56 |
| 13:AM:56:LEU:O | 13:AM:60:VAL:HG23 | 2.04 | 0.56 |
| 25:BA:118:U:OP2 | 61:BA:3886:HOH:O | 2.17 | 0.56 |
| 25:BA:1338:U:H2' | 25:BA:1339:C:C6 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:2348:A:H61 | 46:B0:43:THR:HG22 | 1.70 | 0.56 |
| 45:BZ:158:PRO:O | 45:BZ:161:VAL:HG12 | 2.04 | 0.56 |
| 1:CA:1138:G:C5 | 1:CA:1140:C:H1' | 2.40 | 0.56 |
| 1:CA:1157:A:N6 | 1:CA:1180:A:C4 | 2.72 | 0.56 |
| 1:CA:738:C:H2' | 1:CA:739:C:H6 | 1.70 | 0.56 |
| 10:CJ:65:LEU:HD12 | 14:CN:55:GLY:O | 2.05 | 0.56 |
| 10:CJ:8:LEU:HD23 | 10:CJ:96:ILE:HG23 | 1.87 | 0.56 |
| 25:DA:1636:C:H2' | 25:DA:1637:A:C8 | 2.40 | 0.56 |
| 25:DA:71:A:H5'' | 25:DA:73:A:C8 | 2.40 | 0.56 |
| 25:BA:1211:U:H2' | 25:BA:1212:C:C6 | 2.40 | 0.56 |
| 25:BA:692:C:H2' | 25:BA:693:G:O4' | 2.05 | 0.56 |
| 43:BX:88:LYS:NZ | 43:BX:90:GLU:OE1 | 2.33 | 0.56 |
| 1:CA:1414:U:H3 | 1:CA:1486:G:H1 | 1.53 | 0.56 |
| 1:CA:149:A:H2' | 1:CA:150:C:C6 | 2.40 | 0.56 |
| 4:CD:173:TRP:CZ3 | 4:CD:193:ASP:HB3 | 2.40 | 0.56 |
| 7:CG:106:GLN:O | 7:CG:110:GLN:HG3 | 2.05 | 0.56 |
| 15:CO:25:THR:HG21 | 15:CO:70:LEU:HB2 | 1.87 | 0.56 |
| 32:DI:40:THR:O | 32:DI:44:LEU:HB2 | 2.05 | 0.56 |
| 1:AA:149:A:H2' | 1:AA:150:C:C6 | 2.40 | 0.56 |
| 1:AA:409:G:N2 | 1:AA:433:C:O2 | 2.38 | 0.56 |
| 1:AA:78:G:H1 | 1:AA:92:C:H42 | 1.54 | 0.56 |
| 2:AB:16:HIS:CG | 2:AB:17:PHE:N | 2.70 | 0.56 |
| 31:BH:86:GLU:OE2 | 31:BH:130:ARG:HD3 | 2.06 | 0.56 |
| 37:BR:44:LEU:HD22 | 37:BR:48:VAL:HG23 | 1.87 | 0.56 |
| 1:CA:1318:A:O2' | 19:CS:37:ARG:HB2 | 2.06 | 0.56 |
| 3:CC:56:ASP:O | 3:CC:57:ILE:HD12 | 2.05 | 0.56 |
| 4:CD:31:CYS:SG | 4:CD:32:ALA:N | 2.79 | 0.56 |
| 8:CH:10:LEU:HD22 | 8:CH:83:ILE:HD11 | 1.85 | 0.56 |
| 13:CM:81:LEU:HD22 | 13:CM:88:ARG:HB3 | 1.86 | 0.56 |
| 15:CO:5:LYS:CD | 15:CO:5:LYS:H | 2.17 | 0.56 |
| 16:CP:21:VAL:HG13 | 16:CP:33:ILE:HB | 1.86 | 0.56 |
| 25:DA:2299:G:N2 | 25:DA:2318:G:H8 | 2.02 | 0.56 |
| 1:AA:1025:U:C2 | 1:AA:1036:G:O6 | 2.58 | 0.56 |
| 1:AA:192:U:HO2' | 1:AA:193:C:H6 | 1.52 | 0.56 |
| 1:AA:532:A:O2' | 1:AA:533:A:OP1 | 2.20 | 0.56 |
| 5:AE:103:GLY:O | 5:AE:106:PRO:HD2 | 2.04 | 0.56 |
| 50:B4:56:VAL:HB | 50:B4:60:GLN:HG3 | 1.88 | 0.56 |
| 25:BA:2431:U:O4 | 61:BA:4236:HOH:O | 2.14 | 0.56 |
| 25:BA:2860:A:OP2 | 25:BA:2876:U:H5 | 1.89 | 0.56 |
| 2:CB:120:ALA:O | 2:CB:122:PHE:N | 2.34 | 0.56 |
| 8:CH:68:ARG:NH1 | 8:CH:74:PRO:HB3 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:1470:G:H5'' | 25:DA:1471:A:OP1 | 2.05 | 0.56 |
| 25:DA:1798:U:H5' | 27:DD:259:THR:CG2 | 2.31 | 0.56 |
| 25:DA:1278:A:OP1 | 37:DR:36:THR:HG23 | 2.04 | 0.56 |
| 1:AA:1125:U:H1' | 1:AA:1126:U:O5' | 2.06 | 0.56 |
| 1:AA:193:C:H2' | 1:AA:194:C:C6 | 2.39 | 0.56 |
| 1:AA:538:G:H5'' | 12:AL:114:LYS:HB2 | 1.86 | 0.56 |
| 15:AO:25:THR:HG21 | 15:AO:70:LEU:HB2 | 1.88 | 0.56 |
| 17:AQ:3:LYS:HD2 | 17:AQ:60:ILE:HD11 | 1.87 | 0.56 |
| 18:AR:51:LEU:HD23 | 18:AR:52:PRO:HD2 | 1.87 | 0.56 |
| 25:BA:1066:A:N1 | 25:BA:1186:U:O2' | 2.27 | 0.56 |
| 25:BA:2013:U:H2' | 25:BA:2014:G:H5'' | 1.86 | 0.56 |
| 25:BA:624:C:O2' | 25:BA:628:C:OP1 | 2.16 | 0.56 |
| 25:BA:1000:C:OP1 | 36:BQ:87:LYS:HE3 | 2.05 | 0.56 |
| 1:CA:1207:G:H2' | 1:CA:1208:C:C6 | 2.39 | 0.56 |
| 1:CA:1218:C:H2' | 1:CA:1219:U:C6 | 2.40 | 0.56 |
| 1:CA:1279:A:H5'' | 1:CA:1280:A:OP1 | 2.06 | 0.56 |
| 1:CA:834:C:H2' | 1:CA:835:U:C6 | 2.40 | 0.56 |
| 1:CA:1104:G:H5' | 2:CB:111:ARG:HD2 | 1.86 | 0.56 |
| 2:CB:170:GLU:O | 2:CB:174:VAL:HG23 | 2.04 | 0.56 |
| 53:D7:26:GLY:O | 53:D7:30:VAL:HG23 | 2.05 | 0.56 |
| 25:DA:1292:U:H2' | 25:DA:1293:C:C6 | 2.40 | 0.56 |
| 25:DA:375:C:H2' | 25:DA:376:C:C6 | 2.40 | 0.56 |
| 25:DA:479:A:N3 | 25:DA:481:G:H5'' | 2.20 | 0.56 |
| 25:DA:500:G:N1 | 25:DA:503:A:OP2 | 2.38 | 0.56 |
| 28:DE:143:ASN:HD22 | 28:DE:147:PRO:HD3 | 1.70 | 0.56 |
| 1:AA:1125:U:H3' | 10:AJ:5:ARG:HH22 | 1.70 | 0.56 |
| 1:AA:1202:G:N2 | 14:AN:46:GLU:OE1 | 2.32 | 0.56 |
| 16:AP:18:ARG:NH1 | 16:AP:32:TYR:OH | 2.38 | 0.56 |
| 25:BA:1615:G:P | 27:BD:63:ARG:HH22 | 2.29 | 0.56 |
| 25:BA:2694:U:OP2 | 61:BA:4014:HOH:O | 2.17 | 0.56 |
| 26:BB:50:G:H5'' | 38:BS:61:ASN:HD22 | 1.69 | 0.56 |
| 25:BA:83:A:H5' | 44:BY:8:LYS:HG2 | 1.86 | 0.56 |
| 1:CA:1002:G:N2 | 1:CA:1039:C:N3 | 2.54 | 0.56 |
| 1:CA:38:G:H22 | 1:CA:397:A:H5'' | 1.71 | 0.56 |
| 9:CI:125:TYR:HD1 | 9:CI:126:SER:N | 2.03 | 0.56 |
| 9:CI:6:GLY:H | 9:CI:17:VAL:HG12 | 1.70 | 0.56 |
| 12:CL:74:GLY:O | 12:CL:102:ARG:NH1 | 2.27 | 0.56 |
| 23:CX:8:U:H6 | 23:CX:8:U:O5' | 1.89 | 0.56 |
| 25:DA:1239:G:H2' | 25:DA:1240:U:O4' | 2.06 | 0.56 |
| 25:DA:1359:A:N6 | 25:DA:1372:U:H3 | 2.03 | 0.56 |
| 25:DA:2687:U:H2' | 25:DA:2688:U:O4' | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:DB:95:C:H2' | 26:DB:96:U:C6 | 2.40 | 0.56 |
| 29:DF:157:VAL:HB | 29:DF:194:MET:HG2 | 1.87 | 0.56 |
| 1:AA:1030(D):A:H2' | 1:AA:1031:G:O4' | 2.06 | 0.56 |
| 1:AA:1074:G:O2' | 1:AA:1101:A:N1 | 2.30 | 0.56 |
| 25:BA:1553:A:O2' | 25:BA:1554:A:O4' | 2.24 | 0.56 |
| 28:BE:127:ASP:OD2 | 61:BE:408:HOH:O | 2.18 | 0.56 |
| 25:BA:2481:A:O2' | 36:BQ:56:ARG:HD2 | 2.06 | 0.56 |
| 1:CA:200:G:H2' | 1:CA:201:C:C6 | 2.41 | 0.56 |
| 25:DA:857:C:H4' | 46:D0:23:VAL:HG21 | 1.88 | 0.56 |
| 25:DA:271(H):G:H2' | 25:DA:271(I):G:H8 | 1.69 | 0.56 |
| 25:DA:988:A:N7 | 61:DA:3839:HOH:O | 2.32 | 0.56 |
| 2:AB:231:GLU:HB3 | 2:AB:232:PRO:HD3 | 1.87 | 0.56 |
| 17:AQ:57:VAL:HG12 | 17:AQ:76:LEU:HA | 1.88 | 0.56 |
| 1:AA:1318:A:H4' | 19:AS:10:PHE:CZ | 2.40 | 0.56 |
| 48:B2:32:LEU:HD12 | 48:B2:36:ARG:HH11 | 1.69 | 0.56 |
| 27:BD:206:LEU:HD22 | 27:BD:211:ARG:HG2 | 1.87 | 0.56 |
| 34:BO:2:ILE:HB | 34:BO:33:ALA:HB3 | 1.87 | 0.56 |
| 4:CD:103:ASN:OD1 | 4:CD:114:ARG:NE | 2.37 | 0.56 |
| 59:CX:101:FME:HCN | 25:DA:2451:A:C2 | 2.40 | 0.56 |
| 43:DX:8:ILE:O | 48:D2:36:ARG:NH2 | 2.39 | 0.56 |
| 9:AI:4:TYR:CE1 | 9:AI:88:TYR:HA | 2.41 | 0.56 |
| 14:AN:14:PRO:HG2 | 14:AN:16:PHE:O | 2.06 | 0.56 |
| 14:AN:21:TYR:OH | 14:AN:23:ARG:NH2 | 2.38 | 0.56 |
| 30:BG:179:PRO:HB2 | 50:B4:42:PHE:HE2 | 1.70 | 0.56 |
| 25:BA:1067:A:H8 | 25:BA:1068:G:H5'' | 1.69 | 0.56 |
| 25:BA:1566:U:H2' | 25:BA:1567:G:O4' | 2.06 | 0.56 |
| 25:BA:930:G:H2' | 25:BA:931:C:C6 | 2.41 | 0.56 |
| 30:BG:72:ARG:NH1 | 30:BG:87:PRO:HG3 | 2.21 | 0.56 |
| 31:BH:11:VAL:HG21 | 31:BH:50:VAL:HG23 | 1.88 | 0.56 |
| 31:BH:125:VAL:HG12 | 31:BH:127:GLU:O | 2.05 | 0.56 |
| 1:CA:1125:U:C2 | 10:CJ:38:ILE:HD13 | 2.41 | 0.56 |
| 1:CA:187:C:H2' | 1:CA:188:C:H6 | 1.71 | 0.56 |
| 1:CA:861:G:OP1 | 8:CH:75:ARG:NH2 | 2.38 | 0.56 |
| 25:DA:1338:G:N3 | 25:DA:1393:A:H2 | 2.04 | 0.56 |
| 25:DA:172:C:H2' | 25:DA:173:G:H8 | 1.70 | 0.56 |
| 26:DB:48:A:H2' | 26:DB:49:C:C6 | 2.40 | 0.56 |
| 31:DH:69:ARG:HG3 | 31:DH:70:THR:N | 2.20 | 0.56 |
| 37:DR:88:ARG:NH2 | 37:DR:89:ASP:OD2 | 2.38 | 0.56 |
| 1:AA:1138:G:C6 | 1:AA:1140:C:H1' | 2.41 | 0.56 |
| 1:AA:1504:G:OP1 | 1:AA:1507:A:H4' | 2.06 | 0.56 |
| 1:AA:272:C:H2' | 1:AA:273:A:H8 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:1091:A:O2' | 25:BA:1093:G:C4 | 2.57 | 0.56 |
| 29:BF:185:ASP:OD1 | 29:BF:188:ARG:NH1 | 2.35 | 0.56 |
| 41:BV:21:ARG:HG2 | 41:BV:91:TYR:CD1 | 2.41 | 0.56 |
| 1:CA:1263:C:H2' | 1:CA:1264:C:C6 | 2.41 | 0.56 |
| 1:CA:890:G:O2' | 1:CA:906:G:O6 | 2.19 | 0.56 |
| 11:CK:34:ASP:HB3 | 11:CK:40:ILE:HD11 | 1.88 | 0.56 |
| 11:CK:18:ARG:NH2 | 11:CK:35:PRO:O | 2.32 | 0.56 |
| 19:CS:28:LYS:HB2 | 19:CS:29:ARG:CA | 2.35 | 0.56 |
| 25:DA:1815:A:OP2 | 27:DD:54:ARG:NH2 | 2.37 | 0.56 |
| 25:DA:247:G:H4' | 25:DA:386:G:C5 | 2.40 | 0.56 |
| 34:DO:68:GLU:CB | 34:DO:78:ARG:HB2 | 2.36 | 0.56 |
| 1:AA:1179:A:H2' | 1:AA:1180:A:O4' | 2.06 | 0.56 |
| 4:AD:155:LEU:HD22 | 4:AD:156:GLU:H | 1.70 | 0.56 |
| 33:BN:67:LEU:HD12 | 33:BN:87:LEU:HD13 | 1.87 | 0.56 |
| 8:CH:84:ARG:HD2 | 8:CH:136:GLU:HG2 | 1.87 | 0.56 |
| 9:CI:53:VAL:O | 9:CI:55:ALA:N | 2.39 | 0.56 |
| 12:CL:24:VAL:HG12 | 12:CL:27:LEU:HB2 | 1.86 | 0.56 |
| 30:DG:43:LEU:HD12 | 30:DG:45:GLU:HG3 | 1.88 | 0.56 |
| 1:AA:1030(C):G:H2' | 1:AA:1030(D):A:H8 | 1.70 | 0.55 |
| 1:AA:1369:C:H2' | 1:AA:1370:G:C8 | 2.41 | 0.55 |
| 4:AD:154:ASN:HA | 4:AD:159:ARG:HH21 | 1.71 | 0.55 |
| 25:BA:918:U:OP1 | 36:BQ:5:ARG:HD3 | 2.06 | 0.55 |
| 1:CA:814:A:N7 | 1:CA:816:A:C4 | 2.73 | 0.55 |
| 25:DA:1309:G:HO2' | 25:DA:1611:C:HO2' | 1.53 | 0.55 |
| 25:DA:2359:C:H2' | 25:DA:2360:A:O4' | 2.05 | 0.55 |
| 25:DA:275:G:H2' | 25:DA:276:A:C8 | 2.41 | 0.55 |
| 25:DA:287:C:H2' | 25:DA:288:C:C6 | 2.38 | 0.55 |
| 30:DG:12:TYR:HA | 30:DG:16:ARG:HG2 | 1.88 | 0.55 |
| 1:AA:221:C:H2' | 1:AA:222:U:C6 | 2.38 | 0.55 |
| 1:AA:520:A:N1 | 1:AA:536:C:H1' | 2.21 | 0.55 |
| 8:AH:98:LYS:H | 8:AH:98:LYS:HD3 | 1.71 | 0.55 |
| 15:AO:26:GLU:OE2 | 15:AO:77:ARG:NE | 2.39 | 0.55 |
| 48:B2:1:MET:N | 48:B2:52:ASP:OD2 | 2.38 | 0.55 |
| 25:BA:606:G:OP2 | 40:BU:10:ARG:NH1 | 2.36 | 0.55 |
| 29:BF:101:LEU:O | 29:BF:106:ARG:HD3 | 2.06 | 0.55 |
| 32:BI:72:LEU:C | 32:BI:74:ASN:H | 2.09 | 0.55 |
| 39:BT:95:ARG:NH1 | 39:BT:95:ARG:HG2 | 2.21 | 0.55 |
| 1:CA:138:G:H8 | 1:CA:138:G:H5' | 1.71 | 0.55 |
| 1:CA:444:C:H2' | 1:CA:445:G:C8 | 2.34 | 0.55 |
| 2:CB:189:ASP:HB3 | 2:CB:204:ASN:HA | 1.89 | 0.55 |
| 1:CA:8:A:N6 | 4:CD:209:ARG:HB2 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:CX:59:A:H2' | 23:CX:60:U:H5' | 1.89 | 0.55 |
| 50:D4:46:GLN:C | 50:D4:48:ARG:H | 2.09 | 0.55 |
| 25:DA:1379:A:H4' | 25:DA:1380:G:OP2 | 2.05 | 0.55 |
| 30:DG:101:ILE:HG22 | 30:DG:105:LYS:HE2 | 1.87 | 0.55 |
| 1:AA:437:U:H5' | 4:AD:155:LEU:HD11 | 1.88 | 0.55 |
| 25:BA:231:G:O2' | 25:BA:243:G:O6 | 2.20 | 0.55 |
| 25:BA:2661:U:H2' | 25:BA:2662:U:C6 | 2.41 | 0.55 |
| 25:BA:645:G:H5' | 25:BA:645:G:N3 | 2.22 | 0.55 |
| 25:BA:7:G:H2' | 25:BA:8:A:O4' | 2.06 | 0.55 |
| 61:BA:4299:HOH:O | 37:BR:15:SER:HB3 | 2.06 | 0.55 |
| 3:CC:113:ALA:HB2 | 3:CC:202:ILE:HG13 | 1.87 | 0.55 |
| 55:D9:15:LYS:HE2 | 55:D9:17:ILE:HD13 | 1.89 | 0.55 |
| 27:DD:108:PRO:HB3 | 27:DD:143:HIS:CE1 | 2.40 | 0.55 |
| 2:AB:229:VAL:HG12 | 2:AB:230:VAL:H | 1.70 | 0.55 |
| 1:AA:738:C:OP1 | 6:AF:2:ARG:NH1 | 2.39 | 0.55 |
| 20:AT:45:GLN:HB2 | 20:AT:91:LEU:HD13 | 1.88 | 0.55 |
| 35:BP:62:LEU:O | 54:B8:13:ARG:HD3 | 2.05 | 0.55 |
| 25:BA:1553:A:O2' | 25:BA:1554:A:H8 | 1.88 | 0.55 |
| 25:BA:742:G:OP1 | 25:BA:1426:G:O2' | 2.22 | 0.55 |
| 25:BA:934:A:H4' | 25:BA:935:C:C5 | 2.39 | 0.55 |
| 1:CA:324:G:N7 | 61:CA:4084:HOH:O | 2.33 | 0.55 |
| 3:CC:43:LEU:HD21 | 3:CC:91:LEU:HD13 | 1.89 | 0.55 |
| 5:CE:100:VAL:O | 5:CE:107:ARG:NH2 | 2.40 | 0.55 |
| 25:DA:2357:U:OP1 | 46:D0:20:ARG:HD3 | 2.06 | 0.55 |
| 25:DA:2364:C:H2' | 25:DA:2365:G:O4' | 2.06 | 0.55 |
| 25:DA:286:C:H2' | 25:DA:287:C:H6 | 1.71 | 0.55 |
| 25:DA:906:G:O2' | 36:DQ:67:ARG:NH2 | 2.37 | 0.55 |
| 25:DA:957:A:H5' | 36:DQ:76:LYS:HG3 | 1.88 | 0.55 |
| 1:AA:487:A:H2' | 1:AA:488:C:O4' | 2.06 | 0.55 |
| 12:AL:71:PRO:HG2 | 12:AL:102:ARG:HG3 | 1.88 | 0.55 |
| 25:BA:2053:A:C6 | 25:BA:2510:C:H1' | 2.41 | 0.55 |
| 25:BA:2332:A:H2' | 25:BA:2332:A:N3 | 2.20 | 0.55 |
| 25:BA:2373:A:OP1 | 54:B8:27:THR:OG1 | 2.24 | 0.55 |
| 25:BA:721:G:H1' | 29:BF:74:ARG:HD3 | 1.88 | 0.55 |
| 35:BP:50:ARG:HD3 | 54:B8:7:HIS:CD2 | 2.40 | 0.55 |
| 1:CA:433:C:H2' | 1:CA:434:U:H6 | 1.72 | 0.55 |
| 7:CG:78:ARG:HG2 | 7:CG:79:ARG:HB2 | 1.87 | 0.55 |
| 15:CO:69:TYR:O | 15:CO:73:GLU:HG2 | 2.07 | 0.55 |
| 15:CO:88:ARG:NH2 | 15:CO:88:ARG:HB3 | 2.21 | 0.55 |
| 31:DH:20:ALA:HB1 | 31:DH:21:PRO:HD2 | 1.88 | 0.55 |
| 33:DN:96:GLU:H | 33:DN:96:GLU:CD | 2.10 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DQ:29:PHE:HB2 | 36:DQ:105:GLU:OE2 | 2.06 | 0.55 |
| 1:AA:630:G:H2' | 1:AA:631:G:C8 | 2.41 | 0.55 |
| 2:AB:219:VAL:HA | 2:AB:222:ILE:HD11 | 1.88 | 0.55 |
| 3:AC:130:VAL:HG21 | 3:AC:157:ILE:HG23 | 1.88 | 0.55 |
| 25:BA:1001:G:OP2 | 36:BQ:14:ARG:NH2 | 2.39 | 0.55 |
| 25:BA:1766:G:H3' | 25:BA:1767:A:H5'' | 1.87 | 0.55 |
| 32:BI:133:HIS:ND1 | 32:BI:134:PRO:O | 2.38 | 0.55 |
| 1:CA:130:A:H5' | 17:CQ:63:ARG:HE | 1.71 | 0.55 |
| 1:CA:441:A:H3' | 1:CA:442:C:C6 | 2.40 | 0.55 |
| 2:CB:211:ILE:O | 2:CB:215:LEU:HB2 | 2.07 | 0.55 |
| 6:CF:99:ALA:HB1 | 18:CR:23:LYS:HE3 | 1.88 | 0.55 |
| 1:CA:1320:C:O4' | 19:CS:73:GLU:HG3 | 2.07 | 0.55 |
| 25:DA:2640:G:H1 | 25:DA:2774:C:H42 | 1.55 | 0.55 |
| 25:DA:614(C):A:C4 | 29:DF:180:GLY:HA2 | 2.42 | 0.55 |
| 31:DH:149:ARG:NH1 | 31:DH:167:GLU:OE2 | 2.38 | 0.55 |
| 1:AA:768:A:OP2 | 61:AA:4024:HOH:O | 2.18 | 0.55 |
| 1:AA:833:U:H2' | 1:AA:834:C:H6 | 1.71 | 0.55 |
| 2:AB:163:PHE:HA | 2:AB:185:ILE:HG13 | 1.89 | 0.55 |
| 16:AP:28:ARG:HG2 | 16:AP:29:ASP:OD1 | 2.05 | 0.55 |
| 54:B8:39:LYS:O | 54:B8:43:GLN:HG3 | 2.06 | 0.55 |
| 25:BA:1466:U:HO2' | 25:BA:1467:G:P | 2.29 | 0.55 |
| 1:CA:445:G:H2' | 1:CA:446:G:C8 | 2.42 | 0.55 |
| 8:CH:112:LEU:HA | 8:CH:134:ILE:HG12 | 1.89 | 0.55 |
| 11:CK:85:ARG:HE | 11:CK:111:ASP:HB3 | 1.71 | 0.55 |
| 25:DA:1025:G:O2' | 61:DA:4219:HOH:O | 2.06 | 0.55 |
| 25:DA:2314:C:H2' | 25:DA:2315:G:H8 | 1.72 | 0.55 |
| 25:DA:2541:A:N7 | 61:DA:3938:HOH:O | 2.33 | 0.55 |
| 26:DB:95:C:H2' | 26:DB:96:U:H6 | 1.71 | 0.55 |
| 1:AA:1260:C:OP1 | 1:AA:1284:C:O2' | 2.25 | 0.55 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:N6 | 2.05 | 0.55 |
| 1:AA:727:G:N2 | 1:AA:730:G:OP2 | 2.39 | 0.55 |
| 1:AA:880:C:OP1 | 12:AL:8:ASN:ND2 | 2.37 | 0.55 |
| 1:AA:91:C:H2' | 1:AA:92:C:C6 | 2.42 | 0.55 |
| 4:AD:3:ARG:HE | 4:AD:118:ARG:HD3 | 1.71 | 0.55 |
| 10:AJ:35:SER:CB | 10:AJ:73:ASP:HB2 | 2.29 | 0.55 |
| 23:AX:59:A:H2' | 23:AX:60:U:H5' | 1.88 | 0.55 |
| 25:BA:1232:G:H5'' | 41:BV:81:TYR:CE1 | 2.41 | 0.55 |
| 25:BA:1698:G:OP1 | 37:BR:40:LYS:HE3 | 2.06 | 0.55 |
| 45:BZ:48:PHE:CE1 | 45:BZ:52:SER:HA | 2.41 | 0.55 |
| 1:CA:927:G:H2' | 1:CA:928:G:H8 | 1.72 | 0.55 |
| 9:CI:121:ARG:NH1 | 9:CI:122:ALA:O | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:CM:60:VAL:HG23 | 13:CM:64:TRP:CE3 | 2.42 | 0.55 |
| 47:D1:85:LEU:HB3 | 47:D1:89:GLU:HB3 | 1.88 | 0.55 |
| 25:DA:1805:U:O2 | 27:DD:50:THR:HB | 2.07 | 0.55 |
| 25:DA:668:G:H5' | 25:DA:669:G:OP2 | 2.06 | 0.55 |
| 25:DA:800:A:OP1 | 25:DA:800:A:H8 | 1.90 | 0.55 |
| 27:DD:73:VAL:HG13 | 27:DD:120:GLY:HA3 | 1.88 | 0.55 |
| 1:AA:1008:C:H42 | 1:AA:1021:G:H1 | 1.54 | 0.55 |
| 2:AB:30:ARG:HH21 | 2:AB:194:PRO:HB2 | 1.72 | 0.55 |
| 2:AB:87:ARG:NH2 | 2:AB:220:ASP:OD1 | 2.24 | 0.55 |
| 4:AD:107:ARG:NH2 | 4:AD:194:LEU:HD22 | 2.21 | 0.55 |
| 27:BD:132:PRO:HG2 | 27:BD:135:PHE:CD2 | 2.39 | 0.55 |
| 1:CA:1025:U:H1' | 1:CA:1026:G:C8 | 2.42 | 0.55 |
| 1:CA:1272:G:H2' | 1:CA:1273:G:O4' | 2.06 | 0.55 |
| 1:CA:1346:A:N1 | 1:CA:1374:A:H5'' | 2.22 | 0.55 |
| 1:CA:840:C:H4' | 1:CA:841:U:OP1 | 2.06 | 0.55 |
| 7:CG:69:VAL:HG21 | 7:CG:104:LEU:HD11 | 1.88 | 0.55 |
| 25:DA:1448:G:H4' | 25:DA:1542:A:OP1 | 2.06 | 0.55 |
| 25:DA:1889:A:N1 | 25:DA:2234:G:H1' | 2.22 | 0.55 |
| 42:DW:9:TYR:H | 42:DW:102:HIS:CE1 | 2.25 | 0.55 |
| 45:DZ:52:SER:OG | 45:DZ:53:ILE:N | 2.40 | 0.55 |
| 1:AA:1127:G:H1' | 1:AA:1280:A:C6 | 2.42 | 0.55 |
| 1:AA:1118:C:H1' | 1:AA:1179:A:C4 | 2.42 | 0.55 |
| 2:AB:7:VAL:HG11 | 2:AB:221:LEU:HD23 | 1.89 | 0.55 |
| 46:B0:30:VAL:HG22 | 46:B0:66:VAL:HG22 | 1.89 | 0.55 |
| 25:BA:1639:G:H2' | 25:BA:1640:G:H8 | 1.72 | 0.55 |
| 25:BA:933:C:H4' | 25:BA:933:C:OP1 | 2.05 | 0.55 |
| 29:BF:116:ASP:OD2 | 35:BP:1:MET:HB2 | 2.07 | 0.55 |
| 1:CA:543:C:C2' | 1:CA:544:G:H5' | 2.36 | 0.55 |
| 1:CA:880:C:OP1 | 12:CL:8:ASN:ND2 | 2.40 | 0.55 |
| 49:D3:10:LYS:HB3 | 49:D3:53:LEU:HA | 1.89 | 0.55 |
| 25:DA:1014:U:H2' | 25:DA:1015:G:H8 | 1.72 | 0.55 |
| 25:DA:139(A):G:N7 | 61:DA:4443:HOH:O | 2.33 | 0.55 |
| 25:DA:71:A:N7 | 43:DX:31:HIS:HE1 | 2.04 | 0.55 |
| 25:DA:848:G:N3 | 25:DA:933:A:H1' | 2.21 | 0.55 |
| 35:DP:101:VAL:HA | 35:DP:106:LEU:O | 2.07 | 0.55 |
| 1:AA:1216:G:OP1 | 14:AN:2:ALA:HA | 2.06 | 0.54 |
| 2:AB:178:ARG:NH2 | 8:AH:68:ARG:HH22 | 2.05 | 0.54 |
| 5:AE:15:ARG:HD2 | 5:AE:26:PHE:CD2 | 2.41 | 0.54 |
| 10:AJ:47:PHE:CZ | 14:AN:37:PHE:HE1 | 2.25 | 0.54 |
| 20:AT:47:GLY:HA2 | 20:AT:48:LYS:HB2 | 1.89 | 0.54 |
| 5:CE:78:HIS:CE1 | 5:CE:142:LEU:HA | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:CH:68:ARG:HH11 | 8:CH:68:ARG:HG3 | 1.71 | 0.54 |
| 1:CA:1216:G:H5'' | 14:CN:5:ALA:CB | 2.37 | 0.54 |
| 21:CU:12:LYS:HB3 | 21:CU:22:ARG:HD2 | 1.89 | 0.54 |
| 25:DA:1009:A:OP2 | 61:DA:4091:HOH:O | 2.18 | 0.54 |
| 25:DA:1427:A:H4' | 25:DA:1428:C:O5' | 2.07 | 0.54 |
| 25:DA:19:C:H2' | 25:DA:20:C:H6 | 1.71 | 0.54 |
| 25:DA:253:C:OP2 | 54:D8:5:LYS:NZ | 2.30 | 0.54 |
| 25:DA:1651:G:OP1 | 37:DR:40:LYS:HE3 | 2.07 | 0.54 |
| 1:AA:877:C:H5'' | 8:AH:88:LYS:HD3 | 1.89 | 0.54 |
| 50:B4:63:TYR:N | 50:B4:63:TYR:HD1 | 2.06 | 0.54 |
| 25:BA:1405:A:N1 | 25:BA:1418:U:O4 | 2.40 | 0.54 |
| 33:BN:58:ASP:OD1 | 33:BN:58:ASP:N | 2.37 | 0.54 |
| 1:AA:339:C:OP2 | 34:BO:97:ARG:HD3 | 2.07 | 0.54 |
| 37:BR:97:VAL:HG22 | 37:BR:114:VAL:HG22 | 1.89 | 0.54 |
| 1:CA:1051:C:H2' | 1:CA:1052:U:H6 | 1.71 | 0.54 |
| 1:CA:1072:G:H2' | 1:CA:1073:U:C6 | 2.42 | 0.54 |
| 1:CA:192:U:H2' | 1:CA:193:C:H6 | 1.71 | 0.54 |
| 1:CA:671:G:H2' | 1:CA:672:U:O4' | 2.07 | 0.54 |
| 3:CC:116:VAL:HG21 | 3:CC:202:ILE:HD11 | 1.89 | 0.54 |
| 1:CA:8:A:C6 | 4:CD:209:ARG:HB2 | 2.42 | 0.54 |
| 25:DA:1579:A:H2' | 25:DA:1580:A:C8 | 2.43 | 0.54 |
| 1:AA:96:U:H2' | 1:AA:97:G:H8 | 1.71 | 0.54 |
| 4:AD:103:ASN:O | 4:AD:107:ARG:HG2 | 2.07 | 0.54 |
| 4:AD:172:PRO:HB2 | 4:AD:187:ARG:NH2 | 2.22 | 0.54 |
| 49:B3:55:ARG:NH1 | 49:B3:57:GLU:OE1 | 2.36 | 0.54 |
| 25:BA:1553:A:O2' | 25:BA:1554:A:O5' | 2.25 | 0.54 |
| 38:BS:11:LYS:HD2 | 38:BS:15:ARG:HH12 | 1.73 | 0.54 |
| 40:BU:76:TYR:HH | 40:BU:92:ARG:HH11 | 1.50 | 0.54 |
| 1:CA:1025:U:N3 | 1:CA:1036:G:C6 | 2.75 | 0.54 |
| 5:CE:53:LEU:HD12 | 5:CE:53:LEU:H | 1.73 | 0.54 |
| 9:CI:23:ASN:OD1 | 9:CI:25:LYS:HE3 | 2.08 | 0.54 |
| 52:D6:35:GLU:HG2 | 52:D6:50:ARG:HD3 | 1.88 | 0.54 |
| 25:DA:2887:U:H2' | 25:DA:2888:C:C6 | 2.42 | 0.54 |
| 1:AA:1010:G:N2 | 1:AA:1020:U:O2' | 2.40 | 0.54 |
| 1:AA:105:G:H2' | 1:AA:106:C:C6 | 2.43 | 0.54 |
| 1:AA:986:A:H1' | 19:AS:54:GLY:O | 2.07 | 0.54 |
| 10:AJ:8:LEU:HB2 | 10:AJ:70:ARG:HB2 | 1.90 | 0.54 |
| 25:BA:1003:U:OP2 | 36:BQ:14:ARG:NH1 | 2.41 | 0.54 |
| 25:BA:2044:U:O2' | 25:BA:2629:C:H5' | 2.08 | 0.54 |
| 27:BD:242:ARG:HD3 | 27:BD:242:ARG:N | 2.22 | 0.54 |
| 30:BG:16:ARG:CZ | 30:BG:31:VAL:HG11 | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1120:G:C6 | 1:CA:1154:G:C2 | 2.95 | 0.54 |
| 1:CA:552:U:H2' | 1:CA:553:A:H5' | 1.89 | 0.54 |
| 1:CA:560:U:O2' | 1:CA:561:U:OP2 | 2.22 | 0.54 |
| 4:CD:98:GLU:OE1 | 4:CD:103:ASN:ND2 | 2.39 | 0.54 |
| 1:CA:923:A:OP1 | 5:CE:21:ALA:HB2 | 2.08 | 0.54 |
| 50:D4:2:LYS:HB2 | 50:D4:5:ILE:HD13 | 1.89 | 0.54 |
| 25:DA:2335:A:O2' | 25:DA:2336:A:H5'' | 2.07 | 0.54 |
| 25:DA:918:A:H5'' | 26:DB:98:G:O2' | 2.08 | 0.54 |
| 32:DI:117:GLU:HG3 | 32:DI:118:LYS:H | 1.71 | 0.54 |
| 39:DT:116:ALA:HB1 | 39:DT:121:ILE:HD11 | 1.88 | 0.54 |
| 4:AD:122:ARG:HA | 4:AD:122:ARG:HE | 1.72 | 0.54 |
| 4:AD:18:LYS:HD2 | 4:AD:31:CYS:SG | 2.48 | 0.54 |
| 5:AE:36:ASP:OD2 | 5:AE:40:ARG:HB2 | 2.06 | 0.54 |
| 26:BB:43:C:H5'' | 50:B4:1:MET:HG2 | 1.90 | 0.54 |
| 25:BA:144:C:H5' | 43:BX:2:LYS:HE2 | 1.89 | 0.54 |
| 25:BA:762:G:H2' | 25:BA:763:A:O4' | 2.08 | 0.54 |
| 36:BQ:56:ARG:HG3 | 36:BQ:56:ARG:HH11 | 1.71 | 0.54 |
| 45:BZ:145:GLU:O | 45:BZ:148:ASP:N | 2.39 | 0.54 |
| 1:CA:1015:A:H2' | 1:CA:1016:A:H8 | 1.72 | 0.54 |
| 1:CA:250:A:H4' | 1:CA:251:G:O5' | 2.08 | 0.54 |
| 21:CU:15:ARG:HB2 | 21:CU:15:ARG:HH11 | 1.72 | 0.54 |
| 27:DD:172:TYR:CD1 | 27:DD:186:HIS:HA | 2.43 | 0.54 |
| 34:DO:116:SER:OG | 34:DO:117:LEU:N | 2.40 | 0.54 |
| 1:AA:1095:U:H5'' | 1:AA:1109:C:O2 | 2.07 | 0.54 |
| 1:AA:159:G:N2 | 1:AA:161:A:H3' | 2.22 | 0.54 |
| 1:AA:190:U:H2' | 1:AA:191:G:H8 | 1.70 | 0.54 |
| 5:AE:77:PRO:HD2 | 5:AE:142:LEU:HD22 | 1.89 | 0.54 |
| 25:BA:1475:G:H2' | 25:BA:1476:C:C6 | 2.43 | 0.54 |
| 32:BI:92:VAL:HG11 | 32:BI:144:VAL:HG11 | 1.89 | 0.54 |
| 1:CA:1129:C:H1' | 1:CA:1130:A:N7 | 2.21 | 0.54 |
| 1:CA:1154:G:N7 | 1:CA:1155:G:C8 | 2.76 | 0.54 |
| 9:CI:4:TYR:CZ | 9:CI:88:TYR:HA | 2.43 | 0.54 |
| 49:D3:46:ASN:O | 49:D3:50:VAL:HG22 | 2.07 | 0.54 |
| 25:DA:195:A:OP1 | 35:DP:46:LYS:NZ | 2.37 | 0.54 |
| 25:DA:348:G:H2' | 25:DA:349:G:H8 | 1.72 | 0.54 |
| 44:DY:7:VAL:HG21 | 44:DY:72:VAL:HG12 | 1.90 | 0.54 |
| 10:AJ:49:VAL:HG23 | 14:AN:41:ARG:HD2 | 1.90 | 0.54 |
| 28:BE:59:VAL:HG21 | 28:BE:74:PRO:HB3 | 1.90 | 0.54 |
| 39:BT:5:ALA:O | 39:BT:9:LEU:N | 2.41 | 0.54 |
| 1:CA:1279:A:O2' | 1:CA:1281:U:OP2 | 2.12 | 0.54 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:C6 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CI:4:TYR:CE2 | 9:CI:88:TYR:HD1 | 2.25 | 0.54 |
| 19:CS:17:GLU:O | 19:CS:21:GLU:N | 2.34 | 0.54 |
| 25:DA:1341:U:OP2 | 25:DA:1394:U:O2' | 2.23 | 0.54 |
| 26:DB:50:G:OP1 | 38:DS:63:THR:OG1 | 2.19 | 0.54 |
| 25:DA:607:U:OP1 | 29:DF:102:PRO:HA | 2.08 | 0.54 |
| 29:DF:129:PHE:CD2 | 29:DF:163:VAL:HG21 | 2.43 | 0.54 |
| 1:AA:1316:G:H2' | 1:AA:1318:A:OP2 | 2.07 | 0.54 |
| 1:AA:186:C:H2' | 1:AA:187:C:C6 | 2.42 | 0.54 |
| 1:AA:434:U:H2' | 1:AA:435:C:C6 | 2.42 | 0.54 |
| 1:AA:72:C:H2' | 1:AA:73:G:O4' | 2.08 | 0.54 |
| 1:AA:78:G:C6 | 1:AA:91:C:N4 | 2.75 | 0.54 |
| 5:AE:51:VAL:O | 5:AE:55:VAL:HG23 | 2.08 | 0.54 |
| 25:BA:1471:G:H2' | 25:BA:1472:G:C8 | 2.43 | 0.54 |
| 25:BA:236:G:H4' | 25:BA:413:G:C5 | 2.43 | 0.54 |
| 34:BO:35:VAL:HG11 | 34:BO:103:ALA:CB | 2.36 | 0.54 |
| 1:CA:1169:A:N7 | 1:CA:1170:A:C5 | 2.76 | 0.54 |
| 1:CA:942:G:C2 | 1:CA:1342:C:C2 | 2.96 | 0.54 |
| 1:CA:991:U:O4 | 1:CA:1212:U:H1' | 2.08 | 0.54 |
| 25:DA:1270:C:H5'' | 25:DA:1271:G:H5' | 1.90 | 0.54 |
| 25:DA:340:A:N6 | 25:DA:341:G:C2 | 2.75 | 0.54 |
| 28:DE:24:THR:HG22 | 28:DE:186:GLY:O | 2.07 | 0.54 |
| 38:DS:34:HIS:ND1 | 38:DS:53:SER:OG | 2.33 | 0.54 |
| 4:AD:121:VAL:O | 4:AD:134:ASP:HA | 2.07 | 0.54 |
| 5:AE:76:ILE:HB | 5:AE:77:PRO:HD2 | 1.90 | 0.54 |
| 23:AX:61:C:H2' | 23:AX:62:C:H6 | 1.72 | 0.54 |
| 25:BA:287:G:N7 | 25:BA:448:U:H2' | 2.22 | 0.54 |
| 25:BA:312:C:H2' | 25:BA:313:A:H8 | 1.72 | 0.54 |
| 30:BG:11:TYR:CZ | 30:BG:16:ARG:HD3 | 2.41 | 0.54 |
| 30:BG:143:GLU:OE2 | 50:B4:26:SER:OG | 2.20 | 0.54 |
| 1:CA:1154:G:N7 | 1:CA:1155:G:N9 | 2.55 | 0.54 |
| 1:CA:1479:C:H2' | 1:CA:1480:G:H8 | 1.72 | 0.54 |
| 3:CC:50:ALA:HB1 | 3:CC:72:LYS:O | 2.08 | 0.54 |
| 9:CI:4:TYR:CE1 | 9:CI:88:TYR:HA | 2.42 | 0.54 |
| 25:DA:2268:A:OP1 | 61:DA:4048:HOH:O | 2.18 | 0.54 |
| 25:DA:2331:G:O2' | 46:D0:43:THR:HG22 | 2.08 | 0.54 |
| 25:DA:2706:G:N7 | 61:DA:4124:HOH:O | 2.34 | 0.54 |
| 25:DA:708:C:H42 | 25:DA:723:G:H1 | 1.55 | 0.54 |
| 25:DA:887:A:H5' | 25:DA:888:C:OP1 | 2.07 | 0.54 |
| 1:AA:1064:G:H4' | 1:AA:1065:U:OP1 | 2.07 | 0.54 |
| 1:AA:69:G:H2' | 1:AA:70:G:C8 | 2.43 | 0.54 |
| 3:AC:129:ALA:HB3 | 3:AC:132:ARG:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:AS:61:TYR:CE2 | 19:AS:63:THR:HG23 | 2.44 | 0.54 |
| 25:BA:1067:A:H3' | 25:BA:1067:A:C8 | 2.43 | 0.54 |
| 33:BN:4:TYR:CD2 | 40:BU:100:VAL:HG11 | 2.43 | 0.54 |
| 36:BQ:84:GLY:O | 36:BQ:85:LYS:HB2 | 2.08 | 0.54 |
| 1:CA:841:U:H6 | 1:CA:841:U:OP1 | 1.91 | 0.54 |
| 1:CA:985:C:H2' | 1:CA:986:A:C8 | 2.43 | 0.54 |
| 9:CI:9:ARG:H | 9:CI:79:LEU:HD23 | 1.73 | 0.54 |
| 13:CM:25:ILE:HD11 | 13:CM:66:LEU:HD13 | 1.90 | 0.54 |
| 25:DA:1025:G:C4 | 25:DA:1135:C:H1' | 2.42 | 0.54 |
| 25:DA:529:A:H62 | 25:DA:2041:U:H3 | 1.56 | 0.54 |
| 25:DA:2657:A:O3' | 31:DH:160:LYS:NZ | 2.41 | 0.54 |
| 1:AA:316:G:OP2 | 1:AA:351:G:O2' | 2.24 | 0.53 |
| 2:AB:109:SER:HA | 2:AB:112:VAL:HG13 | 1.90 | 0.53 |
| 6:AF:69:GLU:OE1 | 6:AF:69:GLU:N | 2.39 | 0.53 |
| 25:BA:2474:U:H1' | 25:BA:2503:U:O4 | 2.08 | 0.53 |
| 25:BA:2822:G:N2 | 25:BA:2899:C:O2 | 2.41 | 0.53 |
| 25:BA:479:C:O2 | 25:BA:483:A:O2' | 2.24 | 0.53 |
| 1:CA:1128:C:H1' | 1:CA:1147:C:H42 | 1.73 | 0.53 |
| 1:CA:276:G:H2' | 1:CA:277:C:H5' | 1.90 | 0.53 |
| 1:CA:737:A:H2' | 1:CA:738:C:C6 | 2.43 | 0.53 |
| 10:CJ:77:PRO:O | 10:CJ:81:THR:OG1 | 2.25 | 0.53 |
| 12:CL:36:VAL:HG22 | 12:CL:82:VAL:HG22 | 1.89 | 0.53 |
| 19:CS:20:LEU:HD23 | 19:CS:23:ASN:HD22 | 1.73 | 0.53 |
| 25:DA:2689:U:P | 25:DA:2719:G:H22 | 2.31 | 0.53 |
| 25:DA:997:G:OP1 | 40:DU:92:ARG:HG2 | 2.08 | 0.53 |
| 28:DE:55:ASN:O | 28:DE:58:ARG:HG2 | 2.07 | 0.53 |
| 40:DU:89:GLU:HB2 | 41:DV:50:PRO:HB2 | 1.89 | 0.53 |
| 1:AA:1118:C:H2' | 1:AA:1119:C:C6 | 2.42 | 0.53 |
| 1:AA:1243:C:H2' | 1:AA:1244:C:C6 | 2.43 | 0.53 |
| 1:AA:21:G:H2' | 1:AA:22:G:C8 | 2.43 | 0.53 |
| 2:AB:24:TRP:CZ3 | 2:AB:26:PRO:HA | 2.43 | 0.53 |
| 4:AD:116:GLN:NE2 | 4:AD:157:LEU:HD21 | 2.23 | 0.53 |
| 15:AO:39:LEU:HD13 | 15:AO:56:LEU:HB2 | 1.90 | 0.53 |
| 50:B4:63:TYR:CD1 | 50:B4:63:TYR:N | 2.76 | 0.53 |
| 53:B7:1:MET:H3 | 53:B7:1:MET:HE3 | 1.73 | 0.53 |
| 25:BA:469:A:H1' | 25:BA:1246:C:O4' | 2.08 | 0.53 |
| 25:BA:1346:U:H4' | 25:BA:1347:A:H5' | 1.91 | 0.53 |
| 25:BA:1834:A:O2' | 27:BD:259:THR:HG21 | 2.09 | 0.53 |
| 25:BA:1985:U:H4' | 25:BA:1986:G:OP1 | 2.08 | 0.53 |
| 25:BA:272:U:OP1 | 32:BI:50:ARG:NH2 | 2.42 | 0.53 |
| 1:CA:1118:C:H1' | 1:CA:1179:A:C5 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:192:U:H2' | 1:CA:193:C:C6 | 2.43 | 0.53 |
| 5:CE:52:PRO:HG2 | 5:CE:53:LEU:HD12 | 1.91 | 0.53 |
| 15:CO:56:LEU:O | 15:CO:60:VAL:HG23 | 2.08 | 0.53 |
| 23:CX:19:G:H4' | 23:CX:20:U:OP2 | 2.09 | 0.53 |
| 25:DA:1469:A:H2' | 25:DA:1470:G:O4' | 2.08 | 0.53 |
| 25:DA:1826:G:H4' | 27:DD:242:ARG:NH1 | 2.23 | 0.53 |
| 28:DE:119:ARG:HD2 | 28:DE:120:TRP:CE2 | 2.43 | 0.53 |
| 31:DH:64:LEU:O | 31:DH:68:THR:OG1 | 2.20 | 0.53 |
| 7:AG:111:ARG:NH1 | 7:AG:113:GLU:OE2 | 2.38 | 0.53 |
| 8:AH:34:GLU:OE2 | 8:AH:37:ARG:NH1 | 2.34 | 0.53 |
| 11:AK:98:LEU:O | 11:AK:101:SER:OG | 2.17 | 0.53 |
| 35:BP:121:LYS:HG2 | 35:BP:122:PRO:HD2 | 1.91 | 0.53 |
| 43:BX:11:PRO:HB3 | 43:BX:92:LEU:HD11 | 1.90 | 0.53 |
| 1:CA:557:G:C6 | 1:CA:558:G:C6 | 2.96 | 0.53 |
| 1:CA:598:U:H2' | 1:CA:599:C:C6 | 2.43 | 0.53 |
| 2:CB:16:HIS:HB2 | 2:CB:204:ASN:CB | 2.26 | 0.53 |
| 10:CJ:48:THR:O | 14:CN:34:TYR:OH | 2.27 | 0.53 |
| 18:CR:29:PHE:HE1 | 18:CR:31:LEU:HD13 | 1.72 | 0.53 |
| 31:DH:33:LEU:HD21 | 31:DH:136:ILE:HG13 | 1.90 | 0.53 |
| 31:DH:80:SER:OG | 31:DH:81:GLU:N | 2.40 | 0.53 |
| 1:AA:262:A:C6 | 1:AA:263:A:C6 | 2.96 | 0.53 |
| 1:AA:545:C:H5' | 4:AD:72:GLU:HG2 | 1.90 | 0.53 |
| 25:BA:2642:G:H2' | 25:BA:2643:G:C8 | 2.43 | 0.53 |
| 26:BB:33:G:C2 | 26:BB:50:G:C2 | 2.97 | 0.53 |
| 1:CA:1170:A:O2' | 1:CA:1171:G:C8 | 2.61 | 0.53 |
| 1:CA:1305:G:H22 | 1:CA:1331:G:H1' | 1.73 | 0.53 |
| 1:CA:999:C:N3 | 1:CA:1042:G:C2 | 2.77 | 0.53 |
| 10:CJ:6:ILE:O | 10:CJ:71:LEU:HD12 | 2.08 | 0.53 |
| 13:CM:92:HIS:CE1 | 13:CM:98:VAL:HG11 | 2.44 | 0.53 |
| 23:CX:10:G:N2 | 23:CX:26:G:H1' | 2.24 | 0.53 |
| 25:DA:2557:G:H2' | 25:DA:2558:C:C6 | 2.43 | 0.53 |
| 25:DA:2831:G:OP1 | 28:DE:58:ARG:NH2 | 2.28 | 0.53 |
| 25:DA:300:A:H1' | 25:DA:319:C:H1' | 1.88 | 0.53 |
| 28:DE:163:GLU:HG2 | 28:DE:164:ARG:N | 2.23 | 0.53 |
| 30:DG:41:GLN:HB3 | 30:DG:43:LEU:HD22 | 1.91 | 0.53 |
| 1:AA:352:C:OP2 | 61:AA:4067:HOH:O | 2.19 | 0.53 |
| 1:AA:664:G:N2 | 1:AA:741:G:H1 | 2.06 | 0.53 |
| 1:AA:991:U:N3 | 1:AA:1212:U:H1' | 2.24 | 0.53 |
| 3:AC:121:ALA:HB1 | 3:AC:189:ALA:HB2 | 1.91 | 0.53 |
| 11:AK:48:ILE:O | 11:AK:50:TYR:N | 2.40 | 0.53 |
| 26:BB:78:A:C2 | 26:BB:100:A:C4 | 2.95 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1128:C:H1' | 1:CA:1147:C:N3 | 2.22 | 0.53 |
| 1:CA:1126:U:H4' | 1:CA:1281:U:H1' | 1.91 | 0.53 |
| 1:CA:837:G:H1 | 1:CA:849:C:N4 | 2.06 | 0.53 |
| 47:D1:23:LYS:HB3 | 47:D1:29:GLY:HA3 | 1.91 | 0.53 |
| 25:DA:1816:G:O6 | 27:DD:35:LYS:NZ | 2.23 | 0.53 |
| 25:DA:2849:U:O4 | 39:DT:23:ARG:NH2 | 2.32 | 0.53 |
| 45:DZ:154:ASP:N | 45:DZ:154:ASP:OD1 | 2.42 | 0.53 |
| 1:AA:102:G:H2' | 1:AA:103:C:C6 | 2.43 | 0.53 |
| 1:AA:33:A:H2' | 1:AA:34:C:C6 | 2.44 | 0.53 |
| 2:AB:35:GLU:HB2 | 2:AB:40:HIS:CD2 | 2.44 | 0.53 |
| 4:AD:196:LEU:H | 4:AD:196:LEU:HD12 | 1.73 | 0.53 |
| 18:AR:40:LEU:HD22 | 18:AR:70:ILE:HG12 | 1.90 | 0.53 |
| 25:BA:1293:A:OP1 | 29:BF:95:ARG:NH2 | 2.39 | 0.53 |
| 25:BA:1405:A:N3 | 25:BA:1405:A:H5' | 2.24 | 0.53 |
| 25:BA:1775:C:H5' | 25:BA:1776:G:OP2 | 2.08 | 0.53 |
| 25:BA:2255:U:H2' | 25:BA:2256:U:C6 | 2.44 | 0.53 |
| 25:BA:346:A:H5' | 25:BA:364:A:H1' | 1.89 | 0.53 |
| 25:BA:776:G:H2' | 25:BA:1806:U:H1' | 1.90 | 0.53 |
| 27:BD:148:GLU:HB2 | 27:BD:151:LYS:HD2 | 1.90 | 0.53 |
| 32:BI:108:THR:O | 32:BI:109:ILE:HD12 | 2.09 | 0.53 |
| 35:BP:124:LYS:HG3 | 35:BP:144:GLU:HG2 | 1.91 | 0.53 |
| 44:BY:38:ILE:HD11 | 44:BY:66:PRO:HG3 | 1.90 | 0.53 |
| 1:CA:1104:G:H4' | 2:CB:111:ARG:HH11 | 1.73 | 0.53 |
| 16:CP:5:ARG:NH1 | 16:CP:28:ARG:HA | 2.24 | 0.53 |
| 17:CQ:66:SER:OG | 17:CQ:67:LYS:N | 2.42 | 0.53 |
| 17:CQ:66:SER:O | 17:CQ:70:ARG:NH1 | 2.41 | 0.53 |
| 1:CA:1326:C:H5' | 21:CU:18:TYR:O | 2.09 | 0.53 |
| 25:DA:1914:C:H2' | 25:DA:1915:U:O4' | 2.08 | 0.53 |
| 25:DA:1946:U:H2' | 25:DA:1947:C:C6 | 2.43 | 0.53 |
| 25:DA:2299:G:H22 | 25:DA:2318:G:H8 | 1.56 | 0.53 |
| 25:DA:2510:C:H4' | 61:DA:4416:HOH:O | 2.07 | 0.53 |
| 25:DA:2600:A:C6 | 25:DA:2601:C:N4 | 2.77 | 0.53 |
| 25:DA:2887:U:H2' | 25:DA:2888:C:H6 | 1.73 | 0.53 |
| 25:DA:997:G:O2' | 25:DA:998:C:H5' | 2.08 | 0.53 |
| 45:DZ:53:ILE:HG22 | 45:DZ:71:VAL:O | 2.09 | 0.53 |
| 1:AA:1031:G:H2' | 1:AA:1032:G:H8 | 1.73 | 0.53 |
| 1:AA:1118:C:H1' | 1:AA:1179:A:C5 | 2.44 | 0.53 |
| 1:AA:258:G:H2' | 1:AA:259:G:H8 | 1.73 | 0.53 |
| 1:AA:376:G:O3' | 16:AP:5:ARG:NH2 | 2.41 | 0.53 |
| 1:AA:473:G:C2 | 1:AA:474:G:C5 | 2.97 | 0.53 |
| 1:AA:652:U:O4 | 1:AA:752:G:O2' | 2.22 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:219:VAL:O | 2:AB:222:ILE:HG13 | 2.09 | 0.53 |
| 8:AH:39:LEU:HB3 | 8:AH:45:ILE:HD11 | 1.90 | 0.53 |
| 11:AK:15:ALA:O | 11:AK:79:SER:N | 2.33 | 0.53 |
| 19:AS:22:LEU:HD13 | 19:AS:47:HIS:CD2 | 2.44 | 0.53 |
| 23:AX:23:C:H2' | 23:AX:24:U:C6 | 2.44 | 0.53 |
| 35:BP:65:ARG:HG3 | 54:B8:25:MET:HG3 | 1.91 | 0.53 |
| 25:BA:1660:A:OP1 | 25:BA:1663:C:N4 | 2.39 | 0.53 |
| 37:BR:55:ALA:HB2 | 37:BR:79:LEU:HD13 | 1.90 | 0.53 |
| 1:CA:1182:G:H4' | 1:CA:1183:A:H3' | 1.90 | 0.53 |
| 1:CA:1220:G:O3' | 19:CS:36:ARG:HD3 | 2.09 | 0.53 |
| 1:CA:587:G:N2 | 1:CA:754:C:OP2 | 2.34 | 0.53 |
| 10:CJ:78:ASN:O | 10:CJ:80:LYS:N | 2.41 | 0.53 |
| 12:CL:117:ARG:HB3 | 12:CL:122:THR:HB | 1.89 | 0.53 |
| 48:D2:28:LYS:HD3 | 48:D2:60:LEU:HD11 | 1.91 | 0.53 |
| 25:DA:2286:A:H4' | 25:DA:2287:A:O4' | 2.08 | 0.53 |
| 25:DA:67:U:H2' | 25:DA:68:G:O4' | 2.09 | 0.53 |
| 28:DE:108:SER:HB3 | 28:DE:165:VAL:HG21 | 1.91 | 0.53 |
| 30:DG:96:ARG:O | 30:DG:99:MET:HB3 | 2.09 | 0.53 |
| 1:AA:189(K):U:H2' | 1:AA:189(L):G:C8 | 2.44 | 0.53 |
| 1:AA:243:A:C2 | 1:AA:246:A:C8 | 2.97 | 0.53 |
| 4:AD:119:GLN:HG2 | 4:AD:123:HIS:CD2 | 2.43 | 0.53 |
| 9:AI:8:GLY:HA3 | 9:AI:76:ALA:O | 2.09 | 0.53 |
| 25:BA:1067:A:H2' | 25:BA:1069:U:H5' | 1.89 | 0.53 |
| 25:BA:139:A:C8 | 25:BA:1454:C:O2' | 2.60 | 0.53 |
| 25:BA:326:C:H2' | 25:BA:327:U:H6 | 1.74 | 0.53 |
| 25:BA:407:U:H2' | 25:BA:408:G:H8 | 1.73 | 0.53 |
| 7:CG:51:GLN:O | 7:CG:55:GLY:HA2 | 2.08 | 0.53 |
| 13:CM:89:GLY:O | 13:CM:93:ARG:HG3 | 2.09 | 0.53 |
| 18:CR:61:LYS:O | 18:CR:65:ILE:HG12 | 2.08 | 0.53 |
| 25:DA:1319:G:C6 | 25:DA:1320:C:N4 | 2.77 | 0.53 |
| 25:DA:2189:U:H2' | 25:DA:2190:G:H8 | 1.74 | 0.53 |
| 25:DA:2469:A:C2 | 25:DA:2482:G:C8 | 2.97 | 0.53 |
| 25:DA:2698:U:H2' | 25:DA:2699:C:C6 | 2.44 | 0.53 |
| 25:DA:796:C:H2' | 25:DA:797:C:C6 | 2.44 | 0.53 |
| 25:DA:96:G:H4' | 48:D2:48:HIS:CD2 | 2.43 | 0.53 |
| 1:AA:381:C:N4 | 1:AA:382:A:C2 | 2.77 | 0.53 |
| 1:AA:987:G:H1 | 1:AA:1218:C:H42 | 1.57 | 0.53 |
| 23:AX:23:C:H2' | 23:AX:24:U:H6 | 1.74 | 0.53 |
| 23:AX:59:A:C2' | 23:AX:60:U:H5' | 2.39 | 0.53 |
| 25:BA:1597:C:OP1 | 25:BA:1765:U:O2' | 2.19 | 0.53 |
| 25:BA:2255:U:OP1 | 61:BA:3915:HOH:O | 2.19 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:BI:3:VAL:HG12 | 32:BI:38:LEU:HA | 1.91 | 0.53 |
| 36:BQ:85:LYS:HG2 | 46:B0:7:LEU:HB3 | 1.91 | 0.53 |
| 41:BV:95:LEU:HD13 | 41:BV:97:LYS:HD3 | 1.90 | 0.53 |
| 1:CA:1007:C:C4 | 1:CA:1022:G:N1 | 2.73 | 0.53 |
| 1:CA:1122:U:C4 | 1:CA:1151:A:N1 | 2.77 | 0.53 |
| 1:CA:73:G:C6 | 1:CA:97:G:C6 | 2.97 | 0.53 |
| 25:DA:2712:U:H1' | 25:DA:2712(A):A:C8 | 2.44 | 0.53 |
| 30:DG:63:ILE:HA | 30:DG:143:GLU:HG3 | 1.89 | 0.53 |
| 35:DP:38:GLN:O | 35:DP:39:LYS:HB3 | 2.09 | 0.53 |
| 38:DS:11:LYS:O | 38:DS:15:ARG:HG3 | 2.09 | 0.53 |
| 1:AA:1027:C:C2 | 1:AA:1034:G:N1 | 2.69 | 0.53 |
| 12:AL:60:LEU:HD21 | 12:AL:66:VAL:HG22 | 1.91 | 0.53 |
| 13:AM:37:THR:HG21 | 13:AM:56:LEU:HA | 1.90 | 0.53 |
| 25:BA:851:A:OP1 | 61:BA:4484:HOH:O | 2.19 | 0.53 |
| 32:BI:27:ARG:HD2 | 47:B1:71:TYR:CE1 | 2.44 | 0.53 |
| 32:BI:29:TYR:O | 32:BI:32:PRO:HD2 | 2.09 | 0.53 |
| 1:CA:1095:U:H2' | 1:CA:1096:C:O4' | 2.09 | 0.53 |
| 1:CA:954:G:H2' | 1:CA:955:U:C6 | 2.44 | 0.53 |
| 7:CG:62:PHE:HA | 7:CG:124:LEU:HD22 | 1.90 | 0.53 |
| 1:CA:1360:A:OP2 | 14:CN:35:ARG:NH2 | 2.41 | 0.53 |
| 15:CO:33:THR:HG21 | 15:CO:85:LEU:HD22 | 1.91 | 0.53 |
| 25:DA:687:C:H42 | 25:DA:787:U:H4' | 1.73 | 0.53 |
| 1:AA:975:A:H8 | 1:AA:975:A:H5' | 1.74 | 0.52 |
| 1:AA:1070:U:OP1 | 5:AE:25:ARG:NH1 | 2.38 | 0.52 |
| 52:B6:6:ARG:NH1 | 52:B6:26:ASN:HB2 | 2.24 | 0.52 |
| 25:BA:1653:C:H4' | 25:BA:1654:A:O5' | 2.09 | 0.52 |
| 25:BA:1993:A:C4 | 27:BD:241:PRO:HD3 | 2.45 | 0.52 |
| 27:BD:108:PRO:HG3 | 27:BD:143:HIS:CE1 | 2.43 | 0.52 |
| 1:CA:473:G:H2' | 1:CA:474:G:C8 | 2.45 | 0.52 |
| 1:CA:850:U:H2' | 1:CA:851:G:H5'' | 1.90 | 0.52 |
| 1:CA:983:A:H2 | 1:CA:984:C:C6 | 2.26 | 0.52 |
| 5:CE:90:VAL:O | 5:CE:91:LEU:HD13 | 2.08 | 0.52 |
| 50:D4:46:GLN:HB3 | 50:D4:48:ARG:HG2 | 1.90 | 0.52 |
| 25:DA:1344:G:O2' | 25:DA:1385:G:H2' | 2.09 | 0.52 |
| 25:DA:1858:G:O6 | 61:DA:4292:HOH:O | 2.16 | 0.52 |
| 25:DA:2750:A:H8 | 25:DA:2750:A:OP1 | 1.92 | 0.52 |
| 25:DA:475:U:C4 | 25:DA:481:G:O6 | 2.62 | 0.52 |
| 1:AA:1272:G:H2' | 1:AA:1273:G:O4' | 2.10 | 0.52 |
| 1:AA:154:C:N3 | 1:AA:168:G:N1 | 2.58 | 0.52 |
| 1:AA:56:U:H2' | 1:AA:57:G:H8 | 1.72 | 0.52 |
| 1:AA:923:A:H2' | 1:AA:924:C:C6 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:B8:33:ASN:HA | 54:B8:36:LYS:HD2 | 1.90 | 0.52 |
| 25:BA:1954:A:H2' | 25:BA:1955:G:O4' | 2.09 | 0.52 |
| 25:BA:1952:G:O2' | 25:BA:1990:G:O6 | 2.20 | 0.52 |
| 35:BP:82:GLY:HA2 | 35:BP:113:LYS:O | 2.09 | 0.52 |
| 1:CA:1116:C:H2' | 1:CA:1117:G:H5'' | 1.90 | 0.52 |
| 2:CB:16:HIS:CG | 2:CB:17:PHE:H | 2.28 | 0.52 |
| 2:CB:178:ARG:CZ | 8:CH:74:PRO:HG3 | 2.40 | 0.52 |
| 25:DA:10:G:H2' | 25:DA:11:G:C8 | 2.44 | 0.52 |
| 25:DA:1434:A:H61 | 25:DA:1558:A:N6 | 2.07 | 0.52 |
| 25:DA:2313:C:O2 | 25:DA:2313:C:H2' | 2.09 | 0.52 |
| 25:DA:2646:C:H2' | 25:DA:2647:U:O4' | 2.09 | 0.52 |
| 25:DA:531:C:H5' | 61:DA:4094:HOH:O | 2.09 | 0.52 |
| 31:DH:105:LEU:HD11 | 31:DH:148:ILE:HG23 | 1.91 | 0.52 |
| 32:DI:43:ASN:C | 32:DI:43:ASN:HD22 | 2.12 | 0.52 |
| 43:DX:84:ALA:HB3 | 43:DX:87:GLN:NE2 | 2.24 | 0.52 |
| 1:AA:1005:A:H1' | 1:AA:1036:G:H22 | 1.75 | 0.52 |
| 1:AA:1187:G:H4' | 9:AI:111:ARG:HH11 | 1.73 | 0.52 |
| 1:AA:1256:A:H5'' | 1:AA:1258:G:H1' | 1.92 | 0.52 |
| 8:AH:120:THR:H | 8:AH:123:GLU:HB2 | 1.72 | 0.52 |
| 1:AA:719:C:O2' | 18:AR:49:LYS:HB3 | 2.10 | 0.52 |
| 24:AW:8:2R3:H65 | 24:AW:10:2QY:CE1 | 2.38 | 0.52 |
| 49:B3:59:VAL:O | 49:B3:60:GLU:HG2 | 2.09 | 0.52 |
| 25:BA:1913:G:H2' | 25:BA:1914:C:C6 | 2.45 | 0.52 |
| 30:BG:16:ARG:HE | 30:BG:31:VAL:HG11 | 1.73 | 0.52 |
| 1:CA:1179:A:N1 | 1:CA:1180:A:C8 | 2.78 | 0.52 |
| 1:CA:1376:U:H2' | 1:CA:1377:A:C8 | 2.44 | 0.52 |
| 1:CA:583:A:H2' | 1:CA:584:G:O4' | 2.09 | 0.52 |
| 16:CP:53:VAL:HG13 | 16:CP:79:VAL:HG22 | 1.91 | 0.52 |
| 25:DA:1219:G:H1 | 25:DA:1230:C:H42 | 1.55 | 0.52 |
| 25:DA:2454:G:H1' | 61:DA:3886:HOH:O | 2.08 | 0.52 |
| 32:DI:126:TYR:HB2 | 32:DI:142:VAL:HG23 | 1.92 | 0.52 |
| 36:DQ:56:ARG:CG | 36:DQ:56:ARG:HH11 | 2.22 | 0.52 |
| 40:DU:78:THR:O | 40:DU:117:GLN:NE2 | 2.42 | 0.52 |
| 1:AA:1142:G:H3' | 1:AA:1143:G:H8 | 1.74 | 0.52 |
| 1:AA:364:A:H2' | 1:AA:365:U:C6 | 2.44 | 0.52 |
| 1:AA:558:G:H5'' | 1:AA:559:A:OP2 | 2.10 | 0.52 |
| 2:AB:201:ILE:HG21 | 2:AB:214:ILE:HG21 | 1.91 | 0.52 |
| 25:BA:1221:G:N2 | 25:BA:1223:C:OP2 | 2.43 | 0.52 |
| 26:BB:86:G:H1 | 26:BB:91:C:N4 | 2.08 | 0.52 |
| 34:BO:8:LEU:HB2 | 34:BO:19:ILE:HG13 | 1.91 | 0.52 |
| 25:BA:662:A:H8 | 35:BP:117:GLU:HG3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1237:C:HO2' | 1:CA:1300:G:H1 | 1.55 | 0.52 |
| 1:CA:838:G:H1 | 1:CA:848:C:H42 | 1.56 | 0.52 |
| 4:CD:175:SER:HB3 | 4:CD:186:LEU:HD11 | 1.91 | 0.52 |
| 1:CA:1131:G:OP1 | 9:CI:20:ARG:NH2 | 2.42 | 0.52 |
| 47:D1:73:LEU:HB3 | 47:D1:94:LEU:HD22 | 1.91 | 0.52 |
| 25:DA:184:C:H2' | 25:DA:185:U:H6 | 1.75 | 0.52 |
| 25:DA:2099:U:H5' | 25:DA:2100:G:OP2 | 2.09 | 0.52 |
| 25:DA:2704:C:H2' | 25:DA:2705:A:O4' | 2.09 | 0.52 |
| 25:DA:446:G:OP1 | 40:DU:3:ARG:NH1 | 2.39 | 0.52 |
| 25:DA:991:C:OP1 | 61:DA:4100:HOH:O | 2.19 | 0.52 |
| 27:DD:133:LEU:HA | 27:DD:136:ILE:HD12 | 1.90 | 0.52 |
| 25:DA:2562:U:H1' | 34:DO:23:ARG:HD3 | 1.92 | 0.52 |
| 34:DO:71:ARG:NE | 34:DO:105:GLU:OE2 | 2.42 | 0.52 |
| 38:DS:26:LEU:HD22 | 38:DS:87:PHE:CE1 | 2.44 | 0.52 |
| 40:DU:79:PHE:CZ | 40:DU:83:LEU:HD21 | 2.44 | 0.52 |
| 1:AA:100:C:H2' | 1:AA:101:A:C8 | 2.44 | 0.52 |
| 1:AA:1210:C:H2' | 1:AA:1211:U:H5' | 1.92 | 0.52 |
| 1:AA:503:C:H2' | 1:AA:504:C:H6 | 1.74 | 0.52 |
| 1:AA:985:C:H2' | 1:AA:986:A:C8 | 2.44 | 0.52 |
| 17:AQ:56:VAL:HB | 17:AQ:78:GLU:HB3 | 1.91 | 0.52 |
| 25:BA:2819:A:C6 | 25:BA:2820:A:C6 | 2.98 | 0.52 |
| 1:CA:1004:A:N7 | 1:CA:1037:C:H2' | 2.25 | 0.52 |
| 1:CA:1216:G:H5'' | 14:CN:5:ALA:HB2 | 1.91 | 0.52 |
| 1:CA:1310:G:H5' | 13:CM:77:ASN:ND2 | 2.25 | 0.52 |
| 4:CD:99:SER:O | 4:CD:140:VAL:HG23 | 2.09 | 0.52 |
| 18:CR:33:ASP:OD2 | 18:CR:36:ASN:HB2 | 2.08 | 0.52 |
| 25:DA:1589:C:H2' | 25:DA:1590:U:C6 | 2.44 | 0.52 |
| 25:DA:2751:G:C8 | 31:DH:2:SER:N | 2.77 | 0.52 |
| 30:DG:122:PRO:HG3 | 30:DG:180:PHE:HB3 | 1.92 | 0.52 |
| 32:DI:93:THR:O | 32:DI:97:ILE:HG13 | 2.09 | 0.52 |
| 1:AA:1241:G:H2' | 1:AA:1242:C:C6 | 2.44 | 0.52 |
| 1:AA:134:A:H61 | 16:AP:25:ARG:NH1 | 2.07 | 0.52 |
| 1:AA:148:G:O2' | 1:AA:149:A:H8 | 1.91 | 0.52 |
| 1:AA:195:A:N3 | 1:AA:222:U:O2' | 2.30 | 0.52 |
| 5:AE:78:HIS:HD1 | 8:AH:104:ARG:HD2 | 1.74 | 0.52 |
| 7:AG:113:GLU:HG2 | 7:AG:119:ARG:HG2 | 1.90 | 0.52 |
| 1:AA:520:A:O2' | 12:AL:73:GLU:OE1 | 2.14 | 0.52 |
| 28:BE:47:VAL:HG21 | 28:BE:86:PRO:CD | 2.38 | 0.52 |
| 1:CA:1399:C:C2 | 1:CA:1502:A:N6 | 2.78 | 0.52 |
| 1:CA:358:U:H2' | 1:CA:359:U:H6 | 1.75 | 0.52 |
| 25:DA:1300:U:H4' | 25:DA:1301:A:H5'' | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:1309:G:O2' | 25:DA:1611:C:O2' | 2.27 | 0.52 |
| 25:DA:1857:G:O2' | 25:DA:1885:A:N6 | 2.42 | 0.52 |
| 25:DA:271(H):G:H2' | 25:DA:271(I):G:C8 | 2.45 | 0.52 |
| 25:DA:468:G:H5'' | 29:DF:60:SER:HB2 | 1.90 | 0.52 |
| 25:DA:524:U:H2' | 25:DA:525:U:H6 | 1.73 | 0.52 |
| 25:DA:539:G:H2' | 25:DA:540:C:H6 | 1.73 | 0.52 |
| 25:DA:947:G:N2 | 25:DA:971:C:C2 | 2.78 | 0.52 |
| 31:DH:56:SER:OG | 31:DH:57:ASP:N | 2.40 | 0.52 |
| 37:DR:38:VAL:HG22 | 37:DR:112:ALA:HB2 | 1.92 | 0.52 |
| 38:DS:3:ARG:O | 38:DS:4:LEU:HD23 | 2.10 | 0.52 |
| 41:DV:65:GLY:HA3 | 41:DV:91:TYR:CZ | 2.44 | 0.52 |
| 41:DV:62:LEU:HD11 | 41:DV:95:LEU:HB2 | 1.91 | 0.52 |
| 25:BA:173:C:H2' | 25:BA:174:U:C6 | 2.44 | 0.52 |
| 25:BA:1941:A:H5'' | 25:BA:1942:C:OP2 | 2.10 | 0.52 |
| 25:BA:2897:U:H2' | 25:BA:2898:C:H6 | 1.72 | 0.52 |
| 25:BA:354:A:H2 | 25:BA:1255:A:HO2' | 1.57 | 0.52 |
| 26:BB:76:G:N2 | 26:BB:101:G:O6 | 2.40 | 0.52 |
| 1:CA:1041:A:C6 | 1:CA:1042:G:C6 | 2.98 | 0.52 |
| 6:CF:96:PRO:HB3 | 18:CR:30:ASP:CG | 2.30 | 0.52 |
| 25:DA:2262:U:H4' | 25:DA:2328:A:C2 | 2.45 | 0.52 |
| 25:DA:592:G:O2' | 54:D8:4:MET:HG3 | 2.09 | 0.52 |
| 30:DG:82:LEU:HA | 30:DG:86:MET:SD | 2.49 | 0.52 |
| 33:DN:38:HIS:ND1 | 33:DN:39:ARG:HG3 | 2.25 | 0.52 |
| 45:DZ:152:ALA:O | 45:DZ:155:LEU:HD22 | 2.10 | 0.52 |
| 45:DZ:157:LEU:HB3 | 45:DZ:161:VAL:HG13 | 1.92 | 0.52 |
| 45:DZ:6:LYS:HE2 | 45:DZ:43:GLU:OE1 | 2.09 | 0.52 |
| 1:AA:826:C:H2' | 1:AA:827:U:C6 | 2.44 | 0.52 |
| 4:AD:85:LYS:HG3 | 4:AD:86:LYS:N | 2.24 | 0.52 |
| 6:AF:67:MET:SD | 6:AF:75:LEU:HD13 | 2.50 | 0.52 |
| 15:AO:33:THR:HG21 | 15:AO:85:LEU:HD22 | 1.91 | 0.52 |
| 15:AO:74:ASP:OD2 | 15:AO:77:ARG:HG3 | 2.09 | 0.52 |
| 54:B8:62:LEU:HB3 | 54:B8:65:GLU:HG2 | 1.91 | 0.52 |
| 25:BA:1717:C:O2 | 28:BE:129:HIS:NE2 | 2.34 | 0.52 |
| 25:BA:1814:A:OP1 | 61:BA:4519:HOH:O | 2.18 | 0.52 |
| 25:BA:1993:A:OP2 | 27:BD:242:ARG:NH2 | 2.42 | 0.52 |
| 34:BO:16:ALA:HB2 | 34:BO:52:VAL:HG21 | 1.92 | 0.52 |
| 1:CA:1207:G:H2' | 1:CA:1208:C:H6 | 1.75 | 0.52 |
| 1:CA:192:U:C2' | 1:CA:193:C:H5' | 2.40 | 0.52 |
| 1:CA:792:A:H4' | 1:CA:793:U:O5' | 2.10 | 0.52 |
| 2:CB:76:GLN:HB2 | 2:CB:208:ILE:HG12 | 1.91 | 0.52 |
| 25:DA:348:G:H2' | 25:DA:349:G:C8 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DB:19:G:H2' | 26:DB:20:C:O4' | 2.09 | 0.52 |
| 26:DB:46:A:H2' | 26:DB:47:C:C6 | 2.44 | 0.52 |
| 30:DG:16:ARG:NE | 30:DG:31:VAL:HG11 | 2.25 | 0.52 |
| 45:DZ:8:TYR:HB2 | 45:DZ:38:TYR:CE2 | 2.45 | 0.52 |
| 1:AA:407:G:H2' | 1:AA:408:A:H8 | 1.74 | 0.52 |
| 1:AA:447:G:H2' | 1:AA:485:G:N2 | 2.25 | 0.52 |
| 9:AI:7:THR:O | 9:AI:83:ARG:NH1 | 2.41 | 0.52 |
| 10:AJ:61:GLU:OE2 | 14:AN:45:ARG:NE | 2.35 | 0.52 |
| 23:AX:10:G:N2 | 23:AX:26:G:H1' | 2.25 | 0.52 |
| 50:B4:63:TYR:N | 50:B4:64:GLY:HA2 | 2.25 | 0.52 |
| 25:BA:344:A:OP1 | 29:BF:135:LYS:NZ | 2.41 | 0.52 |
| 29:BF:157:VAL:HB | 29:BF:194:MET:HG2 | 1.91 | 0.52 |
| 32:BI:93:THR:HG22 | 32:BI:119:PRO:HB3 | 1.92 | 0.52 |
| 36:BQ:35:VAL:HG13 | 36:BQ:130:LYS:HB3 | 1.92 | 0.52 |
| 1:CA:1063:C:H5'' | 1:CA:1064:G:H2' | 1.92 | 0.52 |
| 1:CA:1269:A:H2 | 1:CA:1312:G:N3 | 2.08 | 0.52 |
| 1:CA:1323:G:H4' | 1:CA:1363:C:C2 | 2.45 | 0.52 |
| 1:CA:1492:A:H2' | 1:CA:1493:A:H1' | 1.92 | 0.52 |
| 2:CB:56:ARG:NH1 | 2:CB:56:ARG:HB3 | 2.25 | 0.52 |
| 9:CI:78:LYS:HD3 | 9:CI:101:PHE:HD2 | 1.75 | 0.52 |
| 19:CS:28:LYS:HB2 | 19:CS:29:ARG:CB | 2.40 | 0.52 |
| 25:DA:1268:A:H2' | 25:DA:1269:A:O4' | 2.10 | 0.52 |
| 25:DA:2086:U:H2' | 25:DA:2087:G:C8 | 2.45 | 0.52 |
| 25:DA:323:G:O2' | 25:DA:1205:U:N3 | 2.32 | 0.52 |
| 25:DA:72:U:OP2 | 48:D2:29:LYS:NZ | 2.33 | 0.52 |
| 27:DD:69:ARG:NH2 | 27:DD:128:GLY:O | 2.39 | 0.52 |
| 37:DR:56:LYS:NZ | 37:DR:90:ARG:O | 2.43 | 0.52 |
| 43:DX:12:VAL:HG22 | 43:DX:29:TRP:CE2 | 2.45 | 0.52 |
| 1:AA:1328:C:OP1 | 21:AU:21:TYR:OH | 2.25 | 0.52 |
| 2:AB:55:PHE:HA | 2:AB:58:ILE:HD12 | 1.92 | 0.52 |
| 2:AB:60:ASP:O | 2:AB:64:ARG:HB2 | 2.10 | 0.52 |
| 25:BA:2108:U:H2' | 25:BA:2109:G:C8 | 2.45 | 0.52 |
| 25:BA:2784:C:H2' | 25:BA:2785:C:C6 | 2.44 | 0.52 |
| 25:BA:864:C:O2' | 25:BA:886:U:H5'' | 2.10 | 0.52 |
| 31:BH:24:VAL:HG13 | 31:BH:37:VAL:HG21 | 1.91 | 0.52 |
| 9:CI:21:PRO:HA | 9:CI:59:PHE:HA | 1.92 | 0.52 |
| 1:CA:1309:G:H5' | 13:CM:78:ILE:HD11 | 1.92 | 0.52 |
| 20:CT:13:LEU:O | 20:CT:17:ARG:HG3 | 2.10 | 0.52 |
| 25:DA:154:G:O6 | 25:DA:172:C:N4 | 2.43 | 0.52 |
| 25:DA:601:C:O2 | 25:DA:605:C:H4' | 2.10 | 0.52 |
| 25:DA:774:A:H2' | 25:DA:774:A:N3 | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:84:A:N1 | 25:DA:98:G:O2' | 2.41 | 0.52 |
| 25:DA:864:G:C6 | 25:DA:865:C:N4 | 2.78 | 0.52 |
| 26:DB:66:A:H61 | 26:DB:109:C:H5' | 1.75 | 0.52 |
| 28:DE:120:TRP:CE3 | 28:DE:155:LYS:HD3 | 2.45 | 0.52 |
| 29:DF:65:TRP:CZ2 | 29:DF:75:HIS:HD2 | 2.28 | 0.52 |
| 31:DH:106:THR:HG23 | 31:DH:112:PRO:HB3 | 1.92 | 0.52 |
| 40:DU:76:TYR:OH | 40:DU:92:ARG:NH1 | 2.42 | 0.52 |
| 40:DU:78:THR:HG22 | 40:DU:117:GLN:NE2 | 2.24 | 0.52 |
| 1:AA:1223:C:H5'' | 1:AA:1224:G:C5' | 2.40 | 0.51 |
| 1:AA:184:G:H2' | 1:AA:185:A:C8 | 2.42 | 0.51 |
| 1:AA:396:G:O2' | 1:AA:398:C:OP1 | 2.15 | 0.51 |
| 1:AA:503:C:H2' | 1:AA:504:C:C6 | 2.46 | 0.51 |
| 1:AA:657:G:C2 | 1:AA:658:G:C8 | 2.98 | 0.51 |
| 25:BA:239:G:OP2 | 54:B8:13:ARG:NH2 | 2.43 | 0.51 |
| 27:BD:234:GLY:O | 61:BD:402:HOH:O | 2.19 | 0.51 |
| 28:BE:11:MET:HG2 | 28:BE:24:THR:HB | 1.92 | 0.51 |
| 26:BB:91:C:OP2 | 36:BQ:16:ARG:NH1 | 2.42 | 0.51 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:C6 | 2.44 | 0.51 |
| 1:CA:1517:G:H1' | 25:DA:1919:A:O3' | 2.10 | 0.51 |
| 1:CA:15:G:H2' | 1:CA:16:A:H8 | 1.74 | 0.51 |
| 1:CA:652:U:O2' | 1:CA:653:A:OP2 | 2.24 | 0.51 |
| 1:CA:742:G:OP2 | 15:CO:35:ARG:NH2 | 2.40 | 0.51 |
| 1:CA:660:G:H1 | 1:CA:745:C:H42 | 1.58 | 0.51 |
| 12:CL:97:ARG:HB2 | 12:CL:98:TYR:CE2 | 2.45 | 0.51 |
| 25:DA:1529:G:H2' | 25:DA:1530:C:H6 | 1.75 | 0.51 |
| 25:DA:528:A:C2 | 25:DA:2042:A:H2' | 2.45 | 0.51 |
| 26:DB:43:C:H5'' | 50:D4:1:MET:HG2 | 1.91 | 0.51 |
| 32:DI:62:LYS:HG2 | 32:DI:133:HIS:NE2 | 2.25 | 0.51 |
| 39:DT:19:LEU:HD22 | 39:DT:86:ILE:HG13 | 1.92 | 0.51 |
| 39:DT:23:ARG:HG3 | 39:DT:120:ARG:NH1 | 2.24 | 0.51 |
| 1:AA:192:U:O2' | 1:AA:193:C:H6 | 1.92 | 0.51 |
| 1:AA:502:G:C6 | 1:AA:503:C:C4 | 2.98 | 0.51 |
| 1:AA:785:G:C2' | 1:AA:786:G:H5' | 2.41 | 0.51 |
| 1:AA:454:C:OP1 | 16:AP:75:ARG:NH2 | 2.42 | 0.51 |
| 1:AA:235:C:H5' | 17:AQ:70:ARG:HG2 | 1.92 | 0.51 |
| 25:BA:1378:G:OP1 | 61:BA:4471:HOH:O | 2.19 | 0.51 |
| 25:BA:2779:G:H2' | 25:BA:2779:G:N3 | 2.24 | 0.51 |
| 25:BA:611:U:H2' | 25:BA:612:C:C6 | 2.46 | 0.51 |
| 32:BI:72:LEU:HA | 32:BI:75:LEU:HD11 | 1.91 | 0.51 |
| 43:BX:1:MET:HE1 | 48:B2:26:ARG:HH21 | 1.75 | 0.51 |
| 1:CA:1227:A:H8 | 1:CA:1227:A:H3' | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1311:G:H1 | 1:CA:1326:C:H42 | 1.57 | 0.51 |
| 1:CA:1206:G:H4' | 3:CC:192:THR:O | 2.09 | 0.51 |
| 18:CR:52:PRO:O | 18:CR:56:THR:HG23 | 2.10 | 0.51 |
| 20:CT:16:HIS:O | 20:CT:19:SER:OG | 2.17 | 0.51 |
| 25:DA:652(B):A:C2 | 25:DA:655:A:H1' | 2.44 | 0.51 |
| 26:DB:6:C:H2' | 26:DB:7:G:H5'' | 1.92 | 0.51 |
| 28:DE:141:ILE:O | 28:DE:154:LYS:HE2 | 2.10 | 0.51 |
| 1:AA:1399:C:C2 | 1:AA:1502:A:N6 | 2.78 | 0.51 |
| 1:AA:202:U:H3' | 1:AA:203:U:H6 | 1.75 | 0.51 |
| 1:AA:45:U:H2' | 1:AA:46:G:C8 | 2.45 | 0.51 |
| 1:AA:626:U:C2 | 1:AA:627:G:C8 | 2.98 | 0.51 |
| 2:AB:220:ASP:O | 2:AB:223:ILE:HG12 | 2.10 | 0.51 |
| 9:AI:64:THR:HG23 | 9:AI:66:ARG:HD2 | 1.92 | 0.51 |
| 47:B1:3:LYS:HB2 | 47:B1:61:ARG:NH1 | 2.25 | 0.51 |
| 47:B1:91:LYS:O | 47:B1:95:LEU:HD22 | 2.11 | 0.51 |
| 25:BA:1218:G:O2' | 25:BA:1219:A:O5' | 2.28 | 0.51 |
| 25:BA:2372:A:H8 | 25:BA:2372:A:O5' | 1.92 | 0.51 |
| 25:BA:2889:C:OP2 | 61:BA:4427:HOH:O | 2.19 | 0.51 |
| 25:BA:895:G:H2' | 25:BA:896:A:C8 | 2.46 | 0.51 |
| 36:BQ:51:ARG:HD3 | 36:BQ:66:ILE:HD11 | 1.93 | 0.51 |
| 45:BZ:110:GLY:O | 45:BZ:113:ALA:HB3 | 2.10 | 0.51 |
| 1:CA:1121:U:C4 | 1:CA:1122:U:C5 | 2.98 | 0.51 |
| 1:CA:344:A:H4' | 1:CA:345:C:OP2 | 2.10 | 0.51 |
| 2:CB:167:PRO:HG3 | 2:CB:188:ALA:HB2 | 1.92 | 0.51 |
| 3:CC:180:ALA:HB1 | 3:CC:203:PHE:CE1 | 2.46 | 0.51 |
| 10:CJ:22:LYS:HA | 10:CJ:25:GLU:HB2 | 1.93 | 0.51 |
| 47:D1:51:VAL:HG11 | 47:D1:74:VAL:HG21 | 1.92 | 0.51 |
| 25:DA:1563:G:H2' | 25:DA:1564:C:C6 | 2.45 | 0.51 |
| 25:DA:2327:A:H2' | 25:DA:2328:A:C8 | 2.45 | 0.51 |
| 25:DA:2474:C:H5'' | 25:DA:2475:C:OP2 | 2.10 | 0.51 |
| 25:DA:852:G:N2 | 25:DA:926:A:H1' | 2.26 | 0.51 |
| 38:DS:88:ASP:OD1 | 38:DS:90:GLY:N | 2.43 | 0.51 |
| 1:AA:413:G:N2 | 1:AA:428:G:H1' | 2.24 | 0.51 |
| 1:AA:543:C:C2' | 1:AA:544:G:H5' | 2.41 | 0.51 |
| 1:AA:674:G:H2' | 1:AA:675:A:H8 | 1.74 | 0.51 |
| 8:AH:41:ARG:NH2 | 8:AH:123:GLU:OE2 | 2.35 | 0.51 |
| 8:AH:25:ASP:N | 8:AH:25:ASP:OD1 | 2.43 | 0.51 |
| 48:B2:2:LYS:O | 48:B2:6:VAL:HG23 | 2.11 | 0.51 |
| 25:BA:1405:A:N6 | 25:BA:1418:U:H3 | 2.09 | 0.51 |
| 28:BE:2:LYS:HG3 | 28:BE:200:GLU:HB2 | 1.93 | 0.51 |
| 44:BY:99:CYS:HB2 | 44:BY:106:LEU:HD21 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1004:A:H2' | 1:CA:1005:A:H5' | 1.92 | 0.51 |
| 1:CA:1510:U:H2' | 1:CA:1511:G:C8 | 2.44 | 0.51 |
| 1:CA:266:G:H5' | 1:CA:266:G:C8 | 2.46 | 0.51 |
| 8:CH:86:ILE:HG13 | 8:CH:133:LEU:HD22 | 1.92 | 0.51 |
| 8:CH:29:SER:HB3 | 8:CH:32:LYS:HG3 | 1.91 | 0.51 |
| 25:DA:184:C:H2' | 25:DA:185:U:C6 | 2.45 | 0.51 |
| 1:AA:102:G:H2' | 1:AA:103:C:H6 | 1.76 | 0.51 |
| 1:AA:1051:C:H2' | 1:AA:1052:U:C6 | 2.45 | 0.51 |
| 1:AA:671:G:H2' | 1:AA:672:U:O4' | 2.11 | 0.51 |
| 1:AA:865:A:C2 | 1:AA:918:A:H4' | 2.46 | 0.51 |
| 2:AB:208:ILE:HA | 2:AB:211:ILE:HD12 | 1.91 | 0.51 |
| 4:AD:158:ILE:O | 4:AD:162:LEU:N | 2.42 | 0.51 |
| 7:AG:146:GLU:O | 7:AG:149:ARG:HB2 | 2.11 | 0.51 |
| 48:B2:44:LEU:HD23 | 48:B2:47:ASN:HA | 1.93 | 0.51 |
| 19:AS:65:ASN:HA | 50:B4:58:ARG:HG3 | 1.93 | 0.51 |
| 50:B4:61:ARG:HG3 | 50:B4:62:ARG:N | 2.26 | 0.51 |
| 25:BA:549:U:H2' | 25:BA:550:U:C6 | 2.46 | 0.51 |
| 25:BA:559:U:H2' | 25:BA:560:C:C6 | 2.45 | 0.51 |
| 1:CA:1001(A):G:H2' | 1:CA:1002:G:O4' | 2.11 | 0.51 |
| 1:CA:1343:G:H2' | 1:CA:1344:C:C6 | 2.45 | 0.51 |
| 1:CA:392:G:H2' | 1:CA:393:A:H8 | 1.73 | 0.51 |
| 1:CA:424:G:H2' | 1:CA:425:G:H8 | 1.75 | 0.51 |
| 5:CE:40:ARG:NH2 | 5:CE:68:GLU:HA | 2.25 | 0.51 |
| 19:CS:64:GLU:O | 19:CS:67:VAL:HG23 | 2.10 | 0.51 |
| 49:D3:16:PRO:HB2 | 49:D3:18:ASP:OD1 | 2.11 | 0.51 |
| 25:DA:1297:C:H2' | 25:DA:1298:C:H6 | 1.76 | 0.51 |
| 25:DA:1766:U:H2' | 25:DA:1767:C:C6 | 2.44 | 0.51 |
| 25:DA:588:U:H2' | 25:DA:589:C:C6 | 2.45 | 0.51 |
| 25:DA:637:A:H8 | 35:DP:117:GLU:HG3 | 1.74 | 0.51 |
| 1:AA:1144:G:N2 | 1:AA:1146:A:H62 | 2.09 | 0.51 |
| 1:AA:1187:G:H2' | 1:AA:1188:A:C8 | 2.45 | 0.51 |
| 1:AA:714:G:H2' | 1:AA:715:A:C8 | 2.46 | 0.51 |
| 1:AA:747:C:OP2 | 1:AA:748:C:N4 | 2.44 | 0.51 |
| 2:AB:19:HIS:CD2 | 2:AB:206:ASP:HB2 | 2.46 | 0.51 |
| 25:BA:155:C:H6 | 25:BA:155:C:OP2 | 1.94 | 0.51 |
| 25:BA:1647:G:N7 | 61:BA:4116:HOH:O | 2.35 | 0.51 |
| 25:BA:296:U:H2' | 25:BA:297:C:H6 | 1.76 | 0.51 |
| 30:BG:131:TYR:HB3 | 30:BG:159:VAL:HG13 | 1.91 | 0.51 |
| 25:BA:581:G:OP1 | 33:BN:111:PRO:HD2 | 2.11 | 0.51 |
| 1:CA:144:G:H1 | 1:CA:178:C:H42 | 1.59 | 0.51 |
| 1:CA:920:U:H2' | 1:CA:921:U:C6 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:138:LEU:HA | 2:CB:141:GLU:HB3 | 1.92 | 0.51 |
| 13:CM:14:ARG:CZ | 13:CM:42:ALA:HA | 2.40 | 0.51 |
| 1:CA:229:U:O2' | 16:CP:23:ASP:OD2 | 2.26 | 0.51 |
| 25:DA:1709:U:H2' | 25:DA:1710:C:C6 | 2.45 | 0.51 |
| 25:DA:1810:A:H2' | 25:DA:1811:G:O4' | 2.11 | 0.51 |
| 25:DA:2602:A:OP2 | 25:DA:2603:G:H5'' | 2.11 | 0.51 |
| 25:DA:848:G:N9 | 25:DA:933:A:H8 | 2.08 | 0.51 |
| 36:DQ:75:THR:HA | 36:DQ:89:ASN:O | 2.11 | 0.51 |
| 44:DY:44:ILE:HA | 44:DY:63:LYS:O | 2.11 | 0.51 |
| 1:AA:346:G:C6 | 1:AA:348:G:N2 | 2.78 | 0.51 |
| 7:AG:111:ARG:HB3 | 7:AG:113:GLU:OE2 | 2.11 | 0.51 |
| 8:AH:11:THR:HG22 | 8:AH:15:ASN:ND2 | 2.25 | 0.51 |
| 50:B4:62:ARG:HB2 | 50:B4:63:TYR:CD1 | 2.44 | 0.51 |
| 25:BA:2050:U:H2' | 25:BA:2051:G:O4' | 2.11 | 0.51 |
| 34:BO:2:ILE:HD12 | 34:BO:6:THR:HG21 | 1.92 | 0.51 |
| 35:BP:121:LYS:O | 35:BP:123:LEU:N | 2.44 | 0.51 |
| 37:BR:26:LYS:HE2 | 37:BR:70:LEU:O | 2.10 | 0.51 |
| 38:BS:11:LYS:HD2 | 38:BS:15:ARG:NH1 | 2.25 | 0.51 |
| 1:CA:1316:G:O2' | 1:CA:1318:A:N7 | 2.38 | 0.51 |
| 1:CA:596:C:H2' | 1:CA:597:G:H8 | 1.74 | 0.51 |
| 1:CA:620:C:C2 | 4:CD:135:LEU:HG | 2.46 | 0.51 |
| 2:CB:87:ARG:NH2 | 2:CB:220:ASP:OD1 | 2.35 | 0.51 |
| 2:CB:24:TRP:CZ3 | 2:CB:26:PRO:HA | 2.46 | 0.51 |
| 3:CC:100:ALA:O | 3:CC:102:ASN:ND2 | 2.44 | 0.51 |
| 3:CC:42:LEU:O | 3:CC:46:GLU:HG2 | 2.11 | 0.51 |
| 25:DA:2408:U:H6 | 25:DA:2408:U:O5' | 1.94 | 0.51 |
| 25:DA:2849:U:H4' | 25:DA:2868:A:C2 | 2.46 | 0.51 |
| 25:DA:411:G:C5 | 35:DP:72:PRO:HB3 | 2.46 | 0.51 |
| 1:AA:1442:G:H2' | 1:AA:1442(A):G:H5' | 1.93 | 0.51 |
| 1:AA:738:C:H2' | 1:AA:739:C:C6 | 2.46 | 0.51 |
| 1:AA:991:U:C4 | 1:AA:1212:U:H1' | 2.46 | 0.51 |
| 4:AD:3:ARG:HE | 4:AD:118:ARG:CD | 2.24 | 0.51 |
| 4:AD:18:LYS:HG2 | 57:AD:501:SF4:S1 | 2.51 | 0.51 |
| 14:AN:3:ARG:HH21 | 14:AN:3:ARG:HB3 | 1.75 | 0.51 |
| 12:AL:59:ARG:HD3 | 24:AW:10:2QY:C | 2.41 | 0.51 |
| 25:BA:1284:G:OP2 | 61:BA:4767:HOH:O | 2.18 | 0.51 |
| 25:BA:1373:C:O2' | 61:BA:3810:HOH:O | 2.17 | 0.51 |
| 25:BA:8:A:H2' | 25:BA:9:U:H6 | 1.76 | 0.51 |
| 27:BD:132:PRO:HD3 | 27:BD:190:TYR:CZ | 2.46 | 0.51 |
| 45:BZ:150:LEU:HB3 | 45:BZ:171:ILE:HD11 | 1.92 | 0.51 |
| 1:CA:1009:G:H2' | 1:CA:1010:G:O4' | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CA:1002:G:N2 | 1:CA:1039:C:C4 | 2.79 | 0.51 |
| 1:CA:1162:C:N3 | 1:CA:1174:G:N2 | 2.45 | 0.51 |
| 1:CA:1260:C:HO2' | 1:CA:1283:G:HO2' | 1.59 | 0.51 |
| 1:CA:1391:U:H2' | 1:CA:1392:G:C8 | 2.46 | 0.51 |
| 2:CB:84:GLU:OE1 | 2:CB:216:SER:HA | 2.11 | 0.51 |
| 3:CC:164:ARG:NH2 | 3:CC:166:GLU:OE1 | 2.44 | 0.51 |
| 7:CG:107:ALA:O | 7:CG:111:ARG:HG3 | 2.10 | 0.51 |
| 1:CA:568:G:N7 | 12:CL:5:PRO:HD3 | 2.26 | 0.51 |
| 1:CA:980:C:H1' | 14:CN:19:ARG:HA | 1.92 | 0.51 |
| 25:DA:1164:G:H2' | 25:DA:1165:U:C6 | 2.46 | 0.51 |
| 25:DA:1529:G:H2' | 25:DA:1530:C:C6 | 2.45 | 0.51 |
| 25:DA:2293:C:H5' | 38:DS:89:ARG:NH2 | 2.25 | 0.51 |
| 25:DA:2320:A:N3 | 25:DA:2320:A:H2' | 2.24 | 0.51 |
| 25:DA:903:C:H2' | 25:DA:904:C:C6 | 2.46 | 0.51 |
| 25:DA:924:C:H2' | 25:DA:925:C:C6 | 2.46 | 0.51 |
| 2:AB:185:ILE:CG2 | 2:AB:199:TYR:HB2 | 2.41 | 0.51 |
| 1:AA:542:G:P | 4:AD:10:ARG:HH22 | 2.34 | 0.51 |
| 12:AL:34:ARG:HG2 | 12:AL:35:GLY:N | 2.26 | 0.51 |
| 13:AM:49:THR:HB | 13:AM:52:GLU:H | 1.75 | 0.51 |
| 20:AT:87:LYS:O | 20:AT:91:LEU:HG | 2.10 | 0.51 |
| 47:B1:50:ARG:HG2 | 47:B1:59:THR:HB | 1.93 | 0.51 |
| 26:BB:86:G:H1 | 26:BB:91:C:H42 | 1.59 | 0.51 |
| 44:BY:92:ASN:HB3 | 44:BY:94:LYS:N | 2.22 | 0.51 |
| 1:CA:1119:C:H2' | 1:CA:1120:G:C8 | 2.46 | 0.51 |
| 1:CA:599:C:C2' | 1:CA:600:C:H5'' | 2.37 | 0.51 |
| 1:CA:623:C:H2' | 1:CA:624:C:H6 | 1.75 | 0.51 |
| 2:CB:91:PRO:HG3 | 2:CB:154:LEU:HD12 | 1.92 | 0.51 |
| 13:CM:82:MET:HE2 | 13:CM:92:HIS:HB3 | 1.93 | 0.51 |
| 17:CQ:45:HIS:HA | 17:CQ:69:LYS:HE3 | 1.92 | 0.51 |
| 25:DA:1161:C:H2' | 25:DA:1162:G:H8 | 1.76 | 0.51 |
| 25:DA:1639:U:H2' | 25:DA:1640:C:H5'' | 1.92 | 0.51 |
| 25:DA:2850:A:OP2 | 25:DA:2866:U:H5 | 1.94 | 0.51 |
| 25:DA:817:C:H2' | 25:DA:818:G:O4' | 2.11 | 0.51 |
| 25:DA:873:G:N2 | 25:DA:905:U:C2 | 2.78 | 0.51 |
| 25:DA:909:A:H2' | 25:DA:912:C:H5 | 1.76 | 0.51 |
| 25:DA:30:G:OP2 | 40:DU:5:LYS:HE2 | 2.10 | 0.51 |
| 1:AA:394:G:H2' | 1:AA:395:C:H6 | 1.76 | 0.51 |
| 1:AA:474:G:H2' | 1:AA:475:G:C8 | 2.40 | 0.51 |
| 1:AA:693:G:H2' | 1:AA:694:A:C8 | 2.46 | 0.51 |
| 3:AC:11:ARG:NH2 | 3:AC:177:THR:O | 2.39 | 0.51 |
| 49:B3:44:ARG:O | 49:B3:48:GLU:HG3 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1008:U:OP2 | 61:BA:4616:HOH:O | 2.19 | 0.51 |
| 25:BA:1549:U:H2' | 25:BA:1550:C:C6 | 2.46 | 0.51 |
| 25:BA:1921:G:H2' | 25:BA:1921:G:N3 | 2.26 | 0.51 |
| 27:BD:123:ALA:HB3 | 27:BD:131:LEU:HG | 1.93 | 0.51 |
| 30:BG:137:GLU:OE1 | 30:BG:139:LEU:HD11 | 2.11 | 0.51 |
| 1:CA:1005:A:C2 | 1:CA:1026:G:C8 | 2.99 | 0.51 |
| 1:CA:1120:G:C6 | 1:CA:1121:U:C4 | 2.98 | 0.51 |
| 1:CA:1122:U:H3 | 1:CA:1151:A:H2 | 1.59 | 0.51 |
| 1:CA:396:G:O2' | 1:CA:398:C:OP1 | 2.22 | 0.51 |
| 2:CB:162:ILE:O | 2:CB:185:ILE:HG12 | 2.11 | 0.51 |
| 2:CB:60:ASP:O | 2:CB:64:ARG:HG2 | 2.10 | 0.51 |
| 3:CC:35:GLU:OE2 | 3:CC:59:ARG:NH2 | 2.35 | 0.51 |
| 7:CG:76:ARG:HD3 | 7:CG:89:MET:HG3 | 1.93 | 0.51 |
| 16:CP:51:VAL:HG12 | 16:CP:53:VAL:N | 2.26 | 0.51 |
| 25:DA:1833:U:H2' | 25:DA:1834:U:H6 | 1.75 | 0.51 |
| 26:DB:21:G:H2' | 26:DB:22:U:O4' | 2.10 | 0.51 |
| 25:DA:784:A:C5 | 27:DD:229:VAL:HG21 | 2.46 | 0.51 |
| 28:DE:92:THR:O | 28:DE:95:ILE:HG23 | 2.11 | 0.51 |
| 33:DN:4:TYR:CD2 | 40:DU:100:VAL:HG11 | 2.46 | 0.51 |
| 25:DA:1022:G:N7 | 33:DN:66:LYS:HE2 | 2.26 | 0.51 |
| 1:AA:1002:G:H3' | 1:AA:1003:G:C8 | 2.45 | 0.50 |
| 1:AA:1025:U:H3 | 1:AA:1036:G:H1 | 1.60 | 0.50 |
| 7:AG:26:PHE:O | 7:AG:30:ILE:HG13 | 2.11 | 0.50 |
| 1:AA:1348:U:H4' | 9:AI:120:ARG:HD2 | 1.93 | 0.50 |
| 9:AI:23:ASN:ND2 | 9:AI:25:LYS:HG2 | 2.26 | 0.50 |
| 18:AR:59:SER:H | 18:AR:62:GLU:HG3 | 1.76 | 0.50 |
| 23:AX:6:G:H1 | 23:AX:67:C:N4 | 2.09 | 0.50 |
| 50:B4:63:TYR:H | 50:B4:63:TYR:HD1 | 1.57 | 0.50 |
| 25:BA:208:G:H2' | 25:BA:209:G:O4' | 2.11 | 0.50 |
| 25:BA:930:G:O6 | 25:BA:939:C:C2 | 2.64 | 0.50 |
| 25:BA:1846:A:OP2 | 27:BD:54:ARG:NH2 | 2.45 | 0.50 |
| 28:BE:116:VAL:HG13 | 28:BE:122:PHE:HB2 | 1.93 | 0.50 |
| 31:BH:94:TYR:CE2 | 31:BH:160:LYS:HG2 | 2.46 | 0.50 |
| 25:BA:2847:G:H21 | 37:BR:45:ARG:HH12 | 1.59 | 0.50 |
| 1:CA:545:C:OP1 | 4:CD:61:LYS:NZ | 2.42 | 0.50 |
| 1:CA:127:G:OP1 | 1:CA:635:G:H1' | 2.11 | 0.50 |
| 1:CA:758:G:N7 | 61:CA:4152:HOH:O | 2.34 | 0.50 |
| 1:CA:922:G:H2' | 1:CA:923:A:C8 | 2.45 | 0.50 |
| 2:CB:80:ILE:HD13 | 2:CB:80:ILE:O | 2.11 | 0.50 |
| 3:CC:155:GLY:HA3 | 3:CC:196:LEU:HD13 | 1.92 | 0.50 |
| 6:CF:69:GLU:O | 6:CF:72:VAL:HG12 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1060:C:H4' | 10:CJ:51:ARG:HB3 | 1.93 | 0.50 |
| 12:CL:34:ARG:HG3 | 12:CL:105:TYR:CE2 | 2.45 | 0.50 |
| 25:DA:1007:C:P | 33:DN:37:LYS:HZ2 | 2.34 | 0.50 |
| 25:DA:118:A:N3 | 25:DA:178:G:H1' | 2.26 | 0.50 |
| 25:DA:1819:A:H5'' | 27:DD:161:THR:HG21 | 1.93 | 0.50 |
| 25:DA:2847:U:OP1 | 39:DT:98:LYS:NZ | 2.42 | 0.50 |
| 29:DF:154:VAL:HG22 | 29:DF:191:ARG:HB2 | 1.94 | 0.50 |
| 31:DH:117:PRO:HG3 | 31:DH:123:PHE:CD2 | 2.46 | 0.50 |
| 55:B9:25:VAL:HB | 55:B9:34:GLN:HB2 | 1.93 | 0.50 |
| 25:BA:310:C:H2' | 25:BA:311:C:C6 | 2.46 | 0.50 |
| 25:BA:831:A:C5 | 27:BD:229:VAL:HG21 | 2.46 | 0.50 |
| 28:BE:34:VAL:HG21 | 28:BE:78:LEU:HD11 | 1.93 | 0.50 |
| 29:BF:164:ARG:O | 29:BF:168:ARG:HB2 | 2.11 | 0.50 |
| 25:BA:346:A:OP1 | 29:BF:168:ARG:HD2 | 2.11 | 0.50 |
| 26:BB:42:C:C6 | 30:BG:69:ALA:HB2 | 2.46 | 0.50 |
| 35:BP:63:PRO:HD3 | 54:B8:27:THR:HG22 | 1.93 | 0.50 |
| 1:CA:1028:C:O2 | 1:CA:1034:G:H1' | 2.11 | 0.50 |
| 1:CA:1014:A:C2 | 1:CA:1219:U:H1' | 2.46 | 0.50 |
| 1:CA:1241:G:H2' | 1:CA:1242:C:C6 | 2.45 | 0.50 |
| 1:CA:1273:G:H3' | 1:CA:1274:G:C8 | 2.43 | 0.50 |
| 1:CA:509:A:C8 | 1:CA:509:A:H3' | 2.45 | 0.50 |
| 1:CA:91:C:H2' | 1:CA:92:C:C6 | 2.46 | 0.50 |
| 3:CC:181:ASN:ND2 | 3:CC:204:LEU:HD12 | 2.26 | 0.50 |
| 8:CH:73:ASP:OD1 | 8:CH:75:ARG:HD3 | 2.10 | 0.50 |
| 13:CM:80:ARG:HH22 | 19:CS:69:HIS:CE1 | 2.29 | 0.50 |
| 19:CS:28:LYS:HB2 | 19:CS:29:ARG:HA | 1.92 | 0.50 |
| 23:CX:44:A:C6 | 23:CX:45:G:C6 | 3.00 | 0.50 |
| 25:DA:2615:U:H2' | 25:DA:2616:C:H6 | 1.77 | 0.50 |
| 25:DA:581:C:H2' | 25:DA:582:G:C8 | 2.47 | 0.50 |
| 30:DG:97:ASP:O | 30:DG:101:ILE:HG13 | 2.11 | 0.50 |
| 25:DA:2316:C:O2' | 30:DG:128:ARG:NH1 | 2.44 | 0.50 |
| 30:DG:14:GLU:O | 30:DG:17:PRO:HD2 | 2.11 | 0.50 |
| 30:DG:36:LYS:HE3 | 30:DG:95:ARG:NH1 | 2.27 | 0.50 |
| 32:DI:134:PRO:C | 32:DI:136:VAL:H | 2.15 | 0.50 |
| 34:DO:25:LEU:HD12 | 34:DO:38:VAL:HG12 | 1.93 | 0.50 |
| 25:DA:1665:A:H4' | 34:DO:67:LYS:HB2 | 1.93 | 0.50 |
| 35:DP:2:LYS:NZ | 35:DP:4:SER:OG | 2.42 | 0.50 |
| 35:DP:94:GLU:HG3 | 35:DP:124:LYS:HD3 | 1.94 | 0.50 |
| 1:AA:1003:G:C2' | 1:AA:1004:A:H4' | 2.41 | 0.50 |
| 1:AA:1036:G:H5' | 1:AA:1037:C:C5 | 2.41 | 0.50 |
| 1:AA:946:A:O2' | 1:AA:1333:A:N3 | 2.40 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:261:U:OP2 | 20:AT:79:ARG:NH2 | 2.44 | 0.50 |
| 1:AA:308:C:H2' | 1:AA:309:G:C8 | 2.46 | 0.50 |
| 1:AA:985:C:H2' | 1:AA:986:A:H8 | 1.76 | 0.50 |
| 11:AK:34:ASP:HB3 | 11:AK:40:ILE:HD11 | 1.93 | 0.50 |
| 18:AR:59:SER:H | 18:AR:62:GLU:CG | 2.24 | 0.50 |
| 46:B0:27:GLU:HG3 | 46:B0:68:GLU:HA | 1.92 | 0.50 |
| 25:BA:239:G:H2' | 25:BA:240:A:C8 | 2.47 | 0.50 |
| 27:BD:26:LYS:HB3 | 27:BD:83:GLU:HG2 | 1.93 | 0.50 |
| 30:BG:109:VAL:C | 30:BG:112:PRO:HD2 | 2.31 | 0.50 |
| 1:CA:1249:C:O4' | 9:CI:70:LYS:HE2 | 2.11 | 0.50 |
| 1:CA:487:A:H2' | 1:CA:488:C:O4' | 2.11 | 0.50 |
| 1:CA:689:C:OP1 | 11:CK:27:ASN:ND2 | 2.45 | 0.50 |
| 5:CE:100:VAL:HG22 | 5:CE:118:ILE:HG22 | 1.92 | 0.50 |
| 25:DA:454:A:H4' | 25:DA:455:C:OP2 | 2.11 | 0.50 |
| 30:DG:13:GLU:O | 30:DG:15:VAL:N | 2.44 | 0.50 |
| 25:DA:1187:G:H5'' | 41:DV:81:TYR:CE1 | 2.46 | 0.50 |
| 1:AA:1218:C:H2' | 1:AA:1219:U:C6 | 2.46 | 0.50 |
| 1:AA:684:A:H2' | 1:AA:685:G:C8 | 2.46 | 0.50 |
| 9:AI:3:GLN:HG2 | 9:AI:20:ARG:HE | 1.77 | 0.50 |
| 19:AS:52:TYR:HA | 19:AS:56:GLN:O | 2.11 | 0.50 |
| 25:BA:2377:G:O6 | 54:B8:39:LYS:HE3 | 2.11 | 0.50 |
| 25:BA:2062:C:H2' | 25:BA:2063:U:O4' | 2.12 | 0.50 |
| 25:BA:275:C:H2' | 25:BA:276:C:C6 | 2.47 | 0.50 |
| 27:BD:12:SER:HB3 | 27:BD:208:LYS:HB3 | 1.93 | 0.50 |
| 1:CA:1256:A:H61 | 1:CA:1278:U:C1' | 2.23 | 0.50 |
| 1:CA:1270:C:C2' | 1:CA:1271:G:H5' | 2.42 | 0.50 |
| 1:CA:300:A:H1' | 1:CA:565:U:O2 | 2.11 | 0.50 |
| 1:CA:411:A:OP1 | 4:CD:30:LYS:NZ | 2.25 | 0.50 |
| 2:CB:76:GLN:HG3 | 2:CB:206:ASP:O | 2.11 | 0.50 |
| 25:DA:250:G:H2' | 25:DA:251:A:C8 | 2.47 | 0.50 |
| 25:DA:465:G:C6 | 25:DA:466:A:N6 | 2.79 | 0.50 |
| 33:DN:20:GLY:HA2 | 33:DN:61:ARG:NE | 2.27 | 0.50 |
| 7:AG:16:LEU:HD23 | 9:AI:41:VAL:HG12 | 1.92 | 0.50 |
| 8:AH:4:ASP:OD2 | 8:AH:85:ARG:NH1 | 2.36 | 0.50 |
| 9:AI:48:GLU:OE2 | 9:AI:51:ARG:HD2 | 2.12 | 0.50 |
| 52:B6:11:LEU:HB2 | 52:B6:21:TYR:HB2 | 1.92 | 0.50 |
| 25:BA:1093:G:H2' | 25:BA:1156:G:H1 | 1.77 | 0.50 |
| 25:BA:1834:A:H4' | 27:BD:259:THR:HG23 | 1.93 | 0.50 |
| 43:BX:31:HIS:HD2 | 43:BX:33:LYS:N | 2.05 | 0.50 |
| 1:CA:998:G:N2 | 1:CA:1043:C:N3 | 2.48 | 0.50 |
| 1:CA:1072:G:C6 | 1:CA:1073:U:C4 | 3.00 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:170:U:O2' | 1:CA:171:A:H5' | 2.12 | 0.50 |
| 1:CA:757:U:H2' | 1:CA:758:G:O4' | 2.11 | 0.50 |
| 1:CA:977:A:N3 | 1:CA:977:A:H2' | 2.26 | 0.50 |
| 20:CT:42:GLN:O | 20:CT:45:GLN:HB3 | 2.11 | 0.50 |
| 25:DA:2336:A:H61 | 46:D0:43:THR:HG21 | 1.76 | 0.50 |
| 48:D2:1:MET:SD | 48:D2:56:GLN:NE2 | 2.85 | 0.50 |
| 25:DA:1412:A:H2' | 25:DA:1413:G:H8 | 1.72 | 0.50 |
| 25:DA:937:U:H2' | 25:DA:938:G:O4' | 2.12 | 0.50 |
| 27:DD:221:VAL:HG22 | 27:DD:226:MET:CE | 2.42 | 0.50 |
| 29:DF:167:ALA:O | 29:DF:170:LEU:HB2 | 2.11 | 0.50 |
| 43:DX:92:LEU:C | 43:DX:94:GLY:H | 2.15 | 0.50 |
| 1:AA:166:G:C4 | 1:AA:167:G:N7 | 2.79 | 0.50 |
| 1:AA:382:A:N3 | 1:AA:383:A:N7 | 2.59 | 0.50 |
| 1:AA:407:G:OP1 | 4:AD:115:ARG:HD3 | 2.12 | 0.50 |
| 1:AA:36:C:O2' | 1:AA:501:C:OP1 | 2.26 | 0.50 |
| 1:AA:67:C:H2' | 1:AA:68:G:C8 | 2.46 | 0.50 |
| 1:AA:738:C:H2' | 1:AA:739:C:H6 | 1.75 | 0.50 |
| 1:AA:826:C:H2' | 1:AA:827:U:H6 | 1.77 | 0.50 |
| 5:AE:98:THR:HG22 | 5:AE:99:GLY:O | 2.12 | 0.50 |
| 7:AG:69:VAL:HG22 | 7:AG:135:VAL:HG22 | 1.94 | 0.50 |
| 9:AI:53:VAL:HG11 | 9:AI:92:TYR:CE1 | 2.46 | 0.50 |
| 61:BA:3804:HOH:O | 51:B5:15:ARG:HG2 | 2.11 | 0.50 |
| 25:BA:1153:G:N3 | 25:BA:1153:G:H2' | 2.27 | 0.50 |
| 25:BA:2211:U:H2' | 25:BA:2212:G:H5' | 1.92 | 0.50 |
| 32:BI:29:TYR:C | 32:BI:32:PRO:HD2 | 2.31 | 0.50 |
| 33:BN:15:LEU:HD12 | 33:BN:137:LYS:HG2 | 1.94 | 0.50 |
| 41:BV:14:VAL:HA | 41:BV:18:LEU:HD12 | 1.93 | 0.50 |
| 1:CA:1004:A:C8 | 1:CA:1005:A:H4' | 2.47 | 0.50 |
| 1:CA:1093:A:H5'' | 1:CA:1094:G:OP2 | 2.12 | 0.50 |
| 1:CA:276:G:C2' | 1:CA:277:C:H5' | 2.41 | 0.50 |
| 7:CG:16:LEU:H | 7:CG:16:LEU:HD22 | 1.77 | 0.50 |
| 9:CI:9:ARG:O | 9:CI:104:ARG:HG3 | 2.11 | 0.50 |
| 10:CJ:13:HIS:O | 10:CJ:17:ASP:HB2 | 2.12 | 0.50 |
| 11:CK:81:ASP:OD1 | 11:CK:106:LYS:HE2 | 2.12 | 0.50 |
| 20:CT:9:ASN:O | 20:CT:10:LEU:HB2 | 2.11 | 0.50 |
| 25:DA:1328:G:H2' | 25:DA:1330:C:C5 | 2.47 | 0.50 |
| 25:DA:1359:A:N1 | 25:DA:1372:U:C4 | 2.80 | 0.50 |
| 25:DA:1563:G:H2' | 25:DA:1564:C:H6 | 1.77 | 0.50 |
| 25:DA:1697:G:OP2 | 25:DA:1698:A:O2' | 2.24 | 0.50 |
| 25:DA:2262:U:OP2 | 46:D0:19:LYS:HD3 | 2.12 | 0.50 |
| 25:DA:2293:C:H5' | 25:DA:2294:C:OP2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:DE:101:ARG:CZ | 28:DE:171:GLU:HB2 | 2.41 | 0.50 |
| 28:DE:9:VAL:HG22 | 28:DE:25:VAL:HB | 1.94 | 0.50 |
| 40:DU:66:ASN:O | 40:DU:70:ARG:HG3 | 2.12 | 0.50 |
| 41:DV:95:LEU:HD13 | 41:DV:97:LYS:HD3 | 1.93 | 0.50 |
| 1:AA:1066:C:O2' | 1:AA:1067:A:H5' | 2.11 | 0.50 |
| 1:AA:1510:U:H2' | 1:AA:1511:G:C8 | 2.47 | 0.50 |
| 1:AA:397:A:N3 | 1:AA:397:A:H3' | 2.26 | 0.50 |
| 1:AA:491:G:H2' | 1:AA:492:G:O4' | 2.12 | 0.50 |
| 1:AA:872:A:C8 | 1:AA:874:G:C8 | 3.00 | 0.50 |
| 2:AB:71:VAL:HB | 2:AB:164:VAL:HG13 | 1.93 | 0.50 |
| 2:AB:45:GLN:O | 2:AB:49:GLU:HB2 | 2.11 | 0.50 |
| 3:AC:58:GLU:HB2 | 3:AC:65:ALA:HB2 | 1.92 | 0.50 |
| 7:AG:78:ARG:HG2 | 7:AG:79:ARG:HB2 | 1.94 | 0.50 |
| 13:AM:84:ILE:HG13 | 19:AS:74:PHE:HE1 | 1.75 | 0.50 |
| 46:B0:27:GLU:HA | 46:B0:67:VAL:HG12 | 1.94 | 0.50 |
| 25:BA:179:A:N3 | 25:BA:726:C:O2' | 2.37 | 0.50 |
| 27:BD:38:LYS:HE3 | 27:BD:39:LYS:O | 2.12 | 0.50 |
| 1:CA:1095:U:P | 1:CA:1108:G:H1 | 2.35 | 0.50 |
| 9:CI:105:ASP:HB2 | 9:CI:107:ARG:HG3 | 1.93 | 0.50 |
| 42:DW:35:ILE:HG23 | 51:D5:28:PRO:HD2 | 1.93 | 0.50 |
| 25:DA:1153:C:H2' | 25:DA:1154:G:O4' | 2.12 | 0.50 |
| 25:DA:1346:G:OP2 | 61:DA:4263:HOH:O | 2.20 | 0.50 |
| 25:DA:2293:C:H42 | 25:DA:2339:G:H1 | 1.58 | 0.50 |
| 25:DA:2336:A:H61 | 46:D0:43:THR:CG2 | 2.25 | 0.50 |
| 38:DS:25:ARG:NH1 | 38:DS:42:ASP:OD1 | 2.41 | 0.50 |
| 45:DZ:5:LEU:HD13 | 45:DZ:6:LYS:O | 2.12 | 0.50 |
| 1:AA:1269:A:H2 | 1:AA:1312:G:N3 | 2.10 | 0.50 |
| 1:AA:414:A:H2' | 1:AA:415:A:O4' | 2.12 | 0.50 |
| 1:AA:701:C:O2 | 1:AA:703:G:N1 | 2.45 | 0.50 |
| 5:AE:90:VAL:O | 5:AE:91:LEU:HD13 | 2.10 | 0.50 |
| 9:AI:19:LEU:HB3 | 9:AI:59:PHE:HD2 | 1.76 | 0.50 |
| 25:BA:1221:G:H1' | 25:BA:1222:A:O5' | 2.11 | 0.50 |
| 25:BA:1712:A:H4' | 34:BO:67:LYS:HB2 | 1.92 | 0.50 |
| 25:BA:1855:G:OP1 | 27:BD:52:ARG:NH1 | 2.40 | 0.50 |
| 25:BA:225:C:H2' | 25:BA:226:C:C6 | 2.46 | 0.50 |
| 1:CA:1036:G:N7 | 1:CA:1037:C:C2 | 2.80 | 0.50 |
| 1:CA:153:C:H2' | 1:CA:154:C:C6 | 2.47 | 0.50 |
| 1:CA:715:A:H2' | 1:CA:716:A:C8 | 2.47 | 0.50 |
| 5:CE:80:ILE:HG22 | 5:CE:91:LEU:HB2 | 1.94 | 0.50 |
| 13:CM:93:ARG:HD3 | 25:DA:888:C:OP2 | 2.12 | 0.50 |
| 20:CT:43:LEU:O | 20:CT:47:GLY:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:330:A:H2 | 25:DA:1210:A:H2' | 1.76 | 0.50 |
| 25:DA:1406:U:H2' | 25:DA:1407:C:C6 | 2.46 | 0.50 |
| 25:DA:2386:C:H2' | 25:DA:2387:U:C6 | 2.46 | 0.50 |
| 25:DA:2711:A:H5'' | 25:DA:2712:U:H5'' | 1.94 | 0.50 |
| 25:DA:954:G:C5 | 25:DA:955:C:C5 | 2.99 | 0.50 |
| 29:DF:150:GLY:HA2 | 29:DF:172:TRP:CE3 | 2.47 | 0.50 |
| 25:DA:2882:A:OP1 | 37:DR:96:ARG:NE | 2.44 | 0.50 |
| 1:AA:1129:C:O2' | 1:AA:1139:G:N7 | 2.33 | 0.50 |
| 1:AA:1224:G:O2' | 1:AA:1322:C:OP1 | 2.29 | 0.50 |
| 1:AA:137:C:H2' | 1:AA:138:G:H5' | 1.94 | 0.50 |
| 1:AA:174:C:H2' | 1:AA:175:C:H6 | 1.76 | 0.50 |
| 1:AA:203:U:H2' | 1:AA:203:U:OP2 | 2.12 | 0.50 |
| 1:AA:457:C:H2' | 1:AA:458:C:H6 | 1.74 | 0.50 |
| 4:AD:25:ARG:HG2 | 4:AD:25:ARG:O | 2.11 | 0.50 |
| 13:AM:3:ARG:HG3 | 13:AM:4:ILE:H | 1.77 | 0.50 |
| 19:AS:65:ASN:HD22 | 19:AS:65:ASN:N | 2.08 | 0.50 |
| 25:BA:1201:A:OP1 | 40:BU:55:ARG:HD3 | 2.11 | 0.50 |
| 25:BA:1312:G:O5' | 42:BW:15:ARG:NH2 | 2.45 | 0.50 |
| 25:BA:831:A:H5' | 25:BA:832:G:OP1 | 2.12 | 0.50 |
| 25:BA:910:A:H2' | 25:BA:911:G:H8 | 1.77 | 0.50 |
| 27:BD:10:THR:OG1 | 27:BD:13:ARG:HB2 | 2.12 | 0.50 |
| 32:BI:93:THR:OG1 | 32:BI:96:ASP:OD1 | 2.19 | 0.50 |
| 1:CA:501:C:H2' | 1:CA:502:G:C8 | 2.47 | 0.50 |
| 25:DA:1453:U:OP1 | 37:DR:77:ARG:NH1 | 2.36 | 0.50 |
| 25:DA:2302:G:C6 | 25:DA:2303:G:N7 | 2.80 | 0.50 |
| 25:DA:754:C:H2' | 25:DA:755:C:C6 | 2.43 | 0.50 |
| 25:DA:873:G:H2' | 25:DA:874:G:H5'' | 1.94 | 0.50 |
| 25:DA:878:A:N6 | 25:DA:900:A:N7 | 2.60 | 0.50 |
| 26:DB:3:C:H2' | 26:DB:4:C:C6 | 2.47 | 0.50 |
| 27:DD:16:MET:HG3 | 27:DD:206:LEU:O | 2.12 | 0.50 |
| 35:DP:65:ARG:HG3 | 54:D8:25:MET:HG3 | 1.93 | 0.50 |
| 1:AA:1145:C:H4' | 1:AA:1146:A:C5' | 2.41 | 0.49 |
| 1:AA:1241:G:H1 | 1:AA:1296:C:N4 | 2.10 | 0.49 |
| 1:AA:524:G:H2' | 1:AA:525:C:C6 | 2.46 | 0.49 |
| 25:BA:2486:C:H5'' | 25:BA:2487:C:OP2 | 2.12 | 0.49 |
| 25:BA:2899:C:H2' | 25:BA:2900:G:O4' | 2.12 | 0.49 |
| 30:BG:16:ARG:HB2 | 30:BG:17:PRO:HD3 | 1.94 | 0.49 |
| 1:CA:1227:A:H3' | 1:CA:1227:A:C8 | 2.47 | 0.49 |
| 4:CD:26:CYS:HA | 57:CD:501:SF4:S2 | 2.52 | 0.49 |
| 8:CH:64:LYS:HG2 | 8:CH:79:VAL:HG21 | 1.93 | 0.49 |
| 11:CK:20:TYR:CE1 | 11:CK:83:ILE:HD12 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:CO:29:VAL:HG11 | 15:CO:81:LEU:HD21 | 1.94 | 0.49 |
| 18:CR:60:ALA:O | 18:CR:64:ARG:HG3 | 2.12 | 0.49 |
| 48:D2:32:LEU:HD23 | 48:D2:53:LEU:HB3 | 1.94 | 0.49 |
| 38:DS:10:ARG:HH21 | 38:DS:91:PRO:HB2 | 1.77 | 0.49 |
| 1:AA:1210:C:C2' | 1:AA:1211:U:H5' | 2.42 | 0.49 |
| 1:AA:160:A:N1 | 1:AA:343:U:C2 | 2.80 | 0.49 |
| 1:AA:64:G:H4' | 1:AA:65:U:H3' | 1.93 | 0.49 |
| 7:AG:78:ARG:HH21 | 7:AG:156:TRP:HB3 | 1.77 | 0.49 |
| 23:AX:20:U:H5'' | 23:AX:21:A:OP2 | 2.12 | 0.49 |
| 46:B0:27:GLU:HB2 | 46:B0:69:PHE:HD1 | 1.77 | 0.49 |
| 25:BA:1827:U:H2' | 25:BA:1828:C:C6 | 2.47 | 0.49 |
| 1:CA:999:C:C4 | 1:CA:1042:G:C2 | 2.99 | 0.49 |
| 1:CA:1047:G:H5'' | 14:CN:4:LYS:HD3 | 1.93 | 0.49 |
| 1:CA:1176:A:H2' | 1:CA:1177:G:C8 | 2.47 | 0.49 |
| 1:CA:1516:G:N2 | 1:CA:1519:A:OP2 | 2.45 | 0.49 |
| 1:CA:59:A:H5'' | 1:CA:60:A:H5'' | 1.94 | 0.49 |
| 2:CB:230:VAL:HG22 | 2:CB:231:GLU:H | 1.77 | 0.49 |
| 7:CG:47:CYS:O | 7:CG:50:ILE:HG12 | 2.11 | 0.49 |
| 8:CH:124:ALA:O | 8:CH:128:GLY:N | 2.44 | 0.49 |
| 19:CS:27:GLU:HG2 | 19:CS:47:HIS:NE2 | 2.28 | 0.49 |
| 25:DA:1161:C:H2' | 25:DA:1162:G:C8 | 2.46 | 0.49 |
| 25:DA:1651:G:H5' | 37:DR:39:PRO:HG2 | 1.94 | 0.49 |
| 25:DA:1996:C:H4' | 25:DA:1997:G:OP1 | 2.11 | 0.49 |
| 25:DA:608:A:H2' | 25:DA:609:A:C8 | 2.47 | 0.49 |
| 27:DD:71:ASP:HB2 | 27:DD:103:ARG:NH2 | 2.22 | 0.49 |
| 32:DI:140:LEU:HD13 | 32:DI:142:VAL:HG13 | 1.94 | 0.49 |
| 1:AA:1298:C:H4' | 1:AA:1299:A:C4 | 2.46 | 0.49 |
| 1:AA:1492:A:H1' | 25:BA:1935:A:H61 | 1.78 | 0.49 |
| 1:AA:41:G:H2' | 1:AA:42:G:C8 | 2.47 | 0.49 |
| 1:AA:615:C:H2' | 1:AA:616:G:O4' | 2.12 | 0.49 |
| 20:AT:57:ARG:HH22 | 20:AT:100:ILE:HD12 | 1.77 | 0.49 |
| 21:AU:9:ARG:HA | 21:AU:22:ARG:HB2 | 1.94 | 0.49 |
| 25:BA:1222:A:H3' | 25:BA:1223:C:C6 | 2.48 | 0.49 |
| 25:BA:2314:G:C2 | 25:BA:2327:G:C2 | 3.00 | 0.49 |
| 25:BA:296:U:H2' | 25:BA:297:C:C6 | 2.46 | 0.49 |
| 25:BA:354:A:HO2' | 25:BA:355:A:H8 | 1.58 | 0.49 |
| 31:BH:20:ALA:HB1 | 31:BH:21:PRO:HD2 | 1.93 | 0.49 |
| 32:BI:38:LEU:HB2 | 32:BI:40:THR:HG22 | 1.94 | 0.49 |
| 25:BA:1001:G:OP2 | 36:BQ:87:LYS:HE2 | 2.12 | 0.49 |
| 41:BV:98:GLU:OE1 | 41:BV:100:ARG:HD3 | 2.12 | 0.49 |
| 42:BW:18:ARG:NH1 | 42:BW:76:VAL:O | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1057:G:C5 | 1:CA:1204:A:C2 | 3.00 | 0.49 |
| 1:CA:297:G:N2 | 1:CA:300:A:OP2 | 2.45 | 0.49 |
| 1:CA:358:U:H2' | 1:CA:359:U:C6 | 2.47 | 0.49 |
| 1:CA:691:G:H2' | 1:CA:692:U:C6 | 2.46 | 0.49 |
| 7:CG:132:GLY:O | 7:CG:136:LYS:HG2 | 2.12 | 0.49 |
| 10:CJ:11:PHE:CE1 | 10:CJ:67:THR:HG22 | 2.47 | 0.49 |
| 12:CL:54:LYS:O | 12:CL:70:ILE:HG13 | 2.11 | 0.49 |
| 47:D1:7:ILE:HG23 | 47:D1:98:LEU:HD11 | 1.93 | 0.49 |
| 54:D8:3:LYS:HB2 | 54:D8:64:TYR:OH | 2.11 | 0.49 |
| 25:DA:812:C:H2' | 25:DA:813:U:H6 | 1.77 | 0.49 |
| 26:DB:78:A:H2' | 26:DB:79:C:O4' | 2.12 | 0.49 |
| 29:DF:20:LEU:HD22 | 29:DF:21:ALA:H | 1.77 | 0.49 |
| 34:DO:2:ILE:HD12 | 34:DO:6:THR:HG21 | 1.94 | 0.49 |
| 35:DP:84:ASN:OD1 | 35:DP:117:GLU:HB2 | 2.12 | 0.49 |
| 1:AA:391:G:O3' | 16:AP:8:ARG:NH2 | 2.46 | 0.49 |
| 1:AA:757:U:H2' | 1:AA:758:G:O4' | 2.11 | 0.49 |
| 12:AL:25:PRO:HD2 | 12:AL:98:TYR:OH | 2.12 | 0.49 |
| 51:B5:16:ARG:HG2 | 51:B5:16:ARG:HH11 | 1.78 | 0.49 |
| 25:BA:1248:G:O6 | 61:BA:4634:HOH:O | 2.19 | 0.49 |
| 25:BA:1904:C:H2' | 25:BA:1905:G:O4' | 2.13 | 0.49 |
| 25:BA:2827:G:OP1 | 37:BR:99:LYS:HE2 | 2.12 | 0.49 |
| 26:BB:15:A:OP1 | 26:BB:108:U:O2' | 2.24 | 0.49 |
| 29:BF:103:LYS:HA | 29:BF:106:ARG:HG3 | 1.94 | 0.49 |
| 29:BF:31:HIS:HB2 | 35:BP:9:ASN:OD1 | 2.12 | 0.49 |
| 33:BN:96:GLU:H | 33:BN:96:GLU:CD | 2.16 | 0.49 |
| 1:CA:1025:U:O2' | 1:CA:1026:G:H5'' | 2.12 | 0.49 |
| 1:CA:189(L):G:H2' | 1:CA:190:U:H6 | 1.76 | 0.49 |
| 1:CA:1079:G:O3' | 5:CE:14:ARG:NH2 | 2.44 | 0.49 |
| 1:CA:1240:U:OP2 | 7:CG:115:ARG:HA | 2.12 | 0.49 |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:CE1 | 2.47 | 0.49 |
| 13:CM:60:VAL:HG23 | 13:CM:64:TRP:HE3 | 1.77 | 0.49 |
| 16:CP:74:LEU:O | 16:CP:79:VAL:HG23 | 2.13 | 0.49 |
| 24:CW:9:MVA:HG13 | 24:CW:10:2QY:H82 | 1.94 | 0.49 |
| 50:D4:46:GLN:HG3 | 50:D4:48:ARG:HH21 | 1.77 | 0.49 |
| 25:DA:2592:G:N7 | 61:DA:3923:HOH:O | 2.34 | 0.49 |
| 25:DA:816:C:O2' | 25:DA:932:G:O6 | 2.31 | 0.49 |
| 31:DH:27:LYS:HZ3 | 31:DH:32:GLU:HB2 | 1.77 | 0.49 |
| 31:DH:3:ARG:HH22 | 31:DH:5:GLY:H | 1.61 | 0.49 |
| 25:DA:637:A:H2' | 35:DP:117:GLU:OE2 | 2.11 | 0.49 |
| 35:DP:97:PRO:HD3 | 35:DP:126:VAL:O | 2.11 | 0.49 |
| 39:DT:51:ARG:HG3 | 39:DT:98:LYS:HD2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1189:C:H5'' | 1:AA:1190:G:OP2 | 2.13 | 0.49 |
| 1:AA:1243:C:H2' | 1:AA:1244:C:H6 | 1.78 | 0.49 |
| 1:AA:130:A:O2' | 1:AA:131:C:O5' | 2.28 | 0.49 |
| 1:AA:394:G:H2' | 1:AA:395:C:C6 | 2.46 | 0.49 |
| 1:AA:665:A:H1' | 1:AA:733:A:O4' | 2.12 | 0.49 |
| 4:AD:30:LYS:HA | 4:AD:35:ARG:HH11 | 1.78 | 0.49 |
| 25:BA:1298:G:C2 | 25:BA:1299:A:C2 | 3.01 | 0.49 |
| 25:BA:1940:A:O2' | 25:BA:1942:C:N4 | 2.46 | 0.49 |
| 25:BA:2398:C:O2' | 61:BA:3871:HOH:O | 2.20 | 0.49 |
| 25:BA:407:U:H2' | 25:BA:408:G:C8 | 2.47 | 0.49 |
| 25:BA:809:U:H4' | 25:BA:810:G:O5' | 2.12 | 0.49 |
| 40:BU:58:ARG:HA | 40:BU:61:TRP:CE3 | 2.47 | 0.49 |
| 1:CA:1228:C:OP1 | 13:CM:115:LYS:N | 2.33 | 0.49 |
| 4:CD:150:GLU:HA | 4:CD:153:ARG:HE | 1.77 | 0.49 |
| 8:CH:20:TYR:CE2 | 8:CH:75:ARG:HG2 | 2.47 | 0.49 |
| 8:CH:51:VAL:HG11 | 8:CH:60:ARG:NH1 | 2.20 | 0.49 |
| 25:DA:2552:U:C2 | 25:DA:2554:U:H5'' | 2.48 | 0.49 |
| 25:DA:2845:G:H2' | 25:DA:2846:G:H8 | 1.75 | 0.49 |
| 25:DA:315:G:H2' | 25:DA:316:C:C6 | 2.48 | 0.49 |
| 25:DA:684:G:OP1 | 53:D7:16:HIS:ND1 | 2.45 | 0.49 |
| 34:DO:20:MET:HE3 | 34:DO:44:LYS:HE3 | 1.95 | 0.49 |
| 25:DA:1614:A:C2 | 42:DW:93:ALA:HB2 | 2.47 | 0.49 |
| 43:DX:44:GLU:O | 43:DX:48:LYS:N | 2.45 | 0.49 |
| 25:DA:483:A:O2' | 44:DY:49:VAL:O | 2.19 | 0.49 |
| 1:AA:999:C:H2' | 1:AA:1000:U:O4' | 2.13 | 0.49 |
| 1:AA:542:G:H2' | 1:AA:543:C:C6 | 2.47 | 0.49 |
| 1:AA:678:U:H2' | 1:AA:679:C:C6 | 2.47 | 0.49 |
| 2:AB:20:GLU:HG2 | 2:AB:191:ASP:HB3 | 1.94 | 0.49 |
| 5:AE:84:PHE:CE2 | 5:AE:133:TYR:HD2 | 2.31 | 0.49 |
| 13:AM:50:GLU:O | 13:AM:54:VAL:HG22 | 2.13 | 0.49 |
| 25:BA:1825:U:H2' | 25:BA:1826:C:C6 | 2.47 | 0.49 |
| 25:BA:1919:G:H2' | 25:BA:1920:U:O4' | 2.13 | 0.49 |
| 25:BA:207:A:C2 | 25:BA:224:U:H4' | 2.47 | 0.49 |
| 25:BA:2879:G:H2' | 25:BA:2880:C:O4' | 2.13 | 0.49 |
| 25:BA:672:G:H8 | 25:BA:672:G:O5' | 1.96 | 0.49 |
| 1:CA:628:G:H2' | 1:CA:629:G:C8 | 2.48 | 0.49 |
| 2:CB:221:LEU:HD13 | 2:CB:224:GLN:HE22 | 1.76 | 0.49 |
| 9:CI:38:GLN:HG2 | 9:CI:39:GLY:N | 2.27 | 0.49 |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:HE1 | 1.77 | 0.49 |
| 25:DA:1472:A:H2' | 25:DA:1473:G:O4' | 2.13 | 0.49 |
| 25:DA:176:G:O2' | 25:DA:177:G:H5' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:2471:C:N4 | 25:DA:2476:A:O2' | 2.46 | 0.49 |
| 25:DA:807:U:OP1 | 35:DP:36:LYS:NZ | 2.40 | 0.49 |
| 32:DI:70:GLU:O | 32:DI:74:ASN:HB2 | 2.13 | 0.49 |
| 1:CA:1423:G:P | 34:DO:49:ARG:HH12 | 2.34 | 0.49 |
| 1:AA:1015:A:H2' | 1:AA:1016:A:H8 | 1.78 | 0.49 |
| 1:AA:189(C):C:H2' | 1:AA:189(D):C:O4' | 2.12 | 0.49 |
| 1:AA:540:G:H2' | 1:AA:541:G:O4' | 2.12 | 0.49 |
| 2:AB:98:LEU:HB2 | 2:AB:101:MET:SD | 2.52 | 0.49 |
| 9:AI:21:PRO:HA | 9:AI:59:PHE:HA | 1.94 | 0.49 |
| 13:AM:40:ASN:O | 13:AM:43:THR:OG1 | 2.29 | 0.49 |
| 25:BA:1098:C:O5' | 25:BA:1098:C:H6 | 1.96 | 0.49 |
| 25:BA:1552:C:O2' | 25:BA:1553:A:H5' | 2.13 | 0.49 |
| 25:BA:1700:G:H3' | 37:BR:2:ARG:HD3 | 1.93 | 0.49 |
| 25:BA:2507:G:H5'' | 36:BQ:82:ARG:HG2 | 1.93 | 0.49 |
| 27:BD:175:LEU:HD12 | 27:BD:185:VAL:HG21 | 1.95 | 0.49 |
| 1:CA:1012:U:H2' | 1:CA:1013:G:C8 | 2.47 | 0.49 |
| 1:CA:1151:A:H5'' | 10:CJ:41:PRO:HA | 1.95 | 0.49 |
| 1:CA:253:U:H2' | 1:CA:254:G:H8 | 1.77 | 0.49 |
| 1:CA:427:U:H2' | 1:CA:428:G:C8 | 2.48 | 0.49 |
| 1:CA:975:A:H4' | 1:CA:976:G:C5' | 2.40 | 0.49 |
| 2:CB:23:ARG:HB2 | 2:CB:23:ARG:NH1 | 2.28 | 0.49 |
| 1:CA:377:G:OP1 | 16:CP:3:LYS:HD2 | 2.13 | 0.49 |
| 25:DA:1313:U:H2' | 25:DA:1610:A:N1 | 2.27 | 0.49 |
| 25:DA:1899:G:N3 | 25:DA:1899:G:H2' | 2.28 | 0.49 |
| 25:DA:491:G:H2' | 25:DA:492:A:C8 | 2.48 | 0.49 |
| 25:DA:539:G:H2' | 25:DA:540:C:C6 | 2.47 | 0.49 |
| 25:DA:601:C:O2' | 29:DF:104:LYS:NZ | 2.46 | 0.49 |
| 25:DA:895:U:O2' | 25:DA:896:A:H2' | 2.13 | 0.49 |
| 25:DA:2880:C:O3' | 37:DR:90:ARG:NH1 | 2.45 | 0.49 |
| 1:AA:191:G:C6 | 1:AA:192:U:C4 | 3.01 | 0.49 |
| 1:AA:250:A:H4' | 1:AA:251:G:O5' | 2.13 | 0.49 |
| 1:AA:302:G:N3 | 1:AA:556:C:H4' | 2.28 | 0.49 |
| 1:AA:445:G:H2' | 1:AA:446:G:H8 | 1.78 | 0.49 |
| 1:AA:472:A:N6 | 1:AA:473:G:C2 | 2.80 | 0.49 |
| 49:B3:11:SER:OG | 49:B3:13:ILE:HG13 | 2.12 | 0.49 |
| 25:BA:1317:G:OP2 | 61:BA:4516:HOH:O | 2.20 | 0.49 |
| 25:BA:1521:C:H2' | 25:BA:1522:G:C8 | 2.48 | 0.49 |
| 25:BA:1810:U:H2' | 61:BA:4800:HOH:O | 2.11 | 0.49 |
| 25:BA:2316:G:H22 | 25:BA:2324:U:H3 | 1.61 | 0.49 |
| 25:BA:231:G:C8 | 54:B8:5:LYS:HG2 | 2.48 | 0.49 |
| 25:BA:330:U:H2' | 25:BA:331:G:O4' | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:821:A:H2' | 25:BA:821:A:N3 | 2.27 | 0.49 |
| 1:CA:600:C:H2' | 1:CA:601:C:C6 | 2.48 | 0.49 |
| 2:CB:208:ILE:HA | 2:CB:211:ILE:HD12 | 1.95 | 0.49 |
| 14:CN:47:LEU:O | 14:CN:51:GLY:N | 2.44 | 0.49 |
| 25:DA:1434:A:H61 | 25:DA:1558:A:H62 | 1.59 | 0.49 |
| 25:DA:1531:C:N4 | 25:DA:1538:G:H1 | 2.10 | 0.49 |
| 25:DA:2100:G:H2' | 25:DA:2101:G:H5' | 1.94 | 0.49 |
| 25:DA:2649:U:H2' | 25:DA:2650:U:C6 | 2.47 | 0.49 |
| 25:DA:989:G:H4' | 25:DA:990:A:OP1 | 2.12 | 0.49 |
| 25:DA:999:U:O2' | 25:DA:1000:A:H5' | 2.13 | 0.49 |
| 27:DD:228:PRO:HD3 | 27:DD:235:GLY:CA | 2.42 | 0.49 |
| 29:DF:88:VAL:HG21 | 29:DF:91:GLY:HA3 | 1.95 | 0.49 |
| 41:DV:24:LYS:HA | 41:DV:92:THR:OG1 | 2.12 | 0.49 |
| 1:AA:1148:U:H2' | 1:AA:1149:C:O4' | 2.13 | 0.49 |
| 1:AA:308:C:H2' | 1:AA:309:G:H8 | 1.77 | 0.49 |
| 1:AA:438:G:O2' | 1:AA:494:U:O4 | 2.23 | 0.49 |
| 1:AA:542:G:H2' | 1:AA:543:C:H6 | 1.78 | 0.49 |
| 2:AB:20:GLU:O | 2:AB:40:HIS:HB2 | 2.12 | 0.49 |
| 23:AX:8:U:O5' | 23:AX:8:U:H6 | 1.95 | 0.49 |
| 25:BA:1588:G:H5'' | 25:BA:1589:A:OP2 | 2.12 | 0.49 |
| 36:BQ:133:ARG:HG2 | 36:BQ:134:ARG:N | 2.28 | 0.49 |
| 40:BU:24:TYR:HB2 | 40:BU:29:SER:HB3 | 1.95 | 0.49 |
| 1:CA:164:U:H2' | 1:CA:165:C:C6 | 2.47 | 0.49 |
| 1:CA:1129:C:H4' | 9:CI:16:ARG:HH22 | 1.78 | 0.49 |
| 9:CI:49:PRO:HG2 | 9:CI:81:ILE:HG23 | 1.95 | 0.49 |
| 30:DG:7:LEU:HD22 | 30:DG:100:TRP:HE3 | 1.78 | 0.49 |
| 33:DN:104:LYS:HA | 33:DN:107:LEU:HD12 | 1.93 | 0.49 |
| 37:DR:72:ASP:O | 37:DR:76:VAL:HG23 | 2.13 | 0.49 |
| 44:DY:35:TYR:CE2 | 44:DY:69:ALA:HB3 | 2.47 | 0.49 |
| 44:DY:14:LEU:HB2 | 44:DY:75:ILE:HD11 | 1.95 | 0.49 |
| 1:AA:1183:A:H3' | 1:AA:1184:G:H5'' | 1.95 | 0.49 |
| 1:AA:1237:C:O2' | 1:AA:1300:G:N2 | 2.45 | 0.49 |
| 1:AA:276:G:H2' | 1:AA:277:C:H5' | 1.95 | 0.49 |
| 1:AA:392:G:H2' | 1:AA:393:A:H8 | 1.78 | 0.49 |
| 1:AA:864:A:H2' | 1:AA:865:A:C8 | 2.47 | 0.49 |
| 9:AI:15:ALA:HB2 | 9:AI:65:VAL:HG23 | 1.94 | 0.49 |
| 50:B4:20:ASN:ND2 | 50:B4:36:CYS:SG | 2.82 | 0.49 |
| 25:BA:602:G:H2' | 25:BA:603:C:C6 | 2.48 | 0.49 |
| 45:BZ:146:ILE:HA | 45:BZ:147:GLY:HA2 | 1.62 | 0.49 |
| 1:CA:1003:G:H2' | 1:CA:1004:A:H4' | 1.95 | 0.49 |
| 1:CA:532:A:H2 | 1:CA:1207:G:H4' | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CC:36:ASP:O | 3:CC:40:ARG:HG3 | 2.12 | 0.49 |
| 3:CC:29:TYR:OH | 14:CN:54:PRO:O | 2.23 | 0.49 |
| 16:CP:28:ARG:HG3 | 16:CP:29:ASP:N | 2.28 | 0.49 |
| 25:DA:2740:A:C6 | 25:DA:2741:A:C6 | 3.01 | 0.49 |
| 25:DA:321:G:OP2 | 29:DF:135:LYS:HG3 | 2.12 | 0.49 |
| 25:DA:1815:A:P | 27:DD:54:ARG:HH22 | 2.36 | 0.49 |
| 35:DP:38:GLN:HG2 | 35:DP:45:LEU:H | 1.78 | 0.49 |
| 38:DS:15:ARG:O | 38:DS:19:LYS:HG2 | 2.12 | 0.49 |
| 1:AA:1015:A:H8 | 1:AA:1015:A:O5' | 1.96 | 0.48 |
| 1:AA:1145:C:H5'' | 1:AA:1146:A:OP1 | 2.13 | 0.48 |
| 1:AA:1438:G:H2' | 1:AA:1439:C:H6 | 1.77 | 0.48 |
| 1:AA:435:C:H2' | 1:AA:436:C:H6 | 1.77 | 0.48 |
| 1:AA:438:G:OP1 | 4:AD:125:HIS:NE2 | 2.33 | 0.48 |
| 20:AT:9:ASN:ND2 | 20:AT:10:LEU:H | 2.11 | 0.48 |
| 25:BA:1525:G:O2' | 25:BA:1605:A:N1 | 2.43 | 0.48 |
| 25:BA:1615:G:OP2 | 27:BD:63:ARG:NH2 | 2.45 | 0.48 |
| 34:BO:7:TYR:CE1 | 34:BO:20:MET:HB2 | 2.48 | 0.48 |
| 1:CA:1006:C:C4 | 1:CA:1007:C:C5 | 3.01 | 0.48 |
| 1:CA:1051:C:H2' | 1:CA:1052:U:C6 | 2.48 | 0.48 |
| 1:CA:199:G:O2' | 1:CA:200:G:H5' | 2.12 | 0.48 |
| 1:CA:831:U:H3 | 1:CA:855:G:H1 | 1.60 | 0.48 |
| 7:CG:133:GLY:O | 7:CG:137:LYS:N | 2.45 | 0.48 |
| 7:CG:22:LEU:HD13 | 7:CG:97:GLN:OE1 | 2.13 | 0.48 |
| 8:CH:83:ILE:HB | 8:CH:137:VAL:HG13 | 1.95 | 0.48 |
| 12:CL:123:LYS:H | 12:CL:123:LYS:HG2 | 1.37 | 0.48 |
| 54:D8:62:LEU:HB3 | 54:D8:65:GLU:HG2 | 1.94 | 0.48 |
| 54:D8:6:THR:HG22 | 54:D8:63:PRO:HD2 | 1.94 | 0.48 |
| 25:DA:2031:A:N3 | 25:DA:2455:G:O2' | 2.41 | 0.48 |
| 25:DA:2505:G:O6 | 25:DA:2576:G:H2' | 2.13 | 0.48 |
| 25:DA:409:C:O2' | 25:DA:410:G:H5' | 2.12 | 0.48 |
| 25:DA:792:G:OP2 | 61:DA:3818:HOH:O | 2.20 | 0.48 |
| 28:DE:178:GLU:OE2 | 28:DE:178:GLU:N | 2.36 | 0.48 |
| 31:DH:86:GLU:OE1 | 31:DH:130:ARG:HD3 | 2.13 | 0.48 |
| 36:DQ:65:PHE:HB2 | 36:DQ:105:GLU:HB2 | 1.93 | 0.48 |
| 44:DY:49:VAL:HG21 | 44:DY:61:ILE:HG23 | 1.94 | 0.48 |
| 1:AA:1353:G:OP1 | 21:AU:10:ARG:NH1 | 2.45 | 0.48 |
| 1:AA:1513:A:H2' | 1:AA:1514:C:C6 | 2.48 | 0.48 |
| 1:AA:236:G:H2' | 1:AA:237:C:C6 | 2.47 | 0.48 |
| 1:AA:293:G:C6 | 1:AA:294:U:C4 | 3.01 | 0.48 |
| 1:AA:62:U:O2' | 1:AA:379:C:H1' | 2.14 | 0.48 |
| 8:AH:13:ILE:O | 8:AH:17:THR:HG23 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:AJ:5:ARG:HH21 | 10:AJ:73:ASP:CG | 2.17 | 0.48 |
| 25:BA:2444:A:C8 | 47:B1:33:LYS:HD2 | 2.48 | 0.48 |
| 25:BA:1285:G:H2' | 25:BA:1286:U:O4' | 2.13 | 0.48 |
| 25:BA:1314:A:H2' | 25:BA:1315:A:O4' | 2.13 | 0.48 |
| 25:BA:1817:A:H1' | 25:BA:1960:A:N6 | 2.28 | 0.48 |
| 25:BA:839:G:H5'' | 25:BA:840:A:H5' | 1.95 | 0.48 |
| 25:BA:870:G:C6 | 25:BA:882:A:N1 | 2.80 | 0.48 |
| 1:CA:1036:G:H3' | 1:CA:1037:C:O4' | 2.14 | 0.48 |
| 1:CA:730:G:C5 | 1:CA:731:G:H1' | 2.47 | 0.48 |
| 1:CA:736:C:H2' | 1:CA:737:A:C8 | 2.47 | 0.48 |
| 2:CB:105:PHE:CD2 | 2:CB:158:LEU:HG | 2.48 | 0.48 |
| 4:CD:63:LYS:HG3 | 4:CD:198:VAL:HG22 | 1.95 | 0.48 |
| 7:CG:111:ARG:HB3 | 7:CG:113:GLU:OE2 | 2.12 | 0.48 |
| 25:DA:116:C:H2' | 25:DA:117:G:O4' | 2.12 | 0.48 |
| 25:DA:2261:C:O2' | 25:DA:2262:U:H5' | 2.13 | 0.48 |
| 25:DA:2360:A:H2' | 25:DA:2361:A:O4' | 2.13 | 0.48 |
| 25:DA:2391:G:O2' | 25:DA:2422:A:N7 | 2.46 | 0.48 |
| 25:DA:2711:A:OP2 | 61:DA:3973:HOH:O | 2.20 | 0.48 |
| 29:DF:167:ALA:HB1 | 29:DF:173:VAL:HG11 | 1.95 | 0.48 |
| 25:DA:322:A:OP2 | 29:DF:169:ASN:HB2 | 2.13 | 0.48 |
| 31:DH:94:TYR:CE2 | 31:DH:160:LYS:HG2 | 2.48 | 0.48 |
| 32:DI:75:LEU:HD11 | 32:DI:105:HIS:CD2 | 2.47 | 0.48 |
| 37:DR:103:ARG:NH1 | 37:DR:110:PRO:HD3 | 2.28 | 0.48 |
| 1:AA:1051:C:H2' | 1:AA:1052:U:H6 | 1.79 | 0.48 |
| 1:AA:1052:U:H5'' | 1:AA:1053:G:OP2 | 2.13 | 0.48 |
| 1:AA:430:A:OP2 | 4:AD:8:VAL:HG12 | 2.13 | 0.48 |
| 1:AA:437:U:O3' | 4:AD:125:HIS:HE1 | 1.96 | 0.48 |
| 3:AC:52:LEU:HA | 3:AC:70:VAL:HG22 | 1.95 | 0.48 |
| 20:AT:56:MET:HG3 | 20:AT:84:LEU:HD22 | 1.95 | 0.48 |
| 20:AT:9:ASN:HD22 | 20:AT:10:LEU:H | 1.61 | 0.48 |
| 1:AA:1340:A:O2' | 23:AX:31:G:O3' | 2.31 | 0.48 |
| 48:B2:32:LEU:HD23 | 48:B2:53:LEU:HB3 | 1.95 | 0.48 |
| 50:B4:46:GLN:HG2 | 50:B4:48:ARG:HG2 | 1.95 | 0.48 |
| 25:BA:794:U:O2 | 25:BA:2036:A:H1' | 2.13 | 0.48 |
| 25:BA:347:G:C8 | 29:BF:171:PRO:HG3 | 2.48 | 0.48 |
| 25:BA:70:A:H3' | 25:BA:70:A:OP2 | 2.13 | 0.48 |
| 27:BD:72:LYS:HE3 | 27:BD:75:ILE:HD12 | 1.95 | 0.48 |
| 36:BQ:55:VAL:HG12 | 36:BQ:64:ILE:HD12 | 1.96 | 0.48 |
| 44:BY:53:PRO:HA | 44:BY:56:PRO:HD3 | 1.94 | 0.48 |
| 1:CA:1014:A:H2' | 1:CA:1015:A:C8 | 2.49 | 0.48 |
| 1:CA:1038:C:O2' | 1:CA:1039:C:H5' | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1095:U:OP1 | 1:CA:1108:G:N2 | 2.36 | 0.48 |
| 1:CA:1288:A:H2' | 1:CA:1289:A:C8 | 2.49 | 0.48 |
| 1:CA:129(A):G:C6 | 1:CA:189(E):U:H4' | 2.48 | 0.48 |
| 1:CA:460:G:H1' | 1:CA:472:A:H61 | 1.77 | 0.48 |
| 1:CA:48:C:OP2 | 61:CA:4095:HOH:O | 2.20 | 0.48 |
| 1:CA:5:U:H5' | 1:CA:6:G:C5 | 2.48 | 0.48 |
| 13:CM:37:THR:HG21 | 13:CM:56:LEU:HA | 1.94 | 0.48 |
| 25:DA:1916:A:H2' | 25:DA:1917:U:O4' | 2.12 | 0.48 |
| 25:DA:2025:C:H2' | 25:DA:2026:C:C6 | 2.49 | 0.48 |
| 25:DA:328:U:H4' | 44:DY:68:HIS:CD2 | 2.49 | 0.48 |
| 36:DQ:27:VAL:HG11 | 36:DQ:134:ARG:HG3 | 1.95 | 0.48 |
| 38:DS:87:PHE:CZ | 38:DS:102:ALA:HB2 | 2.48 | 0.48 |
| 40:DU:113:ALA:O | 40:DU:117:GLN:HG2 | 2.13 | 0.48 |
| 1:AA:1530:G:H4' | 1:AA:1530:G:OP1 | 2.13 | 0.48 |
| 1:AA:384:G:C2 | 1:AA:385:C:C4 | 3.02 | 0.48 |
| 2:AB:12:GLU:O | 2:AB:15:VAL:HG13 | 2.14 | 0.48 |
| 2:AB:15:VAL:HG11 | 2:AB:213:LEU:HD12 | 1.95 | 0.48 |
| 2:AB:77:ALA:HB2 | 2:AB:211:ILE:HD13 | 1.95 | 0.48 |
| 2:AB:77:ALA:O | 2:AB:81:VAL:HG22 | 2.13 | 0.48 |
| 4:AD:175:SER:OG | 4:AD:184:LYS:HB2 | 2.13 | 0.48 |
| 7:AG:72:ARG:HG3 | 7:AG:142:GLU:OE2 | 2.12 | 0.48 |
| 25:BA:1845:G:H4' | 27:BD:51:VAL:HG21 | 1.96 | 0.48 |
| 25:BA:2601:A:N3 | 61:BA:3847:HOH:O | 2.35 | 0.48 |
| 25:BA:2623:U:H6 | 25:BA:2623:U:H5' | 1.79 | 0.48 |
| 25:BA:596:G:O2' | 25:BA:597:C:H3' | 2.13 | 0.48 |
| 28:BE:179:GLU:HB3 | 28:BE:181:LEU:HD22 | 1.95 | 0.48 |
| 33:BN:28:THR:HG22 | 33:BN:29:LYS:N | 2.29 | 0.48 |
| 36:BQ:54:MET:HG3 | 36:BQ:117:ALA:HB1 | 1.95 | 0.48 |
| 1:CA:1005:A:H8 | 1:CA:1005:A:O5' | 1.96 | 0.48 |
| 1:CA:1007:C:N4 | 1:CA:1022:G:C6 | 2.81 | 0.48 |
| 1:CA:1040:U:C4 | 1:CA:1041:A:C8 | 3.01 | 0.48 |
| 1:CA:1226:C:H4' | 19:CS:80:TYR:CZ | 2.49 | 0.48 |
| 1:CA:1446:U:O2' | 1:CA:1447:A:O5' | 2.31 | 0.48 |
| 1:CA:216:G:H2' | 1:CA:217:C:C6 | 2.49 | 0.48 |
| 1:CA:255:G:OP1 | 17:CQ:69:LYS:NZ | 2.35 | 0.48 |
| 2:CB:127:ILE:HG12 | 2:CB:128:GLU:H | 1.78 | 0.48 |
| 2:CB:71:VAL:HG23 | 2:CB:164:VAL:HA | 1.95 | 0.48 |
| 2:CB:97:TRP:CH2 | 2:CB:173:ALA:HA | 2.49 | 0.48 |
| 6:CF:24:GLU:HG3 | 6:CF:28:ARG:HD3 | 1.95 | 0.48 |
| 16:CP:43:LYS:HA | 16:CP:48:TRP:HB3 | 1.96 | 0.48 |
| 1:CA:986:A:O2' | 19:CS:55:LYS:O | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:1449:A:H5' | 25:DA:1450:G:OP2 | 2.14 | 0.48 |
| 25:DA:1520:G:H3' | 25:DA:1523:U:H6 | 1.78 | 0.48 |
| 25:DA:2001:A:H2' | 25:DA:2002:G:C8 | 2.49 | 0.48 |
| 25:DA:2293:C:OP1 | 25:DA:2377:A:N6 | 2.46 | 0.48 |
| 25:DA:2872:G:C2 | 25:DA:2873:A:N6 | 2.82 | 0.48 |
| 25:DA:330:A:HO2' | 25:DA:331:A:H8 | 1.61 | 0.48 |
| 25:DA:784:A:OP2 | 61:DA:4063:HOH:O | 2.20 | 0.48 |
| 27:DD:242:ARG:N | 27:DD:242:ARG:HD3 | 2.28 | 0.48 |
| 27:DD:58:HIS:HD1 | 27:DD:59:LYS:N | 2.11 | 0.48 |
| 25:DA:614(C):A:N3 | 29:DF:180:GLY:HA2 | 2.29 | 0.48 |
| 30:DG:136:ARG:HD2 | 30:DG:137:GLU:N | 2.28 | 0.48 |
| 31:DH:113:VAL:HG11 | 31:DH:151:ILE:HD13 | 1.94 | 0.48 |
| 32:DI:29:TYR:O | 32:DI:33:ARG:HD2 | 2.14 | 0.48 |
| 1:AA:1131:G:O5' | 1:AA:1131:G:H8 | 1.96 | 0.48 |
| 1:AA:1182:G:C4' | 1:AA:1183:A:H5' | 2.43 | 0.48 |
| 1:AA:1327:C:H2' | 1:AA:1328:C:C6 | 2.48 | 0.48 |
| 1:AA:620:C:H2' | 1:AA:621:A:O4' | 2.14 | 0.48 |
| 1:AA:926:G:C6 | 1:AA:1505:G:C6 | 3.02 | 0.48 |
| 23:AX:19:G:H4' | 23:AX:20:U:OP2 | 2.12 | 0.48 |
| 52:B6:21:TYR:CE2 | 52:B6:38:LYS:HG2 | 2.48 | 0.48 |
| 25:BA:2303:U:O2' | 25:BA:2386:C:O2 | 2.24 | 0.48 |
| 27:BD:68:LYS:HD2 | 27:BD:70:TRP:CH2 | 2.48 | 0.48 |
| 30:BG:56:ALA:HA | 30:BG:153:ARG:NH2 | 2.29 | 0.48 |
| 31:BH:56:SER:OG | 31:BH:58:GLU:HG2 | 2.13 | 0.48 |
| 25:BA:956:A:C5 | 36:BQ:13:GLN:HG3 | 2.49 | 0.48 |
| 34:BO:101:PRO:HG3 | 39:BT:67:SER:OG | 2.13 | 0.48 |
| 1:CA:1003:G:C6 | 1:CA:1004:A:C2 | 3.02 | 0.48 |
| 1:CA:520:A:N1 | 1:CA:536:C:H1' | 2.29 | 0.48 |
| 1:CA:554:C:H2' | 1:CA:555:C:H6 | 1.77 | 0.48 |
| 1:CA:839:U:H5'' | 1:CA:840:C:C5 | 2.48 | 0.48 |
| 2:CB:16:HIS:CG | 2:CB:17:PHE:N | 2.81 | 0.48 |
| 3:CC:34:LEU:HG | 3:CC:38:ARG:HH12 | 1.78 | 0.48 |
| 6:CF:68:PRO:HB2 | 6:CF:71:ARG:HG3 | 1.95 | 0.48 |
| 11:CK:19:ALA:HA | 11:CK:32:ILE:HD13 | 1.96 | 0.48 |
| 11:CK:33:THR:HA | 11:CK:39:PRO:HA | 1.95 | 0.48 |
| 25:DA:2680:C:H5' | 28:DE:189:PRO:HA | 1.96 | 0.48 |
| 25:DA:428:A:H3' | 25:DA:429:A:C8 | 2.48 | 0.48 |
| 25:DA:507:A:H5'' | 25:DA:508:G:H3' | 1.95 | 0.48 |
| 25:DA:934:G:H2' | 25:DA:935:C:H6 | 1.79 | 0.48 |
| 30:DG:41:GLN:NE2 | 30:DG:154:GLY:O | 2.46 | 0.48 |
| 31:DH:26:VAL:HG12 | 31:DH:79:VAL:HG11 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:DO:98:VAL:HG22 | 34:DO:118:ALA:HA | 1.95 | 0.48 |
| 41:DV:30:GLY:H | 41:DV:61:VAL:HG13 | 1.79 | 0.48 |
| 1:AA:1298:C:H2' | 7:AG:114:ARG:NH1 | 2.28 | 0.48 |
| 2:AB:168:THR:OG1 | 2:AB:192:SER:HB3 | 2.13 | 0.48 |
| 2:AB:19:HIS:NE2 | 2:AB:206:ASP:OD2 | 2.46 | 0.48 |
| 7:AG:152:ALA:HB1 | 7:AG:155:ARG:NH2 | 2.28 | 0.48 |
| 10:AJ:57:LYS:HD2 | 10:AJ:60:ARG:HH21 | 1.79 | 0.48 |
| 10:AJ:5:ARG:HD3 | 10:AJ:71:LEU:HD11 | 1.95 | 0.48 |
| 13:AM:15:VAL:O | 13:AM:19:LEU:HD22 | 2.13 | 0.48 |
| 19:AS:3:ARG:NH1 | 19:AS:10:PHE:HB2 | 2.27 | 0.48 |
| 48:B2:32:LEU:HD12 | 48:B2:36:ARG:NH1 | 2.29 | 0.48 |
| 25:BA:1537:G:O2' | 27:BD:101:GLU:HB2 | 2.14 | 0.48 |
| 25:BA:2343:G:O2' | 25:BA:2348:A:N1 | 2.35 | 0.48 |
| 30:BG:102:PHE:HE1 | 30:BG:141:PHE:CE2 | 2.26 | 0.48 |
| 1:CA:1002:G:H1 | 1:CA:1038:C:H42 | 0.67 | 0.48 |
| 1:CA:1169:A:H8 | 1:CA:1169:A:H3' | 1.79 | 0.48 |
| 1:CA:1015:A:H1' | 1:CA:1219:U:H5' | 1.95 | 0.48 |
| 1:CA:1288:A:N1 | 1:CA:1371:G:H1' | 2.29 | 0.48 |
| 1:CA:270:A:H2' | 1:CA:271:C:C6 | 2.48 | 0.48 |
| 1:CA:585:G:N3 | 1:CA:879:C:H4' | 2.29 | 0.48 |
| 2:CB:73:THR:HB | 2:CB:95:GLN:O | 2.14 | 0.48 |
| 7:CG:78:ARG:HH21 | 7:CG:156:TRP:HB3 | 1.78 | 0.48 |
| 8:CH:49:GLU:HG2 | 8:CH:62:TYR:CE2 | 2.45 | 0.48 |
| 9:CI:31:GLN:HB2 | 9:CI:35:GLU:OE2 | 2.13 | 0.48 |
| 10:CJ:42:THR:CG2 | 10:CJ:68:HIS:HD2 | 2.25 | 0.48 |
| 12:CL:34:ARG:HG2 | 12:CL:35:GLY:N | 2.29 | 0.48 |
| 10:CJ:47:PHE:CZ | 14:CN:37:PHE:HE1 | 2.32 | 0.48 |
| 30:DG:101:ILE:HD13 | 50:D4:25:TYR:HB2 | 1.94 | 0.48 |
| 25:DA:1163:G:C2 | 25:DA:1164:G:C8 | 3.01 | 0.48 |
| 25:DA:1666:G:OP1 | 34:DO:66:LYS:HE3 | 2.14 | 0.48 |
| 25:DA:180:G:H5'' | 25:DA:181:A:OP2 | 2.13 | 0.48 |
| 25:DA:784:A:C8 | 25:DA:792:G:C5 | 3.01 | 0.48 |
| 31:DH:24:VAL:HG13 | 31:DH:37:VAL:HG21 | 1.96 | 0.48 |
| 34:DO:120:GLU:HG2 | 34:DO:122:LEU:HG | 1.95 | 0.48 |
| 38:DS:27:SER:HA | 38:DS:88:ASP:HB3 | 1.95 | 0.48 |
| 42:DW:70:TYR:OH | 42:DW:72:LYS:HG3 | 2.14 | 0.48 |
| 1:AA:154:C:H5 | 1:AA:155:C:C5 | 2.31 | 0.48 |
| 1:AA:364:A:H2' | 1:AA:365:U:H6 | 1.79 | 0.48 |
| 3:AC:135:LYS:HE2 | 5:AE:53:LEU:HD11 | 1.95 | 0.48 |
| 10:AJ:68:HIS:CD2 | 10:AJ:68:HIS:H | 2.31 | 0.48 |
| 46:B0:53:MET:HG3 | 46:B0:59:LEU:CD2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:1093:G:H2' | 25:BA:1156:G:N2 | 2.26 | 0.48 |
| 25:BA:1604:C:H5'' | 25:BA:1605:A:OP2 | 2.14 | 0.48 |
| 25:BA:1815:A:H5'' | 61:BA:4186:HOH:O | 2.13 | 0.48 |
| 25:BA:217:A:H2' | 25:BA:219:U:O4' | 2.13 | 0.48 |
| 32:BI:100:ALA:HA | 32:BI:103:ARG:HG2 | 1.94 | 0.48 |
| 25:BA:438:G:C5 | 35:BP:72:PRO:HB3 | 2.49 | 0.48 |
| 1:CA:1137:C:H1' | 1:CA:1138:G:C2 | 2.48 | 0.48 |
| 1:CA:1277:C:O2' | 1:CA:1279:A:H8 | 1.94 | 0.48 |
| 1:CA:1320:C:C1' | 19:CS:73:GLU:HG3 | 2.44 | 0.48 |
| 1:CA:1342:C:H1' | 9:CI:124:GLN:NE2 | 2.28 | 0.48 |
| 1:CA:422:C:H4' | 1:CA:423:G:C4 | 2.48 | 0.48 |
| 1:CA:758:G:H8 | 1:CA:758:G:H5'' | 1.78 | 0.48 |
| 1:CA:999:C:N4 | 1:CA:1042:G:C2 | 2.81 | 0.48 |
| 1:CA:999:C:N4 | 1:CA:1043:C:C4 | 2.81 | 0.48 |
| 25:DA:1041:C:OP1 | 45:DZ:46:LYS:NZ | 2.43 | 0.48 |
| 25:DA:2489:G:C6 | 25:DA:2490:G:C6 | 3.02 | 0.48 |
| 25:DA:78:A:H2' | 25:DA:79:G:H8 | 1.78 | 0.48 |
| 25:DA:2094:G:OP1 | 32:DI:22:LYS:HD2 | 2.14 | 0.48 |
| 26:DB:50:G:OP2 | 38:DS:62:LYS:HD3 | 2.13 | 0.48 |
| 41:DV:6:LYS:HB2 | 41:DV:38:LEU:HD21 | 1.94 | 0.48 |
| 1:AA:1206:G:C6 | 1:AA:1207:G:C5 | 3.01 | 0.48 |
| 3:AC:32:LEU:HD22 | 3:AC:59:ARG:HH12 | 1.79 | 0.48 |
| 16:AP:52:ASP:OD1 | 16:AP:54:GLU:HG3 | 2.14 | 0.48 |
| 13:AM:84:ILE:HD12 | 19:AS:74:PHE:HZ | 1.78 | 0.48 |
| 20:AT:10:LEU:HB3 | 20:AT:12:ALA:H | 1.79 | 0.48 |
| 25:BA:137:G:O2' | 25:BA:138:G:H5' | 2.14 | 0.48 |
| 25:BA:1576:G:O2' | 25:BA:1577:C:H5' | 2.14 | 0.48 |
| 25:BA:2814:C:H2' | 25:BA:2815:C:O4' | 2.14 | 0.48 |
| 25:BA:388:A:H2' | 25:BA:389:G:H8 | 1.77 | 0.48 |
| 25:BA:860:U:H2' | 25:BA:861:C:C6 | 2.48 | 0.48 |
| 27:BD:9:TYR:CZ | 27:BD:13:ARG:HG2 | 2.49 | 0.48 |
| 1:CA:1148:U:H2' | 1:CA:1149:C:O4' | 2.13 | 0.48 |
| 1:CA:1492:A:H2' | 1:CA:1493:A:C1' | 2.43 | 0.48 |
| 1:CA:364:A:H2' | 1:CA:365:U:H6 | 1.79 | 0.48 |
| 1:CA:418:C:H2' | 1:CA:419:C:C6 | 2.48 | 0.48 |
| 1:CA:797:C:O2' | 1:CA:798:G:H5' | 2.13 | 0.48 |
| 4:CD:15:GLU:OE2 | 4:CD:66:ARG:NH1 | 2.46 | 0.48 |
| 10:CJ:8:LEU:CD2 | 10:CJ:96:ILE:HG23 | 2.43 | 0.48 |
| 14:CN:7:ILE:HG12 | 14:CN:8:GLU:N | 2.27 | 0.48 |
| 16:CP:51:VAL:O | 16:CP:53:VAL:HG23 | 2.14 | 0.48 |
| 48:D2:10:LEU:HD22 | 48:D2:14:ARG:NH1 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:1256:G:H5' | 25:DA:1257:C:OP2 | 2.13 | 0.48 |
| 25:DA:1287:A:H5'' | 25:DA:1288:U:OP2 | 2.13 | 0.48 |
| 27:DD:132:PRO:HG2 | 27:DD:135:PHE:CD2 | 2.44 | 0.48 |
| 31:DH:20:ALA:HB3 | 31:DH:23:ARG:HG3 | 1.95 | 0.48 |
| 1:AA:300:A:H2' | 1:AA:301:G:O4' | 2.13 | 0.48 |
| 1:AA:300:A:O2' | 1:AA:564:C:N3 | 2.36 | 0.48 |
| 1:AA:658:G:H2' | 1:AA:659:U:C6 | 2.48 | 0.48 |
| 1:AA:662:G:H2' | 1:AA:663:A:C8 | 2.48 | 0.48 |
| 1:AA:430:A:OP1 | 4:AD:9:CYS:HB2 | 2.13 | 0.48 |
| 1:AA:1286:A:H2 | 21:AU:18:TYR:HH | 1.60 | 0.48 |
| 25:BA:1093:G:HO2' | 25:BA:1094:A:H8 | 1.61 | 0.48 |
| 25:BA:1362:U:H2' | 25:BA:1363:A:C8 | 2.49 | 0.48 |
| 25:BA:905:U:O2 | 25:BA:2280:A:H2' | 2.14 | 0.48 |
| 30:BG:50:ALA:O | 30:BG:52:ILE:N | 2.47 | 0.48 |
| 26:BB:8:U:O3' | 38:BS:25:ARG:NH2 | 2.47 | 0.48 |
| 40:BU:16:LYS:HE2 | 40:BU:16:LYS:HB3 | 1.55 | 0.48 |
| 45:BZ:152:ALA:HA | 45:BZ:155:LEU:HD22 | 1.94 | 0.48 |
| 45:BZ:30:ASN:ND2 | 45:BZ:90:VAL:HB | 2.28 | 0.48 |
| 1:CA:1151:A:O4' | 10:CJ:39:PRO:HB2 | 2.14 | 0.48 |
| 1:CA:1321:C:H5'' | 1:CA:1322:C:H2' | 1.95 | 0.48 |
| 1:CA:1333:A:H2' | 1:CA:1334:G:O4' | 2.13 | 0.48 |
| 1:CA:790:A:H2' | 1:CA:791:G:C8 | 2.49 | 0.48 |
| 6:CF:61:LEU:HD23 | 6:CF:63:TYR:OH | 2.13 | 0.48 |
| 1:CA:192:U:O2' | 20:CT:60:GLU:OE2 | 2.25 | 0.48 |
| 46:D0:27:GLU:HB2 | 46:D0:69:PHE:HD1 | 1.78 | 0.48 |
| 25:DA:1022:G:C6 | 25:DA:1140:C:C4 | 3.01 | 0.48 |
| 25:DA:1794:U:H2' | 25:DA:1795:C:C6 | 2.49 | 0.48 |
| 25:DA:2261:C:H1' | 25:DA:2388:A:N3 | 2.29 | 0.48 |
| 25:DA:2823:A:OP1 | 28:DE:159:HIS:NE2 | 2.42 | 0.48 |
| 25:DA:892:G:H2' | 25:DA:893:C:O4' | 2.14 | 0.48 |
| 34:DO:73:ASP:HB2 | 39:DT:82:LEU:HD13 | 1.96 | 0.48 |
| 34:DO:64:ARG:NH1 | 34:DO:81:ASP:OD1 | 2.47 | 0.48 |
| 45:DZ:19:ARG:HE | 45:DZ:19:ARG:HB2 | 1.44 | 0.48 |
| 1:AA:1028:C:H2' | 1:AA:1029:C:O4' | 2.14 | 0.48 |
| 1:AA:1234:C:C2' | 1:AA:1235:U:H5' | 2.44 | 0.48 |
| 1:AA:1237:C:HO2' | 1:AA:1300:G:H1 | 1.62 | 0.48 |
| 1:AA:376:G:H2' | 1:AA:377:G:H8 | 1.79 | 0.48 |
| 3:AC:113:ALA:HB3 | 3:AC:114:PRO:HD3 | 1.96 | 0.48 |
| 25:BA:1067:A:H3' | 25:BA:1067:A:H8 | 1.79 | 0.48 |
| 25:BA:484:G:C8 | 53:B7:37:LYS:HG2 | 2.49 | 0.48 |
| 26:BB:37:C:C5 | 26:BB:38:C:C5 | 3.02 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BW:86:LEU:HD12 | 42:BW:87:PRO:HD2 | 1.96 | 0.48 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:C8 | 2.49 | 0.48 |
| 2:CB:8:LYS:HD2 | 2:CB:51:LEU:HD13 | 1.96 | 0.48 |
| 6:CF:10:LEU:HD12 | 6:CF:85:VAL:HA | 1.94 | 0.48 |
| 17:CQ:62:SER:OG | 17:CQ:72:ARG:HD3 | 2.13 | 0.48 |
| 47:D1:64:ALA:HA | 47:D1:67:ILE:HG13 | 1.96 | 0.48 |
| 25:DA:1463:C:H2' | 25:DA:1464:C:H6 | 1.78 | 0.48 |
| 25:DA:271(F):C:H2' | 25:DA:271(G):C:H6 | 1.78 | 0.48 |
| 25:DA:729:G:OP2 | 27:DD:13:ARG:NH1 | 2.45 | 0.48 |
| 28:DE:127:ASP:OD2 | 61:DE:408:HOH:O | 2.19 | 0.48 |
| 29:DF:164:ARG:O | 29:DF:168:ARG:HB2 | 2.14 | 0.48 |
| 30:DG:11:TYR:O | 30:DG:16:ARG:HG2 | 2.13 | 0.48 |
| 32:DI:110:ASP:H | 32:DI:130:TYR:HH | 1.55 | 0.48 |
| 38:DS:53:SER:OG | 38:DS:54:LEU:N | 2.47 | 0.48 |
| 1:AA:1030(A):G:H2' | 1:AA:1030(C):G:OP2 | 2.13 | 0.47 |
| 1:AA:606:G:H1' | 1:AA:632:A:H61 | 1.79 | 0.47 |
| 4:AD:12:CYS:SG | 4:AD:19:LEU:N | 2.77 | 0.47 |
| 4:AD:155:LEU:HD22 | 4:AD:156:GLU:N | 2.29 | 0.47 |
| 9:AI:99:LEU:HB3 | 9:AI:101:PHE:HE1 | 1.79 | 0.47 |
| 48:B2:32:LEU:CD1 | 48:B2:36:ARG:HH11 | 2.26 | 0.47 |
| 25:BA:1220:U:OP1 | 25:BA:1222:A:N6 | 2.47 | 0.47 |
| 25:BA:2087:C:H2' | 25:BA:2088:C:C6 | 2.49 | 0.47 |
| 25:BA:2303:U:H2' | 25:BA:2304:C:C6 | 2.49 | 0.47 |
| 25:BA:671:A:H2' | 25:BA:672:G:O4' | 2.14 | 0.47 |
| 25:BA:777:C:OP2 | 61:BA:4592:HOH:O | 2.20 | 0.47 |
| 25:BA:1925:G:OP1 | 27:BD:241:PRO:HB2 | 2.14 | 0.47 |
| 1:CA:1206:G:C6 | 1:CA:1207:G:C5 | 3.03 | 0.47 |
| 1:CA:1262:C:H42 | 1:CA:1273:G:H1 | 1.61 | 0.47 |
| 1:CA:1358:U:OP2 | 1:CA:1359:C:H5 | 1.97 | 0.47 |
| 1:CA:785:G:H2' | 1:CA:786:G:H5' | 1.96 | 0.47 |
| 2:CB:48:MET:HA | 2:CB:51:LEU:HD12 | 1.96 | 0.47 |
| 6:CF:44:GLY:HA2 | 6:CF:59:TYR:CZ | 2.48 | 0.47 |
| 1:CA:671:G:H5' | 6:CF:77:ARG:HH22 | 1.79 | 0.47 |
| 19:CS:27:GLU:HB2 | 19:CS:28:LYS:HE2 | 1.95 | 0.47 |
| 25:DA:1593:G:C2 | 25:DA:1594:G:C4 | 3.02 | 0.47 |
| 25:DA:688:U:H5' | 25:DA:1780:A:C2 | 2.49 | 0.47 |
| 25:DA:253:C:O2' | 61:DA:4187:HOH:O | 2.16 | 0.47 |
| 25:DA:867:C:O2 | 25:DA:913:U:H5' | 2.14 | 0.47 |
| 27:DD:72:LYS:HB3 | 27:DD:75:ILE:HD12 | 1.96 | 0.47 |
| 29:DF:126:VAL:HG21 | 29:DF:129:PHE:CZ | 2.49 | 0.47 |
| 29:DF:53:THR:HG22 | 29:DF:56:GLU:HG3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:910:A:C5 | 36:DQ:13:GLN:HG3 | 2.49 | 0.47 |
| 1:AA:49:U:H3 | 1:AA:362:G:H1' | 1.80 | 0.47 |
| 5:AE:72:GLN:O | 5:AE:75:THR:HG22 | 2.14 | 0.47 |
| 6:AF:44:GLY:HA2 | 6:AF:59:TYR:CE2 | 2.49 | 0.47 |
| 8:AH:96:GLY:H | 8:AH:99:GLU:CD | 2.18 | 0.47 |
| 25:BA:1086:C:H2' | 25:BA:1087:C:O4' | 2.14 | 0.47 |
| 25:BA:1091:A:OP1 | 25:BA:1092:A:H3' | 2.13 | 0.47 |
| 25:BA:1686:U:O2' | 25:BA:1687:C:H5' | 2.14 | 0.47 |
| 25:BA:904:C:H4' | 46:B0:23:VAL:HG21 | 1.96 | 0.47 |
| 28:BE:92:THR:O | 28:BE:95:ILE:HG23 | 2.14 | 0.47 |
| 1:CA:109:A:H2' | 1:CA:326:G:N2 | 2.28 | 0.47 |
| 1:CA:543:C:O2' | 1:CA:544:G:H5' | 2.14 | 0.47 |
| 4:CD:36:ARG:HG3 | 4:CD:38:TYR:CE2 | 2.49 | 0.47 |
| 20:CT:50:GLU:HB2 | 20:CT:99:LEU:HD23 | 1.96 | 0.47 |
| 47:D1:83:GLU:HA | 47:D1:84:GLY:HA2 | 1.62 | 0.47 |
| 25:DA:1149:G:H2' | 25:DA:1150:C:C6 | 2.49 | 0.47 |
| 25:DA:1463:C:H2' | 25:DA:1464:C:C6 | 2.49 | 0.47 |
| 27:DD:275:LYS:HB3 | 27:DD:276:LYS:HA | 1.96 | 0.47 |
| 29:DF:7:TYR:O | 29:DF:22:ALA:N | 2.46 | 0.47 |
| 30:DG:103:LEU:HD22 | 30:DG:178:PHE:HZ | 1.80 | 0.47 |
| 31:DH:87:LEU:HD23 | 31:DH:164:TYR:HA | 1.96 | 0.47 |
| 1:AA:1127:G:H21 | 1:AA:1148:U:H3 | 1.61 | 0.47 |
| 1:AA:146:G:H5'' | 1:AA:146:G:H8 | 1.80 | 0.47 |
| 1:AA:129(A):G:C6 | 1:AA:189(E):U:H4' | 2.50 | 0.47 |
| 2:AB:24:TRP:HD1 | 2:AB:24:TRP:H | 1.62 | 0.47 |
| 14:AN:37:PHE:CE2 | 14:AN:53:LEU:HD13 | 2.50 | 0.47 |
| 19:AS:65:ASN:ND2 | 19:AS:66:MET:HG3 | 2.29 | 0.47 |
| 25:BA:1913:G:H2' | 25:BA:1914:C:H6 | 1.78 | 0.47 |
| 25:BA:2698:G:H5' | 61:BA:4643:HOH:O | 2.15 | 0.47 |
| 25:BA:1740:U:O2' | 27:BD:14:ARG:NH2 | 2.46 | 0.47 |
| 34:BO:64:ARG:NH1 | 34:BO:81:ASP:OD1 | 2.46 | 0.47 |
| 1:CA:1009:G:N2 | 1:CA:1010:G:H1' | 2.30 | 0.47 |
| 1:CA:1157:A:N7 | 1:CA:1180:A:C6 | 2.82 | 0.47 |
| 1:CA:457:C:H2' | 1:CA:458:C:C6 | 2.49 | 0.47 |
| 1:CA:577:G:C8 | 1:CA:816:A:C6 | 3.02 | 0.47 |
| 1:CA:932:C:H2' | 1:CA:933:G:C8 | 2.49 | 0.47 |
| 6:CF:2:ARG:NE | 6:CF:69:GLU:HG2 | 2.29 | 0.47 |
| 12:CL:79:GLU:HB3 | 12:CL:80:HIS:HD2 | 1.78 | 0.47 |
| 20:CT:46:GLU:HG2 | 20:CT:46:GLU:O | 2.13 | 0.47 |
| 25:DA:1027:A:C6 | 25:DA:1126:A:C4 | 3.02 | 0.47 |
| 25:DA:1637:A:H4' | 25:DA:2711:A:O2' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:1786:A:H1' | 25:DA:1938:A:N6 | 2.29 | 0.47 |
| 25:DA:1935:G:H1' | 25:DA:1964:G:N2 | 2.29 | 0.47 |
| 30:DG:114:ILE:HD12 | 30:DG:117:PHE:HD2 | 1.79 | 0.47 |
| 44:DY:9:LYS:HA | 44:DY:10:GLY:HA2 | 1.67 | 0.47 |
| 1:AA:1125:U:O4 | 1:AA:1128:C:C5 | 2.68 | 0.47 |
| 1:AA:430:A:H2' | 1:AA:431:A:O4' | 2.15 | 0.47 |
| 3:AC:123:GLN:HG2 | 3:AC:128:PHE:CD2 | 2.50 | 0.47 |
| 6:AF:99:ALA:O | 18:AR:28:GLU:HG3 | 2.14 | 0.47 |
| 8:AH:6:ILE:HB | 8:AH:85:ARG:NH1 | 2.29 | 0.47 |
| 10:AJ:5:ARG:O | 10:AJ:98:ILE:HA | 2.14 | 0.47 |
| 14:AN:4:LYS:HD3 | 14:AN:7:ILE:CG2 | 2.44 | 0.47 |
| 1:AA:277:C:H5'' | 17:AQ:68:ARG:NH2 | 2.30 | 0.47 |
| 25:BA:2538:G:H5' | 25:BA:2755:C:O2' | 2.13 | 0.47 |
| 25:BA:2643:G:N2 | 25:BA:2800:C:O2 | 2.40 | 0.47 |
| 25:BA:911:G:O2' | 25:BA:912:C:H5' | 2.14 | 0.47 |
| 25:BA:956:A:OP2 | 61:BA:4430:HOH:O | 2.20 | 0.47 |
| 27:BD:132:PRO:HA | 27:BD:190:TYR:HA | 1.96 | 0.47 |
| 28:BE:176:ILE:HB | 28:BE:181:LEU:HB2 | 1.96 | 0.47 |
| 29:BF:7:TYR:CD2 | 29:BF:24:LEU:HB2 | 2.49 | 0.47 |
| 32:BI:110:ASP:HA | 32:BI:111:PRO:HD2 | 1.72 | 0.47 |
| 25:BA:2116:G:OP1 | 32:BI:22:LYS:HD2 | 2.14 | 0.47 |
| 1:CA:1074:G:O2' | 1:CA:1101:A:N1 | 2.37 | 0.47 |
| 1:CA:341:C:H6 | 1:CA:341:C:O5' | 1.98 | 0.47 |
| 1:CA:554:C:H2' | 1:CA:555:C:C6 | 2.49 | 0.47 |
| 2:CB:163:PHE:HA | 2:CB:185:ILE:HG12 | 1.96 | 0.47 |
| 19:CS:30:LEU:CD1 | 19:CS:32:LYS:HG3 | 2.41 | 0.47 |
| 49:D3:3:ARG:HH11 | 49:D3:60:GLU:CB | 2.27 | 0.47 |
| 50:D4:15:ILE:HG23 | 50:D4:21:VAL:HG22 | 1.96 | 0.47 |
| 52:D6:38:LYS:NZ | 52:D6:38:LYS:HB2 | 2.29 | 0.47 |
| 25:DA:118:A:H1' | 25:DA:178:G:O4' | 2.14 | 0.47 |
| 25:DA:1523:U:C2 | 25:DA:1524:G:C8 | 3.01 | 0.47 |
| 25:DA:1528(A):A:C8 | 25:DA:1529:G:C8 | 3.03 | 0.47 |
| 25:DA:1932:A:H2' | 25:DA:1933:G:O4' | 2.14 | 0.47 |
| 25:DA:2303:G:H2' | 25:DA:2304:G:O4' | 2.14 | 0.47 |
| 25:DA:2319:G:C2 | 38:DS:3:ARG:HA | 2.49 | 0.47 |
| 28:DE:72:VAL:HA | 28:DE:73:GLU:CB | 2.43 | 0.47 |
| 29:DF:165:ARG:HG2 | 29:DF:168:ARG:HH21 | 1.79 | 0.47 |
| 31:DH:13:LYS:HA | 31:DH:14:GLY:HA2 | 1.61 | 0.47 |
| 45:DZ:153:SER:HB3 | 45:DZ:167:PRO:HB3 | 1.96 | 0.47 |
| 1:AA:1003:G:H2' | 1:AA:1004:A:H4' | 1.96 | 0.47 |
| 1:AA:1256:A:H5'' | 1:AA:1258:G:C1' | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:481:G:H1' | 1:AA:483:C:N4 | 2.30 | 0.47 |
| 1:AA:685:G:C2 | 1:AA:686:U:C4 | 3.02 | 0.47 |
| 5:AE:69:VAL:HG22 | 5:AE:71:LEU:HD23 | 1.96 | 0.47 |
| 9:AI:49:PRO:HG3 | 9:AI:101:PHE:HD2 | 1.79 | 0.47 |
| 9:AI:28:VAL:HA | 9:AI:63:ILE:HB | 1.97 | 0.47 |
| 25:BA:1828:C:H4' | 27:BD:257:LEU:O | 2.15 | 0.47 |
| 25:BA:2702:C:N4 | 25:BA:2726:A:H1' | 2.29 | 0.47 |
| 25:BA:2795:G:OP2 | 61:BA:4647:HOH:O | 2.20 | 0.47 |
| 25:BA:934:A:O2' | 25:BA:935:C:OP2 | 2.27 | 0.47 |
| 29:BF:195:ASP:HB3 | 29:BF:198:ALA:H | 1.78 | 0.47 |
| 29:BF:110:LEU:HD12 | 29:BF:205:ARG:HG2 | 1.96 | 0.47 |
| 29:BF:7:TYR:HD2 | 29:BF:24:LEU:HB2 | 1.78 | 0.47 |
| 25:BA:83:A:H5'' | 44:BY:8:LYS:HE3 | 1.97 | 0.47 |
| 1:CA:1133:G:N2 | 1:CA:1141:C:N3 | 2.59 | 0.47 |
| 1:CA:834:C:H2' | 1:CA:835:U:H6 | 1.77 | 0.47 |
| 1:CA:954:G:H21 | 1:CA:1227:A:N6 | 2.08 | 0.47 |
| 5:CE:83:GLU:HG2 | 5:CE:88:LYS:HG3 | 1.95 | 0.47 |
| 9:CI:6:GLY:HA3 | 9:CI:80:GLY:O | 2.14 | 0.47 |
| 1:CA:719:C:O2' | 18:CR:49:LYS:HB3 | 2.13 | 0.47 |
| 47:D1:3:LYS:H | 47:D1:61:ARG:HH12 | 1.62 | 0.47 |
| 25:DA:1291:C:H2' | 25:DA:1292:U:C6 | 2.49 | 0.47 |
| 25:DA:1513:C:H2' | 25:DA:1514:U:C6 | 2.49 | 0.47 |
| 25:DA:565:C:H2' | 25:DA:566:U:O4' | 2.15 | 0.47 |
| 25:DA:639:U:H2' | 25:DA:640:C:H6 | 1.79 | 0.47 |
| 25:DA:78:A:H2' | 25:DA:79:G:C8 | 2.49 | 0.47 |
| 25:DA:86:C:H4' | 25:DA:104:U:H1' | 1.96 | 0.47 |
| 28:DE:195:LEU:HG | 28:DE:196:VAL:N | 2.30 | 0.47 |
| 29:DF:160:ASN:HB3 | 29:DF:163:VAL:HB | 1.96 | 0.47 |
| 30:DG:106:LEU:HA | 30:DG:110:ALA:HB3 | 1.95 | 0.47 |
| 25:DA:1012:U:H5 | 33:DN:28:THR:HG21 | 1.79 | 0.47 |
| 35:DP:99:LEU:H | 35:DP:99:LEU:HD23 | 1.79 | 0.47 |
| 36:DQ:59:ARG:C | 36:DQ:61:GLY:H | 2.13 | 0.47 |
| 1:AA:1137:C:H5'' | 1:AA:1138:G:OP1 | 2.15 | 0.47 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.49 | 0.47 |
| 1:AA:567:G:H1' | 61:AA:4081:HOH:O | 2.13 | 0.47 |
| 1:AA:674:G:H2' | 1:AA:675:A:C8 | 2.49 | 0.47 |
| 2:AB:166:ASP:HA | 2:AB:167:PRO:HD3 | 1.73 | 0.47 |
| 2:AB:16:HIS:CB | 2:AB:204:ASN:HB3 | 2.29 | 0.47 |
| 5:AE:33:VAL:HG21 | 5:AE:109:ILE:HA | 1.96 | 0.47 |
| 5:AE:8:GLU:OE1 | 5:AE:63:ARG:NH2 | 2.48 | 0.47 |
| 16:AP:38:TYR:O | 16:AP:49:LEU:HD12 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:AF:97:PHE:HD2 | 18:AR:31:LEU:HD23 | 1.80 | 0.47 |
| 20:AT:58:LYS:O | 20:AT:62:LEU:HB2 | 2.14 | 0.47 |
| 30:BG:67:LYS:H | 50:B4:6:HIS:CE1 | 2.33 | 0.47 |
| 25:BA:12:U:O2 | 25:BA:12:U:H2' | 2.14 | 0.47 |
| 25:BA:1517:G:C6 | 25:BA:1567:G:N7 | 2.83 | 0.47 |
| 25:BA:1549:U:H2' | 25:BA:1550:C:H6 | 1.79 | 0.47 |
| 25:BA:2087:C:H2' | 25:BA:2088:C:H6 | 1.79 | 0.47 |
| 25:BA:2285:A:H2' | 25:BA:2286:A:C8 | 2.49 | 0.47 |
| 25:BA:2325:C:C2' | 25:BA:2326:C:H5' | 2.45 | 0.47 |
| 25:BA:2846:U:C4 | 25:BA:2893:A:N6 | 2.83 | 0.47 |
| 25:BA:1547:C:O4' | 27:BD:100:GLY:HA2 | 2.15 | 0.47 |
| 39:BT:91:ARG:HH11 | 39:BT:120:ARG:NH1 | 2.12 | 0.47 |
| 39:BT:37:GLY:HA2 | 39:BT:38:ASN:HA | 1.66 | 0.47 |
| 1:CA:1023:G:H3' | 1:CA:1024:G:H8 | 1.79 | 0.47 |
| 1:CA:1080:A:H5'' | 1:CA:1081:G:OP2 | 2.15 | 0.47 |
| 1:CA:1217:C:H2' | 1:CA:1218:C:O4' | 2.14 | 0.47 |
| 1:CA:1292:U:C2 | 1:CA:1293:G:C8 | 3.03 | 0.47 |
| 12:CL:119:LYS:O | 12:CL:120:TYR:HB2 | 2.15 | 0.47 |
| 13:CM:82:MET:CE | 13:CM:92:HIS:HB3 | 2.45 | 0.47 |
| 25:DA:1845:G:OP1 | 27:DD:258:LYS:NZ | 2.43 | 0.47 |
| 25:DA:2408:U:H2' | 25:DA:2409:G:C8 | 2.49 | 0.47 |
| 25:DA:735:A:C6 | 25:DA:736:C:C2 | 3.03 | 0.47 |
| 25:DA:900:A:H2' | 25:DA:901:A:O4' | 2.15 | 0.47 |
| 26:DB:43:C:C5 | 26:DB:45:A:N6 | 2.82 | 0.47 |
| 27:DD:71:ASP:OD2 | 27:DD:103:ARG:NH2 | 2.47 | 0.47 |
| 30:DG:103:LEU:HA | 30:DG:106:LEU:HB3 | 1.96 | 0.47 |
| 30:DG:64:THR:HB | 30:DG:94:LEU:HD11 | 1.96 | 0.47 |
| 36:DQ:32:TYR:CE1 | 36:DQ:133:ARG:HG3 | 2.49 | 0.47 |
| 41:DV:5:VAL:CG1 | 41:DV:57:VAL:HG21 | 2.44 | 0.47 |
| 1:AA:676:A:H2' | 1:AA:677:U:C6 | 2.50 | 0.47 |
| 5:AE:12:LEU:HD22 | 5:AE:13:ILE:N | 2.30 | 0.47 |
| 1:AA:1346:A:C8 | 7:AG:10:ARG:NH2 | 2.83 | 0.47 |
| 50:B4:14:ILE:HD12 | 50:B4:24:THR:HG21 | 1.96 | 0.47 |
| 25:BA:1223:C:H2' | 25:BA:1224:C:C6 | 2.49 | 0.47 |
| 25:BA:399:G:H8 | 47:B1:65:SER:O | 1.97 | 0.47 |
| 26:BB:29:A:C2 | 26:BB:30:C:C2 | 3.03 | 0.47 |
| 25:BA:572:A:H61 | 41:BV:18:LEU:HD23 | 1.80 | 0.47 |
| 45:BZ:144:LEU:HD11 | 45:BZ:150:LEU:HD22 | 1.95 | 0.47 |
| 45:BZ:70:LEU:HA | 45:BZ:70:LEU:HD23 | 1.58 | 0.47 |
| 1:CA:337:C:H2' | 1:CA:338:A:C8 | 2.50 | 0.47 |
| 1:CA:410:G:H5'' | 1:CA:411:A:OP1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:622:A:H3' | 1:CA:623:C:C6 | 2.49 | 0.47 |
| 3:CC:140:ARG:NH1 | 3:CC:140:ARG:HB2 | 2.29 | 0.47 |
| 8:CH:6:ILE:O | 8:CH:10:LEU:HG | 2.15 | 0.47 |
| 47:D1:25:LYS:HG3 | 47:D1:31:GLY:HA2 | 1.97 | 0.47 |
| 25:DA:1359:A:C2 | 25:DA:1372:U:O4 | 2.68 | 0.47 |
| 25:DA:2319:G:N2 | 38:DS:3:ARG:HA | 2.29 | 0.47 |
| 25:DA:2508:G:C2 | 25:DA:2582:G:C6 | 3.02 | 0.47 |
| 25:DA:2659:G:N2 | 25:DA:2661:G:H3' | 2.30 | 0.47 |
| 28:DE:143:ASN:HD22 | 28:DE:147:PRO:CD | 2.28 | 0.47 |
| 32:DI:3:VAL:HG12 | 32:DI:38:LEU:HA | 1.96 | 0.47 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:H6 | 1.80 | 0.47 |
| 4:AD:11:LEU:HD23 | 4:AD:66:ARG:HB3 | 1.96 | 0.47 |
| 5:AE:53:LEU:HD12 | 5:AE:53:LEU:H | 1.79 | 0.47 |
| 9:AI:9:ARG:HG2 | 9:AI:14:VAL:HG13 | 1.97 | 0.47 |
| 11:AK:44:SER:OG | 11:AK:47:VAL:HG23 | 2.14 | 0.47 |
| 1:AA:110:C:O2' | 16:AP:25:ARG:O | 2.32 | 0.47 |
| 17:AQ:10:VAL:HG13 | 17:AQ:19:VAL:HB | 1.97 | 0.47 |
| 35:BP:63:PRO:HB2 | 54:B8:30:ARG:NH2 | 2.30 | 0.47 |
| 25:BA:1577:C:H1' | 25:BA:1578:C:OP1 | 2.15 | 0.47 |
| 25:BA:2642:G:H2' | 25:BA:2643:G:H8 | 1.79 | 0.47 |
| 25:BA:908:A:H2' | 25:BA:909:G:O4' | 2.14 | 0.47 |
| 30:BG:11:TYR:CE2 | 30:BG:16:ARG:HD3 | 2.50 | 0.47 |
| 31:BH:86:GLU:OE1 | 31:BH:132:ARG:NH1 | 2.45 | 0.47 |
| 1:CA:1119:C:N3 | 1:CA:1154:G:O6 | 2.48 | 0.47 |
| 1:CA:1137:C:H5' | 1:CA:1138:G:OP1 | 2.15 | 0.47 |
| 1:CA:865:A:C2 | 1:CA:918:A:H4' | 2.50 | 0.47 |
| 1:CA:985:C:H2' | 1:CA:986:A:H8 | 1.80 | 0.47 |
| 2:CB:127:ILE:C | 2:CB:129:GLU:H | 2.16 | 0.47 |
| 6:CF:35:ALA:HA | 6:CF:67:MET:HB3 | 1.96 | 0.47 |
| 9:CI:7:THR:OG1 | 9:CI:83:ARG:NH1 | 2.48 | 0.47 |
| 10:CJ:25:GLU:O | 10:CJ:29:ARG:HD3 | 2.15 | 0.47 |
| 49:D3:6:VAL:HG13 | 49:D3:56:VAL:HG13 | 1.96 | 0.47 |
| 25:DA:1197:G:H5' | 25:DA:1227:G:O2' | 2.14 | 0.47 |
| 25:DA:153:C:OP2 | 47:D1:92:LYS:NZ | 2.46 | 0.47 |
| 1:AA:1251:A:H2' | 1:AA:1252:A:C8 | 2.49 | 0.47 |
| 1:AA:1392:G:C2' | 1:AA:1393:U:H5' | 2.45 | 0.47 |
| 2:AB:162:ILE:HD11 | 2:AB:184:VAL:HG22 | 1.95 | 0.47 |
| 3:AC:112:SER:O | 3:AC:116:VAL:HG23 | 2.14 | 0.47 |
| 47:B1:64:ALA:HA | 47:B1:67:ILE:HG13 | 1.97 | 0.47 |
| 25:BA:1496:A:H5' | 25:BA:1497:G:OP2 | 2.14 | 0.47 |
| 25:BA:1759:C:H2' | 25:BA:1760:U:O4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1833:A:N1 | 25:BA:1853:G:H1' | 2.30 | 0.47 |
| 25:BA:2299:A:H2 | 25:BA:2358:A:H62 | 1.60 | 0.47 |
| 25:BA:623:G:N2 | 25:BA:628:C:O3' | 2.47 | 0.47 |
| 27:BD:16:MET:HG3 | 27:BD:206:LEU:O | 2.15 | 0.47 |
| 25:BA:2584:A:N7 | 28:BE:144:ARG:HD2 | 2.30 | 0.47 |
| 38:BS:24:LEU:HA | 38:BS:24:LEU:HD23 | 1.70 | 0.47 |
| 1:CA:1209:C:O2' | 1:CA:1214:C:N4 | 2.30 | 0.47 |
| 1:CA:1226:C:H4' | 19:CS:80:TYR:OH | 2.14 | 0.47 |
| 1:CA:429:U:H1' | 1:CA:430:A:H5'' | 1.97 | 0.47 |
| 1:CA:441:A:H3' | 1:CA:442:C:H6 | 1.79 | 0.47 |
| 1:CA:452:A:O2' | 1:CA:453:A:OP2 | 2.29 | 0.47 |
| 25:DA:2364:C:OP1 | 46:D0:55:ARG:NH1 | 2.48 | 0.47 |
| 25:DA:2078:C:C4 | 25:DA:2079:U:C4 | 3.02 | 0.47 |
| 25:DA:2315:G:H2' | 25:DA:2316:C:C6 | 2.49 | 0.47 |
| 25:DA:2538:C:H2' | 25:DA:2539:C:H6 | 1.79 | 0.47 |
| 26:DB:79:C:H2' | 26:DB:80:U:O4' | 2.15 | 0.47 |
| 25:DA:1188:U:C4' | 41:DV:79:VAL:HG22 | 2.45 | 0.47 |
| 1:AA:1125:U:N3 | 1:AA:1127:G:C5 | 2.68 | 0.47 |
| 1:AA:172:A:N7 | 1:AA:174:C:C4 | 2.83 | 0.47 |
| 1:AA:276:G:C2' | 1:AA:277:C:H5' | 2.45 | 0.47 |
| 1:AA:435:C:H2' | 1:AA:436:C:C6 | 2.50 | 0.47 |
| 1:AA:652:U:O2' | 1:AA:653:A:OP2 | 2.26 | 0.47 |
| 3:AC:181:ASN:ND2 | 3:AC:204:LEU:HD12 | 2.30 | 0.47 |
| 3:AC:44:GLU:HG2 | 3:AC:52:LEU:HD22 | 1.97 | 0.47 |
| 4:AD:65:ARG:HG2 | 4:AD:75:PHE:CD1 | 2.50 | 0.47 |
| 5:AE:68:GLU:HG2 | 5:AE:70:PRO:HG3 | 1.97 | 0.47 |
| 6:AF:62:TRP:CH2 | 6:AF:64:GLN:HB2 | 2.50 | 0.47 |
| 8:AH:112:LEU:HB3 | 8:AH:133:LEU:HA | 1.97 | 0.47 |
| 11:AK:20:TYR:HB2 | 11:AK:31:THR:HG23 | 1.97 | 0.47 |
| 24:AW:9:MVA:O | 24:AW:10:2QY:CD2 | 2.62 | 0.47 |
| 25:BA:1809:U:H2' | 25:BA:1815:A:N6 | 2.30 | 0.47 |
| 25:BA:2335:G:H2' | 25:BA:2336:C:O4' | 2.15 | 0.47 |
| 25:BA:553:A:C2 | 25:BA:2065:C:H4' | 2.50 | 0.47 |
| 25:BA:932:C:H3' | 25:BA:933:C:C5' | 2.43 | 0.47 |
| 29:BF:101:LEU:HD12 | 29:BF:102:PRO:HD2 | 1.97 | 0.47 |
| 29:BF:150:GLY:HA2 | 29:BF:172:TRP:CE3 | 2.50 | 0.47 |
| 40:BU:78:THR:HG22 | 40:BU:117:GLN:HE22 | 1.80 | 0.47 |
| 1:CA:1154:G:C8 | 1:CA:1155:G:C8 | 3.02 | 0.47 |
| 1:CA:78:G:H2' | 1:CA:79:G:H5' | 1.97 | 0.47 |
| 1:CA:838:G:H1 | 1:CA:848:C:N4 | 2.13 | 0.47 |
| 1:CA:859:A:H2' | 1:CA:860:A:O4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:CA:885:G:O2' | 1:CA:914:A:N1 | 2.38 | 0.47 |
| 1:CA:957:U:H2' | 1:CA:959:A:OP2 | 2.14 | 0.47 |
| 5:CE:104:ALA:HA | 5:CE:107:ARG:HB3 | 1.96 | 0.47 |
| 5:CE:84:PHE:N | 5:CE:87:SER:O | 2.48 | 0.47 |
| 7:CG:138:LYS:HE2 | 7:CG:142:GLU:OE1 | 2.15 | 0.47 |
| 13:CM:16:ASP:N | 13:CM:16:ASP:OD1 | 2.48 | 0.47 |
| 20:CT:50:GLU:HG3 | 20:CT:100:ILE:HD13 | 1.97 | 0.47 |
| 25:DA:585:G:H2' | 25:DA:1251:C:H42 | 1.79 | 0.47 |
| 25:DA:678:C:H2' | 25:DA:679:C:C6 | 2.50 | 0.47 |
| 35:DP:45:LEU:HD23 | 35:DP:45:LEU:HA | 1.51 | 0.47 |
| 39:DT:78:LEU:O | 39:DT:78:LEU:HD13 | 2.14 | 0.47 |
| 40:DU:89:GLU:HB2 | 41:DV:50:PRO:CB | 2.45 | 0.47 |
| 42:DW:59:VAL:HG12 | 42:DW:60:ASN:HD22 | 1.80 | 0.47 |
| 1:AA:1140:C:H2' | 1:AA:1141:C:C6 | 2.49 | 0.47 |
| 1:AA:1176:A:H2' | 1:AA:1177:G:C8 | 2.50 | 0.47 |
| 1:AA:1273:G:H3' | 1:AA:1274:G:H8 | 1.78 | 0.47 |
| 1:AA:159:G:O2' | 1:AA:161:A:N7 | 2.35 | 0.47 |
| 1:AA:458:C:H2' | 1:AA:460:G:C8 | 2.50 | 0.47 |
| 1:AA:499:A:N3 | 1:AA:546:G:N2 | 2.54 | 0.47 |
| 1:AA:735:C:H2' | 1:AA:736:C:H6 | 1.80 | 0.47 |
| 4:AD:173:TRP:HB2 | 4:AD:187:ARG:O | 2.15 | 0.47 |
| 2:AB:178:ARG:HH22 | 8:AH:68:ARG:HH22 | 1.62 | 0.47 |
| 15:AO:24:SER:OG | 15:AO:25:THR:N | 2.48 | 0.47 |
| 25:BA:2745:G:H3' | 25:BA:2746:A:O4' | 2.14 | 0.47 |
| 25:BA:908:A:N3 | 26:BB:79:C:O2' | 2.41 | 0.47 |
| 1:CA:1492:A:H5'' | 1:CA:1493:A:OP2 | 2.15 | 0.47 |
| 1:CA:160:A:H61 | 1:CA:347:G:H1' | 1.80 | 0.47 |
| 4:CD:184:LYS:HE3 | 4:CD:186:LEU:HD23 | 1.96 | 0.47 |
| 7:CG:155:ARG:CZ | 7:CG:155:ARG:HB3 | 2.43 | 0.47 |
| 7:CG:79:ARG:HB3 | 7:CG:80:VAL:H | 1.39 | 0.47 |
| 16:CP:21:VAL:HG22 | 16:CP:33:ILE:HD12 | 1.97 | 0.47 |
| 18:CR:76:LEU:HA | 18:CR:76:LEU:HD12 | 1.74 | 0.47 |
| 25:DA:1509(B):A:H2' | 25:DA:1510:G:H8 | 1.77 | 0.47 |
| 25:DA:19:C:H2' | 25:DA:20:C:C6 | 2.50 | 0.47 |
| 25:DA:10:G:H1' | 25:DA:2801(A):A:C6 | 2.50 | 0.47 |
| 25:DA:489:G:N7 | 42:DW:49:LYS:NZ | 2.61 | 0.47 |
| 25:DA:701:G:N2 | 25:DA:732:C:C2 | 2.82 | 0.47 |
| 25:DA:922:U:H2' | 25:DA:923:C:C6 | 2.50 | 0.47 |
| 25:DA:2227:A:OP1 | 27:DD:263:ARG:HD2 | 2.15 | 0.47 |
| 27:DD:80:ALA:HB3 | 27:DD:94:LEU:HD13 | 1.96 | 0.47 |
| 32:DI:65:ALA:O | 32:DI:69:LYS:N | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DQ:125:LEU:O | 61:DQ:302:HOH:O | 2.20 | 0.47 |
| 43:DX:59:VAL:N | 43:DX:76:ARG:O | 2.33 | 0.47 |
| 1:AA:103:C:OP2 | 20:AT:14:LYS:NZ | 2.30 | 0.46 |
| 1:AA:1129:C:H5'' | 9:AI:16:ARG:HH12 | 1.79 | 0.46 |
| 1:AA:1392:G:N2 | 1:AA:1502:A:C8 | 2.83 | 0.46 |
| 1:AA:1442:G:HO2' | 1:AA:1442(A):G:P | 2.34 | 0.46 |
| 1:AA:189(D):C:O2 | 1:AA:189(H):G:C6 | 2.68 | 0.46 |
| 1:AA:342:C:N3 | 1:AA:348:G:O6 | 2.48 | 0.46 |
| 1:AA:93:G:O2' | 1:AA:96:U:H5' | 2.15 | 0.46 |
| 2:AB:97:TRP:CH2 | 2:AB:173:ALA:HA | 2.49 | 0.46 |
| 6:AF:12:PRO:HG3 | 6:AF:57:GLN:O | 2.15 | 0.46 |
| 7:AG:113:GLU:HG3 | 7:AG:118:VAL:HG12 | 1.97 | 0.46 |
| 8:AH:64:LYS:HG2 | 8:AH:79:VAL:HG21 | 1.98 | 0.46 |
| 10:AJ:27:ALA:HA | 10:AJ:81:THR:CG2 | 2.45 | 0.46 |
| 10:AJ:57:LYS:HD2 | 10:AJ:60:ARG:NH2 | 2.30 | 0.46 |
| 13:AM:16:ASP:N | 13:AM:16:ASP:OD1 | 2.47 | 0.46 |
| 1:AA:189(F):U:O2' | 17:AQ:63:ARG:NH2 | 2.48 | 0.46 |
| 1:AA:103:C:P | 20:AT:17:ARG:HH21 | 2.38 | 0.46 |
| 46:B0:43:THR:O | 46:B0:43:THR:HG23 | 2.14 | 0.46 |
| 25:BA:714:U:O2 | 54:B8:2:PRO:HD2 | 2.14 | 0.46 |
| 25:BA:1229:G:H5' | 49:B3:29:ARG:HH12 | 1.80 | 0.46 |
| 1:CA:1068:G:N2 | 1:CA:1191:A:N3 | 2.55 | 0.46 |
| 1:CA:1310:G:H5' | 13:CM:77:ASN:HD21 | 1.80 | 0.46 |
| 1:CA:1309:G:N2 | 1:CA:1329:A:H1' | 2.30 | 0.46 |
| 1:CA:922:G:N3 | 1:CA:1398:A:H2 | 2.13 | 0.46 |
| 15:CO:39:LEU:HB3 | 15:CO:56:LEU:HD13 | 1.96 | 0.46 |
| 16:CP:55:ARG:O | 16:CP:58:TYR:HB3 | 2.15 | 0.46 |
| 53:D7:24:THR:O | 53:D7:28:ARG:HG3 | 2.15 | 0.46 |
| 35:DP:49:ARG:NH1 | 54:D8:61:LEU:HD23 | 2.30 | 0.46 |
| 25:DA:1151:G:H5'' | 40:DU:81:HIS:CD2 | 2.50 | 0.46 |
| 25:DA:1199:U:H2' | 25:DA:1200:C:C6 | 2.50 | 0.46 |
| 25:DA:1317:A:H2' | 25:DA:1318:C:C6 | 2.50 | 0.46 |
| 25:DA:2302:G:C2 | 25:DA:2303:G:C8 | 3.03 | 0.46 |
| 25:DA:2312:U:C4 | 25:DA:2313:C:H5 | 2.32 | 0.46 |
| 25:DA:2051:A:H5' | 25:DA:2578:G:O4' | 2.14 | 0.46 |
| 25:DA:75:G:H4' | 48:D2:55:ARG:NH1 | 2.30 | 0.46 |
| 25:DA:807:U:OP2 | 35:DP:41:ARG:NH2 | 2.48 | 0.46 |
| 29:DF:29:ASN:HB3 | 29:DF:112:MET:HE1 | 1.97 | 0.46 |
| 30:DG:78:SER:OG | 30:DG:79:ASN:N | 2.48 | 0.46 |
| 35:DP:82:GLY:HA2 | 35:DP:113:LYS:O | 2.15 | 0.46 |
| 35:DP:44:GLY:CA | 35:DP:45:LEU:HB2 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1223:C:OP2 | 19:AS:78:ARG:NH2 | 2.45 | 0.46 |
| 1:AA:646:U:H2' | 1:AA:647:C:C6 | 2.50 | 0.46 |
| 1:AA:918:A:H2' | 1:AA:919:A:C8 | 2.50 | 0.46 |
| 2:AB:174:VAL:O | 2:AB:178:ARG:HB2 | 2.14 | 0.46 |
| 6:AF:35:ALA:HA | 6:AF:67:MET:HB3 | 1.96 | 0.46 |
| 1:AA:1457:G:P | 20:AT:39:LYS:HZ1 | 2.38 | 0.46 |
| 48:B2:37:PHE:O | 48:B2:40:SER:HB3 | 2.14 | 0.46 |
| 25:BA:1688:A:H2' | 25:BA:1689:G:O4' | 2.14 | 0.46 |
| 25:BA:1900:G:H2' | 25:BA:1901:C:C6 | 2.49 | 0.46 |
| 25:BA:329:U:H2' | 25:BA:330:U:C6 | 2.50 | 0.46 |
| 25:BA:768:C:H2' | 25:BA:769:A:C8 | 2.49 | 0.46 |
| 29:BF:106:ARG:HG2 | 29:BF:106:ARG:H | 1.37 | 0.46 |
| 1:CA:1347:G:H22 | 1:CA:1373:G:H2' | 1.77 | 0.46 |
| 1:CA:1516:G:H2' | 1:CA:1518:A:OP2 | 2.15 | 0.46 |
| 1:CA:376:G:H2' | 1:CA:377:G:H8 | 1.80 | 0.46 |
| 1:CA:840:C:H5'' | 1:CA:841:U:H5 | 1.80 | 0.46 |
| 6:CF:5:GLU:HG3 | 6:CF:93:SER:OG | 2.16 | 0.46 |
| 10:CJ:57:LYS:HD2 | 10:CJ:60:ARG:HH21 | 1.81 | 0.46 |
| 25:DA:1221(A):C:C2 | 25:DA:1229:G:C2 | 3.03 | 0.46 |
| 25:DA:1669:A:H5'' | 25:DA:2550:G:OP1 | 2.15 | 0.46 |
| 25:DA:1866:C:H2' | 25:DA:1876:A:O4' | 2.15 | 0.46 |
| 25:DA:2348:U:O4 | 25:DA:2382:G:N1 | 2.48 | 0.46 |
| 25:DA:330:A:H2 | 25:DA:1210:A:HO2' | 1.63 | 0.46 |
| 25:DA:333:G:N3 | 25:DA:333:G:H2' | 2.30 | 0.46 |
| 25:DA:924:C:H2' | 25:DA:925:C:H6 | 1.79 | 0.46 |
| 29:DF:36:VAL:HG11 | 29:DF:183:VAL:HG11 | 1.97 | 0.46 |
| 1:AA:1005:A:H5' | 1:AA:1038:C:H1' | 1.96 | 0.46 |
| 1:AA:1131:G:H2' | 1:AA:1132:C:C6 | 2.50 | 0.46 |
| 1:AA:532:A:O2' | 1:AA:533:A:P | 2.74 | 0.46 |
| 1:AA:616:G:C2 | 1:AA:617:G:C8 | 3.04 | 0.46 |
| 2:AB:55:PHE:HE1 | 2:AB:218:ALA:HA | 1.80 | 0.46 |
| 1:AA:1232:U:OP1 | 9:AI:124:GLN:HG2 | 2.15 | 0.46 |
| 10:AJ:20:ALA:HA | 10:AJ:23:ILE:HG22 | 1.95 | 0.46 |
| 19:AS:20:LEU:HD23 | 19:AS:23:ASN:HD22 | 1.80 | 0.46 |
| 24:AW:9:MVA:HA | 24:AW:10:2QY:H82 | 1.39 | 0.46 |
| 51:B5:42:PRO:HB2 | 51:B5:43:HIS:ND1 | 2.30 | 0.46 |
| 25:BA:2314:G:N2 | 25:BA:2327:G:C4 | 2.84 | 0.46 |
| 25:BA:2389:A:H2' | 25:BA:2390:A:C8 | 2.50 | 0.46 |
| 25:BA:324:A:P | 44:BY:86:ARG:HH22 | 2.38 | 0.46 |
| 25:BA:335:A:C6 | 25:BA:352:U:C4 | 3.04 | 0.46 |
| 25:BA:364:A:H2' | 25:BA:365:G:O4' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:436:C:O2' | 25:BA:437:G:H5' | 2.16 | 0.46 |
| 25:BA:636:G:N2 | 25:BA:640:A:O2' | 2.48 | 0.46 |
| 25:BA:664:U:H2' | 25:BA:665:C:C6 | 2.50 | 0.46 |
| 25:BA:982:U:H2' | 25:BA:983:G:O4' | 2.15 | 0.46 |
| 28:BE:51:PHE:H | 28:BE:75:VAL:CG1 | 2.27 | 0.46 |
| 30:BG:16:ARG:O | 30:BG:20:ILE:HG13 | 2.15 | 0.46 |
| 32:BI:81:VAL:HG21 | 32:BI:88:ILE:HD13 | 1.96 | 0.46 |
| 45:BZ:120:ILE:HB | 45:BZ:171:ILE:HA | 1.97 | 0.46 |
| 1:CA:1003:G:C6 | 1:CA:1004:A:H2 | 2.34 | 0.46 |
| 1:CA:1327:C:H2' | 1:CA:1328:C:C6 | 2.51 | 0.46 |
| 2:CB:163:PHE:HA | 2:CB:185:ILE:O | 2.15 | 0.46 |
| 2:CB:15:VAL:CG1 | 2:CB:209:ARG:HB3 | 2.41 | 0.46 |
| 2:CB:77:ALA:HA | 2:CB:80:ILE:HG22 | 1.96 | 0.46 |
| 5:CE:36:ASP:C | 5:CE:38:GLN:H | 2.18 | 0.46 |
| 13:CM:60:VAL:HG22 | 13:CM:66:LEU:HD11 | 1.96 | 0.46 |
| 25:DA:1593:G:C4 | 25:DA:1594:G:C8 | 3.03 | 0.46 |
| 25:DA:1668:A:H4' | 25:DA:1669:A:O5' | 2.14 | 0.46 |
| 25:DA:1740:G:H2' | 25:DA:1741:A:C8 | 2.51 | 0.46 |
| 25:DA:263:C:H2' | 25:DA:264:C:O4' | 2.15 | 0.46 |
| 25:DA:491:G:H2' | 25:DA:492:A:H8 | 1.80 | 0.46 |
| 25:DA:861:A:C2 | 25:DA:917:A:C4 | 3.03 | 0.46 |
| 25:DA:874:G:H2' | 25:DA:875:G:O4' | 2.15 | 0.46 |
| 26:DB:33:G:C2 | 26:DB:50:G:C2 | 3.04 | 0.46 |
| 26:DB:90:A:N7 | 26:DB:91:C:H1' | 2.30 | 0.46 |
| 29:DF:129:PHE:O | 29:DF:132:VAL:HG13 | 2.15 | 0.46 |
| 30:DG:16:ARG:HB2 | 30:DG:17:PRO:HD3 | 1.98 | 0.46 |
| 40:DU:59:ARG:HB3 | 40:DU:59:ARG:HH11 | 1.80 | 0.46 |
| 40:DU:76:TYR:CZ | 40:DU:80:ILE:HG13 | 2.51 | 0.46 |
| 1:AA:1333:A:H2' | 1:AA:1334:G:O4' | 2.15 | 0.46 |
| 1:AA:391:G:C6 | 1:AA:392:G:C5 | 3.03 | 0.46 |
| 1:AA:814:A:H2' | 1:AA:816:A:H5'' | 1.97 | 0.46 |
| 4:AD:155:LEU:O | 4:AD:158:ILE:HG12 | 2.15 | 0.46 |
| 8:AH:39:LEU:HD12 | 8:AH:39:LEU:HA | 1.79 | 0.46 |
| 9:AI:121:ARG:NH1 | 9:AI:122:ALA:O | 2.49 | 0.46 |
| 15:AO:8:LYS:O | 15:AO:12:ILE:HG13 | 2.16 | 0.46 |
| 25:BA:85:C:H4' | 25:BA:102:U:H1' | 1.97 | 0.46 |
| 25:BA:1217:G:H3' | 25:BA:1218:G:H5' | 1.98 | 0.46 |
| 25:BA:1592:A:H2' | 25:BA:1593:C:O4' | 2.16 | 0.46 |
| 25:BA:2225:U:O4' | 27:BD:151:LYS:HE2 | 2.14 | 0.46 |
| 25:BA:2658:C:OP2 | 25:BA:2745:G:O2' | 2.19 | 0.46 |
| 25:BA:736:A:N3 | 25:BA:826:U:O2' | 2.43 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:926:G:H2' | 25:BA:927:G:C1' | 2.46 | 0.46 |
| 44:BY:30:VAL:O | 44:BY:32:PRO:HD3 | 2.16 | 0.46 |
| 1:CA:1203:C:H2' | 1:CA:1204:A:O4' | 2.16 | 0.46 |
| 1:CA:1238:A:C2 | 1:CA:1303:C:H4' | 2.50 | 0.46 |
| 1:CA:1240:U:O2' | 7:CG:32:ARG:HD3 | 2.16 | 0.46 |
| 2:CB:167:PRO:HD3 | 2:CB:187:LEU:O | 2.15 | 0.46 |
| 3:CC:6:HIS:CD2 | 3:CC:8:ILE:H | 2.32 | 0.46 |
| 14:CN:3:ARG:O | 14:CN:7:ILE:HG23 | 2.15 | 0.46 |
| 54:D8:30:ARG:HD3 | 54:D8:30:ARG:HA | 1.69 | 0.46 |
| 25:DA:1142:U:H2' | 25:DA:1142:U:O2 | 2.15 | 0.46 |
| 25:DA:1259:G:H2' | 25:DA:1260:G:C8 | 2.50 | 0.46 |
| 25:DA:1358:G:O2' | 25:DA:1359:A:H5'' | 2.15 | 0.46 |
| 25:DA:1529:G:O2' | 25:DA:1530:C:H5' | 2.16 | 0.46 |
| 25:DA:1794:U:H2' | 25:DA:1795:C:H6 | 1.80 | 0.46 |
| 25:DA:568:U:H5' | 25:DA:945:A:C2 | 2.50 | 0.46 |
| 25:DA:647:G:H8 | 25:DA:647:G:O5' | 1.99 | 0.46 |
| 25:DA:656:G:H2' | 25:DA:657:U:O4' | 2.14 | 0.46 |
| 25:DA:792:G:H5'' | 25:DA:793:A:H5' | 1.98 | 0.46 |
| 25:DA:857:C:H2' | 25:DA:858:U:C6 | 2.50 | 0.46 |
| 25:DA:888:C:H2' | 25:DA:889:C:N3 | 2.30 | 0.46 |
| 25:DA:889:C:O2' | 25:DA:890:A:H8 | 1.99 | 0.46 |
| 25:DA:956:G:OP1 | 36:DQ:87:LYS:HG3 | 2.16 | 0.46 |
| 1:AA:1149:C:H2' | 1:AA:1150:U:H6 | 1.81 | 0.46 |
| 1:AA:1352:C:H2' | 1:AA:1353:G:C8 | 2.50 | 0.46 |
| 1:AA:186:C:H2' | 1:AA:187:C:H6 | 1.80 | 0.46 |
| 1:AA:59:A:H5'' | 1:AA:60:A:H5'' | 1.97 | 0.46 |
| 1:AA:863:U:H2' | 1:AA:865:A:OP2 | 2.15 | 0.46 |
| 2:AB:16:HIS:CD2 | 2:AB:17:PHE:N | 2.81 | 0.46 |
| 2:AB:84:GLU:HB3 | 2:AB:219:VAL:HG21 | 1.96 | 0.46 |
| 1:AA:437:U:O3' | 4:AD:125:HIS:CE1 | 2.69 | 0.46 |
| 8:AH:97:VAL:HG23 | 8:AH:129:VAL:O | 2.16 | 0.46 |
| 10:AJ:67:THR:O | 10:AJ:67:THR:OG1 | 2.31 | 0.46 |
| 25:BA:696:C:P | 25:BA:696:C:H6 | 2.38 | 0.46 |
| 25:BA:910:A:H2' | 25:BA:911:G:C8 | 2.50 | 0.46 |
| 1:CA:1120:G:N1 | 1:CA:1154:G:N3 | 2.64 | 0.46 |
| 1:CA:1286:A:H2' | 1:CA:1287:A:H4' | 1.96 | 0.46 |
| 1:CA:693:G:H1' | 7:CG:82:GLY:HA3 | 1.97 | 0.46 |
| 2:CB:47:THR:HA | 2:CB:202:PRO:HG2 | 1.98 | 0.46 |
| 3:CC:104:GLN:HE21 | 3:CC:104:GLN:HB3 | 1.58 | 0.46 |
| 5:CE:137:GLU:HG2 | 5:CE:140:ARG:NH1 | 2.29 | 0.46 |
| 6:CF:38:GLU:HB2 | 6:CF:64:GLN:HG2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1240:U:C2 | 7:CG:32:ARG:HD2 | 2.50 | 0.46 |
| 13:CM:15:VAL:HG11 | 13:CM:48:LEU:HD21 | 1.96 | 0.46 |
| 13:CM:33:ALA:HA | 13:CM:59:TYR:CE2 | 2.49 | 0.46 |
| 25:DA:1506:C:H2' | 25:DA:1507:A:H5' | 1.98 | 0.46 |
| 25:DA:2287:A:O2' | 25:DA:2288:A:H3' | 2.15 | 0.46 |
| 25:DA:2747:G:H21 | 25:DA:2757:A:H62 | 1.64 | 0.46 |
| 25:DA:302:C:H2' | 25:DA:303:U:C6 | 2.50 | 0.46 |
| 25:DA:34:C:OP1 | 25:DA:34:C:H6 | 1.99 | 0.46 |
| 29:DF:184:TYR:CE1 | 35:DP:3:LEU:HD21 | 2.50 | 0.46 |
| 31:DH:137:ASP:HB3 | 31:DH:140:LYS:HB3 | 1.95 | 0.46 |
| 33:DN:71:ILE:HG21 | 33:DN:84:LYS:HB3 | 1.98 | 0.46 |
| 40:DU:78:THR:HG22 | 40:DU:117:GLN:HE21 | 1.81 | 0.46 |
| 1:AA:292:G:N7 | 1:AA:293:G:H1' | 2.31 | 0.46 |
| 2:AB:127:ILE:HB | 2:AB:129:GLU:H | 1.79 | 0.46 |
| 25:BA:2901:A:N6 | 25:BA:2902:G:N1 | 2.64 | 0.46 |
| 25:BA:553:A:N1 | 25:BA:2064:A:H2' | 2.30 | 0.46 |
| 25:BA:68:C:O2' | 25:BA:69:G:H5' | 2.16 | 0.46 |
| 25:BA:922:G:H1 | 25:BA:948:C:N4 | 2.13 | 0.46 |
| 1:CA:1145:C:H5'' | 1:CA:1146:A:OP1 | 2.16 | 0.46 |
| 1:CA:1154:G:N7 | 1:CA:1155:G:C5 | 2.83 | 0.46 |
| 1:CA:1154:G:O6 | 1:CA:1155:G:N1 | 2.48 | 0.46 |
| 1:CA:1401:G:C2 | 1:CA:1402:C:H1' | 2.51 | 0.46 |
| 1:CA:25:C:H2' | 1:CA:26:A:C8 | 2.51 | 0.46 |
| 1:CA:323:U:H2' | 1:CA:324:G:O4' | 2.16 | 0.46 |
| 1:CA:32:A:C2 | 1:CA:33:A:C4 | 3.04 | 0.46 |
| 2:CB:17:PHE:HB2 | 2:CB:44:LEU:CD1 | 2.46 | 0.46 |
| 4:CD:191:ARG:O | 4:CD:191:ARG:HD2 | 2.16 | 0.46 |
| 7:CG:12:LEU:HD12 | 7:CG:12:LEU:H | 1.80 | 0.46 |
| 9:CI:26:VAL:HG22 | 9:CI:61:ALA:HB3 | 1.97 | 0.46 |
| 16:CP:6:LEU:HD23 | 16:CP:17:TYR:CG | 2.51 | 0.46 |
| 19:CS:22:LEU:HB3 | 19:CS:27:GLU:HG3 | 1.97 | 0.46 |
| 20:CT:33:ILE:HG13 | 20:CT:62:LEU:HD22 | 1.96 | 0.46 |
| 13:CM:3:ARG:CA | 50:D4:34:GLU:HG2 | 2.43 | 0.46 |
| 25:DA:1341:U:OP1 | 25:DA:1397:U:N3 | 2.40 | 0.46 |
| 25:DA:1364:G:P | 47:D1:3:LYS:HG3 | 2.55 | 0.46 |
| 25:DA:1589:C:H2' | 25:DA:1590:U:H6 | 1.80 | 0.46 |
| 29:DF:53:THR:HG23 | 29:DF:55:GLY:N | 2.26 | 0.46 |
| 38:DS:38:GLN:HB2 | 38:DS:47:THR:HG23 | 1.96 | 0.46 |
| 45:DZ:54:HIS:CG | 45:DZ:101:PRO:HG3 | 2.51 | 0.46 |
| 1:AA:1270:C:H2' | 1:AA:1271:G:H5' | 1.98 | 0.46 |
| 1:AA:346:G:OP1 | 39:BT:41:ARG:NH2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:877:C:OP1 | 8:AH:88:LYS:NZ | 2.34 | 0.46 |
| 1:AA:865:A:H2 | 1:AA:918:A:H4' | 1.79 | 0.46 |
| 3:AC:58:GLU:O | 3:AC:59:ARG:HG3 | 2.15 | 0.46 |
| 24:AW:3:004:C | 24:AW:4:PRO:O | 2.63 | 0.46 |
| 25:BA:1071:G:C4 | 25:BA:1180:C:H1' | 2.50 | 0.46 |
| 30:BG:102:PHE:CE1 | 30:BG:141:PHE:HE2 | 2.25 | 0.46 |
| 36:BQ:21:THR:HG21 | 36:BQ:101:ARG:HB2 | 1.98 | 0.46 |
| 1:CA:1126:U:H6 | 1:CA:1281:U:O2 | 1.98 | 0.46 |
| 1:CA:232:G:H1' | 1:CA:262:A:N1 | 2.30 | 0.46 |
| 1:CA:918:A:H2' | 1:CA:919:A:C8 | 2.50 | 0.46 |
| 3:CC:106:VAL:HG11 | 3:CC:115:LEU:HD21 | 1.98 | 0.46 |
| 5:CE:7:GLU:OE1 | 5:CE:37:ARG:NH2 | 2.47 | 0.46 |
| 9:CI:14:VAL:HG22 | 9:CI:66:ARG:O | 2.16 | 0.46 |
| 9:CI:99:LEU:HB3 | 9:CI:101:PHE:HE1 | 1.81 | 0.46 |
| 46:D0:82:ARG:HA | 46:D0:83:PRO:HD3 | 1.73 | 0.46 |
| 51:D5:40:LYS:HD3 | 51:D5:41:PRO:O | 2.16 | 0.46 |
| 25:DA:1324:G:C2 | 25:DA:1331:A:C2 | 3.04 | 0.46 |
| 25:DA:1371:G:H2' | 25:DA:1372:U:H5 | 1.80 | 0.46 |
| 25:DA:1420:U:HO2' | 25:DA:1421:G:P | 2.39 | 0.46 |
| 25:DA:2443:C:H2' | 25:DA:2444:G:H8 | 1.80 | 0.46 |
| 25:DA:2885:C:O2' | 51:D5:34:PRO:HG3 | 2.14 | 0.46 |
| 28:DE:36:ARG:HD3 | 28:DE:85:ASN:HD21 | 1.80 | 0.46 |
| 36:DQ:32:TYR:OH | 36:DQ:111:GLU:OE1 | 2.29 | 0.46 |
| 34:DO:120:GLU:HB2 | 39:DT:68:TYR:HE2 | 1.81 | 0.46 |
| 43:DX:41:ASN:O | 43:DX:45:THR:HG23 | 2.15 | 0.46 |
| 1:AA:676:A:H2' | 1:AA:677:U:H6 | 1.79 | 0.46 |
| 1:AA:658:G:C2 | 1:AA:749:C:N3 | 2.83 | 0.46 |
| 2:AB:54:THR:HG22 | 2:AB:58:ILE:HD11 | 1.97 | 0.46 |
| 3:AC:115:LEU:O | 3:AC:118:GLN:HG2 | 2.15 | 0.46 |
| 3:AC:148:GLY:HA3 | 3:AC:172:ARG:O | 2.16 | 0.46 |
| 5:AE:77:PRO:HG2 | 5:AE:78:HIS:CD2 | 2.51 | 0.46 |
| 25:BA:1233:U:C2' | 25:BA:1234:A:H5' | 2.45 | 0.46 |
| 25:BA:1465:A:O2' | 25:BA:1467:G:N7 | 2.44 | 0.46 |
| 25:BA:1662:A:H4' | 25:BA:1663:C:OP2 | 2.15 | 0.46 |
| 25:BA:279:G:H5'' | 25:BA:279:G:H8 | 1.81 | 0.46 |
| 31:BH:71:LEU:HA | 31:BH:71:LEU:HD12 | 1.70 | 0.46 |
| 1:CA:1151:A:O2' | 1:CA:1152:A:H8 | 1.98 | 0.46 |
| 1:CA:1491:G:H3' | 1:CA:1492:A:C8 | 2.50 | 0.46 |
| 1:CA:174:C:H2' | 1:CA:175:C:H6 | 1.81 | 0.46 |
| 1:CA:283:C:H2' | 1:CA:284:G:O4' | 2.15 | 0.46 |
| 1:CA:96:U:O2' | 1:CA:97:G:H5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:CF:22:GLU:O | 6:CF:26:ILE:HG13 | 2.16 | 0.46 |
| 19:CS:20:LEU:HA | 19:CS:23:ASN:HD22 | 1.81 | 0.46 |
| 50:D4:46:GLN:HG2 | 50:D4:48:ARG:HE | 1.81 | 0.46 |
| 25:DA:1198:U:H2' | 25:DA:1199:U:C6 | 2.50 | 0.46 |
| 25:DA:1773:A:C5 | 25:DA:1829:A:H1' | 2.51 | 0.46 |
| 25:DA:32:C:O2' | 25:DA:33:U:H5' | 2.16 | 0.46 |
| 25:DA:492:A:H2' | 25:DA:493:G:O4' | 2.16 | 0.46 |
| 26:DB:31:C:C2' | 26:DB:32:C:H5' | 2.45 | 0.46 |
| 30:DG:170:ARG:HH21 | 30:DG:180:PHE:CB | 2.28 | 0.46 |
| 41:DV:64:HIS:CD2 | 41:DV:92:THR:HG1 | 2.33 | 0.46 |
| 1:AA:1068:G:N7 | 1:AA:1094:G:H2' | 2.31 | 0.46 |
| 1:AA:597:G:H5'' | 1:AA:598:U:OP2 | 2.16 | 0.46 |
| 1:AA:736:C:H2' | 1:AA:737:A:C8 | 2.51 | 0.46 |
| 1:AA:920:U:H2' | 1:AA:921:U:C6 | 2.51 | 0.46 |
| 7:AG:69:VAL:HG12 | 7:AG:100:ALA:HA | 1.96 | 0.46 |
| 9:AI:27:THR:O | 9:AI:63:ILE:N | 2.49 | 0.46 |
| 25:BA:1008:U:H2' | 25:BA:1009:C:C6 | 2.51 | 0.46 |
| 25:BA:1096:A:N3 | 25:BA:1096:A:H2' | 2.30 | 0.46 |
| 25:BA:1199:C:H2' | 25:BA:1200:G:O4' | 2.16 | 0.46 |
| 25:BA:160:G:O2' | 25:BA:161:C:H5' | 2.16 | 0.46 |
| 25:BA:593:G:H2' | 25:BA:2052:A:C5 | 2.50 | 0.46 |
| 25:BA:2786:C:H2' | 25:BA:2787:C:C6 | 2.51 | 0.46 |
| 40:BU:66:ASN:O | 40:BU:70:ARG:HG3 | 2.15 | 0.46 |
| 40:BU:95:LEU:HA | 40:BU:95:LEU:HD12 | 1.78 | 0.46 |
| 1:CA:1118:C:H1' | 1:CA:1179:A:C4 | 2.51 | 0.46 |
| 1:CA:89:C:H2' | 1:CA:90:U:O4' | 2.16 | 0.46 |
| 2:CB:145:LEU:O | 2:CB:149:LEU:HB2 | 2.15 | 0.46 |
| 2:CB:19:HIS:HB2 | 2:CB:204:ASN:HB2 | 1.98 | 0.46 |
| 7:CG:50:ILE:HD11 | 7:CG:58:PRO:HA | 1.98 | 0.46 |
| 17:CQ:41:LYS:NZ | 17:CQ:92:ARG:HH21 | 2.14 | 0.46 |
| 52:D6:19:ARG:N | 52:D6:19:ARG:HD2 | 2.30 | 0.46 |
| 55:D9:17:ILE:HD12 | 55:D9:17:ILE:HA | 1.76 | 0.46 |
| 25:DA:1163:G:O2' | 25:DA:1164:G:H5' | 2.16 | 0.46 |
| 25:DA:1417:C:H2' | 25:DA:1418:G:O4' | 2.16 | 0.46 |
| 25:DA:189:G:H2' | 25:DA:205:G:N2 | 2.30 | 0.46 |
| 25:DA:2228:G:C6 | 25:DA:2229:C:C4 | 3.04 | 0.46 |
| 25:DA:704:G:H1' | 25:DA:726:G:H22 | 1.81 | 0.46 |
| 25:DA:2831:G:P | 28:DE:58:ARG:HH22 | 2.38 | 0.46 |
| 36:DQ:111:GLU:O | 36:DQ:115:MET:HG2 | 2.16 | 0.46 |
| 1:AA:658:G:H2' | 1:AA:659:U:H6 | 1.80 | 0.46 |
| 1:AA:78:G:C2 | 1:AA:91:C:N3 | 2.84 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:30:SER:O | 10:AJ:81:THR:HG23 | 2.16 | 0.46 |
| 25:BA:1171:G:H5' | 55:B9:37:GLY:HA2 | 1.98 | 0.46 |
| 25:BA:1629:C:H2' | 25:BA:1630:A:H8 | 1.81 | 0.46 |
| 25:BA:1854:G:OP1 | 27:BD:54:ARG:NH1 | 2.48 | 0.46 |
| 25:BA:2812:A:N3 | 25:BA:2904:U:H1' | 2.31 | 0.46 |
| 25:BA:508:A:H5'' | 25:BA:509:A:OP1 | 2.16 | 0.46 |
| 25:BA:751:G:O2' | 25:BA:773:G:N2 | 2.35 | 0.46 |
| 27:BD:182:LEU:HA | 27:BD:182:LEU:HD23 | 1.65 | 0.46 |
| 28:BE:143:ASN:HD22 | 28:BE:147:PRO:HD3 | 1.81 | 0.46 |
| 32:BI:104:GLN:HG3 | 32:BI:105:HIS:HD2 | 1.80 | 0.46 |
| 25:BA:1264:G:OP2 | 40:BU:19:LYS:HE3 | 2.15 | 0.46 |
| 44:BY:15:VAL:HG21 | 44:BY:42:VAL:HG11 | 1.99 | 0.46 |
| 1:CA:1077:G:C2 | 1:CA:1081:G:C6 | 3.04 | 0.46 |
| 1:CA:1305:G:O2' | 1:CA:1331:G:N2 | 2.49 | 0.46 |
| 1:CA:923:A:H2' | 1:CA:924:C:C6 | 2.51 | 0.46 |
| 1:CA:983:A:H3' | 1:CA:983:A:N3 | 2.31 | 0.46 |
| 16:CP:40:ASP:O | 16:CP:48:TRP:HB2 | 2.16 | 0.46 |
| 25:DA:2354:G:OP1 | 46:D0:32:ARG:NH2 | 2.49 | 0.46 |
| 25:DA:1885:A:H2' | 25:DA:1886:C:O4' | 2.17 | 0.46 |
| 25:DA:2207:G:H3' | 25:DA:2208:A:H5'' | 1.98 | 0.46 |
| 25:DA:2461:C:H2' | 25:DA:2462:U:C6 | 2.51 | 0.46 |
| 33:DN:19:GLU:HA | 33:DN:59:LYS:HB2 | 1.97 | 0.46 |
| 36:DQ:108:GLY:HA3 | 45:DZ:116:VAL:HG13 | 1.96 | 0.46 |
| 45:DZ:70:LEU:HA | 45:DZ:70:LEU:HD23 | 1.79 | 0.46 |
| 1:AA:1424:C:H2' | 1:AA:1425:U:O4' | 2.15 | 0.45 |
| 1:AA:752:G:H4' | 15:AO:69:TYR:OH | 2.16 | 0.45 |
| 4:AD:190:ASP:N | 4:AD:190:ASP:OD1 | 2.49 | 0.45 |
| 4:AD:30:LYS:HA | 4:AD:35:ARG:NH1 | 2.31 | 0.45 |
| 11:AK:99:GLN:HG3 | 11:AK:105:VAL:HG11 | 1.97 | 0.45 |
| 11:AK:31:THR:HA | 11:AK:42:TRP:HA | 1.98 | 0.45 |
| 26:BB:48:A:H4' | 38:BS:95:HIS:CD2 | 2.42 | 0.45 |
| 26:BB:75:G:H8 | 26:BB:75:G:H5'' | 1.80 | 0.45 |
| 27:BD:72:LYS:HB3 | 27:BD:75:ILE:HD12 | 1.99 | 0.45 |
| 36:BQ:85:LYS:HD3 | 46:B0:7:LEU:HG | 1.98 | 0.45 |
| 42:BW:71:VAL:HA | 42:BW:107:LEU:HD12 | 1.98 | 0.45 |
| 1:CA:1058:G:N2 | 10:CJ:53:PRO:HG3 | 2.31 | 0.45 |
| 1:CA:1243:C:H2' | 1:CA:1244:C:H6 | 1.81 | 0.45 |
| 1:CA:433:C:H2' | 1:CA:434:U:C6 | 2.49 | 0.45 |
| 1:CA:931:C:H42 | 1:CA:1386:G:H1 | 1.64 | 0.45 |
| 3:CC:183:ASP:N | 3:CC:202:ILE:O | 2.46 | 0.45 |
| 4:CD:20:TYR:CD1 | 4:CD:26:CYS:HB3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:77:C:O2' | 48:D2:14:ARG:NH2 | 2.49 | 0.45 |
| 25:DA:1405:U:H2' | 25:DA:1406:U:H6 | 1.77 | 0.45 |
| 25:DA:1707:G:H2' | 25:DA:1708:C:C6 | 2.51 | 0.45 |
| 25:DA:2065:C:H2' | 25:DA:2066:C:H6 | 1.80 | 0.45 |
| 25:DA:1783:A:H5' | 25:DA:2608:G:H4' | 1.98 | 0.45 |
| 25:DA:556:G:C6 | 25:DA:557:U:C4 | 3.04 | 0.45 |
| 33:DN:30:ILE:O | 33:DN:34:LEU:HD22 | 2.16 | 0.45 |
| 36:DQ:42:ILE:HG22 | 36:DQ:47:ILE:HG13 | 1.98 | 0.45 |
| 38:DS:77:ALA:HB1 | 38:DS:82:ILE:HB | 1.97 | 0.45 |
| 39:DT:61:PHE:CE1 | 39:DT:76:PHE:HB2 | 2.51 | 0.45 |
| 44:DY:19:LYS:HE2 | 44:DY:20:TYR:CE1 | 2.51 | 0.45 |
| 1:AA:923:A:OP1 | 5:AE:21:ALA:HB2 | 2.15 | 0.45 |
| 1:AA:958:A:C6 | 1:AA:959:A:N1 | 2.84 | 0.45 |
| 11:AK:84:VAL:HG11 | 11:AK:91:ARG:HD2 | 1.97 | 0.45 |
| 19:AS:38:SER:O | 19:AS:70:LYS:HD3 | 2.17 | 0.45 |
| 25:BA:1702:A:H3' | 25:BA:1703:C:H6 | 1.81 | 0.45 |
| 27:BD:43:ARG:HA | 27:BD:48:ARG:O | 2.16 | 0.45 |
| 28:BE:144:ARG:HB3 | 28:BE:145:LYS:H | 1.36 | 0.45 |
| 29:BF:8:GLN:OE1 | 29:BF:19:GLU:HG2 | 2.17 | 0.45 |
| 30:BG:97:ASP:O | 30:BG:101:ILE:HG13 | 2.16 | 0.45 |
| 31:BH:174:GLY:O | 31:BH:175:LYS:HB3 | 2.16 | 0.45 |
| 39:BT:29:ARG:HB2 | 39:BT:46:GLU:HG3 | 1.97 | 0.45 |
| 45:BZ:136:PHE:O | 45:BZ:137:ILE:HG13 | 2.17 | 0.45 |
| 1:CA:1004:A:H3' | 1:CA:1005:A:O4' | 2.16 | 0.45 |
| 1:CA:1329:A:P | 13:CM:28:ALA:HB3 | 2.57 | 0.45 |
| 1:CA:689:C:O4' | 1:CA:704:A:H2 | 1.99 | 0.45 |
| 2:CB:51:LEU:HD23 | 2:CB:201:ILE:HD12 | 1.97 | 0.45 |
| 5:CE:33:VAL:HG13 | 5:CE:112:LEU:HD12 | 1.98 | 0.45 |
| 25:DA:94(A):G:N2 | 48:D2:47:ASN:OD1 | 2.40 | 0.45 |
| 25:DA:1266:G:O4' | 42:DW:15:ARG:NH2 | 2.48 | 0.45 |
| 25:DA:1321:A:H2' | 25:DA:1322:A:O4' | 2.16 | 0.45 |
| 25:DA:858:U:O2 | 25:DA:2268:A:H2' | 2.16 | 0.45 |
| 25:DA:2443:C:H2' | 25:DA:2444:G:C8 | 2.51 | 0.45 |
| 25:DA:428:A:H3' | 25:DA:429:A:H8 | 1.81 | 0.45 |
| 25:DA:57:C:H2' | 25:DA:58:G:O4' | 2.16 | 0.45 |
| 25:DA:776:G:C8 | 25:DA:793:A:C2 | 3.04 | 0.45 |
| 25:DA:881:G:C2 | 25:DA:882:G:C4 | 3.03 | 0.45 |
| 29:DF:31:HIS:NE2 | 29:DF:35:GLU:OE2 | 2.49 | 0.45 |
| 30:DG:61:ALA:HA | 30:DG:66:GLN:O | 2.15 | 0.45 |
| 34:DO:4:PRO:O | 34:DO:5:GLN:HB2 | 2.17 | 0.45 |
| 38:DS:30:ARG:HD3 | 38:DS:98:VAL:HG22 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:DV:62:LEU:CD1 | 41:DV:95:LEU:HB2 | 2.46 | 0.45 |
| 45:DZ:6:LYS:HE3 | 45:DZ:8:TYR:OH | 2.16 | 0.45 |
| 1:AA:1030:C:H5' | 1:AA:1030(A):G:O5' | 2.16 | 0.45 |
| 1:AA:1082:G:H2' | 1:AA:1083:U:O4' | 2.16 | 0.45 |
| 1:AA:181:G:N1 | 1:AA:195:A:C8 | 2.84 | 0.45 |
| 1:AA:355:C:C4 | 1:AA:356:A:N7 | 2.84 | 0.45 |
| 1:AA:660:G:H2' | 1:AA:661:G:H8 | 1.82 | 0.45 |
| 4:AD:107:ARG:HD2 | 4:AD:107:ARG:HA | 1.72 | 0.45 |
| 5:AE:44:GLY:HA3 | 5:AE:62:ALA:HB2 | 1.99 | 0.45 |
| 19:AS:12:ASP:OD1 | 19:AS:37:ARG:HD2 | 2.16 | 0.45 |
| 1:AA:323:U:OP1 | 20:AT:23:ARG:HA | 2.16 | 0.45 |
| 25:BA:471:C:H2' | 25:BA:472:G:O4' | 2.16 | 0.45 |
| 29:BF:184:TYR:O | 29:BF:188:ARG:HG3 | 2.16 | 0.45 |
| 45:BZ:28:MET:HA | 45:BZ:88:PHE:O | 2.16 | 0.45 |
| 1:CA:1007:C:N3 | 1:CA:1022:G:C2 | 2.83 | 0.45 |
| 1:CA:1194:U:H2' | 1:CA:1195:C:C6 | 2.51 | 0.45 |
| 1:CA:1323:G:H2' | 1:CA:1324:A:C8 | 2.52 | 0.45 |
| 1:CA:1342:C:H4' | 9:CI:125:TYR:HB3 | 1.97 | 0.45 |
| 1:CA:1479:C:H2' | 1:CA:1480:G:C8 | 2.51 | 0.45 |
| 1:CA:243:A:C2 | 1:CA:246:A:C8 | 3.05 | 0.45 |
| 1:CA:299:G:H2' | 1:CA:300:A:C8 | 2.50 | 0.45 |
| 1:CA:790:A:C6 | 1:CA:791:G:C6 | 3.05 | 0.45 |
| 3:CC:28:GLN:HB3 | 3:CC:32:LEU:HD23 | 1.96 | 0.45 |
| 12:CL:117:ARG:NH2 | 12:CL:124:LYS:HB2 | 2.31 | 0.45 |
| 19:CS:22:LEU:HD23 | 19:CS:28:LYS:HA | 1.98 | 0.45 |
| 20:CT:89:ARG:O | 20:CT:93:GLU:HB2 | 2.15 | 0.45 |
| 25:DA:987:G:O2' | 25:DA:1000:A:N3 | 2.44 | 0.45 |
| 25:DA:858:U:H1' | 25:DA:2268:A:H2' | 1.97 | 0.45 |
| 25:DA:2335:A:C8 | 25:DA:2337:G:N7 | 2.84 | 0.45 |
| 25:DA:2439:A:C8 | 25:DA:2439:A:H5' | 2.50 | 0.45 |
| 25:DA:2693:A:H2' | 25:DA:2694:G:H8 | 1.81 | 0.45 |
| 25:DA:903:C:H2' | 25:DA:904:C:H6 | 1.80 | 0.45 |
| 36:DQ:56:ARG:HG3 | 36:DQ:56:ARG:HH11 | 1.81 | 0.45 |
| 1:AA:1035:A:H2 | 1:AA:1036:G:N7 | 2.15 | 0.45 |
| 1:AA:1523:G:OP1 | 11:AK:123:LYS:HD2 | 2.16 | 0.45 |
| 1:AA:299:G:C6 | 1:AA:300:A:C6 | 3.04 | 0.45 |
| 4:AD:15:GLU:HG2 | 4:AD:63:LYS:HB3 | 1.99 | 0.45 |
| 15:AO:74:ASP:CG | 15:AO:77:ARG:HG3 | 2.37 | 0.45 |
| 50:B4:59:PHE:C | 50:B4:61:ARG:H | 2.18 | 0.45 |
| 54:B8:30:ARG:HA | 54:B8:30:ARG:HD3 | 1.58 | 0.45 |
| 25:BA:1825:U:H2' | 25:BA:1826:C:H6 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1882:U:H3 | 25:BA:1913:G:H1 | 1.64 | 0.45 |
| 25:BA:2117:C:H2' | 25:BA:2118:U:O4' | 2.16 | 0.45 |
| 25:BA:270:C:H6 | 25:BA:270:C:O5' | 1.99 | 0.45 |
| 26:BB:32:C:C2 | 26:BB:51:G:N2 | 2.85 | 0.45 |
| 31:BH:159:GLU:HG3 | 31:BH:169:VAL:HG11 | 1.99 | 0.45 |
| 25:BA:1183:G:H2' | 33:BN:106:MET:HE2 | 1.98 | 0.45 |
| 43:BX:26:TYR:CE2 | 43:BX:89:ILE:HG13 | 2.51 | 0.45 |
| 1:CA:186:C:H2' | 1:CA:187:C:C6 | 2.51 | 0.45 |
| 1:CA:35:G:C6 | 1:CA:36:C:N4 | 2.85 | 0.45 |
| 1:CA:35:G:C5 | 1:CA:36:C:C4 | 3.04 | 0.45 |
| 1:CA:474:G:H2' | 1:CA:475:G:C8 | 2.47 | 0.45 |
| 1:CA:685:G:C2 | 1:CA:686:U:C4 | 3.04 | 0.45 |
| 1:CA:872:A:C4 | 1:CA:874:G:N7 | 2.85 | 0.45 |
| 1:CA:757:U:O2' | 1:CA:879:C:O2 | 2.32 | 0.45 |
| 1:CA:927:G:H2' | 1:CA:928:G:C8 | 2.52 | 0.45 |
| 3:CC:179:ARG:O | 3:CC:206:GLU:HA | 2.16 | 0.45 |
| 1:CA:1186:G:O3' | 9:CI:113:LYS:NZ | 2.49 | 0.45 |
| 7:CG:153:HIS:CE1 | 11:CK:58:PRO:HD2 | 2.50 | 0.45 |
| 16:CP:22:THR:HA | 16:CP:33:ILE:HG13 | 1.99 | 0.45 |
| 46:D0:72:ARG:O | 46:D0:75:LEU:HB2 | 2.16 | 0.45 |
| 25:DA:140:G:N2 | 25:DA:1596:A:H4' | 2.31 | 0.45 |
| 25:DA:747:U:O2 | 25:DA:2014:A:H1' | 2.17 | 0.45 |
| 31:DH:163:TYR:CE2 | 31:DH:169:VAL:HG22 | 2.52 | 0.45 |
| 32:DI:129:THR:HG22 | 32:DI:139:GLN:HE22 | 1.80 | 0.45 |
| 35:DP:52:GLU:OE2 | 54:D8:57:ARG:NH1 | 2.46 | 0.45 |
| 45:DZ:45:ASP:OD2 | 45:DZ:49:ARG:HD2 | 2.16 | 0.45 |
| 1:AA:1030(C):G:N7 | 1:AA:1031:G:N2 | 2.65 | 0.45 |
| 1:AA:1225:A:H2' | 1:AA:1226:C:C5 | 2.51 | 0.45 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:H62 | 1.64 | 0.45 |
| 1:AA:202:U:H3' | 1:AA:203:U:C6 | 2.51 | 0.45 |
| 1:AA:433:C:H2' | 1:AA:434:U:C6 | 2.49 | 0.45 |
| 1:AA:303:A:HO2' | 1:AA:555:C:HO2' | 1.57 | 0.45 |
| 5:AE:78:HIS:NE2 | 5:AE:142:LEU:HA | 2.32 | 0.45 |
| 7:AG:103:TRP:CH2 | 7:AG:141:VAL:HG21 | 2.52 | 0.45 |
| 8:AH:53:VAL:HG12 | 8:AH:54:ASP:OD1 | 2.16 | 0.45 |
| 8:AH:28:ALA:HA | 8:AH:59:LEU:HG | 1.98 | 0.45 |
| 9:AI:99:LEU:HB3 | 9:AI:101:PHE:CE1 | 2.52 | 0.45 |
| 52:B6:11:LEU:HB3 | 52:B6:49:HIS:HB3 | 1.99 | 0.45 |
| 34:BO:104:ARG:NH2 | 39:BT:43:GLN:OE1 | 2.50 | 0.45 |
| 36:BQ:34:LEU:HD11 | 36:BQ:129:THR:HB | 1.99 | 0.45 |
| 38:BS:10:ARG:O | 38:BS:14:VAL:HG13 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BZ:8:TYR:HB2 | 45:BZ:38:TYR:CE2 | 2.51 | 0.45 |
| 1:CA:489:C:H2' | 1:CA:490:G:H8 | 1.81 | 0.45 |
| 2:CB:180:LEU:HD23 | 2:CB:180:LEU:HA | 1.69 | 0.45 |
| 3:CC:73:PRO:O | 3:CC:77:ILE:HG12 | 2.16 | 0.45 |
| 4:CD:43:HIS:CA | 4:CD:46:LYS:HG3 | 2.45 | 0.45 |
| 13:CM:8:GLU:HG2 | 30:DG:146:TYR:HD2 | 1.81 | 0.45 |
| 14:CN:32:SER:O | 14:CN:40:CYS:HA | 2.17 | 0.45 |
| 25:DA:139(A):G:O2' | 25:DA:140:G:H5' | 2.17 | 0.45 |
| 25:DA:1927:A:H2' | 25:DA:1928:A:C8 | 2.52 | 0.45 |
| 25:DA:2564:A:OP1 | 25:DA:2648:C:H4' | 2.16 | 0.45 |
| 25:DA:506:G:O3' | 25:DA:507:A:H8 | 2.00 | 0.45 |
| 25:DA:714:U:O2 | 25:DA:716:A:C8 | 2.70 | 0.45 |
| 26:DB:33:G:C2' | 26:DB:34:U:H5' | 2.47 | 0.45 |
| 25:DA:1803:A:H4' | 27:DD:259:THR:HG23 | 1.98 | 0.45 |
| 31:DH:20:ALA:HB3 | 31:DH:23:ARG:CG | 2.46 | 0.45 |
| 38:DS:36:TYR:CD1 | 38:DS:36:TYR:N | 2.85 | 0.45 |
| 43:DX:26:TYR:CE2 | 43:DX:89:ILE:HG13 | 2.51 | 0.45 |
| 45:DZ:131:ARG:HD2 | 45:DZ:131:ARG:H | 1.81 | 0.45 |
| 1:AA:130:A:H5' | 17:AQ:63:ARG:HE | 1.81 | 0.45 |
| 1:AA:473:G:H2' | 1:AA:474:G:C8 | 2.52 | 0.45 |
| 3:AC:58:GLU:HB2 | 3:AC:65:ALA:CB | 2.46 | 0.45 |
| 5:AE:137:GLU:HG2 | 5:AE:140:ARG:NH1 | 2.30 | 0.45 |
| 6:AF:81:ILE:HD11 | 27:BD:125:ILE:HB | 1.99 | 0.45 |
| 7:AG:50:ILE:CD1 | 7:AG:58:PRO:HA | 2.41 | 0.45 |
| 8:AH:121:ASP:OD1 | 8:AH:121:ASP:N | 2.49 | 0.45 |
| 1:AA:1179:A:O3' | 9:AI:103:THR:HB | 2.16 | 0.45 |
| 1:AA:1309:G:OP1 | 13:AM:88:ARG:NH1 | 2.49 | 0.45 |
| 47:B1:86:SER:N | 47:B1:89:GLU:HG3 | 2.31 | 0.45 |
| 25:BA:1003:U:HO2' | 25:BA:1004:A:P | 2.40 | 0.45 |
| 25:BA:1314:A:C2 | 25:BA:2035:A:C4 | 3.05 | 0.45 |
| 25:BA:1938:A:H2' | 25:BA:1939:U:O4' | 2.17 | 0.45 |
| 29:BF:7:TYR:O | 29:BF:21:ALA:HA | 2.16 | 0.45 |
| 45:BZ:74:VAL:HG22 | 45:BZ:86:VAL:HG12 | 1.99 | 0.45 |
| 1:CA:1504:G:OP1 | 1:CA:1507:A:H4' | 2.17 | 0.45 |
| 1:CA:840:C:H5'' | 1:CA:848:C:O2 | 2.17 | 0.45 |
| 1:CA:959:A:O2' | 1:CA:984:C:O2' | 2.14 | 0.45 |
| 4:CD:108:LEU:HD12 | 4:CD:108:LEU:HA | 1.68 | 0.45 |
| 8:CH:63:LEU:HA | 8:CH:63:LEU:HD13 | 1.85 | 0.45 |
| 9:CI:47:LEU:HD22 | 9:CI:50:LEU:HD21 | 1.99 | 0.45 |
| 9:CI:16:ARG:HB2 | 9:CI:64:THR:HB | 1.99 | 0.45 |
| 1:CA:881:G:P | 12:CL:12:ARG:HH22 | 2.40 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:CM:47:ASP:N | 13:CM:47:ASP:OD1 | 2.50 | 0.45 |
| 17:CQ:94:ASN:O | 17:CQ:98:LEU:HD13 | 2.16 | 0.45 |
| 18:CR:56:THR:HB | 18:CR:58:LEU:HD23 | 1.98 | 0.45 |
| 25:DA:1539:G:H2' | 25:DA:1540:U:C6 | 2.52 | 0.45 |
| 25:DA:198:C:H5' | 25:DA:2244:U:OP1 | 2.17 | 0.45 |
| 25:DA:222:A:C2 | 25:DA:233:A:H5'' | 2.52 | 0.45 |
| 25:DA:2658:C:O3' | 31:DH:158:HIS:HE1 | 1.98 | 0.45 |
| 25:DA:646:A:H2' | 25:DA:647:G:O4' | 2.16 | 0.45 |
| 25:DA:955:C:OP1 | 36:DQ:87:LYS:HE3 | 2.16 | 0.45 |
| 27:DD:2:ALA:O | 27:DD:3:VAL:HB | 2.16 | 0.45 |
| 28:DE:77:ILE:HD13 | 28:DE:195:LEU:HD13 | 1.98 | 0.45 |
| 29:DF:33:LEU:HB3 | 35:DP:6:LEU:HD21 | 1.99 | 0.45 |
| 37:DR:60:LEU:HA | 37:DR:60:LEU:HD23 | 1.77 | 0.45 |
| 38:DS:26:LEU:HD22 | 38:DS:87:PHE:CD1 | 2.51 | 0.45 |
| 40:DU:49:HIS:HA | 40:DU:52:ARG:HB3 | 1.97 | 0.45 |
| 1:AA:109:A:H2' | 1:AA:326:G:N2 | 2.32 | 0.45 |
| 1:AA:1123:A:H61 | 1:AA:1149:C:N4 | 2.15 | 0.45 |
| 1:AA:1125:U:HO2' | 1:AA:1126:U:P | 2.39 | 0.45 |
| 1:AA:419:C:OP1 | 1:AA:513:C:O2' | 2.27 | 0.45 |
| 1:AA:974:A:OP2 | 14:AN:29:ARG:NH2 | 2.50 | 0.45 |
| 5:AE:36:ASP:OD1 | 5:AE:38:GLN:N | 2.37 | 0.45 |
| 11:AK:70:LYS:HB2 | 11:AK:70:LYS:NZ | 2.31 | 0.45 |
| 25:BA:1410:G:OP2 | 47:B1:3:LYS:HG3 | 2.16 | 0.45 |
| 25:BA:1002:A:N1 | 25:BA:2470:G:H4' | 2.32 | 0.45 |
| 25:BA:561:A:H2' | 25:BA:562:C:C6 | 2.52 | 0.45 |
| 25:BA:943:C:H6 | 25:BA:943:C:O5' | 2.00 | 0.45 |
| 26:BB:14:U:OP2 | 26:BB:70:C:O2' | 2.29 | 0.45 |
| 28:BE:51:PHE:O | 28:BE:75:VAL:HG13 | 2.16 | 0.45 |
| 29:BF:181:LEU:HA | 29:BF:181:LEU:HD12 | 1.71 | 0.45 |
| 31:BH:13:LYS:HA | 31:BH:14:GLY:HA2 | 1.78 | 0.45 |
| 36:BQ:54:MET:HB3 | 36:BQ:64:ILE:HD11 | 1.99 | 0.45 |
| 44:BY:55:TYR:CD2 | 44:BY:55:TYR:N | 2.84 | 0.45 |
| 45:BZ:45:ASP:OD1 | 45:BZ:49:ARG:HD2 | 2.16 | 0.45 |
| 1:CA:1427:U:H2' | 1:CA:1428:A:C8 | 2.52 | 0.45 |
| 1:CA:584:G:H2' | 1:CA:585:G:C8 | 2.51 | 0.45 |
| 1:CA:624:C:H2' | 1:CA:625:G:H8 | 1.82 | 0.45 |
| 2:CB:17:PHE:HB2 | 2:CB:44:LEU:HD12 | 1.97 | 0.45 |
| 3:CC:52:LEU:HD23 | 3:CC:68:VAL:HG13 | 1.98 | 0.45 |
| 4:CD:10:ARG:HB2 | 4:CD:40:PRO:HG3 | 1.99 | 0.45 |
| 10:CJ:55:LYS:HE3 | 10:CJ:56:HIS:HE2 | 1.82 | 0.45 |
| 14:CN:6:LEU:HB3 | 14:CN:23:ARG:NH2 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:CN:2:ALA:HB1 | 14:CN:6:LEU:HD13 | 1.97 | 0.45 |
| 1:CA:376:G:H5'' | 16:CP:5:ARG:HB2 | 1.99 | 0.45 |
| 20:CT:43:LEU:HB3 | 20:CT:52:ALA:HB2 | 1.99 | 0.45 |
| 51:D5:41:PRO:HG2 | 51:D5:44:THR:OG1 | 2.16 | 0.45 |
| 25:DA:1003:G:N2 | 25:DA:1153:C:C2 | 2.84 | 0.45 |
| 25:DA:1138:G:H2' | 25:DA:1139:G:O4' | 2.16 | 0.45 |
| 25:DA:1291:C:H2' | 25:DA:1292:U:H6 | 1.82 | 0.45 |
| 25:DA:11:G:C2' | 25:DA:12:U:H5' | 2.43 | 0.45 |
| 25:DA:1786:A:C4 | 25:DA:1938:A:C6 | 3.04 | 0.45 |
| 25:DA:1876:A:H2' | 25:DA:1877:A:H8 | 1.77 | 0.45 |
| 25:DA:2019:A:OP2 | 51:D5:9:LYS:NZ | 2.30 | 0.45 |
| 25:DA:2370:G:H2' | 25:DA:2371:G:C8 | 2.51 | 0.45 |
| 25:DA:362:U:O2' | 25:DA:363:G:H5' | 2.17 | 0.45 |
| 25:DA:729:G:C5 | 27:DD:208:LYS:HB2 | 2.51 | 0.45 |
| 25:DA:919:G:C6 | 25:DA:920:G:C5 | 3.05 | 0.45 |
| 27:DD:268:ARG:HD3 | 27:DD:269:PHE:CE2 | 2.51 | 0.45 |
| 43:DX:53:LYS:NZ | 43:DX:55:ASN:OD1 | 2.32 | 0.45 |
| 1:AA:1002:G:H5'' | 1:AA:1003:G:OP2 | 2.17 | 0.45 |
| 1:AA:1258:G:O2' | 1:AA:1259:C:H5' | 2.17 | 0.45 |
| 1:AA:1285:A:O5' | 1:AA:1285:A:H8 | 1.99 | 0.45 |
| 1:AA:1351:U:O4 | 9:AI:118:LYS:NZ | 2.49 | 0.45 |
| 1:AA:1511:G:H2' | 1:AA:1512:U:O4' | 2.17 | 0.45 |
| 1:AA:44:G:C2 | 1:AA:45:U:H1' | 2.50 | 0.45 |
| 1:AA:721:G:C6 | 1:AA:733:A:C2 | 3.04 | 0.45 |
| 1:AA:991:U:H1' | 1:AA:993:G:C8 | 2.52 | 0.45 |
| 2:AB:95:GLN:HB3 | 2:AB:147:LYS:HZ2 | 1.82 | 0.45 |
| 4:AD:189:PRO:HB3 | 4:AD:193:ASP:HB3 | 1.99 | 0.45 |
| 4:AD:5:ILE:O | 4:AD:5:ILE:HD13 | 2.17 | 0.45 |
| 7:AG:26:PHE:CE2 | 7:AG:30:ILE:HD11 | 2.51 | 0.45 |
| 8:AH:7:ALA:HB2 | 8:AH:85:ARG:HD2 | 1.98 | 0.45 |
| 16:AP:56:ALA:O | 16:AP:60:LEU:HD23 | 2.17 | 0.45 |
| 6:AF:60:PHE:CE2 | 18:AR:78:LEU:HD21 | 2.52 | 0.45 |
| 25:BA:1715:A:H4' | 25:BA:1716:A:O5' | 2.16 | 0.45 |
| 25:BA:1735:U:O2 | 25:BA:1747:A:H5' | 2.17 | 0.45 |
| 25:BA:2092:G:H2' | 25:BA:2093:A:O4' | 2.16 | 0.45 |
| 25:BA:2289:G:OP2 | 46:B0:10:THR:HG21 | 2.16 | 0.45 |
| 25:BA:211:A:H5'' | 25:BA:448:U:OP1 | 2.16 | 0.45 |
| 35:BP:46:LYS:HE3 | 35:BP:46:LYS:HB3 | 1.77 | 0.45 |
| 26:BB:106:G:OP1 | 45:BZ:31:ARG:HG2 | 2.17 | 0.45 |
| 1:CA:1106:G:H2' | 1:CA:1107:C:H6 | 1.82 | 0.45 |
| 1:CA:1118:C:C2 | 1:CA:1119:C:H5 | 2.35 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1403:C:H6 | 1:CA:1403:C:O5' | 1.99 | 0.45 |
| 1:CA:21:G:H2' | 1:CA:22:G:C8 | 2.52 | 0.45 |
| 1:CA:615:C:H2' | 1:CA:616:G:O4' | 2.16 | 0.45 |
| 4:CD:132:ARG:NH2 | 4:CD:134:ASP:OD2 | 2.49 | 0.45 |
| 6:CF:61:LEU:HB3 | 6:CF:63:TYR:CE1 | 2.49 | 0.45 |
| 9:CI:4:TYR:HB2 | 9:CI:19:LEU:HB2 | 1.99 | 0.45 |
| 1:CA:130:A:H5' | 17:CQ:63:ARG:NE | 2.32 | 0.45 |
| 1:CA:130:A:OP2 | 17:CQ:63:ARG:NE | 2.44 | 0.45 |
| 23:CX:67:C:C2' | 23:CX:68:C:H5' | 2.46 | 0.45 |
| 25:DA:1006:C:C2 | 25:DA:1138:G:N2 | 2.85 | 0.45 |
| 25:DA:1336:A:H2' | 25:DA:1337:G:C8 | 2.52 | 0.45 |
| 25:DA:1477:A:H2' | 25:DA:1478:G:O4' | 2.16 | 0.45 |
| 25:DA:1710:C:H2' | 25:DA:1711:C:C6 | 2.51 | 0.45 |
| 25:DA:1857:G:C6 | 25:DA:1858:G:N1 | 2.85 | 0.45 |
| 25:DA:2261:C:C5 | 46:D0:16:SER:HB3 | 2.52 | 0.45 |
| 25:DA:2528:U:O2' | 25:DA:2529:G:H3' | 2.16 | 0.45 |
| 25:DA:64:A:O3' | 43:DX:71:GLY:HA3 | 2.17 | 0.45 |
| 26:DB:17:C:H2' | 26:DB:18:G:O4' | 2.16 | 0.45 |
| 27:DD:148:GLU:CB | 27:DD:151:LYS:HD2 | 2.45 | 0.45 |
| 27:DD:58:HIS:ND1 | 27:DD:59:LYS:N | 2.65 | 0.45 |
| 29:DF:120:GLU:HB3 | 29:DF:122:LYS:HG2 | 1.99 | 0.45 |
| 37:DR:28:LEU:HD23 | 37:DR:28:LEU:HA | 1.85 | 0.45 |
| 39:DT:95:ARG:HG2 | 39:DT:95:ARG:NH1 | 2.31 | 0.45 |
| 1:AA:303:A:O2' | 1:AA:555:C:O2' | 2.34 | 0.45 |
| 4:AD:13:ARG:HB3 | 4:AD:38:TYR:O | 2.17 | 0.45 |
| 1:AA:921:U:O2 | 5:AE:19:MET:HB2 | 2.17 | 0.45 |
| 6:AF:11:ASN:HB3 | 6:AF:14:LEU:HG | 1.99 | 0.45 |
| 52:B6:19:ARG:NH2 | 52:B6:52:VAL:HG11 | 2.32 | 0.45 |
| 25:BA:163:C:H2' | 25:BA:164:G:O4' | 2.17 | 0.45 |
| 25:BA:1834:A:C8 | 25:BA:1835:C:C5 | 3.04 | 0.45 |
| 25:BA:211:A:H3' | 25:BA:448:U:H5' | 1.99 | 0.45 |
| 25:BA:2299:A:C4 | 25:BA:2301:G:C8 | 3.05 | 0.45 |
| 25:BA:2624:C:H2' | 25:BA:2625:U:H5' | 1.99 | 0.45 |
| 26:BB:50:G:O5' | 26:BB:50:G:H8 | 2.00 | 0.45 |
| 1:CA:1106:G:H2' | 1:CA:1107:C:C6 | 2.51 | 0.45 |
| 2:CB:81:VAL:O | 2:CB:85:ALA:N | 2.49 | 0.45 |
| 4:CD:17:VAL:HG11 | 4:CD:197:PRO:CG | 2.47 | 0.45 |
| 4:CD:79:PHE:HE1 | 4:CD:204:ILE:HD13 | 1.81 | 0.45 |
| 9:CI:53:VAL:HG21 | 9:CI:92:TYR:OH | 2.17 | 0.45 |
| 1:CA:35:G:O2' | 12:CL:118:SER:O | 2.34 | 0.45 |
| 49:D3:6:VAL:HG12 | 49:D3:56:VAL:HG22 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:D3:8:LEU:O | 49:D3:32:GLN:N | 2.38 | 0.45 |
| 25:DA:1525:G:H2' | 25:DA:1526:G:H8 | 1.82 | 0.45 |
| 25:DA:193:U:O3' | 25:DA:803:U:H4' | 2.17 | 0.45 |
| 25:DA:2699:C:H2' | 25:DA:2700:C:O4' | 2.17 | 0.45 |
| 25:DA:652(B):A:H2 | 25:DA:655:A:H1' | 1.82 | 0.45 |
| 25:DA:804:A:H5'' | 25:DA:805:G:OP1 | 2.17 | 0.45 |
| 28:DE:119:ARG:HB3 | 28:DE:120:TRP:CD1 | 2.52 | 0.45 |
| 28:DE:1:MET:HB3 | 28:DE:83:ASP:O | 2.16 | 0.45 |
| 25:DA:587:C:OP2 | 35:DP:21:ARG:NH2 | 2.50 | 0.45 |
| 1:AA:192:U:O2' | 1:AA:193:C:C6 | 2.68 | 0.45 |
| 1:AA:452:A:O2' | 1:AA:453:A:OP2 | 2.29 | 0.45 |
| 2:AB:71:VAL:HA | 2:AB:93:VAL:HG23 | 1.99 | 0.45 |
| 5:AE:127:ASN:HA | 5:AE:128:PRO:HD3 | 1.85 | 0.45 |
| 1:AA:1347:G:H5'' | 9:AI:107:ARG:HB3 | 1.99 | 0.45 |
| 9:AI:18:PHE:O | 9:AI:61:ALA:HA | 2.17 | 0.45 |
| 13:AM:84:ILE:N | 13:AM:85:GLY:HA2 | 2.32 | 0.45 |
| 17:AQ:26:GLN:HE21 | 17:AQ:37:LYS:HG2 | 1.81 | 0.45 |
| 25:BA:2274:U:P | 46:B0:19:LYS:HZ3 | 2.40 | 0.45 |
| 46:B0:43:THR:OG1 | 46:B0:46:LYS:HG2 | 2.16 | 0.45 |
| 54:B8:54:GLU:O | 54:B8:58:ILE:HG13 | 2.17 | 0.45 |
| 25:BA:1321:A:N1 | 25:BA:1341:C:O2' | 2.48 | 0.45 |
| 25:BA:217:A:OP1 | 35:BP:76:LYS:NZ | 2.42 | 0.45 |
| 25:BA:2211:U:C2' | 25:BA:2212:G:H5' | 2.47 | 0.45 |
| 25:BA:2473:C:H2' | 25:BA:2474:U:C6 | 2.51 | 0.45 |
| 25:BA:254:A:H1' | 25:BA:255:G:O4' | 2.17 | 0.45 |
| 25:BA:2660:C:H2' | 25:BA:2661:U:C6 | 2.53 | 0.45 |
| 25:BA:2784:C:H2' | 25:BA:2785:C:H6 | 1.82 | 0.45 |
| 27:BD:180:GLY:HA3 | 27:BD:275:LYS:HD2 | 1.98 | 0.45 |
| 30:BG:115:ARG:HB3 | 30:BG:136:ARG:HH22 | 1.81 | 0.45 |
| 40:BU:85:LYS:HE2 | 40:BU:85:LYS:HB3 | 1.78 | 0.45 |
| 1:CA:1038:C:H2' | 1:CA:1039:C:C6 | 2.52 | 0.45 |
| 1:CA:1066:C:O2' | 1:CA:1067:A:H5' | 2.17 | 0.45 |
| 1:CA:1136:U:O5' | 1:CA:1137:C:C4 | 2.69 | 0.45 |
| 1:CA:1289:A:H2 | 1:CA:1372:U:O4' | 2.00 | 0.45 |
| 1:CA:1237:C:H3' | 1:CA:1336:C:H41 | 1.82 | 0.45 |
| 1:CA:1366:C:H2' | 1:CA:1367:C:C6 | 2.51 | 0.45 |
| 1:CA:590:C:H2' | 1:CA:591:U:C6 | 2.52 | 0.45 |
| 9:CI:77:ILE:O | 9:CI:81:ILE:HG22 | 2.17 | 0.45 |
| 13:CM:87:TYR:O | 13:CM:91:ARG:HG2 | 2.17 | 0.45 |
| 1:CA:1227:A:N3 | 19:CS:83:HIS:HB3 | 2.32 | 0.45 |
| 54:D8:54:GLU:O | 54:D8:58:ILE:HG13 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 25:DA:1575:C:H2' | 25:DA:1576:U:H6 | 1.81 | 0.45 |
| 25:DA:1652:A:C2' | 25:DA:1653:G:H5' | 2.47 | 0.45 |
| 25:DA:1817:G:H2' | 25:DA:1818:U:H5' | 1.98 | 0.45 |
| 25:DA:2002:G:OP2 | 61:DA:3782:HOH:O | 2.21 | 0.45 |
| 25:DA:2242:G:H2' | 25:DA:2243:U:O4' | 2.17 | 0.45 |
| 25:DA:453:C:O2 | 25:DA:457:A:O2' | 2.35 | 0.45 |
| 25:DA:652(D):C:N4 | 25:DA:652(U):G:H1 | 2.10 | 0.45 |
| 28:DE:176:ILE:HB | 28:DE:181:LEU:HB2 | 1.98 | 0.45 |
| 38:DS:23:ARG:NH2 | 38:DS:84:GLN:HG2 | 2.32 | 0.45 |
| 38:DS:57:LYS:HB2 | 38:DS:57:LYS:HE2 | 1.79 | 0.45 |
| 44:DY:49:VAL:CG2 | 44:DY:61:ILE:HG23 | 2.47 | 0.45 |
| 1:AA:590:C:H2' | 1:AA:591:U:H6 | 1.81 | 0.44 |
| 4:AD:61:LYS:NZ | 4:AD:72:GLU:OE2 | 2.48 | 0.44 |
| 1:AA:1187:G:H4' | 9:AI:111:ARG:NH1 | 2.31 | 0.44 |
| 49:B3:43:ILE:O | 49:B3:47:VAL:HG23 | 2.18 | 0.44 |
| 54:B8:42:ARG:HD2 | 61:B8:203:HOH:O | 2.17 | 0.44 |
| 25:BA:1032:C:C2' | 25:BA:1033:G:H5' | 2.47 | 0.44 |
| 25:BA:659:C:H2' | 25:BA:660:C:C6 | 2.52 | 0.44 |
| 25:BA:722:A:C8 | 25:BA:851:A:C6 | 3.05 | 0.44 |
| 42:BW:84:ARG:HG3 | 42:BW:98:LYS:HD2 | 1.99 | 0.44 |
| 36:BQ:135:ASP:OD2 | 45:BZ:49:ARG:NH2 | 2.50 | 0.44 |
| 1:CA:1009:G:N2 | 1:CA:1021:G:H1' | 2.32 | 0.44 |
| 1:CA:1030(A):G:HO2' | 1:CA:1030(B):C:H5 | 1.61 | 0.44 |
| 1:CA:1118:C:H2' | 1:CA:1119:C:H6 | 1.82 | 0.44 |
| 1:CA:1166:G:H1' | 1:CA:1171:G:H22 | 1.81 | 0.44 |
| 1:CA:1192:C:OP2 | 3:CC:4:LYS:NZ | 2.45 | 0.44 |
| 1:CA:1291:G:C6 | 1:CA:1292:U:C4 | 3.05 | 0.44 |
| 1:CA:791:G:C5 | 1:CA:792:A:N7 | 2.85 | 0.44 |
| 3:CC:12:LEU:HD23 | 3:CC:16:ARG:HB3 | 1.98 | 0.44 |
| 3:CC:66:VAL:HB | 3:CC:101:LEU:HA | 1.99 | 0.44 |
| 7:CG:56:GLN:O | 7:CG:58:PRO:HD3 | 2.17 | 0.44 |
| 11:CK:44:SER:OG | 11:CK:47:VAL:HG23 | 2.17 | 0.44 |
| 1:CA:953:G:N7 | 13:CM:104:ARG:NH1 | 2.65 | 0.44 |
| 21:CU:22:ARG:HA | 21:CU:23:PRO:HD3 | 1.74 | 0.44 |
| 24:CW:4:PRO:O | 24:CW:5:MVA:HG23 | 2.17 | 0.44 |
| 23:CX:40:C:H2' | 23:CX:41:C:C6 | 2.46 | 0.44 |
| 25:DA:931:G:O2' | 49:D3:24:LYS:HD3 | 2.16 | 0.44 |
| 54:D8:34:TRP:CG | 54:D8:35:GLN:N | 2.85 | 0.44 |
| 25:DA:1022:G:C5 | 25:DA:1140:C:C4 | 3.06 | 0.44 |
| 25:DA:1489:U:O3' | 25:DA:1490:A:H8 | 2.00 | 0.44 |
| 25:DA:1540:U:O2' | 25:DA:1541:G:H5' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:1857:G:C6 | 25:DA:1858:G:C6 | 3.05 | 0.44 |
| 25:DA:39:C:H2' | 25:DA:40:C:C6 | 2.52 | 0.44 |
| 25:DA:614:U:H4' | 25:DA:614(C):A:N6 | 2.32 | 0.44 |
| 25:DA:911:A:H2' | 36:DQ:9:TYR:CZ | 2.53 | 0.44 |
| 31:DH:86:GLU:CD | 31:DH:130:ARG:HD3 | 2.38 | 0.44 |
| 32:DI:27:ARG:HD2 | 47:D1:71:TYR:CE1 | 2.52 | 0.44 |
| 40:DU:65:ILE:CD1 | 40:DU:95:LEU:HB3 | 2.47 | 0.44 |
| 40:DU:76:TYR:HH | 40:DU:92:ARG:NH1 | 2.15 | 0.44 |
| 42:DW:18:ARG:NH1 | 42:DW:76:VAL:O | 2.50 | 0.44 |
| 1:AA:1068:G:OP2 | 1:AA:1068:G:H8 | 2.00 | 0.44 |
| 1:AA:384:G:H2' | 1:AA:385:C:C6 | 2.51 | 0.44 |
| 1:AA:922:G:C6 | 1:AA:923:A:C6 | 3.04 | 0.44 |
| 2:AB:115:LEU:HD13 | 2:AB:145:LEU:HB3 | 1.98 | 0.44 |
| 4:AD:122:ARG:O | 4:AD:134:ASP:HB2 | 2.18 | 0.44 |
| 4:AD:177:ASP:OD2 | 4:AD:180:GLY:HA3 | 2.16 | 0.44 |
| 6:AF:21:LEU:O | 6:AF:24:GLU:HB3 | 2.16 | 0.44 |
| 9:AI:85:LEU:HB3 | 9:AI:92:TYR:HD2 | 1.82 | 0.44 |
| 20:AT:92:LEU:HA | 20:AT:92:LEU:HD23 | 1.80 | 0.44 |
| 49:B3:46:ASN:O | 49:B3:50:VAL:HG22 | 2.17 | 0.44 |
| 51:B5:33:CYS:HB2 | 51:B5:40:LYS:HD2 | 1.98 | 0.44 |
| 51:B5:48:GLU:HA | 51:B5:48:GLU:OE1 | 2.16 | 0.44 |
| 25:BA:597:C:H1' | 25:BA:2077:C:C6 | 2.53 | 0.44 |
| 30:BG:34:LEU:HA | 30:BG:34:LEU:HD23 | 1.76 | 0.44 |
| 31:BH:93:GLY:O | 31:BH:95:ARG:NH2 | 2.50 | 0.44 |
| 36:BQ:32:TYR:OH | 36:BQ:111:GLU:OE1 | 2.15 | 0.44 |
| 36:BQ:137:TYR:O | 36:BQ:141:GLN:HG2 | 2.16 | 0.44 |
| 43:BX:24:GLY:O | 43:BX:83:VAL:HG22 | 2.17 | 0.44 |
| 1:CA:1005:A:H3' | 1:CA:1006:C:O4' | 2.17 | 0.44 |
| 1:CA:1119:C:C4 | 1:CA:1154:G:O6 | 2.71 | 0.44 |
| 1:CA:1118:C:C2 | 1:CA:1119:C:C5 | 3.06 | 0.44 |
| 1:CA:1209:C:HO2' | 1:CA:1214:C:H42 | 1.61 | 0.44 |
| 1:CA:269:C:H2' | 1:CA:270:A:C8 | 2.51 | 0.44 |
| 1:CA:719:C:N4 | 18:CR:71:LYS:HE2 | 2.32 | 0.44 |
| 1:CA:738:C:H2' | 1:CA:739:C:C6 | 2.50 | 0.44 |
| 2:CB:74:LYS:HZ2 | 2:CB:166:ASP:HB2 | 1.82 | 0.44 |
| 3:CC:58:GLU:O | 3:CC:59:ARG:HG3 | 2.16 | 0.44 |
| 4:CD:43:HIS:ND1 | 4:CD:46:LYS:HE3 | 2.32 | 0.44 |
| 8:CH:17:THR:HA | 8:CH:65:TYR:HE2 | 1.82 | 0.44 |
| 9:CI:51:ARG:HG2 | 9:CI:56:LEU:CD2 | 2.46 | 0.44 |
| 10:CJ:23:ILE:HD12 | 10:CJ:85:LEU:HD22 | 2.00 | 0.44 |
| 13:CM:78:ILE:HD12 | 13:CM:92:HIS:NE2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:1420:U:O2' | 25:DA:1421:G:OP1 | 2.31 | 0.44 |
| 25:DA:1527:G:H2' | 25:DA:1542:A:N1 | 2.32 | 0.44 |
| 25:DA:2714:G:P | 61:DA:3973:HOH:O | 2.75 | 0.44 |
| 25:DA:949:C:H2' | 25:DA:950:G:C8 | 2.51 | 0.44 |
| 28:DE:150:VAL:CG1 | 28:DE:154:LYS:HG3 | 2.45 | 0.44 |
| 38:DS:36:TYR:OH | 38:DS:54:LEU:HD22 | 2.17 | 0.44 |
| 1:AA:109:A:C6 | 1:AA:326:G:C6 | 3.06 | 0.44 |
| 1:AA:272:C:H2' | 1:AA:273:A:C8 | 2.52 | 0.44 |
| 1:AA:977:A:H1' | 1:AA:982:U:O4 | 2.17 | 0.44 |
| 3:AC:26:LYS:HA | 14:AN:36:PHE:HE1 | 1.81 | 0.44 |
| 6:AF:1:MET:HA | 6:AF:67:MET:O | 2.18 | 0.44 |
| 8:AH:121:ASP:HB2 | 8:AH:125:ARG:NH1 | 2.31 | 0.44 |
| 14:AN:13:THR:HA | 14:AN:14:PRO:HD3 | 1.85 | 0.44 |
| 3:AC:26:LYS:HA | 14:AN:36:PHE:CE1 | 2.52 | 0.44 |
| 19:AS:48:THR:HG22 | 19:AS:61:TYR:HA | 1.99 | 0.44 |
| 1:AA:1456:G:O3' | 20:AT:39:LYS:NZ | 2.51 | 0.44 |
| 25:BA:11:G:C2' | 25:BA:12:U:H5' | 2.42 | 0.44 |
| 25:BA:1709:C:H1' | 25:BA:2699:U:H5'' | 1.99 | 0.44 |
| 25:BA:1778:G:H2' | 25:BA:1779:G:H5'' | 1.99 | 0.44 |
| 25:BA:288:U:H2' | 25:BA:288:U:H6 | 1.56 | 0.44 |
| 25:BA:701:A:H2 | 25:BA:702:A:C2 | 2.36 | 0.44 |
| 31:BH:69:ARG:HG3 | 31:BH:70:THR:N | 2.32 | 0.44 |
| 32:BI:93:THR:H | 32:BI:96:ASP:CG | 2.21 | 0.44 |
| 33:BN:138:LEU:HA | 33:BN:138:LEU:HD23 | 1.53 | 0.44 |
| 36:BQ:135:ASP:O | 36:BQ:139:GLU:HG3 | 2.17 | 0.44 |
| 1:CA:1004:A:H62 | 1:CA:1037:C:H2' | 1.81 | 0.44 |
| 1:CA:1339:A:H2' | 1:CA:1340:A:O4' | 2.18 | 0.44 |
| 1:CA:186:C:H2' | 1:CA:187:C:H6 | 1.83 | 0.44 |
| 1:CA:671:G:N2 | 1:CA:735:C:O2 | 2.49 | 0.44 |
| 1:CA:811:C:O2' | 1:CA:901:A:N1 | 2.48 | 0.44 |
| 2:CB:7:VAL:HG12 | 2:CB:8:LYS:HG2 | 1.99 | 0.44 |
| 3:CC:150:LYS:HD2 | 3:CC:201:TYR:HD2 | 1.82 | 0.44 |
| 1:CA:7:G:O2' | 5:CE:120:THR:O | 2.35 | 0.44 |
| 6:CF:72:VAL:O | 6:CF:75:LEU:HB3 | 2.18 | 0.44 |
| 7:CG:78:ARG:NH2 | 7:CG:79:ARG:HH22 | 2.16 | 0.44 |
| 10:CJ:16:LEU:HD23 | 10:CJ:16:LEU:HA | 1.88 | 0.44 |
| 18:CR:36:ASN:OD1 | 18:CR:39:VAL:HG23 | 2.17 | 0.44 |
| 48:D2:3:LEU:HD23 | 48:D2:3:LEU:HA | 1.72 | 0.44 |
| 52:D6:11:LEU:HA | 52:D6:11:LEU:HD23 | 1.80 | 0.44 |
| 25:DA:1223:G:N2 | 25:DA:1226:A:OP2 | 2.44 | 0.44 |
| 25:DA:1448:G:H1' | 25:DA:1528:A:N1 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:2044:C:C2 | 25:DA:2625:G:C2 | 3.05 | 0.44 |
| 25:DA:341:G:H2' | 25:DA:342:G:O4' | 2.17 | 0.44 |
| 25:DA:583:G:OP2 | 40:DU:10:ARG:NH1 | 2.50 | 0.44 |
| 25:DA:953:A:O2' | 25:DA:954:G:H5' | 2.18 | 0.44 |
| 30:DG:114:ILE:HD12 | 30:DG:117:PHE:CD2 | 2.52 | 0.44 |
| 30:DG:110:ALA:HA | 30:DG:140:ILE:O | 2.17 | 0.44 |
| 31:DH:149:ARG:NH1 | 31:DH:154:PRO:HG2 | 2.32 | 0.44 |
| 33:DN:16:ILE:HB | 33:DN:54:VAL:HG22 | 1.99 | 0.44 |
| 35:DP:62:LEU:O | 54:D8:13:ARG:HD3 | 2.17 | 0.44 |
| 36:DQ:77:LYS:HE3 | 36:DQ:84:GLY:O | 2.17 | 0.44 |
| 45:DZ:11:GLU:HB3 | 45:DZ:12:GLY:H | 1.53 | 0.44 |
| 1:AA:149:A:H2' | 1:AA:150:C:H6 | 1.81 | 0.44 |
| 1:AA:144:G:H1 | 1:AA:178:C:H42 | 1.64 | 0.44 |
| 1:AA:410:G:H5'' | 1:AA:411:A:OP1 | 2.17 | 0.44 |
| 2:AB:47:THR:O | 2:AB:51:LEU:N | 2.40 | 0.44 |
| 3:AC:43:LEU:HD21 | 3:AC:91:LEU:HD13 | 1.99 | 0.44 |
| 7:AG:56:GLN:O | 7:AG:58:PRO:HD3 | 2.17 | 0.44 |
| 25:BA:2348:A:H61 | 46:B0:43:THR:HG21 | 1.81 | 0.44 |
| 25:BA:2101:U:OP1 | 47:B1:21:ARG:NH2 | 2.51 | 0.44 |
| 50:B4:40:HIS:HA | 50:B4:41:PRO:HD2 | 1.84 | 0.44 |
| 25:BA:2042:A:O2' | 25:BA:2043:C:H5' | 2.17 | 0.44 |
| 25:BA:2425:G:H2' | 25:BA:2426:G:O4' | 2.18 | 0.44 |
| 25:BA:41:C:H2' | 25:BA:42:G:O4' | 2.17 | 0.44 |
| 25:BA:768:C:H2' | 25:BA:769:A:H8 | 1.82 | 0.44 |
| 25:BA:927:G:C2 | 25:BA:928:G:C8 | 3.05 | 0.44 |
| 28:BE:51:PHE:CD2 | 28:BE:52:LEU:HG | 2.51 | 0.44 |
| 29:BF:28:ILE:O | 29:BF:30:PRO:HD3 | 2.17 | 0.44 |
| 31:BH:87:LEU:HD23 | 31:BH:164:TYR:HA | 1.99 | 0.44 |
| 37:BR:65:LEU:HD13 | 37:BR:65:LEU:HA | 1.59 | 0.44 |
| 45:BZ:120:ILE:HD13 | 45:BZ:120:ILE:N | 2.33 | 0.44 |
| 1:CA:1001(A):G:N3 | 1:CA:1002:G:H1' | 2.32 | 0.44 |
| 1:CA:1091:U:H2' | 1:CA:1093:A:OP2 | 2.18 | 0.44 |
| 1:CA:1223:C:H5'' | 1:CA:1224:G:C5' | 2.43 | 0.44 |
| 1:CA:1243:C:H2' | 1:CA:1244:C:C6 | 2.53 | 0.44 |
| 1:CA:189(L):G:H2' | 1:CA:190:U:C6 | 2.52 | 0.44 |
| 1:CA:633:G:H2' | 1:CA:634:C:C6 | 2.53 | 0.44 |
| 2:CB:9:GLU:HA | 2:CB:48:MET:SD | 2.58 | 0.44 |
| 3:CC:6:HIS:HA | 3:CC:7:PRO:HD3 | 1.83 | 0.44 |
| 8:CH:98:LYS:HE3 | 8:CH:98:LYS:HB2 | 1.66 | 0.44 |
| 50:D4:16:CYS:SG | 50:D4:17:GLY:N | 2.90 | 0.44 |
| 50:D4:46:GLN:HG3 | 50:D4:48:ARG:NH2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:D9:2:LYS:HE2 | 55:D9:31:LYS:O | 2.17 | 0.44 |
| 25:DA:1005:C:H4' | 25:DA:1012:U:C6 | 2.52 | 0.44 |
| 25:DA:1041:C:H42 | 25:DA:1114:G:H1 | 1.64 | 0.44 |
| 25:DA:2708:G:H1' | 37:DR:71:GLN:NE2 | 2.32 | 0.44 |
| 25:DA:2734:A:H2' | 25:DA:2735:G:O4' | 2.17 | 0.44 |
| 25:DA:2745:C:C4 | 25:DA:2746:U:C4 | 3.04 | 0.44 |
| 25:DA:2881:C:H2' | 25:DA:2882:A:O4' | 2.18 | 0.44 |
| 25:DA:675:A:C6 | 25:DA:676:A:C6 | 3.05 | 0.44 |
| 25:DA:192:C:O2' | 25:DA:802:A:N3 | 2.44 | 0.44 |
| 30:DG:11:TYR:HA | 30:DG:15:VAL:HB | 2.00 | 0.44 |
| 30:DG:70:VAL:HA | 30:DG:90:LEU:HD23 | 2.00 | 0.44 |
| 1:AA:1030(B):C:H2' | 1:AA:1030(C):G:H5' | 2.00 | 0.44 |
| 1:AA:1289:A:N1 | 1:AA:1371:G:O2' | 2.42 | 0.44 |
| 1:AA:1376:U:H2' | 1:AA:1377:A:C8 | 2.51 | 0.44 |
| 1:AA:392:G:H2' | 1:AA:393:A:C8 | 2.53 | 0.44 |
| 1:AA:500:G:N2 | 1:AA:546:G:H1' | 2.32 | 0.44 |
| 2:AB:145:LEU:O | 2:AB:149:LEU:HB2 | 2.18 | 0.44 |
| 3:AC:6:HIS:HD2 | 3:AC:8:ILE:H | 1.65 | 0.44 |
| 7:AG:50:ILE:HD11 | 7:AG:58:PRO:CA | 2.40 | 0.44 |
| 15:AO:54:ARG:O | 15:AO:58:MET:HG3 | 2.17 | 0.44 |
| 20:AT:16:HIS:O | 20:AT:19:SER:OG | 2.24 | 0.44 |
| 25:BA:1002:A:H5' | 36:BQ:76:LYS:HG3 | 1.98 | 0.44 |
| 25:BA:1044:C:OP2 | 40:BU:92:ARG:NH2 | 2.51 | 0.44 |
| 25:BA:1096:A:H3' | 25:BA:1097:G:H8 | 1.82 | 0.44 |
| 25:BA:2340:A:H2' | 25:BA:2341:G:H8 | 1.83 | 0.44 |
| 25:BA:2410:U:H2' | 25:BA:2411:G:C8 | 2.53 | 0.44 |
| 25:BA:2418:U:OP1 | 61:BA:4136:HOH:O | 2.21 | 0.44 |
| 25:BA:2545:A:H2' | 25:BA:2546:A:O4' | 2.17 | 0.44 |
| 25:BA:640:A:C4 | 29:BF:180:GLY:HA2 | 2.53 | 0.44 |
| 25:BA:851:A:H5'' | 25:BA:852:G:OP1 | 2.17 | 0.44 |
| 25:BA:964:A:H5'' | 26:BB:98:G:O2' | 2.18 | 0.44 |
| 30:BG:43:LEU:HB3 | 30:BG:44:GLY:H | 1.52 | 0.44 |
| 32:BI:99:GLU:O | 32:BI:103:ARG:NH1 | 2.50 | 0.44 |
| 25:BA:2116:G:P | 32:BI:22:LYS:HD2 | 2.57 | 0.44 |
| 44:BY:20:TYR:CE1 | 44:BY:43:ASN:HA | 2.52 | 0.44 |
| 45:BZ:161:VAL:HG13 | 45:BZ:161:VAL:O | 2.18 | 0.44 |
| 1:CA:1004:A:C6 | 1:CA:1038:C:C6 | 3.06 | 0.44 |
| 1:CA:1024:G:H2' | 1:CA:1024:G:N3 | 2.33 | 0.44 |
| 1:CA:1259:C:C4 | 1:CA:1260:C:H1' | 2.53 | 0.44 |
| 1:CA:397:A:H3' | 1:CA:397:A:N3 | 2.32 | 0.44 |
| 1:CA:620:C:H2' | 1:CA:621:A:O4' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:66:G:C2 | 1:CA:67:C:C6 | 3.05 | 0.44 |
| 7:CG:69:VAL:HG21 | 7:CG:104:LEU:CD1 | 2.48 | 0.44 |
| 7:CG:26:PHE:CE2 | 7:CG:30:ILE:HD11 | 2.52 | 0.44 |
| 1:CA:1346:A:H5'' | 9:CI:120:ARG:HH12 | 1.83 | 0.44 |
| 10:CJ:30:SER:O | 10:CJ:81:THR:HG23 | 2.17 | 0.44 |
| 13:CM:16:ASP:HB3 | 13:CM:34:LEU:CD1 | 2.46 | 0.44 |
| 25:DA:652(D):C:H2' | 25:DA:652(E):G:O4' | 2.17 | 0.44 |
| 25:DA:817:C:O2' | 25:DA:839:U:H5'' | 2.18 | 0.44 |
| 26:DB:70:C:H2' | 26:DB:71:C:H6 | 1.83 | 0.44 |
| 29:DF:102:PRO:HB2 | 29:DF:105:VAL:HG23 | 2.00 | 0.44 |
| 29:DF:64:ILE:HG21 | 29:DF:78:ILE:HG23 | 1.98 | 0.44 |
| 36:DQ:137:TYR:CE1 | 45:DZ:83:PRO:HG3 | 2.52 | 0.44 |
| 25:DA:2318:G:N2 | 38:DS:3:ARG:NH1 | 2.66 | 0.44 |
| 41:DV:35:LEU:HB2 | 41:DV:57:VAL:HG23 | 1.99 | 0.44 |
| 1:AA:1346:A:C8 | 1:AA:1348:U:O2 | 2.71 | 0.44 |
| 1:AA:444:C:H2' | 1:AA:445:G:C8 | 2.50 | 0.44 |
| 1:AA:457:C:H2' | 1:AA:458:C:C5 | 2.53 | 0.44 |
| 1:AA:62:U:OP1 | 1:AA:385:C:O2' | 2.35 | 0.44 |
| 2:AB:113:HIS:HA | 2:AB:116:GLU:HB2 | 2.00 | 0.44 |
| 2:AB:155:LEU:HD21 | 2:AB:159:PRO:HG3 | 1.98 | 0.44 |
| 4:AD:188:LEU:H | 4:AD:188:LEU:HD23 | 1.82 | 0.44 |
| 12:AL:57:LYS:HG2 | 12:AL:65:GLU:OE2 | 2.18 | 0.44 |
| 13:AM:49:THR:HG22 | 13:AM:51:ALA:H | 1.82 | 0.44 |
| 14:AN:26:ARG:NH2 | 14:AN:47:LEU:HD21 | 2.33 | 0.44 |
| 16:AP:6:LEU:HD23 | 16:AP:17:TYR:CD2 | 2.52 | 0.44 |
| 16:AP:75:ARG:HA | 16:AP:80:PHE:HD2 | 1.82 | 0.44 |
| 25:BA:927:G:C2' | 25:BA:928:G:H5' | 2.48 | 0.44 |
| 25:BA:939:C:O2' | 25:BA:940:C:H5' | 2.16 | 0.44 |
| 28:BE:111:ARG:HG3 | 28:BE:160:TYR:CD2 | 2.53 | 0.44 |
| 31:BH:28:GLY:HA3 | 31:BH:79:VAL:HB | 2.00 | 0.44 |
| 40:BU:50:ARG:HG2 | 40:BU:53:ARG:NH2 | 2.33 | 0.44 |
| 1:CA:1036:G:N7 | 1:CA:1037:C:O2 | 2.51 | 0.44 |
| 1:CA:1380:U:C4 | 7:CG:3:ARG:HG2 | 2.52 | 0.44 |
| 1:CA:292:G:C5 | 1:CA:293:G:H1' | 2.53 | 0.44 |
| 1:CA:407:G:N2 | 1:CA:436:C:C2 | 2.86 | 0.44 |
| 1:CA:472:A:C2 | 1:CA:473:G:H1' | 2.53 | 0.44 |
| 1:CA:692:U:O2' | 1:CA:694:A:N7 | 2.37 | 0.44 |
| 2:CB:172:ILE:O | 2:CB:176:GLU:HG3 | 2.18 | 0.44 |
| 2:CB:16:HIS:CB | 2:CB:210:SER:HB3 | 2.42 | 0.44 |
| 2:CB:96:ARG:NH1 | 2:CB:98:LEU:HD13 | 2.33 | 0.44 |
| 7:CG:40:ALA:HB1 | 9:CI:41:VAL:HG21 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:CG:42:ILE:HD13 | 7:CG:116:ALA:HB3 | 1.99 | 0.44 |
| 25:DA:108:U:H2' | 25:DA:109:G:C8 | 2.52 | 0.44 |
| 25:DA:1027:A:N6 | 25:DA:1126:A:C4 | 2.86 | 0.44 |
| 25:DA:1721:G:H8 | 25:DA:1741:A:N6 | 2.12 | 0.44 |
| 25:DA:2318:G:H21 | 38:DS:3:ARG:HD3 | 1.83 | 0.44 |
| 25:DA:2461:C:H2' | 25:DA:2462:U:H6 | 1.83 | 0.44 |
| 25:DA:311:A:C8 | 25:DA:332:A:N7 | 2.85 | 0.44 |
| 25:DA:815:C:C2 | 25:DA:1193:G:C2 | 3.05 | 0.44 |
| 29:DF:33:LEU:HD22 | 29:DF:112:MET:HE3 | 2.00 | 0.44 |
| 30:DG:170:ARG:HD3 | 30:DG:170:ARG:C | 2.38 | 0.44 |
| 26:DB:31:C:H4' | 30:DG:29:TRP:CZ2 | 2.52 | 0.44 |
| 44:DY:90:LEU:HD23 | 44:DY:92:ASN:HB2 | 1.99 | 0.44 |
| 1:AA:1291:G:H2' | 1:AA:1292:U:C6 | 2.53 | 0.44 |
| 1:AA:376:G:H2' | 1:AA:377:G:C8 | 2.52 | 0.44 |
| 1:AA:720:C:H6 | 1:AA:720:C:O5' | 2.01 | 0.44 |
| 1:AA:799:G:H5'' | 1:AA:799:G:H8 | 1.82 | 0.44 |
| 2:AB:163:PHE:HA | 2:AB:185:ILE:O | 2.17 | 0.44 |
| 1:AA:1060:C:N4 | 3:AC:2:GLY:HA3 | 2.32 | 0.44 |
| 3:AC:47:LEU:HD12 | 3:AC:68:VAL:HG11 | 1.98 | 0.44 |
| 3:AC:77:ILE:H | 3:AC:77:ILE:HG12 | 1.70 | 0.44 |
| 4:AD:20:TYR:HD1 | 4:AD:26:CYS:HB3 | 1.82 | 0.44 |
| 13:AM:4:ILE:HB | 13:AM:57:ARG:HG3 | 1.99 | 0.44 |
| 20:AT:34:LYS:HE2 | 20:AT:34:LYS:HB2 | 1.69 | 0.44 |
| 26:BB:12:C:H2' | 46:B0:73:GLY:HA3 | 1.99 | 0.44 |
| 35:BP:59:LEU:HD21 | 54:B8:10:ALA:HA | 1.99 | 0.44 |
| 25:BA:254:A:C8 | 25:BA:255:G:H1' | 2.53 | 0.44 |
| 25:BA:276:C:O3' | 32:BI:42:SER:OG | 2.36 | 0.44 |
| 25:BA:442:A:H2' | 25:BA:443:C:C6 | 2.53 | 0.44 |
| 25:BA:648:G:H2' | 25:BA:649:C:C6 | 2.52 | 0.44 |
| 28:BE:181:LEU:HD12 | 28:BE:181:LEU:HA | 1.79 | 0.44 |
| 26:BB:31:C:H4' | 30:BG:29:TRP:CH2 | 2.51 | 0.44 |
| 1:CA:60:A:N6 | 1:CA:110:C:N3 | 2.64 | 0.44 |
| 1:CA:430:A:H2' | 1:CA:431:A:O4' | 2.18 | 0.44 |
| 1:CA:767:A:H2' | 1:CA:768:A:O4' | 2.16 | 0.44 |
| 1:CA:1191:A:OP2 | 3:CC:3:ASN:ND2 | 2.50 | 0.44 |
| 4:CD:64:LEU:HD22 | 4:CD:198:VAL:HG11 | 1.99 | 0.44 |
| 5:CE:51:VAL:O | 5:CE:55:VAL:HG23 | 2.17 | 0.44 |
| 7:CG:131:LYS:HG2 | 7:CG:132:GLY:H | 1.83 | 0.44 |
| 8:CH:13:ILE:O | 8:CH:17:THR:HG23 | 2.18 | 0.44 |
| 8:CH:36:LEU:HA | 8:CH:36:LEU:HD23 | 1.89 | 0.44 |
| 11:CK:85:ARG:HA | 11:CK:112:THR:OG1 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:CS:14:HIS:O | 19:CS:18:LYS:HG3 | 2.18 | 0.44 |
| 46:D0:40:GLN:HE21 | 46:D0:57:PHE:HB3 | 1.83 | 0.44 |
| 25:DA:460:A:P | 53:D7:41:ARG:HH22 | 2.41 | 0.44 |
| 35:DP:64:LYS:HA | 54:D8:13:ARG:HB3 | 2.00 | 0.44 |
| 25:DA:2294:C:OP2 | 38:DS:89:ARG:NH2 | 2.41 | 0.44 |
| 25:DA:2410:G:H2' | 25:DA:2411:A:O4' | 2.17 | 0.44 |
| 25:DA:2556:C:H2' | 25:DA:2557:G:O4' | 2.18 | 0.44 |
| 25:DA:984:A:H5'' | 25:DA:985:C:H5 | 1.81 | 0.44 |
| 45:DZ:141:VAL:O | 45:DZ:144:LEU:HB2 | 2.18 | 0.44 |
| 45:DZ:5:LEU:HD22 | 45:DZ:6:LYS:H | 1.83 | 0.44 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:C8 | 2.53 | 0.44 |
| 1:AA:1084:G:C5 | 1:AA:1085:U:C4 | 3.06 | 0.44 |
| 1:AA:1125:U:O2' | 1:AA:1126:U:P | 2.75 | 0.44 |
| 1:AA:1134:G:N3 | 1:AA:1134:G:H2' | 2.33 | 0.44 |
| 1:AA:1198:G:C6 | 1:AA:1199:U:C4 | 3.06 | 0.44 |
| 1:AA:1258:G:H2' | 1:AA:1259:C:C6 | 2.52 | 0.44 |
| 1:AA:456:C:H2' | 1:AA:457:C:C6 | 2.53 | 0.44 |
| 1:AA:532:A:H5' | 3:AC:161:GLU:OE2 | 2.18 | 0.44 |
| 3:AC:175:LEU:HD21 | 3:AC:201:TYR:CE2 | 2.52 | 0.44 |
| 3:AC:58:GLU:H | 3:AC:65:ALA:HB3 | 1.83 | 0.44 |
| 10:AJ:40:LEU:HB2 | 10:AJ:69:ASN:HB3 | 2.00 | 0.44 |
| 11:AK:85:ARG:HA | 11:AK:112:THR:OG1 | 2.18 | 0.44 |
| 1:AA:1456:G:N1 | 20:AT:51:GLU:OE1 | 2.51 | 0.44 |
| 47:B1:51:VAL:HG11 | 47:B1:74:VAL:HG21 | 1.99 | 0.44 |
| 52:B6:9:LEU:HD21 | 52:B6:25:LYS:HB3 | 1.98 | 0.44 |
| 25:BA:2336:C:H5'' | 25:BA:2337:G:H5' | 2.00 | 0.44 |
| 25:BA:2850:C:H4' | 37:BR:53:HIS:CE1 | 2.53 | 0.44 |
| 25:BA:926:G:H2' | 25:BA:927:G:O4' | 2.17 | 0.44 |
| 27:BD:145:VAL:HG12 | 27:BD:146:GLU:O | 2.18 | 0.44 |
| 33:BN:30:ILE:HG22 | 33:BN:34:LEU:HD22 | 2.00 | 0.44 |
| 1:CA:1005:A:H2 | 1:CA:1026:G:C8 | 2.36 | 0.44 |
| 1:CA:1068:G:H8 | 1:CA:1068:G:OP2 | 2.00 | 0.44 |
| 1:CA:1142:G:C2 | 1:CA:1143:G:H1' | 2.52 | 0.44 |
| 1:CA:1277:C:HO2' | 1:CA:1279:A:H1' | 1.83 | 0.44 |
| 1:CA:922:G:C6 | 1:CA:923:A:C6 | 3.05 | 0.44 |
| 1:CA:933:G:C6 | 1:CA:1385:G:C6 | 3.05 | 0.44 |
| 2:CB:230:VAL:HG13 | 2:CB:231:GLU:O | 2.18 | 0.44 |
| 3:CC:33:LEU:HD21 | 14:CN:53:LEU:CD2 | 2.48 | 0.44 |
| 4:CD:39:PRO:O | 4:CD:44:GLY:HA3 | 2.18 | 0.44 |
| 9:CI:53:VAL:C | 9:CI:55:ALA:H | 2.20 | 0.44 |
| 13:CM:82:MET:O | 13:CM:93:ARG:NH2 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:CT:14:LYS:O | 20:CT:18:GLN:HG3 | 2.18 | 0.44 |
| 25:DA:1115:G:H8 | 25:DA:1115:G:OP2 | 2.01 | 0.44 |
| 25:DA:2251:G:OP1 | 61:DA:4599:HOH:O | 2.21 | 0.44 |
| 25:DA:55:G:H2' | 25:DA:56:A:H8 | 1.83 | 0.44 |
| 25:DA:863:A:O2' | 25:DA:864:G:H5' | 2.18 | 0.44 |
| 25:DA:875:G:C2 | 25:DA:903:C:C2 | 3.06 | 0.44 |
| 26:DB:42:C:O2' | 30:DG:66:GLN:HG2 | 2.18 | 0.44 |
| 27:DD:77:ALA:HB2 | 27:DD:97:TYR:CD2 | 2.52 | 0.44 |
| 31:DH:150:ALA:HA | 31:DH:153:LYS:HG3 | 2.00 | 0.44 |
| 36:DQ:27:VAL:O | 36:DQ:29:PHE:N | 2.51 | 0.44 |
| 1:AA:1164:G:H2' | 1:AA:1165:C:H6 | 1.82 | 0.44 |
| 1:AA:539:A:H2' | 1:AA:540:G:C8 | 2.52 | 0.44 |
| 1:AA:600:C:H2' | 1:AA:601:C:H6 | 1.83 | 0.44 |
| 1:AA:78:G:N1 | 1:AA:91:C:N4 | 2.66 | 0.44 |
| 4:AD:106:TYR:HE2 | 4:AD:112:VAL:O | 2.01 | 0.44 |
| 4:AD:88:VAL:O | 4:AD:92:VAL:HG23 | 2.18 | 0.44 |
| 1:AA:8:A:H5' | 5:AE:101:ILE:HG22 | 2.00 | 0.44 |
| 6:AF:48:LEU:HD22 | 18:AR:77:GLY:HA3 | 1.99 | 0.44 |
| 10:AJ:31:GLY:HA2 | 10:AJ:32:ALA:HA | 1.46 | 0.44 |
| 20:AT:42:GLN:NE2 | 20:AT:46:GLU:OE2 | 2.51 | 0.44 |
| 25:BA:1091:A:H2' | 25:BA:1091:A:N3 | 2.31 | 0.44 |
| 25:BA:1157:A:N3 | 25:BA:1158:G:H1' | 2.33 | 0.44 |
| 25:BA:1749:G:H2' | 25:BA:1750:G:O4' | 2.17 | 0.44 |
| 25:BA:1805:C:O5' | 25:BA:1805:C:H6 | 2.01 | 0.44 |
| 25:BA:2214:G:H5' | 25:BA:2215:G:OP2 | 2.18 | 0.44 |
| 25:BA:2614:A:N7 | 46:B0:3:HIS:CE1 | 2.86 | 0.44 |
| 31:BH:126:PRO:HB2 | 31:BH:127:GLU:H | 1.51 | 0.44 |
| 25:BA:2830:A:OP1 | 37:BR:2:ARG:NH2 | 2.51 | 0.44 |
| 37:BR:72:ASP:OD2 | 37:BR:75:LEU:HB2 | 2.18 | 0.44 |
| 38:BS:103:GLU:O | 38:BS:107:GLU:HG3 | 2.18 | 0.44 |
| 25:BA:63:A:O3' | 43:BX:71:GLY:HA3 | 2.18 | 0.44 |
| 1:CA:1324:A:H5' | 1:CA:1362:C:O2' | 2.18 | 0.44 |
| 1:CA:142:G:H2' | 1:CA:143:A:C8 | 2.53 | 0.44 |
| 1:CA:165:C:O5' | 1:CA:165:C:H6 | 2.01 | 0.44 |
| 1:CA:713:G:H2' | 1:CA:714:G:C8 | 2.53 | 0.44 |
| 3:CC:153:VAL:HA | 3:CC:197:GLY:O | 2.17 | 0.44 |
| 7:CG:51:GLN:HB3 | 7:CG:51:GLN:HE21 | 1.63 | 0.44 |
| 14:CN:26:ARG:HB3 | 14:CN:43:CYS:SG | 2.57 | 0.44 |
| 19:CS:28:LYS:HD2 | 19:CS:47:HIS:HA | 2.00 | 0.44 |
| 12:CL:36:VAL:HG23 | 24:CW:10:2QY:CE1 | 2.47 | 0.44 |
| 25:DA:271(F):C:H2' | 25:DA:271(G):C:C6 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:2854:G:H2' | 25:DA:2855:C:C6 | 2.52 | 0.44 |
| 33:DN:138:LEU:HA | 33:DN:138:LEU:HD23 | 1.75 | 0.44 |
| 39:DT:88:ILE:HG21 | 39:DT:91:ARG:NE | 2.33 | 0.44 |
| 1:AA:10:A:OP2 | 5:AE:126:ARG:HD2 | 2.17 | 0.43 |
| 1:AA:1427:U:H2' | 1:AA:1428:A:C8 | 2.53 | 0.43 |
| 1:AA:266:G:O3' | 17:AQ:67:LYS:HB2 | 2.18 | 0.43 |
| 1:AA:346:G:H3' | 1:AA:346:G:N3 | 2.33 | 0.43 |
| 1:AA:106:C:O2' | 1:AA:379:C:H5'' | 2.17 | 0.43 |
| 1:AA:404:U:H2' | 1:AA:405:U:C6 | 2.53 | 0.43 |
| 4:AD:110:PHE:CD1 | 4:AD:110:PHE:N | 2.86 | 0.43 |
| 8:AH:25:ASP:HA | 8:AH:60:ARG:HA | 1.99 | 0.43 |
| 8:AH:94:TYR:HD1 | 8:AH:132:GLU:HA | 1.83 | 0.43 |
| 14:AN:45:ARG:HG2 | 14:AN:49:HIS:HD2 | 1.83 | 0.43 |
| 19:AS:50:ALA:HA | 19:AS:58:VAL:O | 2.18 | 0.43 |
| 25:BA:1188:A:C4 | 25:BA:1190:G:C8 | 3.05 | 0.43 |
| 25:BA:1319:U:H4' | 25:BA:1321:A:OP2 | 2.18 | 0.43 |
| 25:BA:1617:A:H2' | 25:BA:1618:A:C8 | 2.53 | 0.43 |
| 25:BA:171:A:H2' | 25:BA:172:C:O4' | 2.18 | 0.43 |
| 25:BA:174:U:H4' | 25:BA:207:A:H4' | 2.00 | 0.43 |
| 25:BA:1874:C:H6 | 25:BA:1874:C:O5' | 2.01 | 0.43 |
| 25:BA:2804:C:H6 | 25:BA:2804:C:OP2 | 2.01 | 0.43 |
| 25:BA:31:C:C4 | 25:BA:32:C:C5 | 3.05 | 0.43 |
| 25:BA:588:C:H2' | 25:BA:589:U:O4' | 2.18 | 0.43 |
| 26:BB:33:G:C2' | 26:BB:34:U:H5' | 2.47 | 0.43 |
| 1:CA:1017:G:H2' | 1:CA:1018:C:O4' | 2.17 | 0.43 |
| 1:CA:1066:C:H2' | 1:CA:1067:A:C8 | 2.53 | 0.43 |
| 1:CA:380:G:C2 | 1:CA:384:G:C6 | 3.06 | 0.43 |
| 1:CA:579:G:C6 | 1:CA:580:U:C4 | 3.06 | 0.43 |
| 1:CA:89:C:C4 | 1:CA:90:U:C5 | 3.05 | 0.43 |
| 1:CA:926:G:C6 | 1:CA:1505:G:C6 | 3.06 | 0.43 |
| 1:CA:93:G:O2' | 1:CA:96:U:H5' | 2.18 | 0.43 |
| 4:CD:112:VAL:HG22 | 4:CD:116:GLN:OE1 | 2.18 | 0.43 |
| 5:CE:102:ALA:HB2 | 5:CE:120:THR:HG21 | 2.00 | 0.43 |
| 5:CE:84:PHE:CE2 | 5:CE:133:TYR:HD2 | 2.36 | 0.43 |
| 15:CO:54:ARG:O | 15:CO:57:LEU:HB2 | 2.18 | 0.43 |
| 17:CQ:41:LYS:HZ2 | 17:CQ:92:ARG:HH21 | 1.65 | 0.43 |
| 23:CX:59:A:C2' | 23:CX:60:U:H5' | 2.47 | 0.43 |
| 25:DA:1384:A:N3 | 25:DA:1405:U:H1' | 2.32 | 0.43 |
| 25:DA:1942:C:OP2 | 25:DA:1943:U:O2' | 2.20 | 0.43 |
| 25:DA:1991:U:H2' | 25:DA:1992:G:H5'' | 1.99 | 0.43 |
| 25:DA:2197:U:H1' | 25:DA:2198:A:C8 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:271(S):G:C2' | 25:DA:271(T):C:H5' | 2.47 | 0.43 |
| 25:DA:479:A:O2' | 25:DA:481:G:H5' | 2.18 | 0.43 |
| 25:DA:644:A:H4' | 25:DA:645:C:N4 | 2.33 | 0.43 |
| 25:DA:777:A:H2' | 25:DA:778:G:H8 | 1.83 | 0.43 |
| 27:DD:206:LEU:HD23 | 27:DD:206:LEU:HA | 1.68 | 0.43 |
| 27:DD:206:LEU:CD2 | 27:DD:211:ARG:HG2 | 2.46 | 0.43 |
| 29:DF:196:LEU:HA | 29:DF:196:LEU:HD23 | 1.66 | 0.43 |
| 30:DG:54:GLU:O | 30:DG:57:ALA:HB3 | 2.17 | 0.43 |
| 39:DT:16:ARG:HD2 | 39:DT:18:ASP:OD1 | 2.18 | 0.43 |
| 40:DU:16:LYS:HB3 | 40:DU:16:LYS:HE2 | 1.78 | 0.43 |
| 45:DZ:67:LEU:HA | 45:DZ:68:PRO:HD3 | 1.64 | 0.43 |
| 1:AA:428:G:O4' | 1:AA:430:A:C8 | 2.72 | 0.43 |
| 1:AA:432:A:OP2 | 1:AA:433:C:N4 | 2.43 | 0.43 |
| 2:AB:230:VAL:HG22 | 2:AB:231:GLU:H | 1.83 | 0.43 |
| 17:AQ:50:LYS:HD2 | 17:AQ:51:TYR:CZ | 2.53 | 0.43 |
| 25:BA:1072:U:H4' | 25:BA:1073:A:OP1 | 2.18 | 0.43 |
| 25:BA:1899:A:H5' | 25:BA:1900:G:OP2 | 2.18 | 0.43 |
| 25:BA:400:U:H1' | 25:BA:450:A:N3 | 2.34 | 0.43 |
| 25:BA:733:G:OP2 | 25:BA:733:G:H4' | 2.18 | 0.43 |
| 32:BI:10:GLU:O | 32:BI:12:LEU:N | 2.51 | 0.43 |
| 36:BQ:12:GLN:HG2 | 36:BQ:73:PRO:HD2 | 2.00 | 0.43 |
| 38:BS:35:ILE:HG12 | 38:BS:101:LEU:HD12 | 2.00 | 0.43 |
| 25:BA:1042:A:H4' | 40:BU:91:ASP:OD2 | 2.17 | 0.43 |
| 43:BX:40:LYS:HE2 | 61:BX:3103:HOH:O | 2.17 | 0.43 |
| 1:CA:1133:G:C2' | 1:CA:1134:G:H8 | 2.30 | 0.43 |
| 1:CA:1237:C:O2' | 1:CA:1300:G:N1 | 2.43 | 0.43 |
| 1:CA:1224:G:O2' | 1:CA:1322:C:OP1 | 2.26 | 0.43 |
| 1:CA:245:C:O2 | 1:CA:283:C:N3 | 2.51 | 0.43 |
| 1:CA:848:C:H2' | 1:CA:849:C:O4' | 2.18 | 0.43 |
| 1:CA:960:U:O2 | 1:CA:960:U:H2' | 2.17 | 0.43 |
| 3:CC:12:LEU:HA | 3:CC:16:ARG:HB3 | 2.00 | 0.43 |
| 3:CC:155:GLY:O | 3:CC:157:ILE:HG13 | 2.19 | 0.43 |
| 18:CR:66:LEU:O | 18:CR:70:ILE:HG13 | 2.18 | 0.43 |
| 19:CS:20:LEU:HA | 19:CS:23:ASN:ND2 | 2.34 | 0.43 |
| 24:CW:1:2QZ:CG2 | 24:CW:10:2QY:H83 | 2.48 | 0.43 |
| 25:DA:1268:A:C2 | 25:DA:2013:A:C4 | 3.06 | 0.43 |
| 25:DA:2274:A:C5 | 25:DA:2276:G:C8 | 3.05 | 0.43 |
| 25:DA:307:G:H21 | 25:DA:330:A:H62 | 1.66 | 0.43 |
| 25:DA:657:U:H2' | 25:DA:658:C:C6 | 2.52 | 0.43 |
| 25:DA:880:G:N2 | 25:DA:898:C:H1' | 2.33 | 0.43 |
| 25:DA:910:A:H2' | 25:DA:2264:C:O2' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DE:70:ALA:O | 28:DE:72:VAL:N | 2.42 | 0.43 |
| 29:DF:123:LEU:HD12 | 29:DF:124:LEU:N | 2.32 | 0.43 |
| 35:DP:47:ASP:HA | 35:DP:48:PRO:HD3 | 1.80 | 0.43 |
| 36:DQ:66:ILE:HG12 | 36:DQ:104:PHE:HE2 | 1.82 | 0.43 |
| 1:AA:1034:G:H5'' | 1:AA:1035:A:OP2 | 2.18 | 0.43 |
| 1:AA:1234:C:O2' | 1:AA:1235:U:H5' | 2.19 | 0.43 |
| 1:AA:180:U:O2' | 1:AA:181:G:H5' | 2.18 | 0.43 |
| 1:AA:375:U:C2 | 1:AA:376:G:C8 | 3.06 | 0.43 |
| 1:AA:400:C:H5'' | 4:AD:73:ARG:NH2 | 2.32 | 0.43 |
| 1:AA:414:A:C5 | 1:AA:431:A:C2 | 3.06 | 0.43 |
| 1:AA:584:G:H1 | 1:AA:757:U:H3 | 1.65 | 0.43 |
| 3:AC:24:ALA:HB1 | 3:AC:28:GLN:O | 2.19 | 0.43 |
| 4:AD:129:ASN:OD1 | 4:AD:145:GLU:N | 2.45 | 0.43 |
| 5:AE:52:PRO:HG2 | 5:AE:53:LEU:HD12 | 1.99 | 0.43 |
| 6:AF:22:GLU:OE2 | 6:AF:82:ARG:HG2 | 2.18 | 0.43 |
| 7:AG:22:LEU:HD13 | 7:AG:97:GLN:OE1 | 2.18 | 0.43 |
| 9:AI:53:VAL:C | 9:AI:55:ALA:H | 2.17 | 0.43 |
| 50:B4:62:ARG:C | 50:B4:64:GLY:HA2 | 2.38 | 0.43 |
| 25:BA:1541:A:C6 | 25:BA:1542:A:C6 | 3.06 | 0.43 |
| 25:BA:2307:C:C2' | 25:BA:2308:U:H5' | 2.48 | 0.43 |
| 25:BA:2671:G:O2' | 31:BH:175:LYS:NZ | 2.50 | 0.43 |
| 25:BA:2858:G:C8 | 39:BT:97:ALA:HB2 | 2.53 | 0.43 |
| 25:BA:609:A:H5' | 29:BF:89:VAL:HG21 | 1.99 | 0.43 |
| 25:BA:843:C:H2' | 25:BA:844:C:C6 | 2.54 | 0.43 |
| 27:BD:77:ALA:O | 27:BD:116:GLN:HG3 | 2.18 | 0.43 |
| 29:BF:81:PRO:HA | 29:BF:87:GLY:O | 2.17 | 0.43 |
| 37:BR:38:VAL:HB | 37:BR:39:PRO:HD3 | 2.00 | 0.43 |
| 45:BZ:126:VAL:HG13 | 45:BZ:161:VAL:HG23 | 1.99 | 0.43 |
| 1:CA:1119:C:H2' | 1:CA:1120:G:H8 | 1.82 | 0.43 |
| 1:CA:1134:G:H2' | 1:CA:1135:U:H5' | 2.00 | 0.43 |
| 1:CA:791:G:C6 | 1:CA:792:A:N7 | 2.86 | 0.43 |
| 2:CB:100:GLY:HA2 | 2:CB:103:THR:OG1 | 2.18 | 0.43 |
| 2:CB:95:GLN:HB2 | 2:CB:148:TYR:HD1 | 1.83 | 0.43 |
| 2:CB:187:LEU:HD13 | 2:CB:205:ASP:HA | 2.01 | 0.43 |
| 5:CE:93:PRO:HG2 | 8:CH:105:ARG:NE | 2.33 | 0.43 |
| 5:CE:148:VAL:HG21 | 8:CH:107:LEU:HD12 | 2.00 | 0.43 |
| 10:CJ:89:ASP:O | 10:CJ:91:PRO:HD3 | 2.18 | 0.43 |
| 16:CP:74:LEU:HD23 | 16:CP:79:VAL:HG11 | 2.00 | 0.43 |
| 19:CS:28:LYS:CB | 19:CS:29:ARG:HA | 2.48 | 0.43 |
| 9:CI:128:ARG:NH2 | 23:CX:33:U:OP2 | 2.50 | 0.43 |
| 49:D3:7:LYS:HG3 | 49:D3:34:GLU:HG3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:D8:50:LEU:HD23 | 54:D8:50:LEU:HA | 1.75 | 0.43 |
| 55:D9:13:LYS:HD3 | 55:D9:28:GLU:OE2 | 2.17 | 0.43 |
| 25:DA:1907:G:C2 | 25:DA:1908:C:C2 | 3.07 | 0.43 |
| 25:DA:2494:G:C4 | 25:DA:2495:G:C8 | 3.06 | 0.43 |
| 25:DA:2776:A:C6 | 25:DA:2782:G:H1' | 2.54 | 0.43 |
| 29:DF:11:VAL:HG21 | 29:DF:20:LEU:HB2 | 1.99 | 0.43 |
| 31:DH:54:ARG:HD3 | 31:DH:65:HIS:ND1 | 2.34 | 0.43 |
| 32:DI:48:GLU:OE2 | 32:DI:52:ARG:HD3 | 2.18 | 0.43 |
| 32:DI:61:ARG:HA | 32:DI:61:ARG:HD3 | 1.81 | 0.43 |
| 32:DI:92:VAL:CG2 | 32:DI:120:ILE:HB | 2.48 | 0.43 |
| 39:DT:53:ARG:HD3 | 39:DT:60:THR:OG1 | 2.18 | 0.43 |
| 40:DU:61:TRP:CH2 | 40:DU:93:LYS:HB2 | 2.53 | 0.43 |
| 1:AA:1162:C:H2' | 1:AA:1163:C:C6 | 2.53 | 0.43 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:N1 | 2.04 | 0.43 |
| 1:AA:170:U:O2' | 1:AA:171:A:H5' | 2.17 | 0.43 |
| 1:AA:298:A:C6 | 1:AA:299:G:C2 | 3.06 | 0.43 |
| 1:AA:442:C:H5' | 1:AA:443:C:OP2 | 2.18 | 0.43 |
| 1:AA:630:G:O2' | 1:AA:631:G:H5' | 2.18 | 0.43 |
| 2:AB:118:LEU:HD11 | 2:AB:141:GLU:HG2 | 2.01 | 0.43 |
| 3:AC:110:ASN:O | 3:AC:141:VAL:HG22 | 2.19 | 0.43 |
| 4:AD:184:LYS:HB3 | 4:AD:184:LYS:HZ2 | 1.83 | 0.43 |
| 6:AF:92:LYS:HB2 | 6:AF:92:LYS:HE2 | 1.83 | 0.43 |
| 1:AA:1125:U:C3' | 10:AJ:5:ARG:HH22 | 2.30 | 0.43 |
| 12:AL:77:LEU:HD21 | 12:AL:107:ALA:HA | 1.99 | 0.43 |
| 16:AP:68:ASP:O | 16:AP:71:ARG:HG2 | 2.17 | 0.43 |
| 47:B1:23:LYS:HB3 | 47:B1:29:GLY:HA3 | 1.99 | 0.43 |
| 47:B1:3:LYS:HB2 | 47:B1:61:ARG:HH11 | 1.83 | 0.43 |
| 48:B2:63:VAL:O | 48:B2:66:GLU:HB2 | 2.18 | 0.43 |
| 51:B5:40:LYS:HE2 | 51:B5:40:LYS:HB2 | 1.88 | 0.43 |
| 25:BA:1721:G:H1' | 25:BA:1723:A:N6 | 2.33 | 0.43 |
| 25:BA:715:G:H5' | 25:BA:716:G:OP2 | 2.18 | 0.43 |
| 33:BN:38:HIS:HD1 | 33:BN:38:HIS:H | 1.66 | 0.43 |
| 45:BZ:150:LEU:HB3 | 45:BZ:171:ILE:CD1 | 2.48 | 0.43 |
| 1:CA:1105:A:C2 | 1:CA:1106:G:N7 | 2.86 | 0.43 |
| 1:CA:1122:U:C4 | 1:CA:1123:A:N7 | 2.87 | 0.43 |
| 6:CF:25:ILE:CD1 | 6:CF:82:ARG:HH21 | 2.31 | 0.43 |
| 7:CG:94:ARG:O | 7:CG:97:GLN:HB3 | 2.19 | 0.43 |
| 8:CH:33:GLU:HG2 | 8:CH:48:TYR:CE2 | 2.53 | 0.43 |
| 9:CI:46:ALA:HA | 9:CI:78:LYS:HB2 | 2.01 | 0.43 |
| 11:CK:99:GLN:C | 11:CK:101:SER:H | 2.21 | 0.43 |
| 12:CL:75:HIS:ND1 | 12:CL:77:LEU:HB2 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:CS:12:ASP:OD2 | 19:CS:38:SER:OG | 2.36 | 0.43 |
| 46:D0:24:LYS:O | 46:D0:25:ARG:HD3 | 2.18 | 0.43 |
| 53:D7:22:MET:HA | 53:D7:28:ARG:HG2 | 2.00 | 0.43 |
| 25:DA:999:U:H3' | 25:DA:1154:G:O6 | 2.19 | 0.43 |
| 25:DA:2249:U:O4 | 61:DA:3947:HOH:O | 2.21 | 0.43 |
| 25:DA:644:A:H4' | 25:DA:645:C:C4 | 2.53 | 0.43 |
| 25:DA:729:G:C6 | 27:DD:208:LYS:HB2 | 2.53 | 0.43 |
| 26:DB:46:A:C5 | 26:DB:47:C:C4 | 3.06 | 0.43 |
| 27:DD:221:VAL:HG22 | 27:DD:226:MET:HE3 | 2.00 | 0.43 |
| 29:DF:36:VAL:HG11 | 29:DF:183:VAL:CG1 | 2.48 | 0.43 |
| 45:DZ:30:ASN:ND2 | 45:DZ:90:VAL:HB | 2.33 | 0.43 |
| 1:AA:147:G:C6 | 1:AA:148:G:C5 | 3.07 | 0.43 |
| 1:AA:353:A:H5' | 1:AA:353:A:H8 | 1.84 | 0.43 |
| 1:AA:416:G:C6 | 1:AA:417:C:C4 | 3.06 | 0.43 |
| 1:AA:631:G:H2' | 1:AA:632:A:H8 | 1.82 | 0.43 |
| 2:AB:146:GLN:O | 2:AB:150:SER:HB3 | 2.19 | 0.43 |
| 8:AH:110:ALA:HB3 | 8:AH:121:ASP:HB3 | 2.00 | 0.43 |
| 47:B1:82:LEU:HA | 47:B1:85:LEU:HD12 | 2.01 | 0.43 |
| 53:B7:24:THR:HG22 | 53:B7:26:GLY:N | 2.32 | 0.43 |
| 25:BA:1183:G:H2' | 25:BA:1184:G:O4' | 2.18 | 0.43 |
| 25:BA:1324:A:OP1 | 37:BR:36:THR:HG22 | 2.18 | 0.43 |
| 25:BA:2768:C:C4 | 55:B9:19:ARG:NH1 | 2.86 | 0.43 |
| 26:BB:73:A:C4 | 26:BB:105:A:C2 | 3.06 | 0.43 |
| 26:BB:66:A:H61 | 26:BB:109:C:H5' | 1.82 | 0.43 |
| 1:CA:1038:C:C2' | 1:CA:1039:C:H5' | 2.49 | 0.43 |
| 1:CA:1118:C:H2' | 1:CA:1119:C:C6 | 2.53 | 0.43 |
| 1:CA:35:G:C5 | 1:CA:36:C:N4 | 2.86 | 0.43 |
| 1:CA:401:C:H1' | 1:CA:622:A:H1' | 2.01 | 0.43 |
| 1:CA:683:G:C6 | 1:CA:684:A:C5 | 3.07 | 0.43 |
| 1:CA:688:G:H5' | 11:CK:46:GLY:C | 2.39 | 0.43 |
| 1:CA:545:C:H5' | 4:CD:72:GLU:CB | 2.49 | 0.43 |
| 19:CS:31:ILE:HG22 | 19:CS:33:THR:HG22 | 2.00 | 0.43 |
| 25:DA:443:A:H1' | 25:DA:1201:C:O4' | 2.18 | 0.43 |
| 25:DA:1784:A:H4' | 25:DA:1785:A:O5' | 2.19 | 0.43 |
| 25:DA:1859:A:N6 | 25:DA:1883:G:O2' | 2.52 | 0.43 |
| 25:DA:1970:A:OP2 | 61:DA:3905:HOH:O | 2.20 | 0.43 |
| 25:DA:483:A:O4' | 44:DY:48:ALA:HB1 | 2.18 | 0.43 |
| 26:DB:46:A:H2' | 26:DB:47:C:H6 | 1.84 | 0.43 |
| 30:DG:25:TYR:HB3 | 30:DG:30:GLU:CB | 2.47 | 0.43 |
| 35:DP:100:LEU:HD12 | 35:DP:112:LEU:HD11 | 1.99 | 0.43 |
| 37:DR:92:GLY:HA2 | 37:DR:94:TYR:CZ | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1030:C:H3' | 1:AA:1030(A):G:H4' | 2.01 | 0.43 |
| 1:AA:1142:G:H3' | 1:AA:1143:G:C8 | 2.53 | 0.43 |
| 1:AA:246:A:N1 | 1:AA:278:G:O2' | 2.39 | 0.43 |
| 1:AA:598:U:H2' | 1:AA:599:C:H6 | 1.84 | 0.43 |
| 1:AA:6:G:O2' | 1:AA:7:G:H5' | 2.18 | 0.43 |
| 1:AA:93:G:H2' | 1:AA:96:U:O4' | 2.19 | 0.43 |
| 3:AC:123:GLN:HG2 | 3:AC:128:PHE:HD2 | 1.84 | 0.43 |
| 6:AF:86:ARG:O | 6:AF:87:ARG:HG2 | 2.19 | 0.43 |
| 7:AG:27:ILE:CD1 | 7:AG:40:ALA:HA | 2.47 | 0.43 |
| 7:AG:50:ILE:HD12 | 7:AG:50:ILE:O | 2.19 | 0.43 |
| 23:AX:66:C:H2' | 23:AX:67:C:O4' | 2.17 | 0.43 |
| 23:AX:6:G:N2 | 23:AX:68:C:C2 | 2.86 | 0.43 |
| 49:B3:18:ASP:N | 49:B3:18:ASP:OD1 | 2.51 | 0.43 |
| 49:B3:4:LEU:O | 49:B3:36:VAL:HA | 2.18 | 0.43 |
| 50:B4:59:PHE:HA | 50:B4:61:ARG:HG2 | 2.00 | 0.43 |
| 25:BA:2306:C:OP2 | 38:BS:89:ARG:NH2 | 2.46 | 0.43 |
| 25:BA:2661:U:H2' | 25:BA:2662:U:H6 | 1.84 | 0.43 |
| 25:BA:403:C:H42 | 25:BA:425:G:H1 | 1.65 | 0.43 |
| 26:BB:24:G:N7 | 26:BB:56:G:H2' | 2.34 | 0.43 |
| 32:BI:87:LYS:HE3 | 32:BI:87:LYS:HB2 | 1.85 | 0.43 |
| 34:BO:2:ILE:HG23 | 34:BO:6:THR:HG21 | 2.01 | 0.43 |
| 1:CA:1032:G:H2' | 1:CA:1033:G:C8 | 2.54 | 0.43 |
| 1:CA:1071:C:H2' | 1:CA:1072:G:H8 | 1.84 | 0.43 |
| 1:CA:1093:A:N3 | 1:CA:1109:C:O2' | 2.47 | 0.43 |
| 1:CA:1134:G:N3 | 1:CA:1134:G:H2' | 2.32 | 0.43 |
| 1:CA:1151:A:C4 | 1:CA:1152:A:N7 | 2.87 | 0.43 |
| 1:CA:1312:G:O6 | 19:CS:2:PRO:HD2 | 2.18 | 0.43 |
| 1:CA:500:G:C6 | 1:CA:546:G:C2 | 3.07 | 0.43 |
| 1:CA:724:G:C2 | 1:CA:725:G:C8 | 3.06 | 0.43 |
| 3:CC:12:LEU:HD23 | 3:CC:12:LEU:HA | 1.86 | 0.43 |
| 4:CD:52:SER:O | 4:CD:56:VAL:HG23 | 2.19 | 0.43 |
| 7:CG:23:VAL:HG13 | 7:CG:43:PHE:CE2 | 2.53 | 0.43 |
| 10:CJ:11:PHE:CD1 | 10:CJ:67:THR:HG22 | 2.54 | 0.43 |
| 13:CM:15:VAL:O | 13:CM:19:LEU:HD22 | 2.19 | 0.43 |
| 13:CM:88:ARG:HG3 | 13:CM:98:VAL:HG12 | 2.00 | 0.43 |
| 23:CX:61:C:H2' | 23:CX:62:C:H6 | 1.82 | 0.43 |
| 47:D1:95:LEU:O | 47:D1:98:LEU:HB2 | 2.18 | 0.43 |
| 50:D4:62:ARG:HD3 | 50:D4:62:ARG:H | 1.83 | 0.43 |
| 25:DA:517:C:OP1 | 51:D5:16:ARG:NH2 | 2.51 | 0.43 |
| 55:D9:17:ILE:HG21 | 55:D9:26:ILE:HD11 | 2.01 | 0.43 |
| 25:DA:2330:G:H2' | 25:DA:2331:G:O4' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:1955:U:O4 | 25:DA:2554:U:H5 | 2.01 | 0.43 |
| 25:DA:271(X):G:C2 | 25:DA:271(Y):U:O4 | 2.71 | 0.43 |
| 25:DA:2636:U:H1' | 25:DA:2783:G:N2 | 2.34 | 0.43 |
| 26:DB:5:C:OP1 | 26:DB:61:G:O2' | 2.34 | 0.43 |
| 28:DE:147:PRO:HB2 | 28:DE:149:ARG:HG2 | 2.01 | 0.43 |
| 30:DG:179:PRO:HG3 | 50:D4:43:TYR:OH | 2.18 | 0.43 |
| 31:DH:169:VAL:HG12 | 31:DH:171:LEU:HD22 | 2.00 | 0.43 |
| 42:DW:88:ARG:NH1 | 42:DW:94:ASP:OD2 | 2.52 | 0.43 |
| 1:AA:1343:G:O2' | 9:AI:121:ARG:HD2 | 2.19 | 0.43 |
| 1:AA:389:A:C6 | 1:AA:390:C:H1' | 2.53 | 0.43 |
| 1:AA:436:C:H5'' | 4:AD:156:GLU:OE2 | 2.19 | 0.43 |
| 1:AA:625:G:O2' | 1:AA:626:U:H5' | 2.17 | 0.43 |
| 2:AB:124:SER:HB3 | 2:AB:125:PRO:HA | 2.01 | 0.43 |
| 6:AF:82:ARG:HB3 | 6:AF:85:VAL:HG23 | 2.00 | 0.43 |
| 10:AJ:81:THR:O | 10:AJ:85:LEU:HG | 2.18 | 0.43 |
| 21:AU:22:ARG:HA | 21:AU:23:PRO:HD3 | 1.65 | 0.43 |
| 25:BA:1034:A:H8 | 25:BA:1034:A:O5' | 2.02 | 0.43 |
| 25:BA:1095:C:H2' | 25:BA:1096:A:H8 | 1.84 | 0.43 |
| 25:BA:1558:G:H2' | 25:BA:1559:C:C6 | 2.54 | 0.43 |
| 25:BA:199:C:H2' | 25:BA:200:A:C8 | 2.54 | 0.43 |
| 25:BA:2843:G:H4' | 25:BA:2844:G:OP2 | 2.19 | 0.43 |
| 25:BA:316:C:C2 | 25:BA:373:G:C2 | 3.07 | 0.43 |
| 26:BB:96:U:H2' | 26:BB:97:G:C8 | 2.54 | 0.43 |
| 27:BD:206:LEU:HD23 | 27:BD:206:LEU:HA | 1.78 | 0.43 |
| 1:CA:1015:A:C6 | 1:CA:1016:A:C6 | 3.07 | 0.43 |
| 1:CA:1052:U:H5'' | 1:CA:1053:G:OP2 | 2.17 | 0.43 |
| 1:CA:1125:U:H2' | 1:CA:1127:G:N7 | 2.34 | 0.43 |
| 1:CA:1323:G:H4' | 1:CA:1363:C:N3 | 2.32 | 0.43 |
| 1:CA:445:G:H2' | 1:CA:446:G:H8 | 1.83 | 0.43 |
| 1:CA:937:A:H1' | 1:CA:1379:G:N2 | 2.34 | 0.43 |
| 3:CC:112:SER:O | 3:CC:115:LEU:HB2 | 2.19 | 0.43 |
| 4:CD:67:ILE:HG22 | 4:CD:68:TYR:CD1 | 2.54 | 0.43 |
| 8:CH:121:ASP:OD1 | 8:CH:121:ASP:N | 2.50 | 0.43 |
| 9:CI:96:LEU:HD22 | 9:CI:101:PHE:HB2 | 2.00 | 0.43 |
| 10:CJ:16:LEU:HD13 | 10:CJ:70:ARG:CG | 2.47 | 0.43 |
| 12:CL:34:ARG:HB3 | 12:CL:34:ARG:HE | 1.37 | 0.43 |
| 17:CQ:56:VAL:O | 17:CQ:77:VAL:HB | 2.19 | 0.43 |
| 48:D2:65:ASN:OD1 | 48:D2:69:ARG:NH1 | 2.49 | 0.43 |
| 25:DA:108:U:H2' | 25:DA:109:G:H8 | 1.84 | 0.43 |
| 25:DA:1475:G:C2 | 25:DA:1517:G:C2 | 3.06 | 0.43 |
| 25:DA:154:G:C6 | 25:DA:173:G:C6 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:2027:G:H2' | 25:DA:2028:U:O4' | 2.19 | 0.43 |
| 25:DA:242:G:H5'' | 54:D8:64:TYR:CE2 | 2.54 | 0.43 |
| 25:DA:2464:C:C2 | 25:DA:2487:G:C2 | 3.07 | 0.43 |
| 25:DA:2537:U:H2' | 25:DA:2538:C:C6 | 2.54 | 0.43 |
| 25:DA:2645:G:H4' | 25:DA:2732:G:O3' | 2.19 | 0.43 |
| 25:DA:1462:C:H4' | 25:DA:2703:C:H5' | 2.00 | 0.43 |
| 25:DA:31:C:H5' | 25:DA:1239:G:OP1 | 2.19 | 0.43 |
| 25:DA:702:G:C2 | 25:DA:731:C:C2 | 3.06 | 0.43 |
| 25:DA:763:G:H1' | 25:DA:765:G:O4' | 2.18 | 0.43 |
| 25:DA:844:C:C5 | 25:DA:845:G:C6 | 3.06 | 0.43 |
| 25:DA:863:A:H2' | 25:DA:864:G:C8 | 2.53 | 0.43 |
| 25:DA:952:G:C6 | 25:DA:953:A:N7 | 2.87 | 0.43 |
| 26:DB:28:C:H2' | 26:DB:29:A:O4' | 2.19 | 0.43 |
| 28:DE:181:LEU:HD12 | 28:DE:181:LEU:HA | 1.58 | 0.43 |
| 31:DH:3:ARG:HB3 | 31:DH:3:ARG:NH1 | 2.34 | 0.43 |
| 35:DP:96:THR:N | 35:DP:99:LEU:HD21 | 2.24 | 0.43 |
| 25:DA:863:A:OP1 | 36:DQ:22:LYS:HG3 | 2.18 | 0.43 |
| 42:DW:14:PRO:HG2 | 42:DW:78:GLU:CG | 2.46 | 0.43 |
| 45:DZ:121:HIS:HB3 | 45:DZ:123:ASP:O | 2.18 | 0.43 |
| 1:AA:113:G:H2' | 1:AA:114:U:C6 | 2.54 | 0.43 |
| 1:AA:1187:G:H2' | 1:AA:1188:A:H8 | 1.84 | 0.43 |
| 1:AA:312:C:H2' | 1:AA:313:A:H8 | 1.83 | 0.43 |
| 1:AA:637:G:C6 | 1:AA:638:G:C5 | 3.06 | 0.43 |
| 1:AA:975:A:H4' | 1:AA:976:G:C5' | 2.44 | 0.43 |
| 2:AB:180:LEU:O | 2:AB:181:PHE:HB2 | 2.18 | 0.43 |
| 4:AD:163:GLU:O | 4:AD:166:LYS:HG2 | 2.19 | 0.43 |
| 9:AI:19:LEU:HB3 | 9:AI:59:PHE:CD2 | 2.52 | 0.43 |
| 3:AC:12:LEU:HD11 | 14:AN:51:GLY:CA | 2.48 | 0.43 |
| 25:BA:866:A:C4 | 25:BA:1234:A:C2 | 3.06 | 0.43 |
| 25:BA:1854:G:N2 | 61:BA:3835:HOH:O | 2.41 | 0.43 |
| 25:BA:2418:U:OP2 | 25:BA:2418:U:H2' | 2.19 | 0.43 |
| 32:BI:93:THR:O | 32:BI:97:ILE:HG13 | 2.18 | 0.43 |
| 33:BN:48:MET:H | 33:BN:48:MET:HG3 | 1.70 | 0.43 |
| 36:BQ:58:PHE:HB3 | 36:BQ:61:GLY:O | 2.18 | 0.43 |
| 38:BS:14:VAL:O | 38:BS:18:ILE:HG12 | 2.17 | 0.43 |
| 40:BU:104:GLN:H | 40:BU:104:GLN:CD | 2.22 | 0.43 |
| 1:CA:1005:A:N6 | 1:CA:1024:G:O2' | 2.51 | 0.43 |
| 1:CA:1178:G:H2' | 1:CA:1180:A:OP2 | 2.18 | 0.43 |
| 1:CA:1385:G:C6 | 1:CA:1386:G:C5 | 3.07 | 0.43 |
| 1:CA:452:A:C2 | 1:CA:453:A:C4 | 3.06 | 0.43 |
| 1:CA:473:G:O2' | 1:CA:474:G:H5' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:961:U:OP2 | 1:CA:1223:C:O2' | 2.31 | 0.43 |
| 7:CG:111:ARG:HB2 | 7:CG:119:ARG:HD2 | 2.00 | 0.43 |
| 7:CG:65:ALA:HB3 | 7:CG:124:LEU:HD23 | 2.01 | 0.43 |
| 8:CH:37:ARG:NH2 | 8:CH:38:ILE:HG12 | 2.34 | 0.43 |
| 19:CS:23:ASN:OD1 | 19:CS:47:HIS:NE2 | 2.51 | 0.43 |
| 50:D4:59:PHE:HA | 50:D4:60:GLN:C | 2.39 | 0.43 |
| 25:DA:1005:C:C2 | 25:DA:1143:A:C5 | 3.06 | 0.43 |
| 25:DA:1578:U:H2' | 25:DA:1578:U:O2 | 2.18 | 0.43 |
| 25:DA:1759:A:H4' | 25:DA:2715:C:O4' | 2.19 | 0.43 |
| 25:DA:2318:G:H21 | 38:DS:3:ARG:CD | 2.31 | 0.43 |
| 25:DA:2409:G:H2' | 25:DA:2410:G:O4' | 2.18 | 0.43 |
| 25:DA:2494:G:C5 | 25:DA:2495:G:N7 | 2.87 | 0.43 |
| 25:DA:2563:U:O2 | 25:DA:2565:A:H8 | 2.01 | 0.43 |
| 25:DA:2679:A:C2 | 25:DA:2729:G:C2 | 3.07 | 0.43 |
| 25:DA:537:C:H2' | 25:DA:538:G:O4' | 2.19 | 0.43 |
| 25:DA:616:G:C2 | 25:DA:618:C:C2 | 3.06 | 0.43 |
| 25:DA:706:A:H2' | 25:DA:707:G:O4' | 2.19 | 0.43 |
| 25:DA:898:C:H6 | 25:DA:898:C:H3' | 1.84 | 0.43 |
| 26:DB:11:C:H3' | 26:DB:12:C:C6 | 2.54 | 0.43 |
| 28:DE:1:MET:O | 28:DE:84:PHE:HB2 | 2.19 | 0.43 |
| 25:DA:2094:G:P | 32:DI:22:LYS:HD2 | 2.59 | 0.43 |
| 45:DZ:161:VAL:O | 45:DZ:161:VAL:HG13 | 2.19 | 0.43 |
| 1:AA:114:U:H1' | 1:AA:353:A:H1' | 2.00 | 0.43 |
| 1:AA:1443:G:C2 | 1:AA:1460:A:N3 | 2.87 | 0.43 |
| 1:AA:161:A:H2' | 1:AA:162:A:H8 | 1.82 | 0.43 |
| 1:AA:298:A:H5'' | 1:AA:299:G:OP2 | 2.18 | 0.43 |
| 1:AA:309:G:H1' | 1:AA:608:A:C2 | 2.54 | 0.43 |
| 1:AA:327:A:C4 | 1:AA:329:A:C8 | 3.07 | 0.43 |
| 1:AA:357:G:O2' | 1:AA:358:U:H5' | 2.19 | 0.43 |
| 1:AA:433:C:H6 | 1:AA:433:C:O5' | 2.02 | 0.43 |
| 1:AA:601:C:O2 | 1:AA:637:G:N2 | 2.27 | 0.43 |
| 1:AA:625:G:C2' | 1:AA:626:U:H5' | 2.48 | 0.43 |
| 1:AA:901:A:C5 | 1:AA:902:G:H1' | 2.54 | 0.43 |
| 1:AA:958:A:C2 | 19:AS:55:LYS:HB2 | 2.54 | 0.43 |
| 2:AB:155:LEU:HD11 | 2:AB:159:PRO:HD3 | 2.01 | 0.43 |
| 3:AC:34:LEU:O | 3:AC:34:LEU:HD12 | 2.19 | 0.43 |
| 4:AD:23:GLY:HA3 | 4:AD:112:VAL:HB | 2.01 | 0.43 |
| 8:AH:40:ALA:HA | 8:AH:45:ILE:HG13 | 2.00 | 0.43 |
| 12:AL:85:ILE:HD12 | 12:AL:98:TYR:HB3 | 2.00 | 0.43 |
| 25:BA:1073:A:C2 | 25:BA:2500:A:H5' | 2.53 | 0.43 |
| 25:BA:1176:U:O2 | 25:BA:2047:C:H5'' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:1766:G:H3' | 25:BA:1767:A:C5' | 2.47 | 0.43 |
| 25:BA:2576:A:C2 | 25:BA:2659:U:H4' | 2.54 | 0.43 |
| 25:BA:302:A:H8 | 25:BA:302:A:P | 2.42 | 0.43 |
| 28:BE:73:GLU:HG3 | 28:BE:73:GLU:H | 1.54 | 0.43 |
| 29:BF:11:VAL:HG22 | 29:BF:125:LEU:HB2 | 2.00 | 0.43 |
| 29:BF:149:ASP:OD1 | 29:BF:149:ASP:N | 2.45 | 0.43 |
| 30:BG:150:ASP:OD2 | 30:BG:151:ALA:N | 2.52 | 0.43 |
| 36:BQ:37:LEU:HD21 | 36:BQ:130:LYS:HE2 | 2.00 | 0.43 |
| 39:BT:81:PRO:HG2 | 39:BT:82:LEU:HD12 | 2.01 | 0.43 |
| 42:BW:20:VAL:O | 42:BW:23:LEU:HB2 | 2.19 | 0.43 |
| 44:BY:91:GLU:CD | 44:BY:91:GLU:N | 2.72 | 0.43 |
| 45:BZ:19:ARG:HB2 | 45:BZ:19:ARG:HE | 1.65 | 0.43 |
| 45:BZ:44:PHE:CZ | 45:BZ:86:VAL:HG11 | 2.53 | 0.43 |
| 1:CA:1157:A:N6 | 1:CA:1180:A:N3 | 2.67 | 0.43 |
| 1:CA:402:G:C2' | 1:CA:403:C:H5' | 2.49 | 0.43 |
| 3:CC:16:ARG:HD2 | 3:CC:16:ARG:HA | 1.80 | 0.43 |
| 5:CE:12:LEU:HD22 | 5:CE:13:ILE:N | 2.33 | 0.43 |
| 25:DA:1332:G:OP1 | 61:DA:4077:HOH:O | 2.21 | 0.43 |
| 25:DA:1665:A:C4' | 34:DO:67:LYS:HB2 | 2.48 | 0.43 |
| 25:DA:1711:C:H2' | 25:DA:1712:C:C6 | 2.53 | 0.43 |
| 25:DA:2000:G:N7 | 61:DA:4008:HOH:O | 2.36 | 0.43 |
| 25:DA:2648:C:H2' | 25:DA:2649:U:C6 | 2.54 | 0.43 |
| 25:DA:322:A:P | 29:DF:169:ASN:HB2 | 2.59 | 0.43 |
| 25:DA:536:A:H2' | 25:DA:537:C:C6 | 2.54 | 0.43 |
| 25:DA:881:G:H1 | 25:DA:895:U:H3 | 1.67 | 0.43 |
| 28:DE:163:GLU:HG2 | 28:DE:164:ARG:H | 1.83 | 0.43 |
| 30:DG:23:PHE:HB2 | 30:DG:25:TYR:CZ | 2.53 | 0.43 |
| 31:DH:95:ARG:HB2 | 31:DH:128:PRO:HB2 | 2.01 | 0.43 |
| 36:DQ:42:ILE:HD13 | 36:DQ:97:VAL:CG2 | 2.49 | 0.43 |
| 37:DR:96:ARG:HD3 | 37:DR:98:LEU:HD11 | 2.00 | 0.43 |
| 39:DT:88:ILE:HG13 | 39:DT:91:ARG:NH2 | 2.34 | 0.43 |
| 1:AA:1362:C:H2' | 1:AA:1363:C:H5'' | 2.00 | 0.43 |
| 1:AA:309:G:O2' | 1:AA:607:A:N1 | 2.48 | 0.43 |
| 1:AA:687:A:N3 | 1:AA:688:G:H1' | 2.33 | 0.43 |
| 2:AB:192:SER:O | 2:AB:194:PRO:HD3 | 2.18 | 0.43 |
| 4:AD:45:GLN:HB3 | 4:AD:45:GLN:HE21 | 1.59 | 0.43 |
| 13:AM:40:ASN:OD1 | 13:AM:42:ALA:HB3 | 2.19 | 0.43 |
| 16:AP:22:THR:HA | 16:AP:33:ILE:HG12 | 2.00 | 0.43 |
| 20:AT:90:GLN:O | 20:AT:93:GLU:HB3 | 2.19 | 0.43 |
| 50:B4:59:PHE:HA | 50:B4:61:ARG:H | 1.83 | 0.43 |
| 25:BA:1752:G:C6 | 25:BA:1753:U:C4 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:2070:G:C5 | 25:BA:2071:G:C8 | 3.07 | 0.43 |
| 25:BA:2490:A:H2' | 25:BA:2491:G:O4' | 2.19 | 0.43 |
| 25:BA:2830:A:O2' | 25:BA:2831:A:OP1 | 2.37 | 0.43 |
| 25:BA:64:C:H2' | 25:BA:65:C:H6 | 1.83 | 0.43 |
| 26:BB:1:U:H2' | 26:BB:2:C:C6 | 2.53 | 0.43 |
| 31:BH:89:ILE:O | 31:BH:129:THR:HG22 | 2.19 | 0.43 |
| 32:BI:65:ALA:HB1 | 32:BI:136:VAL:HG11 | 1.99 | 0.43 |
| 36:BQ:39:PRO:HA | 36:BQ:97:VAL:O | 2.19 | 0.43 |
| 45:BZ:5:LEU:O | 45:BZ:59:LEU:HA | 2.19 | 0.43 |
| 1:CA:1198:G:H2' | 1:CA:1199:U:C6 | 2.54 | 0.43 |
| 1:CA:1375:A:O2' | 7:CG:29:LYS:NZ | 2.50 | 0.43 |
| 1:CA:80:G:N2 | 1:CA:90:U:H1' | 2.34 | 0.43 |
| 4:CD:19:LEU:O | 4:CD:21:LEU:N | 2.51 | 0.43 |
| 5:CE:11:ILE:HB | 5:CE:31:LEU:HB3 | 2.00 | 0.43 |
| 5:CE:92:LYS:HA | 5:CE:93:PRO:HD2 | 1.84 | 0.43 |
| 7:CG:101:LEU:O | 7:CG:104:LEU:HB2 | 2.18 | 0.43 |
| 11:CK:48:ILE:C | 11:CK:50:TYR:H | 2.21 | 0.43 |
| 12:CL:55:VAL:HG12 | 12:CL:69:TYR:HA | 2.01 | 0.43 |
| 13:CM:97:PRO:HB3 | 13:CM:101:GLN:OE1 | 2.19 | 0.43 |
| 15:CO:4:THR:OG1 | 15:CO:7:GLU:OE1 | 2.27 | 0.43 |
| 15:CO:82:ILE:HB | 15:CO:87:ILE:HB | 2.01 | 0.43 |
| 1:CA:261:U:C5 | 20:CT:79:ARG:CZ | 3.02 | 0.43 |
| 48:D2:35:LEU:HA | 48:D2:35:LEU:HD23 | 1.80 | 0.43 |
| 54:D8:22:VAL:CG2 | 54:D8:59:LYS:HG3 | 2.48 | 0.43 |
| 25:DA:1169:G:O5' | 25:DA:1169:G:H8 | 2.01 | 0.43 |
| 25:DA:196:A:N3 | 25:DA:196:A:H2' | 2.34 | 0.43 |
| 25:DA:2257:U:H2' | 25:DA:2258:C:C6 | 2.54 | 0.43 |
| 25:DA:2302:G:C6 | 25:DA:2315:G:C6 | 3.06 | 0.43 |
| 25:DA:1638:C:H5'' | 25:DA:2710:C:O2' | 2.19 | 0.43 |
| 25:DA:538:G:H2' | 25:DA:539:G:H8 | 1.83 | 0.43 |
| 25:DA:55:G:H2' | 25:DA:56:A:C8 | 2.54 | 0.43 |
| 25:DA:601:C:O2' | 25:DA:605:C:H5'' | 2.19 | 0.43 |
| 25:DA:854:G:H2' | 25:DA:855:G:C8 | 2.48 | 0.43 |
| 25:DA:927:G:H2' | 25:DA:928:G:C8 | 2.53 | 0.43 |
| 27:DD:139:GLY:H | 27:DD:165:ILE:HB | 1.84 | 0.43 |
| 30:DG:16:ARG:HA | 30:DG:16:ARG:HD2 | 1.69 | 0.43 |
| 25:DA:2310:A:H61 | 30:DG:79:ASN:ND2 | 2.17 | 0.43 |
| 30:DG:76:SER:CB | 30:DG:84:LYS:H | 2.32 | 0.43 |
| 25:DA:2675:A:H4' | 34:DO:29:ASN:ND2 | 2.34 | 0.43 |
| 34:DO:34:THR:O | 34:DO:37:ASP:HB2 | 2.19 | 0.43 |
| 1:AA:1129:C:H1' | 1:AA:1130:A:N7 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1445:C:C4 | 1:AA:1446:U:C4 | 3.07 | 0.42 |
| 1:AA:453:A:C5 | 1:AA:454:C:C4 | 3.07 | 0.42 |
| 3:AC:44:GLU:HG2 | 3:AC:52:LEU:CD2 | 2.49 | 0.42 |
| 8:AH:73:ASP:OD2 | 8:AH:75:ARG:NH1 | 2.52 | 0.42 |
| 9:AI:64:THR:CG2 | 9:AI:66:ARG:HD2 | 2.49 | 0.42 |
| 25:BA:1702:A:H3' | 25:BA:1703:C:C6 | 2.53 | 0.42 |
| 25:BA:2331:G:C8 | 25:BA:2332:A:C2 | 3.07 | 0.42 |
| 25:BA:2658:C:H2' | 25:BA:2659:U:O4' | 2.19 | 0.42 |
| 25:BA:771:U:H2' | 25:BA:772:G:O4' | 2.18 | 0.42 |
| 26:BB:4:C:H2' | 26:BB:5:C:O4' | 2.19 | 0.42 |
| 30:BG:96:ARG:O | 30:BG:99:MET:HB3 | 2.19 | 0.42 |
| 25:BA:1712:A:C4' | 34:BO:67:LYS:HB2 | 2.49 | 0.42 |
| 1:CA:1317:C:OP1 | 14:CN:17:LYS:HG2 | 2.19 | 0.42 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:H6 | 1.82 | 0.42 |
| 1:CA:1445:C:C2 | 1:CA:1458:G:C2 | 3.07 | 0.42 |
| 1:CA:414:A:C5 | 1:CA:431:A:C2 | 3.07 | 0.42 |
| 1:CA:491:G:C2 | 1:CA:492:G:C4 | 3.07 | 0.42 |
| 1:CA:939:G:H2' | 1:CA:940:C:C6 | 2.54 | 0.42 |
| 7:CG:69:VAL:HG22 | 7:CG:135:VAL:HG22 | 2.01 | 0.42 |
| 1:CA:664:G:H5'' | 18:CR:64:ARG:NH2 | 2.33 | 0.42 |
| 25:DA:2076:U:H6 | 25:DA:2076:U:O5' | 2.02 | 0.42 |
| 25:DA:272(B):G:H2' | 25:DA:272(C):G:C8 | 2.54 | 0.42 |
| 25:DA:879:G:C8 | 25:DA:880:G:C8 | 3.07 | 0.42 |
| 26:DB:28:C:OP1 | 38:DS:36:TYR:OH | 2.34 | 0.42 |
| 29:DF:138:GLU:O | 29:DF:141:ALA:HB3 | 2.19 | 0.42 |
| 30:DG:109:VAL:O | 30:DG:113:ARG:HB2 | 2.19 | 0.42 |
| 30:DG:33:ARG:O | 30:DG:161:THR:HG23 | 2.18 | 0.42 |
| 33:DN:96:GLU:N | 33:DN:96:GLU:OE2 | 2.46 | 0.42 |
| 29:DF:31:HIS:HB2 | 35:DP:9:ASN:OD1 | 2.19 | 0.42 |
| 1:AA:1100:C:O2' | 1:AA:1102:A:OP1 | 2.34 | 0.42 |
| 1:AA:1446:U:O2' | 1:AA:1447:A:O5' | 2.38 | 0.42 |
| 1:AA:317:G:C6 | 1:AA:318:G:C5 | 3.07 | 0.42 |
| 1:AA:39:G:C6 | 1:AA:40:C:C4 | 3.07 | 0.42 |
| 1:AA:410:G:N1 | 1:AA:431:A:OP2 | 2.48 | 0.42 |
| 2:AB:54:THR:HG21 | 2:AB:201:ILE:HD11 | 2.00 | 0.42 |
| 2:AB:54:THR:HG23 | 2:AB:199:TYR:HB3 | 2.00 | 0.42 |
| 4:AD:110:PHE:HD1 | 4:AD:110:PHE:N | 2.16 | 0.42 |
| 4:AD:15:GLU:OE2 | 4:AD:66:ARG:NH1 | 2.52 | 0.42 |
| 4:AD:13:ARG:HB2 | 4:AD:40:PRO:HD3 | 2.00 | 0.42 |
| 8:AH:51:VAL:HG21 | 8:AH:60:ARG:HB2 | 2.00 | 0.42 |
| 10:AJ:16:LEU:HD21 | 10:AJ:70:ARG:CG | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:6:THR:HG23 | 12:AL:9:GLN:OE1 | 2.19 | 0.42 |
| 20:AT:30:LYS:HA | 20:AT:33:ILE:HD12 | 2.00 | 0.42 |
| 51:B5:16:ARG:O | 51:B5:20:ARG:HG3 | 2.19 | 0.42 |
| 54:B8:39:LYS:HA | 54:B8:42:ARG:NH1 | 2.34 | 0.42 |
| 25:BA:21:A:H2' | 25:BA:22:C:O4' | 2.19 | 0.42 |
| 25:BA:2442:A:N3 | 25:BA:2442:A:H2' | 2.33 | 0.42 |
| 25:BA:311:C:H2' | 25:BA:312:C:C6 | 2.51 | 0.42 |
| 25:BA:873:U:H2' | 25:BA:875:U:O4' | 2.19 | 0.42 |
| 26:BB:37:C:C5 | 26:BB:38:C:C4 | 3.06 | 0.42 |
| 34:BO:115:VAL:HG13 | 34:BO:121:VAL:HG21 | 2.00 | 0.42 |
| 38:BS:6:ALA:O | 38:BS:10:ARG:HB2 | 2.18 | 0.42 |
| 45:BZ:15:PRO:O | 45:BZ:19:ARG:HB2 | 2.19 | 0.42 |
| 1:CA:1390:U:H2' | 1:CA:1391:U:C6 | 2.54 | 0.42 |
| 1:CA:339:C:H2' | 1:CA:340:U:C6 | 2.54 | 0.42 |
| 1:CA:382:A:H2' | 1:CA:383:A:H8 | 1.78 | 0.42 |
| 2:CB:23:ARG:HB2 | 2:CB:23:ARG:HH11 | 1.82 | 0.42 |
| 1:CA:1205:U:O2' | 3:CC:195:VAL:HG23 | 2.19 | 0.42 |
| 5:CE:10:MET:HG2 | 5:CE:13:ILE:HD11 | 2.00 | 0.42 |
| 13:CM:23:TYR:CD2 | 13:CM:70:LEU:HD13 | 2.54 | 0.42 |
| 17:CQ:5:VAL:O | 17:CQ:6:LEU:HD13 | 2.19 | 0.42 |
| 23:CX:22:G:H2' | 23:CX:23:C:C6 | 2.54 | 0.42 |
| 25:DA:77:C:H5'' | 48:D2:10:LEU:HD21 | 2.01 | 0.42 |
| 25:DA:1412:A:C2 | 25:DA:1591:G:C2 | 3.07 | 0.42 |
| 25:DA:1514:U:H2' | 25:DA:1515:G:C8 | 2.55 | 0.42 |
| 25:DA:1515:G:H2' | 25:DA:1516:C:C6 | 2.55 | 0.42 |
| 25:DA:2193:G:H2' | 25:DA:2194:G:C8 | 2.54 | 0.42 |
| 25:DA:2408:U:H2' | 25:DA:2409:G:H8 | 1.84 | 0.42 |
| 25:DA:532:A:N7 | 25:DA:2021:C:O2' | 2.42 | 0.42 |
| 25:DA:754:C:H4' | 25:DA:1272:A:N6 | 2.34 | 0.42 |
| 25:DA:768:G:C6 | 25:DA:769:G:C5 | 3.07 | 0.42 |
| 25:DA:945:A:C4 | 25:DA:2448:A:C2 | 3.07 | 0.42 |
| 28:DE:14:ILE:HB | 39:DT:14:TYR:CE2 | 2.54 | 0.42 |
| 29:DF:37:VAL:HA | 29:DF:40:GLN:HB2 | 2.00 | 0.42 |
| 30:DG:121:ASN:HB3 | 30:DG:124:SER:HB2 | 2.00 | 0.42 |
| 34:DO:7:TYR:CZ | 34:DO:44:LYS:HG3 | 2.54 | 0.42 |
| 42:DW:46:PHE:O | 42:DW:50:VAL:HG23 | 2.19 | 0.42 |
| 25:DA:1338:G:N7 | 43:DX:62:LYS:NZ | 2.64 | 0.42 |
| 45:DZ:7:ALA:O | 45:DZ:62:PRO:HD3 | 2.19 | 0.42 |
| 1:AA:1006:C:H2' | 1:AA:1007:C:O4' | 2.19 | 0.42 |
| 1:AA:1091:U:H2' | 1:AA:1093:A:OP2 | 2.19 | 0.42 |
| 1:AA:1114:C:H42 | 1:AA:1186:G:H1 | 1.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:64:VAL:HG13 | 3:AC:99:VAL:HA | 2.01 | 0.42 |
| 4:AD:119:GLN:HG2 | 4:AD:123:HIS:NE2 | 2.35 | 0.42 |
| 7:AG:51:GLN:O | 7:AG:55:GLY:HA2 | 2.19 | 0.42 |
| 9:AI:3:GLN:CG | 9:AI:20:ARG:HE | 2.32 | 0.42 |
| 12:AL:24:VAL:CG1 | 12:AL:27:LEU:HD22 | 2.44 | 0.42 |
| 1:AA:310:G:H5'' | 16:AP:31:LYS:HB2 | 2.02 | 0.42 |
| 19:AS:64:GLU:O | 19:AS:67:VAL:HG23 | 2.19 | 0.42 |
| 50:B4:8:LYS:HB3 | 50:B4:8:LYS:HE2 | 1.70 | 0.42 |
| 25:BA:1766:G:H8 | 25:BA:1770:A:H62 | 1.66 | 0.42 |
| 25:BA:287:G:O2' | 25:BA:448:U:OP2 | 2.26 | 0.42 |
| 33:BN:42:TRP:CE3 | 40:BU:63:VAL:HG11 | 2.54 | 0.42 |
| 36:BQ:14:ARG:HG2 | 36:BQ:41:TRP:HH2 | 1.83 | 0.42 |
| 25:BA:2695:C:OP1 | 39:BT:53:ARG:NH2 | 2.52 | 0.42 |
| 43:BX:12:VAL:HG22 | 43:BX:29:TRP:CE2 | 2.54 | 0.42 |
| 45:BZ:111:VAL:HG12 | 45:BZ:112:ARG:N | 2.34 | 0.42 |
| 1:CA:1122:U:C5 | 1:CA:1123:A:N7 | 2.88 | 0.42 |
| 1:CA:448:A:P | 1:CA:485:G:H22 | 2.42 | 0.42 |
| 1:CA:9:G:O6 | 1:CA:558:G:H2' | 2.20 | 0.42 |
| 1:CA:833:U:H2' | 1:CA:834:C:C6 | 2.54 | 0.42 |
| 2:CB:187:LEU:HD23 | 2:CB:201:ILE:HG22 | 2.00 | 0.42 |
| 1:CA:19:C:H5'' | 5:CE:86:ALA:HB3 | 2.02 | 0.42 |
| 8:CH:28:ALA:HB3 | 8:CH:57:PRO:HB2 | 2.02 | 0.42 |
| 1:CA:1014:A:H4' | 19:CS:14:HIS:CE1 | 2.54 | 0.42 |
| 47:D1:52:ARG:NH2 | 47:D1:57:GLU:HB2 | 2.34 | 0.42 |
| 50:D4:64:GLY:C | 50:D4:66:SER:N | 2.71 | 0.42 |
| 25:DA:1167:U:O2 | 25:DA:1183:G:N2 | 2.52 | 0.42 |
| 25:DA:180:G:H5'' | 25:DA:181:A:P | 2.59 | 0.42 |
| 25:DA:2275:C:H5' | 25:DA:2275:C:H6 | 1.84 | 0.42 |
| 25:DA:289:A:H2' | 25:DA:290:G:C8 | 2.54 | 0.42 |
| 25:DA:652(D):C:C2' | 25:DA:652(E):G:H5' | 2.49 | 0.42 |
| 25:DA:660:G:H5' | 29:DF:99:TYR:CD2 | 2.55 | 0.42 |
| 25:DA:760:G:H2' | 25:DA:761:A:O4' | 2.19 | 0.42 |
| 25:DA:934:G:H2' | 25:DA:935:C:C6 | 2.55 | 0.42 |
| 25:DA:837:C:N3 | 25:DA:941:A:N6 | 2.67 | 0.42 |
| 29:DF:184:TYR:O | 29:DF:188:ARG:HG3 | 2.20 | 0.42 |
| 38:DS:69:VAL:O | 38:DS:72:ALA:HB3 | 2.18 | 0.42 |
| 1:AA:1086:U:C2' | 1:AA:1087:G:H5' | 2.49 | 0.42 |
| 1:AA:1316:G:N2 | 1:AA:1318:A:H3' | 2.34 | 0.42 |
| 1:AA:1405:G:O4' | 1:AA:1519:A:H4' | 2.20 | 0.42 |
| 1:AA:1524:C:OP1 | 11:AK:120:ARG:NH1 | 2.50 | 0.42 |
| 1:AA:922:G:H2' | 1:AA:923:A:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:998:G:H2' | 1:AA:999:C:C6 | 2.55 | 0.42 |
| 8:AH:104:ARG:HG3 | 8:AH:138:TRP:CD2 | 2.54 | 0.42 |
| 16:AP:6:LEU:HB3 | 16:AP:17:TYR:CD2 | 2.54 | 0.42 |
| 16:AP:34:GLU:OE2 | 16:AP:55:ARG:NH2 | 2.39 | 0.42 |
| 25:BA:2760:G:C2 | 25:BA:2769:U:C5 | 3.07 | 0.42 |
| 25:BA:776:G:OP2 | 27:BD:13:ARG:NH1 | 2.45 | 0.42 |
| 25:BA:895:G:O6 | 25:BA:974:G:H2' | 2.20 | 0.42 |
| 30:BG:86:MET:HA | 30:BG:87:PRO:HD3 | 1.90 | 0.42 |
| 31:BH:17:VAL:HG21 | 31:BH:50:VAL:HG21 | 2.01 | 0.42 |
| 39:BT:7:ILE:O | 39:BT:11:GLU:HG3 | 2.19 | 0.42 |
| 45:BZ:111:VAL:HG12 | 45:BZ:112:ARG:H | 1.84 | 0.42 |
| 1:CA:1023:G:C4 | 1:CA:1024:G:C8 | 3.07 | 0.42 |
| 1:CA:1005:A:H1' | 1:CA:1036:G:C6 | 2.55 | 0.42 |
| 1:CA:1120:G:C6 | 1:CA:1154:G:N2 | 2.87 | 0.42 |
| 1:CA:1210:C:H2' | 1:CA:1211:U:H5'' | 2.01 | 0.42 |
| 1:CA:35:G:H2' | 1:CA:36:C:C6 | 2.55 | 0.42 |
| 1:CA:383:A:H5'' | 1:CA:384:G:OP2 | 2.20 | 0.42 |
| 1:CA:473:G:H2' | 1:CA:474:G:H8 | 1.81 | 0.42 |
| 1:CA:540:G:H2' | 1:CA:541:G:O4' | 2.19 | 0.42 |
| 1:CA:590:C:H2' | 1:CA:591:U:H6 | 1.84 | 0.42 |
| 1:CA:97:G:O2' | 1:CA:98:G:O4' | 2.35 | 0.42 |
| 2:CB:130:ARG:HA | 2:CB:131:PRO:HD3 | 1.80 | 0.42 |
| 4:CD:90:GLY:HA2 | 4:CD:204:ILE:HD11 | 2.01 | 0.42 |
| 6:CF:76:ALA:O | 6:CF:80:ARG:HG3 | 2.20 | 0.42 |
| 9:CI:33:PHE:CE1 | 9:CI:43:ALA:HB1 | 2.46 | 0.42 |
| 9:CI:99:LEU:HB3 | 9:CI:101:PHE:CE1 | 2.54 | 0.42 |
| 16:CP:53:VAL:O | 16:CP:57:ARG:HB2 | 2.19 | 0.42 |
| 51:D5:48:GLU:O | 51:D5:60:VAL:HG11 | 2.20 | 0.42 |
| 52:D6:11:LEU:HB2 | 52:D6:21:TYR:HB2 | 2.00 | 0.42 |
| 25:DA:1418:G:O5' | 25:DA:1418:G:H8 | 2.03 | 0.42 |
| 25:DA:1517:G:C6 | 25:DA:1518:U:C4 | 3.07 | 0.42 |
| 25:DA:2298:A:C8 | 25:DA:2299:G:C8 | 3.07 | 0.42 |
| 25:DA:2419:U:H2' | 25:DA:2420:C:C6 | 2.54 | 0.42 |
| 25:DA:2477:C:N4 | 55:D9:10:ILE:HG23 | 2.34 | 0.42 |
| 25:DA:836:G:H2' | 25:DA:837:C:C6 | 2.53 | 0.42 |
| 25:DA:871:U:H5'' | 36:DQ:69:PHE:CE2 | 2.54 | 0.42 |
| 27:DD:134:ARG:NH1 | 27:DD:188:GLU:OE2 | 2.51 | 0.42 |
| 29:DF:110:LEU:HD21 | 29:DF:181:LEU:HG | 2.00 | 0.42 |
| 31:DH:88:LEU:HD23 | 31:DH:165:ALA:HA | 2.01 | 0.42 |
| 34:DO:2:ILE:HB | 34:DO:33:ALA:HB3 | 2.01 | 0.42 |
| 38:DS:24:LEU:HD23 | 38:DS:24:LEU:HA | 1.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:DS:78:LEU:HD11 | 38:DS:108:GLY:O | 2.18 | 0.42 |
| 1:AA:1129:C:N4 | 1:AA:1143:G:N1 | 2.40 | 0.42 |
| 1:AA:1486:G:H2' | 1:AA:1487:G:C1' | 2.50 | 0.42 |
| 1:AA:448:A:H2' | 1:AA:449:C:C6 | 2.54 | 0.42 |
| 1:AA:575:G:O2' | 1:AA:821:G:H5' | 2.19 | 0.42 |
| 2:AB:170:GLU:O | 2:AB:174:VAL:HG23 | 2.20 | 0.42 |
| 1:AA:406:G:N2 | 4:AD:119:GLN:HE22 | 2.18 | 0.42 |
| 19:AS:19:VAL:O | 19:AS:22:LEU:HB2 | 2.19 | 0.42 |
| 47:B1:98:LEU:HA | 47:B1:98:LEU:HD23 | 1.88 | 0.42 |
| 50:B4:53:GLU:O | 50:B4:56:VAL:HG13 | 2.20 | 0.42 |
| 25:BA:2245:U:H2' | 25:BA:2246:G:C8 | 2.54 | 0.42 |
| 25:BA:904:C:N4 | 25:BA:905:U:O4 | 2.52 | 0.42 |
| 26:BB:16:G:C6 | 26:BB:69:G:C2 | 3.08 | 0.42 |
| 28:BE:49:LEU:HA | 28:BE:49:LEU:HD12 | 1.89 | 0.42 |
| 34:BO:10:VAL:HG21 | 34:BO:16:ALA:HB3 | 2.01 | 0.42 |
| 37:BR:83:ILE:O | 37:BR:86:ARG:HG2 | 2.20 | 0.42 |
| 1:CA:1023:G:H3' | 1:CA:1024:G:C8 | 2.54 | 0.42 |
| 1:CA:1179:A:C6 | 1:CA:1180:A:C8 | 3.07 | 0.42 |
| 1:CA:373:A:H2' | 1:CA:374:A:H8 | 1.84 | 0.42 |
| 1:CA:391:G:C6 | 1:CA:392:G:C5 | 3.07 | 0.42 |
| 1:CA:460:G:C6 | 1:CA:470:C:H5'' | 2.53 | 0.42 |
| 1:CA:622:A:H3' | 1:CA:623:C:H6 | 1.84 | 0.42 |
| 1:CA:973:G:H3' | 1:CA:974:A:H5'' | 2.01 | 0.42 |
| 4:CD:110:PHE:N | 4:CD:110:PHE:CD1 | 2.87 | 0.42 |
| 5:CE:40:ARG:HH21 | 5:CE:68:GLU:HA | 1.82 | 0.42 |
| 16:CP:5:ARG:HH12 | 16:CP:28:ARG:HA | 1.84 | 0.42 |
| 24:CW:9:MVA:CB | 24:CW:10:2QY:H82 | 2.49 | 0.42 |
| 24:CW:9:MVA:O | 24:CW:10:2QY:CD2 | 2.63 | 0.42 |
| 25:DA:1636:C:H2' | 25:DA:1637:A:H8 | 1.80 | 0.42 |
| 25:DA:1790:C:H5'' | 25:DA:1791:A:OP1 | 2.19 | 0.42 |
| 25:DA:1815:A:P | 27:DD:54:ARG:NH2 | 2.92 | 0.42 |
| 25:DA:2005:A:H5'' | 25:DA:2006:C:OP2 | 2.20 | 0.42 |
| 25:DA:2055:C:H5' | 25:DA:2056:G:O5' | 2.19 | 0.42 |
| 25:DA:829:A:N7 | 25:DA:2248:C:H5' | 2.35 | 0.42 |
| 25:DA:2298:A:N6 | 25:DA:2321:G:H1 | 2.18 | 0.42 |
| 25:DA:2740:A:C6 | 25:DA:2764:A:C8 | 3.07 | 0.42 |
| 25:DA:319:C:N4 | 25:DA:320:A:C6 | 2.87 | 0.42 |
| 25:DA:442:G:O4' | 29:DF:46:ARG:HG3 | 2.19 | 0.42 |
| 25:DA:576:U:H2' | 25:DA:577:G:C8 | 2.55 | 0.42 |
| 25:DA:608:A:C6 | 25:DA:609:A:C6 | 3.07 | 0.42 |
| 25:DA:900:A:C2' | 25:DA:901:A:H8 | 2.32 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DP:6:LEU:HA | 35:DP:6:LEU:HD23 | 1.76 | 0.42 |
| 35:DP:83:VAL:O | 35:DP:115:LEU:N | 2.44 | 0.42 |
| 36:DQ:18:LYS:HE3 | 36:DQ:18:LYS:HB2 | 1.91 | 0.42 |
| 38:DS:103:GLU:O | 38:DS:107:GLU:HG3 | 2.20 | 0.42 |
| 45:DZ:122:ARG:HH11 | 45:DZ:122:ARG:HG2 | 1.84 | 0.42 |
| 45:DZ:95:PRO:HA | 45:DZ:129:SER:HA | 2.00 | 0.42 |
| 45:DZ:150:LEU:HD12 | 45:DZ:150:LEU:HA | 1.58 | 0.42 |
| 1:AA:1041:A:C2' | 1:AA:1042:G:H5' | 2.49 | 0.42 |
| 1:AA:271:C:H2' | 1:AA:272:C:C6 | 2.54 | 0.42 |
| 4:AD:158:ILE:HB | 4:AD:162:LEU:HD12 | 2.01 | 0.42 |
| 1:AA:1346:A:H5'' | 9:AI:120:ARG:NH1 | 2.34 | 0.42 |
| 13:AM:20:THR:C | 13:AM:22:ILE:H | 2.21 | 0.42 |
| 14:AN:45:ARG:HG2 | 14:AN:49:HIS:CD2 | 2.53 | 0.42 |
| 15:AO:5:LYS:CD | 15:AO:5:LYS:H | 2.31 | 0.42 |
| 23:AX:19:G:C5 | 23:AX:57:A:C2 | 3.07 | 0.42 |
| 48:B2:3:LEU:HA | 48:B2:3:LEU:HD23 | 1.76 | 0.42 |
| 25:BA:1308:A:OP1 | 42:BW:99:ARG:NH1 | 2.49 | 0.42 |
| 25:BA:196:A:H2' | 25:BA:197:C:O4' | 2.18 | 0.42 |
| 25:BA:2703:C:O3' | 25:BA:2881:C:H4' | 2.20 | 0.42 |
| 25:BA:354:A:H2 | 25:BA:1255:A:O2' | 2.02 | 0.42 |
| 27:BD:33:LEU:HA | 27:BD:33:LEU:HD23 | 1.81 | 0.42 |
| 30:BG:145:THR:OG1 | 30:BG:148:MET:SD | 2.73 | 0.42 |
| 30:BG:125:PHE:HB3 | 30:BG:166:ASP:OD1 | 2.20 | 0.42 |
| 1:CA:1002:G:N3 | 1:CA:1003:G:N7 | 2.67 | 0.42 |
| 1:CA:999:C:C2 | 1:CA:1042:G:N2 | 2.87 | 0.42 |
| 1:CA:1057:G:C4 | 1:CA:1204:A:C2 | 3.07 | 0.42 |
| 1:CA:1145:C:H4' | 1:CA:1146:A:C5' | 2.48 | 0.42 |
| 1:CA:837:G:H2' | 1:CA:838:G:C8 | 2.55 | 0.42 |
| 1:CA:881:G:H2' | 1:CA:882:C:O4' | 2.19 | 0.42 |
| 2:CB:61:LEU:HD23 | 2:CB:68:ILE:HD11 | 2.01 | 0.42 |
| 4:CD:173:TRP:CE2 | 4:CD:189:PRO:HG3 | 2.54 | 0.42 |
| 4:CD:81:GLU:O | 4:CD:85:LYS:HB2 | 2.20 | 0.42 |
| 1:CA:735:C:H5' | 18:CR:71:LYS:HD3 | 2.00 | 0.42 |
| 25:DA:1479:G:C6 | 25:DA:1480:G:C5 | 3.08 | 0.42 |
| 25:DA:1510:G:O5' | 25:DA:1510:G:H8 | 2.03 | 0.42 |
| 25:DA:172:C:H2' | 25:DA:173:G:C8 | 2.52 | 0.42 |
| 25:DA:1844:C:OP1 | 27:DD:257:LEU:HD23 | 2.19 | 0.42 |
| 25:DA:2046:G:H2' | 25:DA:2047:U:C6 | 2.53 | 0.42 |
| 25:DA:2399:G:C6 | 25:DA:2400:G:C5 | 3.07 | 0.42 |
| 25:DA:14:A:C6 | 25:DA:526:A:C2 | 3.08 | 0.42 |
| 25:DA:994:C:O2' | 25:DA:996:A:OP1 | 2.30 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DB:15:A:O4' | 26:DB:110:G:C8 | 2.73 | 0.42 |
| 26:DB:24:G:H4' | 26:DB:25:A:N7 | 2.35 | 0.42 |
| 29:DF:32:LEU:HD11 | 29:DF:105:VAL:HG13 | 2.00 | 0.42 |
| 29:DF:51:THR:HG23 | 29:DF:92:PRO:HG2 | 2.01 | 0.42 |
| 1:AA:1001:A:N6 | 1:AA:1001(A):G:O6 | 2.53 | 0.42 |
| 1:AA:1047:G:O3' | 14:AN:4:LYS:HB2 | 2.20 | 0.42 |
| 1:AA:1236:A:H2' | 1:AA:1237:C:C6 | 2.55 | 0.42 |
| 1:AA:1438:G:H2' | 1:AA:1439:C:C6 | 2.54 | 0.42 |
| 1:AA:341:C:O2' | 1:AA:342:C:H5' | 2.20 | 0.42 |
| 1:AA:68:G:H22 | 1:AA:101:A:H2 | 1.67 | 0.42 |
| 1:AA:840:C:H4' | 1:AA:841:U:OP1 | 2.20 | 0.42 |
| 2:AB:156:LYS:HE2 | 2:AB:156:LYS:HB3 | 1.81 | 0.42 |
| 2:AB:102:LEU:HB3 | 2:AB:180:LEU:CD1 | 2.50 | 0.42 |
| 3:AC:19:GLU:HB3 | 3:AC:40:ARG:NH2 | 2.35 | 0.42 |
| 3:AC:23:TYR:CG | 3:AC:24:ALA:N | 2.87 | 0.42 |
| 4:AD:121:VAL:HA | 4:AD:126:ILE:HG13 | 2.01 | 0.42 |
| 9:AI:4:TYR:CZ | 9:AI:88:TYR:HD1 | 2.38 | 0.42 |
| 49:B3:3:ARG:HD3 | 49:B3:60:GLU:OE2 | 2.20 | 0.42 |
| 25:BA:2887:G:O2' | 25:BA:2888:U:H5' | 2.18 | 0.42 |
| 25:BA:416:G:N1 | 35:BP:70:GLN:HG3 | 2.34 | 0.42 |
| 39:BT:16:ARG:HD2 | 39:BT:18:ASP:OD1 | 2.20 | 0.42 |
| 43:BX:92:LEU:C | 43:BX:94:GLY:N | 2.71 | 0.42 |
| 1:CA:1002:G:N2 | 1:CA:1038:C:C2 | 2.82 | 0.42 |
| 1:CA:1002:G:H5'' | 1:CA:1003:G:OP2 | 2.19 | 0.42 |
| 1:CA:1002:G:C2 | 1:CA:1038:C:N3 | 2.83 | 0.42 |
| 1:CA:1158:C:H2' | 1:CA:1160:G:H5' | 2.02 | 0.42 |
| 1:CA:1239:A:H62 | 1:CA:1299:A:N6 | 2.16 | 0.42 |
| 1:CA:149:A:H2' | 1:CA:150:C:H6 | 1.83 | 0.42 |
| 1:CA:189:G:C5 | 1:CA:189(A):C:C4 | 3.07 | 0.42 |
| 1:CA:811:C:H4' | 1:CA:900:A:N6 | 2.34 | 0.42 |
| 1:CA:865:A:H2 | 1:CA:918:A:H4' | 1.83 | 0.42 |
| 2:CB:28:PHE:CD1 | 2:CB:31:TYR:HB2 | 2.55 | 0.42 |
| 2:CB:69:LEU:HD12 | 2:CB:70:PHE:H | 1.84 | 0.42 |
| 2:CB:78:GLN:O | 2:CB:94:ASN:ND2 | 2.52 | 0.42 |
| 18:CR:24:ALA:C | 18:CR:26:LEU:H | 2.23 | 0.42 |
| 25:DA:1425:G:H2' | 25:DA:1426:G:O4' | 2.19 | 0.42 |
| 25:DA:2009:G:O2' | 25:DA:2010:G:H5' | 2.20 | 0.42 |
| 25:DA:2307:G:OP1 | 25:DA:2307:G:H8 | 2.03 | 0.42 |
| 25:DA:2319:G:H22 | 38:DS:3:ARG:HE | 1.68 | 0.42 |
| 25:DA:2348:U:OP2 | 54:D8:42:ARG:NH2 | 2.52 | 0.42 |
| 25:DA:2510:C:C4 | 25:DA:2511:U:C4 | 3.08 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:824:A:H2' | 25:DA:825:C:O4' | 2.19 | 0.42 |
| 26:DB:45:A:H2' | 26:DB:46:A:H8 | 1.84 | 0.42 |
| 27:DD:145:VAL:HG12 | 27:DD:146:GLU:O | 2.18 | 0.42 |
| 25:DA:1654:A:O2' | 28:DE:113:PHE:O | 2.30 | 0.42 |
| 30:DG:170:ARG:HD3 | 30:DG:170:ARG:O | 2.19 | 0.42 |
| 31:DH:118:PRO:HD2 | 31:DH:121:ILE:HB | 2.00 | 0.42 |
| 31:DH:42:ARG:NH1 | 31:DH:53:GLU:OE2 | 2.52 | 0.42 |
| 25:DA:864:G:OP2 | 36:DQ:22:LYS:HE2 | 2.20 | 0.42 |
| 38:DS:68:GLN:HE21 | 38:DS:68:GLN:HA | 1.85 | 0.42 |
| 1:AA:1057:G:OP2 | 61:AA:4014:HOH:O | 2.22 | 0.42 |
| 1:AA:1503:A:OP1 | 1:AA:1503:A:H8 | 2.03 | 0.42 |
| 2:AB:119:GLU:OE2 | 2:AB:153:ARG:NH2 | 2.53 | 0.42 |
| 2:AB:141:GLU:O | 2:AB:145:LEU:HB2 | 2.20 | 0.42 |
| 3:AC:121:ALA:O | 3:AC:125:GLU:HG3 | 2.19 | 0.42 |
| 3:AC:32:LEU:HD22 | 3:AC:59:ARG:NH1 | 2.34 | 0.42 |
| 6:AF:63:TYR:CD1 | 6:AF:63:TYR:N | 2.88 | 0.42 |
| 48:B2:18:PRO:HA | 48:B2:21:LEU:HB2 | 2.02 | 0.42 |
| 25:BA:1273:G:OP1 | 40:BU:13:LYS:HG2 | 2.19 | 0.42 |
| 25:BA:2326:C:H2' | 25:BA:2327:G:C8 | 2.55 | 0.42 |
| 25:BA:753:A:H2' | 25:BA:754:G:O4' | 2.20 | 0.42 |
| 25:BA:83:A:C5' | 44:BY:8:LYS:HG2 | 2.49 | 0.42 |
| 25:BA:950:C:H2' | 25:BA:951:U:H6 | 1.83 | 0.42 |
| 26:BB:6:C:C2 | 26:BB:116:G:N2 | 2.88 | 0.42 |
| 28:BE:3:GLY:HA3 | 28:BE:81:ILE:HD12 | 2.01 | 0.42 |
| 31:BH:167:GLU:HA | 31:BH:168:PRO:HD3 | 1.86 | 0.42 |
| 32:BI:130:TYR:HB3 | 32:BI:138:ILE:HB | 2.02 | 0.42 |
| 35:BP:135:LEU:HD23 | 35:BP:135:LEU:HA | 1.86 | 0.42 |
| 25:BA:589:U:OP1 | 35:BP:29:LYS:HD2 | 2.19 | 0.42 |
| 38:BS:58:LEU:HD23 | 38:BS:58:LEU:HA | 1.83 | 0.42 |
| 1:CA:1095:U:H5'' | 1:CA:1109:C:O2 | 2.20 | 0.42 |
| 1:CA:991:U:C4 | 1:CA:1212:U:H1' | 2.54 | 0.42 |
| 1:CA:1292:U:O2' | 1:CA:1293:G:H5' | 2.20 | 0.42 |
| 1:CA:1522:U:H2' | 1:CA:1523:G:H8 | 1.84 | 0.42 |
| 1:CA:15:G:H2' | 1:CA:16:A:C8 | 2.53 | 0.42 |
| 1:CA:176:C:H2' | 1:CA:177:C:C6 | 2.54 | 0.42 |
| 1:CA:683:G:H2' | 1:CA:684:A:C8 | 2.55 | 0.42 |
| 1:CA:741:G:H2' | 1:CA:742:G:O4' | 2.20 | 0.42 |
| 1:CA:938:A:N6 | 1:CA:939:G:C6 | 2.88 | 0.42 |
| 1:CA:947:G:H2' | 1:CA:948:C:O4' | 2.20 | 0.42 |
| 2:CB:20:GLU:HG3 | 2:CB:191:ASP:HB3 | 2.02 | 0.42 |
| 8:CH:5:PRO:O | 8:CH:8:ASP:HB3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CI:95:LYS:HA | 9:CI:99:LEU:HD13 | 2.00 | 0.42 |
| 16:CP:21:VAL:CG1 | 16:CP:34:GLU:HB3 | 2.50 | 0.42 |
| 19:CS:50:ALA:HA | 19:CS:58:VAL:O | 2.20 | 0.42 |
| 20:CT:39:LYS:HB2 | 20:CT:39:LYS:HE3 | 1.90 | 0.42 |
| 24:CW:8:2R3:H62 | 24:CW:9:MVA:HN1 | 1.62 | 0.42 |
| 25:DA:1364:G:OP2 | 47:D1:3:LYS:HG3 | 2.20 | 0.42 |
| 25:DA:1184:G:OP1 | 49:D3:30:ARG:HD2 | 2.19 | 0.42 |
| 50:D4:60:GLN:HA | 50:D4:62:ARG:HG2 | 2.02 | 0.42 |
| 54:D8:26:LYS:HG2 | 54:D8:48:PHE:CD1 | 2.55 | 0.42 |
| 25:DA:1015:G:O2' | 25:DA:1016:G:H5' | 2.20 | 0.42 |
| 25:DA:1375:C:H2' | 25:DA:1376:C:H6 | 1.84 | 0.42 |
| 25:DA:571:A:N6 | 25:DA:2499:C:O3' | 2.53 | 0.42 |
| 25:DA:2590:A:O2' | 25:DA:2591:C:H5' | 2.20 | 0.42 |
| 25:DA:9:U:O4 | 25:DA:2629:A:H2 | 2.02 | 0.42 |
| 25:DA:13:A:N1 | 25:DA:525:U:H2' | 2.34 | 0.42 |
| 25:DA:530:G:O4' | 25:DA:530:G:N3 | 2.53 | 0.42 |
| 25:DA:959:A:C6 | 25:DA:960:A:C6 | 3.08 | 0.42 |
| 27:DD:13:ARG:HD2 | 27:DD:13:ARG:HA | 1.43 | 0.42 |
| 27:DD:127:VAL:HA | 27:DD:193:VAL:HG22 | 2.01 | 0.42 |
| 29:DF:154:VAL:HG22 | 29:DF:191:ARG:CB | 2.49 | 0.42 |
| 30:DG:45:GLU:C | 30:DG:47:LYS:H | 2.23 | 0.42 |
| 1:AA:1256:A:C2 | 1:AA:1277:C:N4 | 2.88 | 0.42 |
| 1:AA:1277:C:H1' | 1:AA:1282:C:C2 | 2.55 | 0.42 |
| 1:AA:352:C:O2' | 1:AA:354:G:OP1 | 2.28 | 0.42 |
| 1:AA:357:G:C2 | 1:AA:358:U:C5 | 3.08 | 0.42 |
| 1:AA:589:C:O2' | 1:AA:590:C:H5' | 2.20 | 0.42 |
| 1:AA:657:G:C2 | 1:AA:750:G:C5 | 3.08 | 0.42 |
| 1:AA:66:G:O3' | 1:AA:199:G:H4' | 2.20 | 0.42 |
| 1:AA:977:A:H2' | 1:AA:978:A:H5'' | 2.01 | 0.42 |
| 1:AA:1060:C:H41 | 3:AC:2:GLY:HA3 | 1.85 | 0.42 |
| 9:AI:110:GLU:OE2 | 9:AI:113:LYS:NZ | 2.49 | 0.42 |
| 17:AQ:27:PHE:CZ | 17:AQ:36:ILE:HD11 | 2.55 | 0.42 |
| 6:AF:96:PRO:HB3 | 18:AR:30:ASP:CG | 2.39 | 0.42 |
| 23:AX:19:G:C4 | 23:AX:57:A:C2 | 3.07 | 0.42 |
| 25:BA:1370:G:C4 | 25:BA:1374:G:O6 | 2.72 | 0.42 |
| 25:BA:1387:U:OP1 | 25:BA:1443:U:N3 | 2.47 | 0.42 |
| 25:BA:1522:G:N2 | 25:BA:1565:G:C4 | 2.87 | 0.42 |
| 25:BA:1629:C:C2 | 25:BA:1630:A:C8 | 3.08 | 0.42 |
| 25:BA:1790:A:H1' | 25:BA:2723:A:C2 | 2.55 | 0.42 |
| 25:BA:1898:A:H2' | 25:BA:1899:A:C8 | 2.54 | 0.42 |
| 25:BA:2623:U:H2' | 51:B5:2:ALA:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:2860:A:C2 | 25:BA:2861:A:C4 | 3.08 | 0.42 |
| 25:BA:439:A:O5' | 25:BA:439:A:H8 | 2.03 | 0.42 |
| 32:BI:6:LEU:HG | 32:BI:36:ALA:HA | 2.01 | 0.42 |
| 34:BO:7:TYR:CZ | 34:BO:44:LYS:HG3 | 2.55 | 0.42 |
| 45:BZ:67:LEU:HA | 45:BZ:68:PRO:HD3 | 1.72 | 0.42 |
| 1:CA:160:A:H2' | 1:CA:161:A:C8 | 2.55 | 0.42 |
| 1:CA:472:A:H2' | 1:CA:473:G:O4' | 2.20 | 0.42 |
| 1:CA:576:G:N2 | 1:CA:760:G:OP2 | 2.53 | 0.42 |
| 1:CA:677:U:H1' | 11:CK:119:CYS:SG | 2.60 | 0.42 |
| 1:CA:714:G:H2' | 1:CA:715:A:C8 | 2.55 | 0.42 |
| 1:CA:951:G:C6 | 1:CA:952:U:C4 | 3.08 | 0.42 |
| 6:CF:80:ARG:NH1 | 6:CF:88:VAL:O | 2.53 | 0.42 |
| 19:CS:27:GLU:HG2 | 19:CS:47:HIS:HE2 | 1.83 | 0.42 |
| 25:DA:144:C:H2' | 25:DA:145:G:C8 | 2.50 | 0.42 |
| 25:DA:1912:A:C8 | 25:DA:1918:A:C2 | 3.08 | 0.42 |
| 25:DA:2298:A:N7 | 25:DA:2299:G:C4 | 2.88 | 0.42 |
| 25:DA:244:A:C2 | 25:DA:255:A:C4 | 3.08 | 0.42 |
| 25:DA:2821:A:C2 | 25:DA:2822:G:C4 | 3.08 | 0.42 |
| 25:DA:459:U:H4' | 53:D7:40:TRP:CZ3 | 2.55 | 0.42 |
| 25:DA:537:C:H1' | 33:DN:45:ASN:HD21 | 1.85 | 0.42 |
| 25:DA:595:C:H2' | 25:DA:596:G:O4' | 2.19 | 0.42 |
| 30:DG:128:ARG:HE | 30:DG:128:ARG:HB2 | 1.55 | 0.42 |
| 40:DU:79:PHE:O | 40:DU:83:LEU:HD22 | 2.20 | 0.42 |
| 1:AA:1162:C:H2' | 1:AA:1163:C:H6 | 1.85 | 0.42 |
| 1:AA:1277:C:H2' | 1:AA:1279:A:C8 | 2.53 | 0.42 |
| 1:AA:1308:U:H5'' | 13:AM:98:VAL:CG2 | 2.49 | 0.42 |
| 1:AA:192:U:C2 | 1:AA:193:C:C5 | 3.08 | 0.42 |
| 1:AA:22:G:H2' | 1:AA:23:C:C6 | 2.55 | 0.42 |
| 1:AA:55:A:C5 | 1:AA:56:U:C5 | 3.08 | 0.42 |
| 1:AA:673:G:N2 | 1:AA:674:G:C2 | 2.88 | 0.42 |
| 1:AA:684:A:H2' | 1:AA:685:G:H8 | 1.84 | 0.42 |
| 1:AA:890:G:O2' | 1:AA:906:G:O6 | 2.31 | 0.42 |
| 2:AB:158:LEU:HA | 2:AB:159:PRO:HD3 | 1.88 | 0.42 |
| 3:AC:175:LEU:HD21 | 3:AC:201:TYR:HE2 | 1.85 | 0.42 |
| 3:AC:22:TRP:CD1 | 3:AC:59:ARG:HD2 | 2.54 | 0.42 |
| 5:AE:20:GLN:NE2 | 5:AE:21:ALA:O | 2.53 | 0.42 |
| 15:AO:61:GLY:O | 15:AO:65:ARG:HG3 | 2.19 | 0.42 |
| 16:AP:71:ARG:O | 16:AP:75:ARG:N | 2.30 | 0.42 |
| 49:B3:26:LEU:O | 49:B3:35:ARG:NE | 2.51 | 0.42 |
| 25:BA:1224:C:O2' | 25:BA:1225:C:H5' | 2.20 | 0.42 |
| 25:BA:2376:C:H2' | 25:BA:2377:G:O4' | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2450:U:O2' | 25:BA:2452:C:OP1 | 2.30 | 0.42 |
| 25:BA:2517:G:O6 | 25:BA:2588:G:H2' | 2.19 | 0.42 |
| 25:BA:2673:G:H2' | 25:BA:2674:A:C8 | 2.55 | 0.42 |
| 25:BA:2677:A:C2 | 25:BA:2678:C:C2 | 3.08 | 0.42 |
| 25:BA:374:U:H2' | 25:BA:375:G:O4' | 2.20 | 0.42 |
| 25:BA:738:C:O2' | 25:BA:739:C:H5' | 2.20 | 0.42 |
| 25:BA:801:C:H2' | 25:BA:802:C:C6 | 2.55 | 0.42 |
| 25:BA:831:A:C8 | 25:BA:839:G:C5 | 3.08 | 0.42 |
| 27:BD:145:VAL:HB | 27:BD:155:LEU:HB2 | 2.02 | 0.42 |
| 28:BE:178:GLU:OE2 | 28:BE:178:GLU:N | 2.47 | 0.42 |
| 25:BA:2797:C:O2' | 28:BE:42:ASP:OD1 | 2.22 | 0.42 |
| 37:BR:117:VAL:HG12 | 37:BR:118:GLU:N | 2.34 | 0.42 |
| 39:BT:101:PHE:HD2 | 39:BT:105:LEU:HD11 | 1.84 | 0.42 |
| 40:BU:112:ARG:H | 40:BU:112:ARG:HG2 | 1.53 | 0.42 |
| 1:CA:1188:A:H2' | 1:CA:1189:C:O4' | 2.19 | 0.42 |
| 1:CA:1228:C:H4' | 13:CM:116:THR:HA | 2.01 | 0.42 |
| 1:CA:1270:C:H2' | 1:CA:1271:G:H5' | 2.02 | 0.42 |
| 1:CA:1298:C:H4' | 1:CA:1299:A:C4 | 2.54 | 0.42 |
| 1:CA:226:G:C2 | 1:CA:227:G:C8 | 3.08 | 0.42 |
| 1:CA:59:A:H5" | 1:CA:60:A:C5' | 2.49 | 0.42 |
| 1:CA:952:U:O2' | 1:CA:965:A:N6 | 2.52 | 0.42 |
| 4:CD:135:LEU:O | 4:CD:137:SER:N | 2.53 | 0.42 |
| 1:CA:1291:G:H4' | 9:CI:39:GLY:HA3 | 2.02 | 0.42 |
| 9:CI:96:LEU:HD23 | 9:CI:96:LEU:HA | 1.92 | 0.42 |
| 19:CS:29:ARG:O | 19:CS:31:ILE:HG13 | 2.19 | 0.42 |
| 24:CW:9:MVA:HN3 | 24:CW:10:2QY:CE2 | 2.49 | 0.42 |
| 51:D5:49:CYS:SG | 51:D5:51:TYR:HB2 | 2.59 | 0.42 |
| 25:DA:1024:G:O5' | 25:DA:1024:G:H8 | 2.02 | 0.42 |
| 25:DA:1275:A:N1 | 25:DA:1295:C:O2' | 2.39 | 0.42 |
| 25:DA:1575:C:H2' | 25:DA:1576:U:C6 | 2.55 | 0.42 |
| 25:DA:190:A:OP2 | 47:D1:39:LYS:HE3 | 2.19 | 0.42 |
| 25:DA:597:U:H2' | 25:DA:598:G:C8 | 2.55 | 0.42 |
| 25:DA:776:G:C8 | 25:DA:793:A:N3 | 2.88 | 0.42 |
| 27:DD:228:PRO:HD3 | 27:DD:235:GLY:HA3 | 2.02 | 0.42 |
| 31:DH:130:ARG:HH11 | 31:DH:132:ARG:NH2 | 2.18 | 0.42 |
| 32:DI:14:ASP:OD1 | 32:DI:15:VAL:N | 2.53 | 0.42 |
| 32:DI:4:ILE:HG12 | 32:DI:18:VAL:HG22 | 2.01 | 0.42 |
| 34:DO:69:ILE:HD13 | 34:DO:69:ILE:H | 1.85 | 0.42 |
| 36:DQ:133:ARG:HG2 | 36:DQ:134:ARG:N | 2.34 | 0.42 |
| 41:DV:58:VAL:O | 41:DV:97:LYS:N | 2.38 | 0.42 |
| 1:AA:503:C:O2' | 1:AA:504:C:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:622:A:H3' | 1:AA:623:C:C6 | 2.55 | 0.41 |
| 1:AA:767:A:H2' | 1:AA:768:A:O4' | 2.20 | 0.41 |
| 2:AB:219:VAL:HA | 2:AB:222:ILE:CD1 | 2.49 | 0.41 |
| 4:AD:81:GLU:OE2 | 4:AD:139:ARG:NH2 | 2.53 | 0.41 |
| 12:AL:124:LYS:HA | 12:AL:125:PRO:HD3 | 1.77 | 0.41 |
| 25:BA:202:A:H2' | 25:BA:203:G:O4' | 2.19 | 0.41 |
| 25:BA:2798:C:H2' | 25:BA:2799:U:C6 | 2.55 | 0.41 |
| 25:BA:310:C:H2' | 25:BA:311:C:H6 | 1.85 | 0.41 |
| 25:BA:312:C:H2' | 25:BA:313:A:C8 | 2.53 | 0.41 |
| 25:BA:518:G:H2' | 25:BA:519:G:O4' | 2.20 | 0.41 |
| 31:BH:37:VAL:HG13 | 31:BH:68:THR:CG2 | 2.50 | 0.41 |
| 34:BO:120:GLU:OE1 | 39:BT:67:SER:OG | 2.27 | 0.41 |
| 35:BP:6:LEU:HD23 | 35:BP:6:LEU:HA | 1.71 | 0.41 |
| 43:BX:31:HIS:HD2 | 43:BX:33:LYS:HB2 | 1.84 | 0.41 |
| 44:BY:1:MET:HE2 | 44:BY:1:MET:HB2 | 1.89 | 0.41 |
| 45:BZ:111:VAL:C | 45:BZ:113:ALA:N | 2.71 | 0.41 |
| 1:CA:61:G:C5 | 1:CA:107:G:C2 | 3.08 | 0.41 |
| 1:CA:1105:A:C2 | 1:CA:1106:G:C8 | 3.08 | 0.41 |
| 1:CA:1245:A:H61 | 1:CA:1292:U:H3 | 1.68 | 0.41 |
| 1:CA:189(K):U:H2' | 1:CA:189(L):G:C8 | 2.55 | 0.41 |
| 1:CA:447:G:H2' | 1:CA:485:G:N2 | 2.35 | 0.41 |
| 1:CA:538:G:OP2 | 12:CL:115:LYS:HB2 | 2.18 | 0.41 |
| 1:CA:922:G:H2' | 1:CA:923:A:H8 | 1.85 | 0.41 |
| 4:CD:110:PHE:N | 4:CD:110:PHE:HD1 | 2.18 | 0.41 |
| 4:CD:88:VAL:O | 4:CD:92:VAL:HG23 | 2.20 | 0.41 |
| 10:CJ:23:ILE:HD13 | 10:CJ:23:ILE:HA | 1.74 | 0.41 |
| 11:CK:43:SER:HA | 11:CK:47:VAL:HG21 | 2.02 | 0.41 |
| 13:CM:80:ARG:O | 13:CM:84:ILE:HG23 | 2.20 | 0.41 |
| 10:CJ:49:VAL:HG23 | 14:CN:41:ARG:HD2 | 2.00 | 0.41 |
| 15:CO:76:GLU:HA | 15:CO:76:GLU:OE1 | 2.20 | 0.41 |
| 21:CU:9:ARG:O | 21:CU:13:ILE:HG13 | 2.20 | 0.41 |
| 25:DA:1032:A:O3' | 55:D9:16:VAL:HG11 | 2.19 | 0.41 |
| 25:DA:1138:G:O2' | 33:DN:105:GLY:HA3 | 2.20 | 0.41 |
| 25:DA:1339:G:H5'' | 43:DX:16:LYS:HD3 | 2.01 | 0.41 |
| 25:DA:1366:A:H2' | 25:DA:1367:A:O4' | 2.20 | 0.41 |
| 25:DA:1954:G:N2 | 25:DA:1956:U:C2 | 2.89 | 0.41 |
| 25:DA:1833:U:O2' | 25:DA:1969:A:N1 | 2.37 | 0.41 |
| 25:DA:2376:A:N3 | 38:DS:106:ARG:NH2 | 2.60 | 0.41 |
| 25:DA:2758:A:C2 | 25:DA:2759:G:H1' | 2.55 | 0.41 |
| 25:DA:275:G:H2' | 25:DA:276:A:H8 | 1.83 | 0.41 |
| 25:DA:30:G:H2' | 25:DA:31:C:H6 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:489:G:H2' | 25:DA:491:G:O4' | 2.20 | 0.41 |
| 25:DA:590:A:H2' | 25:DA:591:C:C6 | 2.54 | 0.41 |
| 25:DA:623:G:C2 | 25:DA:624:C:C2 | 3.08 | 0.41 |
| 25:DA:721:C:H2' | 25:DA:722:A:C8 | 2.55 | 0.41 |
| 25:DA:884:C:H5' | 25:DA:885:C:OP2 | 2.20 | 0.41 |
| 25:DA:848:G:C4 | 25:DA:933:A:H8 | 2.38 | 0.41 |
| 32:DI:127:VAL:O | 32:DI:128:LEU:HD23 | 2.19 | 0.41 |
| 35:DP:85:LEU:HG | 35:DP:115:LEU:O | 2.20 | 0.41 |
| 36:DQ:43:THR:OG1 | 36:DQ:45:GLN:HG2 | 2.20 | 0.41 |
| 42:DW:31:GLU:O | 42:DW:34:ASN:HB2 | 2.20 | 0.41 |
| 43:DX:46:ALA:O | 48:D2:30:ARG:NH2 | 2.50 | 0.41 |
| 1:AA:1004:A:C8 | 1:AA:1037:C:C2 | 3.09 | 0.41 |
| 1:AA:1020:U:H2' | 1:AA:1021:G:C8 | 2.55 | 0.41 |
| 1:AA:1118:C:OP1 | 9:AI:104:ARG:NH1 | 2.48 | 0.41 |
| 1:AA:1325:C:O2' | 1:AA:1326:C:H5' | 2.19 | 0.41 |
| 1:AA:342:C:N3 | 1:AA:348:G:C6 | 2.87 | 0.41 |
| 1:AA:545:C:H5' | 4:AD:72:GLU:CB | 2.51 | 0.41 |
| 1:AA:20:U:H1' | 1:AA:916:G:N2 | 2.34 | 0.41 |
| 4:AD:138:TYR:HE1 | 4:AD:140:VAL:HA | 1.85 | 0.41 |
| 8:AH:21:LYS:O | 8:AH:65:TYR:OH | 2.24 | 0.41 |
| 8:AH:34:GLU:CD | 8:AH:37:ARG:HH22 | 2.23 | 0.41 |
| 49:B3:31:LEU:HD23 | 49:B3:31:LEU:HA | 1.88 | 0.41 |
| 25:BA:1889:G:H21 | 25:BA:1905:G:H2' | 1.84 | 0.41 |
| 25:BA:2285:A:O2' | 25:BA:2286:A:H5' | 2.20 | 0.41 |
| 25:BA:233:A:C2 | 25:BA:244:A:C4 | 3.08 | 0.41 |
| 38:BS:61:ASN:O | 38:BS:65:VAL:HG23 | 2.19 | 0.41 |
| 45:BZ:121:HIS:HB3 | 45:BZ:123:ASP:O | 2.20 | 0.41 |
| 1:CA:1245:A:H2' | 1:CA:1246:C:O4' | 2.20 | 0.41 |
| 1:CA:137:C:H2' | 1:CA:138:G:H5' | 2.00 | 0.41 |
| 1:CA:189(C):C:H2' | 1:CA:189(D):C:O4' | 2.20 | 0.41 |
| 1:CA:44:G:H2' | 1:CA:45:U:O4' | 2.20 | 0.41 |
| 1:CA:557:G:N1 | 1:CA:558:G:C2 | 2.88 | 0.41 |
| 1:CA:833:U:H2' | 1:CA:834:C:H6 | 1.85 | 0.41 |
| 1:CA:991:U:H3' | 1:CA:1212:U:N3 | 2.35 | 0.41 |
| 3:CC:11:ARG:HB3 | 3:CC:15:THR:HB | 2.00 | 0.41 |
| 1:CA:407:G:O2' | 4:CD:116:GLN:HG3 | 2.20 | 0.41 |
| 4:CD:8:VAL:HA | 4:CD:11:LEU:HD13 | 2.02 | 0.41 |
| 6:CF:89:MET:HG2 | 6:CF:91:VAL:HG23 | 2.02 | 0.41 |
| 15:CO:15:PHE:CZ | 15:CO:84:LYS:HG2 | 2.55 | 0.41 |
| 23:CX:19:G:C4 | 23:CX:57:A:C2 | 3.08 | 0.41 |
| 53:D7:12:ARG:NH2 | 53:D7:44:PRO:HB3 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:1026:U:H4' | 25:DA:1027:A:OP1 | 2.20 | 0.41 |
| 25:DA:1399:C:O2' | 25:DA:1400:G:H5' | 2.20 | 0.41 |
| 25:DA:2058:A:N7 | 61:DA:3842:HOH:O | 2.37 | 0.41 |
| 25:DA:2070:G:C2 | 25:DA:2442:C:C2 | 3.08 | 0.41 |
| 25:DA:2416:C:H2' | 25:DA:2417:C:H6 | 1.85 | 0.41 |
| 25:DA:1782:C:O4' | 25:DA:2609:U:C2 | 2.73 | 0.41 |
| 25:DA:2022:U:O2' | 25:DA:2617:C:H5' | 2.19 | 0.41 |
| 25:DA:442:G:H21 | 29:DF:48:THR:HB | 1.86 | 0.41 |
| 25:DA:826:U:H5'' | 25:DA:2428:G:O3' | 2.20 | 0.41 |
| 25:DA:843:G:C2 | 25:DA:936:C:C2 | 3.08 | 0.41 |
| 26:DB:33:G:C6 | 26:DB:34:U:C4 | 3.08 | 0.41 |
| 27:DD:232:PRO:HG2 | 27:DD:248:SER:O | 2.20 | 0.41 |
| 27:DD:68:LYS:O | 27:DD:69:ARG:HB2 | 2.20 | 0.41 |
| 30:DG:117:PHE:CE1 | 30:DG:119:GLY:HA2 | 2.55 | 0.41 |
| 30:DG:178:PHE:HA | 30:DG:179:PRO:HD2 | 1.87 | 0.41 |
| 31:DH:123:PHE:CD1 | 31:DH:133:VAL:HG22 | 2.56 | 0.41 |
| 41:DV:40:LEU:HD11 | 41:DV:55:ALA:HB2 | 2.01 | 0.41 |
| 43:DX:72:LYS:HG2 | 43:DX:73:ARG:O | 2.20 | 0.41 |
| 36:DQ:141:GLN:NE2 | 45:DZ:74:VAL:O | 2.42 | 0.41 |
| 1:AA:1001(A):G:C5 | 1:AA:1002:G:C8 | 3.08 | 0.41 |
| 1:AA:1039:C:N4 | 1:AA:1040:U:O4 | 2.53 | 0.41 |
| 1:AA:1085:U:OP2 | 61:AA:4121:HOH:O | 2.22 | 0.41 |
| 1:AA:1162:C:C2 | 1:AA:1175:G:C2 | 3.09 | 0.41 |
| 1:AA:258:G:N3 | 1:AA:259:G:C8 | 2.89 | 0.41 |
| 1:AA:575:G:HO2' | 1:AA:821:G:H5' | 1.85 | 0.41 |
| 3:AC:19:GLU:HB3 | 3:AC:40:ARG:HH21 | 1.85 | 0.41 |
| 4:AD:71:SER:OG | 4:AD:74:GLN:HB2 | 2.21 | 0.41 |
| 10:AJ:38:ILE:HA | 10:AJ:39:PRO:HD3 | 1.85 | 0.41 |
| 16:AP:55:ARG:HA | 16:AP:55:ARG:HD2 | 1.89 | 0.41 |
| 19:AS:31:ILE:O | 19:AS:49:ILE:HG23 | 2.20 | 0.41 |
| 23:AX:8:U:O2 | 23:AX:21:A:H2 | 2.03 | 0.41 |
| 48:B2:10:LEU:HD23 | 48:B2:10:LEU:HA | 1.90 | 0.41 |
| 50:B4:56:VAL:HB | 50:B4:57:GLU:H | 1.65 | 0.41 |
| 25:BA:2038:U:H1' | 51:B5:6:VAL:HG13 | 2.02 | 0.41 |
| 55:B9:17:ILE:HD12 | 55:B9:17:ILE:HA | 1.81 | 0.41 |
| 25:BA:1722:C:H2' | 25:BA:1723:A:O4' | 2.20 | 0.41 |
| 25:BA:1775:C:H6 | 25:BA:1775:C:H5'' | 1.85 | 0.41 |
| 25:BA:2455:C:OP1 | 29:BF:68:LYS:HD3 | 2.20 | 0.41 |
| 25:BA:324:A:H2' | 25:BA:358:C:H1' | 2.02 | 0.41 |
| 25:BA:442:A:H2' | 25:BA:443:C:H6 | 1.85 | 0.41 |
| 25:BA:694:G:N1 | 25:BA:696:C:O2 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:895:G:N9 | 25:BA:978:A:H8 | 2.18 | 0.41 |
| 32:BI:102:SER:HA | 32:BI:106:GLY:HA3 | 2.01 | 0.41 |
| 39:BT:16:ARG:NH1 | 39:BT:18:ASP:OD2 | 2.53 | 0.41 |
| 39:BT:88:ILE:HG21 | 39:BT:91:ARG:NE | 2.35 | 0.41 |
| 1:CA:1151:A:C2 | 1:CA:1152:A:C5 | 3.08 | 0.41 |
| 1:CA:1155:G:N7 | 1:CA:1156:G:C5 | 2.88 | 0.41 |
| 1:CA:1260:C:O5' | 1:CA:1284:C:H4' | 2.20 | 0.41 |
| 1:CA:1309:G:H2' | 1:CA:1310:G:O4' | 2.20 | 0.41 |
| 1:CA:445:G:C6 | 1:CA:490:G:C6 | 3.09 | 0.41 |
| 1:CA:663:A:C2' | 1:CA:664:G:H5' | 2.49 | 0.41 |
| 1:CA:964:A:N3 | 1:CA:969:A:O2' | 2.34 | 0.41 |
| 13:CM:29:ARG:NH1 | 13:CM:64:TRP:HB3 | 2.35 | 0.41 |
| 17:CQ:53:LEU:HD23 | 17:CQ:82:MET:HE1 | 2.01 | 0.41 |
| 18:CR:35:ARG:O | 18:CR:37:VAL:N | 2.51 | 0.41 |
| 24:CW:1:2QZ:CB | 24:CW:10:2QY:H83 | 2.49 | 0.41 |
| 24:CW:8:2R3:H69 | 24:CW:8:2R3:H67 | 1.72 | 0.41 |
| 47:D1:23:LYS:HB2 | 47:D1:23:LYS:HE3 | 1.70 | 0.41 |
| 48:D2:21:LEU:HA | 48:D2:21:LEU:HD23 | 1.86 | 0.41 |
| 25:DA:254:G:N7 | 54:D8:5:LYS:HE2 | 2.35 | 0.41 |
| 25:DA:1639:U:C2' | 25:DA:1640:C:H5'' | 2.51 | 0.41 |
| 25:DA:2030:A:H4' | 25:DA:2031:A:C8 | 2.55 | 0.41 |
| 25:DA:2319:G:H4' | 25:DA:2320:A:OP1 | 2.19 | 0.41 |
| 25:DA:2517:C:C6 | 25:DA:2542:A:N7 | 2.88 | 0.41 |
| 25:DA:2892:A:H2' | 25:DA:2893:G:H5' | 2.02 | 0.41 |
| 25:DA:340:A:H2' | 25:DA:341:G:O4' | 2.19 | 0.41 |
| 25:DA:729:G:O5' | 27:DD:208:LYS:NZ | 2.54 | 0.41 |
| 25:DA:79:G:C4 | 25:DA:80:G:C8 | 3.08 | 0.41 |
| 25:DA:674:G:C1' | 29:DF:74:ARG:HD3 | 2.50 | 0.41 |
| 31:DH:71:LEU:HA | 31:DH:71:LEU:HD12 | 1.78 | 0.41 |
| 35:DP:16:ARG:HH11 | 35:DP:16:ARG:HD2 | 1.73 | 0.41 |
| 36:DQ:106:VAL:HG21 | 36:DQ:114:ALA:HB1 | 2.02 | 0.41 |
| 36:DQ:72:LYS:HB3 | 36:DQ:94:VAL:HG23 | 2.01 | 0.41 |
| 37:DR:21:TYR:OH | 37:DR:43:GLU:HG2 | 2.21 | 0.41 |
| 37:DR:65:LEU:HA | 37:DR:65:LEU:HD12 | 1.65 | 0.41 |
| 41:DV:25:LEU:H | 41:DV:92:THR:HG1 | 1.65 | 0.41 |
| 43:DX:43:VAL:HG21 | 43:DX:81:VAL:HG11 | 2.03 | 0.41 |
| 45:DZ:5:LEU:HD22 | 45:DZ:6:LYS:N | 2.35 | 0.41 |
| 1:AA:1349:A:OP2 | 9:AI:118:LYS:HE3 | 2.20 | 0.41 |
| 1:AA:258:G:H2' | 1:AA:259:G:C8 | 2.55 | 0.41 |
| 4:AD:190:ASP:H | 4:AD:193:ASP:HB2 | 1.86 | 0.41 |
| 8:AH:28:ALA:HB3 | 8:AH:57:PRO:HB2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:AS:22:LEU:HD13 | 19:AS:47:HIS:HD2 | 1.85 | 0.41 |
| 50:B4:68:ARG:HB3 | 50:B4:69:LYS:H | 1.43 | 0.41 |
| 25:BA:1506:G:H5'' | 25:BA:1507:A:OP2 | 2.20 | 0.41 |
| 25:BA:223:C:H2' | 25:BA:224:U:C6 | 2.56 | 0.41 |
| 25:BA:2303:U:OP1 | 25:BA:2392:C:O2' | 2.25 | 0.41 |
| 25:BA:469:A:H5'' | 25:BA:470:C:OP1 | 2.19 | 0.41 |
| 29:BF:129:PHE:CD2 | 29:BF:163:VAL:HG21 | 2.56 | 0.41 |
| 30:BG:6:ALA:HB3 | 30:BG:104:GLU:OE2 | 2.20 | 0.41 |
| 34:BO:4:PRO:O | 34:BO:5:GLN:HB2 | 2.20 | 0.41 |
| 35:BP:27:HIS:O | 35:BP:31:ALA:HA | 2.19 | 0.41 |
| 39:BT:101:PHE:CD2 | 39:BT:105:LEU:HD11 | 2.56 | 0.41 |
| 1:CA:1001:A:N6 | 1:CA:1001(A):G:O6 | 2.53 | 0.41 |
| 1:CA:1077:G:N1 | 1:CA:1081:G:C6 | 2.89 | 0.41 |
| 1:CA:865:A:H5' | 1:CA:1078:U:O4 | 2.20 | 0.41 |
| 1:CA:1120:G:O5' | 1:CA:1120:G:H8 | 2.02 | 0.41 |
| 1:CA:1266:G:N2 | 1:CA:1268:A:H3' | 2.35 | 0.41 |
| 1:CA:328:C:H4' | 1:CA:329:A:H5' | 2.02 | 0.41 |
| 1:CA:438:G:O2' | 1:CA:494:U:O4 | 2.32 | 0.41 |
| 1:CA:558:G:H5'' | 1:CA:559:A:OP2 | 2.20 | 0.41 |
| 1:CA:727:G:N2 | 1:CA:730:G:OP2 | 2.51 | 0.41 |
| 1:CA:971:G:OP1 | 1:CA:971:G:H3' | 2.19 | 0.41 |
| 2:CB:192:SER:O | 2:CB:194:PRO:HD3 | 2.20 | 0.41 |
| 2:CB:213:LEU:HD22 | 2:CB:214:ILE:HD13 | 2.02 | 0.41 |
| 4:CD:100:ARG:HG2 | 4:CD:137:SER:HA | 2.01 | 0.41 |
| 5:CE:137:GLU:HA | 5:CE:140:ARG:HB3 | 2.02 | 0.41 |
| 5:CE:81:GLU:OE1 | 5:CE:88:LYS:HE2 | 2.20 | 0.41 |
| 8:CH:58:TYR:O | 8:CH:59:LEU:HD23 | 2.21 | 0.41 |
| 18:CR:26:LEU:HA | 18:CR:26:LEU:HD13 | 1.93 | 0.41 |
| 25:DA:1364:G:C8 | 47:D1:3:LYS:HD2 | 2.55 | 0.41 |
| 54:D8:56:GLU:HA | 54:D8:59:LYS:HE3 | 2.02 | 0.41 |
| 25:DA:1313:U:H2' | 25:DA:1610:A:C2 | 2.55 | 0.41 |
| 25:DA:2023:G:H4' | 25:DA:2617:C:O3' | 2.20 | 0.41 |
| 25:DA:45:C:H2' | 25:DA:47:C:C6 | 2.56 | 0.41 |
| 26:DB:33:G:N3 | 26:DB:50:G:C2 | 2.88 | 0.41 |
| 26:DB:90:A:C5 | 26:DB:91:C:H1' | 2.56 | 0.41 |
| 28:DE:166:THR:HG21 | 28:DE:199:ARG:HH22 | 1.85 | 0.41 |
| 30:DG:17:PRO:HA | 30:DG:20:ILE:HD12 | 2.01 | 0.41 |
| 35:DP:38:GLN:O | 35:DP:39:LYS:CB | 2.69 | 0.41 |
| 25:DA:996:A:H4' | 40:DU:91:ASP:OD2 | 2.20 | 0.41 |
| 42:DW:79:GLY:CA | 42:DW:100:THR:HG22 | 2.51 | 0.41 |
| 1:AA:1376:U:H2' | 1:AA:1377:A:H8 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:404:U:H2' | 1:AA:405:U:H6 | 1.86 | 0.41 |
| 1:AA:512:U:H2' | 1:AA:513:C:C6 | 2.56 | 0.41 |
| 2:AB:80:ILE:HD11 | 2:AB:212:GLN:HA | 2.01 | 0.41 |
| 2:AB:36:ARG:C | 2:AB:38:GLY:H | 2.23 | 0.41 |
| 3:AC:152:ILE:O | 3:AC:198:VAL:HA | 2.20 | 0.41 |
| 5:AE:31:LEU:HD23 | 5:AE:31:LEU:HA | 1.80 | 0.41 |
| 6:AF:62:TRP:CD1 | 18:AR:35:ARG:HD2 | 2.56 | 0.41 |
| 5:AE:78:HIS:CE1 | 8:AH:104:ARG:NH1 | 2.89 | 0.41 |
| 9:AI:128:ARG:NH2 | 23:AX:33:U:OP2 | 2.53 | 0.41 |
| 19:AS:20:LEU:HD13 | 50:B4:69:LYS:HE2 | 2.03 | 0.41 |
| 25:BA:1047:A:H2' | 25:BA:1048:G:O4' | 2.20 | 0.41 |
| 25:BA:1074:A:N6 | 25:BA:1171:G:H2' | 2.35 | 0.41 |
| 25:BA:1155:C:C5 | 25:BA:1156:G:C6 | 3.09 | 0.41 |
| 25:BA:1520:G:C6 | 25:BA:1521:C:N3 | 2.89 | 0.41 |
| 25:BA:1530:G:N2 | 25:BA:1552:C:C2 | 2.88 | 0.41 |
| 30:BG:77:ILE:HG21 | 30:BG:80:PHE:CD2 | 2.56 | 0.41 |
| 33:BN:10:GLU:OE1 | 33:BN:11:PRO:HD2 | 2.21 | 0.41 |
| 36:BQ:137:TYR:HB3 | 45:BZ:76:LEU:HD21 | 2.01 | 0.41 |
| 38:BS:110:LEU:HD12 | 38:BS:110:LEU:HA | 1.70 | 0.41 |
| 40:BU:18:LEU:HD23 | 40:BU:18:LEU:HA | 1.89 | 0.41 |
| 44:BY:106:LEU:O | 44:BY:107:ASP:HB2 | 2.20 | 0.41 |
| 44:BY:9:LYS:HA | 44:BY:10:GLY:HA2 | 1.80 | 0.41 |
| 1:CA:919:A:O2' | 1:CA:1080:A:N1 | 2.50 | 0.41 |
| 1:CA:1127:G:H2' | 1:CA:1128:C:C6 | 2.55 | 0.41 |
| 1:CA:1179:A:C6 | 1:CA:1180:A:N7 | 2.89 | 0.41 |
| 1:CA:1227:A:C3' | 1:CA:1227:A:C8 | 3.03 | 0.41 |
| 1:CA:1264:C:C2 | 1:CA:1272:G:N2 | 2.88 | 0.41 |
| 1:CA:1460:A:H2' | 1:CA:1461:G:O4' | 2.21 | 0.41 |
| 1:CA:325:A:H2' | 1:CA:326:G:O4' | 2.20 | 0.41 |
| 1:CA:53:A:N6 | 1:CA:54:C:C4 | 2.88 | 0.41 |
| 1:CA:868:C:H2' | 1:CA:869:G:O4' | 2.21 | 0.41 |
| 2:CB:7:VAL:HB | 2:CB:8:LYS:H | 1.72 | 0.41 |
| 4:CD:171:GLY:HA2 | 4:CD:172:PRO:HD3 | 1.93 | 0.41 |
| 4:CD:153:ARG:HB2 | 4:CD:181:MET:SD | 2.61 | 0.41 |
| 13:CM:91:ARG:HA | 13:CM:91:ARG:HD2 | 1.93 | 0.41 |
| 16:CP:55:ARG:O | 16:CP:58:TYR:N | 2.51 | 0.41 |
| 20:CT:26:ASN:OD1 | 20:CT:71:THR:HG23 | 2.21 | 0.41 |
| 46:D0:19:LYS:NZ | 46:D0:19:LYS:H | 2.18 | 0.41 |
| 25:DA:1790:C:O3' | 25:DA:1791:A:C8 | 2.73 | 0.41 |
| 25:DA:2297:C:C6 | 25:DA:2297:C:H3' | 2.55 | 0.41 |
| 25:DA:2472:G:H2' | 25:DA:2475:C:H42 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:343:C:H2' | 25:DA:344:G:H8 | 1.85 | 0.41 |
| 25:DA:372:G:O2' | 25:DA:373:U:OP2 | 2.37 | 0.41 |
| 25:DA:632:A:H2' | 25:DA:633:A:C8 | 2.55 | 0.41 |
| 25:DA:705:A:H2' | 25:DA:706:A:O4' | 2.21 | 0.41 |
| 25:DA:966:G:C6 | 25:DA:967:C:N4 | 2.88 | 0.41 |
| 26:DB:3:C:H2' | 26:DB:4:C:H6 | 1.84 | 0.41 |
| 28:DE:167:VAL:HG11 | 28:DE:189:PRO:HD3 | 2.02 | 0.41 |
| 30:DG:18:GLU:HG2 | 30:DG:175:LEU:HD21 | 2.01 | 0.41 |
| 43:DX:26:TYR:HB3 | 43:DX:92:LEU:CD2 | 2.51 | 0.41 |
| 1:AA:1005:A:H1' | 1:AA:1036:G:N2 | 2.35 | 0.41 |
| 1:AA:376:G:OP1 | 16:AP:5:ARG:HB2 | 2.20 | 0.41 |
| 1:AA:538:G:O2' | 1:AA:539:A:H5' | 2.21 | 0.41 |
| 1:AA:628:G:H2' | 1:AA:629:G:C8 | 2.55 | 0.41 |
| 2:AB:137:ARG:NH1 | 2:AB:137:ARG:HB3 | 2.36 | 0.41 |
| 2:AB:30:ARG:HG3 | 2:AB:31:TYR:CD1 | 2.55 | 0.41 |
| 2:AB:48:MET:HA | 2:AB:51:LEU:HD12 | 2.03 | 0.41 |
| 4:AD:59:ARG:NH2 | 4:AD:66:ARG:NH1 | 2.68 | 0.41 |
| 17:AQ:62:SER:CB | 17:AQ:72:ARG:HD3 | 2.49 | 0.41 |
| 19:AS:15:LEU:HD12 | 19:AS:15:LEU:HA | 1.96 | 0.41 |
| 47:B1:11:ARG:HD2 | 47:B1:11:ARG:HH11 | 1.70 | 0.41 |
| 53:B7:24:THR:HG22 | 53:B7:26:GLY:H | 1.86 | 0.41 |
| 25:BA:1421:C:H2' | 25:BA:1422:C:H6 | 1.85 | 0.41 |
| 25:BA:2555:G:H2' | 25:BA:2556:G:C8 | 2.55 | 0.41 |
| 25:BA:999:G:N3 | 25:BA:2286:A:C2 | 2.88 | 0.41 |
| 36:BQ:41:TRP:CD1 | 36:BQ:96:VAL:HG22 | 2.55 | 0.41 |
| 45:BZ:151:HIS:C | 45:BZ:153:SER:N | 2.73 | 0.41 |
| 1:CA:1111:A:H2' | 1:CA:1112:C:C6 | 2.56 | 0.41 |
| 1:CA:429:U:H3' | 4:CD:9:CYS:SG | 2.61 | 0.41 |
| 1:CA:749:C:O2' | 1:CA:750:G:H5' | 2.20 | 0.41 |
| 2:CB:200:ILE:O | 2:CB:200:ILE:HG12 | 2.21 | 0.41 |
| 4:CD:15:GLU:CG | 4:CD:63:LYS:HB3 | 2.46 | 0.41 |
| 8:CH:82:HIS:NE2 | 8:CH:84:ARG:HG2 | 2.36 | 0.41 |
| 11:CK:33:THR:OG1 | 11:CK:34:ASP:O | 2.31 | 0.41 |
| 19:CS:41:VAL:HG12 | 19:CS:43:GLU:N | 2.30 | 0.41 |
| 24:CW:4:PRO:HA | 24:CW:5:MVA:HN1 | 1.33 | 0.41 |
| 23:CX:43:A:C2 | 23:CX:44:A:C4 | 3.09 | 0.41 |
| 25:DA:1525:G:H2' | 25:DA:1526:G:C8 | 2.56 | 0.41 |
| 25:DA:1580:A:OP2 | 25:DA:1580:A:H8 | 2.04 | 0.41 |
| 25:DA:1788:C:H2' | 25:DA:1789:A:O4' | 2.20 | 0.41 |
| 25:DA:1854:A:H2' | 25:DA:1855:G:O4' | 2.20 | 0.41 |
| 25:DA:2640:G:H1 | 25:DA:2774:C:N4 | 2.17 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:301:G:C4 | 25:DA:302:C:C5 | 3.08 | 0.41 |
| 25:DA:705:A:H1' | 27:DD:9:TYR:CE1 | 2.55 | 0.41 |
| 29:DF:110:LEU:HA | 29:DF:110:LEU:HD23 | 1.79 | 0.41 |
| 38:DS:29:PHE:CD1 | 38:DS:30:ARG:N | 2.89 | 0.41 |
| 43:DX:84:ALA:O | 43:DX:87:GLN:HG3 | 2.21 | 0.41 |
| 1:AA:1258:G:H1 | 1:AA:1277:C:H42 | 1.68 | 0.41 |
| 1:AA:1339:A:H2' | 1:AA:1340:A:O4' | 2.21 | 0.41 |
| 1:AA:1508:G:H2' | 1:AA:1509:C:O4' | 2.21 | 0.41 |
| 7:AG:104:LEU:HD13 | 7:AG:104:LEU:HA | 1.88 | 0.41 |
| 9:AI:23:ASN:ND2 | 9:AI:25:LYS:HE3 | 2.36 | 0.41 |
| 13:AM:49:THR:OG1 | 13:AM:52:GLU:OE1 | 2.28 | 0.41 |
| 49:B3:15:TYR:HA | 49:B3:16:PRO:HD3 | 1.88 | 0.41 |
| 51:B5:35:GLU:HG3 | 51:B5:51:TYR:CD2 | 2.56 | 0.41 |
| 25:BA:1362:U:H2' | 25:BA:1363:A:H8 | 1.85 | 0.41 |
| 25:BA:816:G:H5' | 25:BA:1425:A:N6 | 2.36 | 0.41 |
| 25:BA:1505:C:H4' | 25:BA:1506:G:O5' | 2.19 | 0.41 |
| 25:BA:642:G:H5' | 29:BF:205:ARG:HD2 | 2.02 | 0.41 |
| 30:BG:139:LEU:HG | 30:BG:139:LEU:H | 1.53 | 0.41 |
| 32:BI:30:LEU:HD23 | 32:BI:30:LEU:HA | 1.70 | 0.41 |
| 1:CA:1039:C:N4 | 1:CA:1040:U:O4 | 2.54 | 0.41 |
| 1:CA:10:A:O2' | 1:CA:11:G:H5' | 2.20 | 0.41 |
| 1:CA:1191:A:OP1 | 3:CC:4:LYS:HG3 | 2.20 | 0.41 |
| 1:CA:991:U:N3 | 1:CA:1212:U:O2 | 2.53 | 0.41 |
| 1:CA:1245:A:H2' | 1:CA:1246:C:C6 | 2.56 | 0.41 |
| 1:CA:1258:G:O2' | 1:CA:1259:C:H5' | 2.21 | 0.41 |
| 1:CA:647:C:C2' | 1:CA:648:A:H5' | 2.50 | 0.41 |
| 1:CA:892:A:O2' | 1:CA:1415:G:H4' | 2.21 | 0.41 |
| 1:CA:955:U:O2' | 19:CS:83:HIS:HD2 | 2.03 | 0.41 |
| 2:CB:185:ILE:HA | 2:CB:199:TYR:O | 2.21 | 0.41 |
| 7:CG:69:VAL:HG12 | 7:CG:69:VAL:O | 2.21 | 0.41 |
| 13:CM:20:THR:C | 13:CM:22:ILE:H | 2.23 | 0.41 |
| 3:CC:18:TRP:NE1 | 14:CN:53:LEU:O | 2.53 | 0.41 |
| 15:CO:64:ARG:HH11 | 15:CO:68:ARG:NH2 | 2.17 | 0.41 |
| 1:CA:664:G:P | 18:CR:64:ARG:HH12 | 2.44 | 0.41 |
| 24:CW:3:004:O | 24:CW:6:2R1:N | 2.53 | 0.41 |
| 23:CX:30:G:C4 | 23:CX:31:G:C8 | 3.09 | 0.41 |
| 48:D2:8:LYS:HA | 48:D2:8:LYS:HD2 | 1.92 | 0.41 |
| 37:DR:33:ARG:NH2 | 51:D5:57:VAL:O | 2.49 | 0.41 |
| 25:DA:1341:U:H3' | 25:DA:1397:U:O2 | 2.21 | 0.41 |
| 25:DA:1487:G:H2' | 25:DA:1488:G:H8 | 1.85 | 0.41 |
| 25:DA:1850:G:C6 | 25:DA:1851:U:C4 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:2320:A:H4' | 25:DA:2321:G:N7 | 2.36 | 0.41 |
| 25:DA:2328:A:H2' | 25:DA:2329:G:C8 | 2.56 | 0.41 |
| 25:DA:2337:G:C2 | 25:DA:2338:G:C8 | 3.08 | 0.41 |
| 25:DA:2467:C:C5 | 25:DA:2468:G:C6 | 3.08 | 0.41 |
| 25:DA:2488:A:O2' | 25:DA:2489:G:H5' | 2.21 | 0.41 |
| 25:DA:2836:U:C4 | 25:DA:2883:A:N6 | 2.88 | 0.41 |
| 25:DA:375:C:H2' | 25:DA:376:C:H6 | 1.84 | 0.41 |
| 25:DA:784:A:H5' | 25:DA:785:G:OP1 | 2.20 | 0.41 |
| 25:DA:811:U:H2' | 35:DP:21:ARG:HA | 2.02 | 0.41 |
| 25:DA:910:A:C6 | 25:DA:911:A:C6 | 3.08 | 0.41 |
| 26:DB:5:C:OP1 | 26:DB:62:C:H5' | 2.21 | 0.41 |
| 26:DB:83:G:H5'' | 49:D3:52:HIS:CE1 | 2.55 | 0.41 |
| 31:DH:3:ARG:NH2 | 31:DH:5:GLY:H | 2.19 | 0.41 |
| 40:DU:81:HIS:O | 40:DU:84:LYS:HB3 | 2.21 | 0.41 |
| 41:DV:43:GLU:N | 41:DV:43:GLU:OE2 | 2.54 | 0.41 |
| 43:DX:31:HIS:HA | 43:DX:32:PRO:HD3 | 1.87 | 0.41 |
| 45:DZ:144:LEU:HD23 | 45:DZ:144:LEU:HA | 1.89 | 0.41 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:C6 | 2.56 | 0.41 |
| 1:AA:178:C:H2' | 1:AA:179:A:O4' | 2.21 | 0.41 |
| 1:AA:872:A:C4 | 1:AA:874:G:N7 | 2.88 | 0.41 |
| 2:AB:109:SER:O | 2:AB:112:VAL:HG22 | 2.20 | 0.41 |
| 2:AB:71:VAL:HG13 | 2:AB:93:VAL:HG21 | 2.02 | 0.41 |
| 3:AC:12:LEU:HD23 | 3:AC:12:LEU:HA | 1.96 | 0.41 |
| 4:AD:79:PHE:HE1 | 4:AD:204:ILE:HD13 | 1.86 | 0.41 |
| 13:AM:17:VAL:O | 13:AM:20:THR:OG1 | 2.19 | 0.41 |
| 13:AM:3:ARG:CG | 13:AM:8:GLU:HA | 2.51 | 0.41 |
| 14:AN:12:ARG:HG2 | 14:AN:13:THR:N | 2.35 | 0.41 |
| 48:B2:41:ILE:HG12 | 48:B2:41:ILE:H | 1.67 | 0.41 |
| 50:B4:18:CYS:SG | 50:B4:20:ASN:HB2 | 2.61 | 0.41 |
| 50:B4:15:ILE:HB | 50:B4:32:TYR:CD1 | 2.55 | 0.41 |
| 25:BA:1051:C:O2 | 25:BA:1189:A:C6 | 2.74 | 0.41 |
| 25:BA:1652:G:H5'' | 25:BA:1653:C:OP1 | 2.21 | 0.41 |
| 25:BA:1821:C:H5'' | 25:BA:1822:A:OP1 | 2.20 | 0.41 |
| 25:BA:2120:U:C4 | 25:BA:2121:U:C5 | 3.09 | 0.41 |
| 25:BA:2219:U:H1' | 25:BA:2220:A:C8 | 2.55 | 0.41 |
| 25:BA:771:U:C4 | 25:BA:772:G:C5 | 3.09 | 0.41 |
| 25:BA:785:G:C6 | 25:BA:786:G:C2 | 3.07 | 0.41 |
| 25:BA:776:G:C6 | 27:BD:208:LYS:HB2 | 2.56 | 0.41 |
| 30:BG:137:GLU:HG2 | 30:BG:152:LEU:HD22 | 2.03 | 0.41 |
| 30:BG:7:LEU:HD23 | 30:BG:7:LEU:HA | 1.85 | 0.41 |
| 44:BY:68:HIS:CE1 | 44:BY:70:SER:HB3 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1218:C:OP2 | 14:CN:9:LYS:NZ | 2.31 | 0.41 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:H6 | 1.84 | 0.41 |
| 1:CA:1442:G:H2' | 1:CA:1442(A):G:H5' | 2.02 | 0.41 |
| 1:CA:202:U:O2' | 1:CA:203:U:O5' | 2.19 | 0.41 |
| 1:CA:292:G:N7 | 1:CA:293:G:H1' | 2.35 | 0.41 |
| 1:CA:541:G:H2' | 1:CA:542:G:H8 | 1.85 | 0.41 |
| 1:CA:678:U:H2' | 1:CA:679:C:C6 | 2.56 | 0.41 |
| 3:CC:180:ALA:HA | 3:CC:206:GLU:HB3 | 2.02 | 0.41 |
| 1:CA:437:U:C5' | 4:CD:155:LEU:HD11 | 2.50 | 0.41 |
| 4:CD:38:TYR:HA | 4:CD:39:PRO:HD3 | 1.92 | 0.41 |
| 7:CG:26:PHE:CD2 | 7:CG:30:ILE:HD11 | 2.56 | 0.41 |
| 8:CH:97:VAL:O | 8:CH:100:ILE:HG13 | 2.21 | 0.41 |
| 9:CI:54:ASP:O | 9:CI:56:LEU:N | 2.44 | 0.41 |
| 10:CJ:21:GLN:O | 10:CJ:25:GLU:HG2 | 2.20 | 0.41 |
| 10:CJ:6:ILE:HD13 | 10:CJ:98:ILE:HD11 | 2.02 | 0.41 |
| 10:CJ:8:LEU:HB3 | 10:CJ:16:LEU:CD2 | 2.51 | 0.41 |
| 11:CK:81:ASP:OD1 | 11:CK:106:LYS:HB2 | 2.21 | 0.41 |
| 51:D5:19:ARG:HH11 | 51:D5:19:ARG:HD2 | 1.74 | 0.41 |
| 52:D6:21:TYR:CE1 | 52:D6:38:LYS:HG2 | 2.55 | 0.41 |
| 25:DA:1274:A:N3 | 25:DA:1297:C:H1' | 2.35 | 0.41 |
| 25:DA:1486:A:O2' | 25:DA:1487:G:H5' | 2.21 | 0.41 |
| 25:DA:1649:G:C2' | 25:DA:1650:G:H5' | 2.51 | 0.41 |
| 25:DA:1664:A:OP1 | 61:DA:4384:HOH:O | 2.21 | 0.41 |
| 25:DA:527:C:H5' | 25:DA:527:C:O2 | 2.21 | 0.41 |
| 25:DA:932:G:H4' | 25:DA:933:A:O5' | 2.21 | 0.41 |
| 25:DA:990:A:N1 | 25:DA:1186:G:O2' | 2.52 | 0.41 |
| 27:DD:182:LEU:HD23 | 27:DD:182:LEU:HA | 1.90 | 0.41 |
| 25:DA:2590:A:OP2 | 27:DD:238:GLY:HA2 | 2.20 | 0.41 |
| 28:DE:31:CYS:HA | 28:DE:32:PRO:HD2 | 1.83 | 0.41 |
| 25:DA:2638:G:P | 28:DE:82:ARG:NH2 | 2.94 | 0.41 |
| 30:DG:43:LEU:HB3 | 30:DG:44:GLY:H | 1.48 | 0.41 |
| 31:DH:3:ARG:CD | 31:DH:54:ARG:HH12 | 2.34 | 0.41 |
| 34:DO:29:ASN:OD1 | 34:DO:29:ASN:N | 2.54 | 0.41 |
| 38:DS:19:LYS:H | 38:DS:19:LYS:HG2 | 1.59 | 0.41 |
| 39:DT:27:THR:O | 39:DT:89:VAL:HG22 | 2.20 | 0.41 |
| 41:DV:31:ALA:O | 41:DV:61:VAL:HG12 | 2.20 | 0.41 |
| 44:DY:5:MET:HE1 | 44:DY:32:PRO:HA | 2.03 | 0.41 |
| 1:AA:1058:G:H2' | 1:AA:1059:C:O4' | 2.20 | 0.41 |
| 1:AA:1084:G:H2' | 1:AA:1085:U:C5 | 2.56 | 0.41 |
| 1:AA:1136:U:H5'' | 1:AA:1137:C:C4 | 2.56 | 0.41 |
| 1:AA:1304:G:C6 | 1:AA:1305:G:N1 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1516:G:H2' | 1:AA:1518:A:OP2 | 2.20 | 0.41 |
| 1:AA:509:A:O4' | 4:AD:58:LEU:HD12 | 2.21 | 0.41 |
| 1:AA:872:A:C5 | 1:AA:874:G:C8 | 3.09 | 0.41 |
| 3:AC:82:GLU:O | 3:AC:85:ARG:HB2 | 2.21 | 0.41 |
| 13:AM:108:ARG:HA | 13:AM:108:ARG:HD3 | 1.83 | 0.41 |
| 14:AN:46:GLU:O | 14:AN:50:LYS:HG3 | 2.21 | 0.41 |
| 17:AQ:81:ARG:HD2 | 17:AQ:81:ARG:HA | 1.86 | 0.41 |
| 30:BG:109:VAL:HG13 | 50:B4:33:VAL:HG11 | 2.03 | 0.41 |
| 25:BA:2119:C:H2' | 25:BA:2120:U:O4' | 2.21 | 0.41 |
| 25:BA:415:G:O2' | 25:BA:416:G:N7 | 2.43 | 0.41 |
| 25:BA:496:A:H5'' | 25:BA:496:A:C8 | 2.56 | 0.41 |
| 25:BA:870:G:C6 | 25:BA:882:A:C6 | 3.09 | 0.41 |
| 32:BI:14:ASP:OD1 | 32:BI:15:VAL:N | 2.54 | 0.41 |
| 34:BO:108:GLU:HG3 | 34:BO:108:GLU:H | 1.63 | 0.41 |
| 43:BX:92:LEU:O | 43:BX:94:GLY:N | 2.51 | 0.41 |
| 1:CA:1154:G:H8 | 1:CA:1154:G:H2' | 1.35 | 0.41 |
| 1:CA:1256:A:H2 | 1:CA:1277:C:H42 | 1.67 | 0.41 |
| 1:CA:939:G:N2 | 1:CA:1344:C:N3 | 2.59 | 0.41 |
| 1:CA:1493:A:O2' | 1:CA:1494:G:O5' | 2.34 | 0.41 |
| 1:CA:1511:G:H2' | 1:CA:1512:U:O4' | 2.20 | 0.41 |
| 1:CA:454:C:OP2 | 1:CA:455:C:N4 | 2.52 | 0.41 |
| 1:CA:500:G:N2 | 1:CA:546:G:H1' | 2.36 | 0.41 |
| 1:CA:601:C:C2 | 1:CA:638:G:N2 | 2.88 | 0.41 |
| 1:CA:22:G:H4' | 1:CA:885:G:C8 | 2.56 | 0.41 |
| 1:CA:919:A:H8 | 1:CA:919:A:O5' | 2.03 | 0.41 |
| 1:CA:952:U:C5 | 13:CM:104:ARG:NH1 | 2.89 | 0.41 |
| 2:CB:219:VAL:O | 2:CB:223:ILE:HG23 | 2.21 | 0.41 |
| 2:CB:52:GLU:HG2 | 2:CB:56:ARG:NH2 | 2.30 | 0.41 |
| 2:CB:56:ARG:CB | 2:CB:56:ARG:HH11 | 2.31 | 0.41 |
| 8:CH:20:TYR:HE2 | 8:CH:75:ARG:HG2 | 1.85 | 0.41 |
| 9:CI:106:ALA:O | 9:CI:108:VAL:HG23 | 2.21 | 0.41 |
| 9:CI:23:ASN:HD22 | 9:CI:23:ASN:H | 1.68 | 0.41 |
| 13:CM:3:ARG:C | 13:CM:3:ARG:HD2 | 2.41 | 0.41 |
| 19:CS:58:VAL:HA | 19:CS:59:PRO:HD2 | 1.80 | 0.41 |
| 25:DA:1348:G:O6 | 25:DA:1349:A:N6 | 2.54 | 0.41 |
| 25:DA:1607:C:H5'' | 25:DA:1608:A:H5' | 2.03 | 0.41 |
| 25:DA:1804:C:O5' | 25:DA:1804:C:H6 | 2.02 | 0.41 |
| 25:DA:2274:A:C6 | 25:DA:2276:G:C8 | 3.09 | 0.41 |
| 25:DA:2416:C:O5' | 25:DA:2416:C:H6 | 2.04 | 0.41 |
| 25:DA:2516:G:C6 | 25:DA:2517:C:C4 | 3.09 | 0.41 |
| 25:DA:2505:G:H2' | 25:DA:2576:G:O6 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:2627:G:N3 | 25:DA:2781:A:H2 | 2.19 | 0.41 |
| 25:DA:2840:C:H2' | 25:DA:2841:C:C6 | 2.56 | 0.41 |
| 26:DB:48:A:H4' | 38:DS:95:HIS:CD2 | 2.53 | 0.41 |
| 27:DD:175:LEU:HD12 | 27:DD:185:VAL:HG21 | 2.03 | 0.41 |
| 27:DD:182:LEU:O | 27:DD:271:ILE:N | 2.47 | 0.41 |
| 30:DG:91:ARG:HB3 | 30:DG:91:ARG:HE | 1.53 | 0.41 |
| 33:DN:114:ARG:HD2 | 33:DN:114:ARG:HH11 | 1.75 | 0.41 |
| 33:DN:36:GLY:HA3 | 33:DN:49:GLY:HA2 | 2.03 | 0.41 |
| 40:DU:88:ILE:HG22 | 40:DU:90:VAL:HG23 | 2.03 | 0.41 |
| 43:DX:27:THR:OG1 | 43:DX:80:ILE:HG12 | 2.21 | 0.41 |
| 25:DA:335:C:H4' | 44:DY:73:ARG:CD | 2.51 | 0.41 |
| 45:DZ:156:LYS:NZ | 45:DZ:158:PRO:HD3 | 2.35 | 0.41 |
| 45:DZ:125:LEU:HG | 45:DZ:164:ALA:HB3 | 2.01 | 0.41 |
| 1:AA:1168:A:C6 | 1:AA:1169:A:C6 | 3.09 | 0.41 |
| 1:AA:138:G:H2' | 1:AA:139:G:O4' | 2.21 | 0.41 |
| 1:AA:146:G:C4 | 1:AA:147:G:C8 | 3.08 | 0.41 |
| 1:AA:717:C:H6 | 1:AA:717:C:H5'' | 1.86 | 0.41 |
| 1:AA:741:G:H2' | 1:AA:742:G:O4' | 2.21 | 0.41 |
| 1:AA:857:C:H2' | 1:AA:858:G:O4' | 2.21 | 0.41 |
| 2:AB:211:ILE:H | 2:AB:211:ILE:HG13 | 1.69 | 0.41 |
| 2:AB:71:VAL:HG12 | 2:AB:170:GLU:HG2 | 2.03 | 0.41 |
| 4:AD:85:LYS:HG3 | 4:AD:86:LYS:H | 1.85 | 0.41 |
| 7:AG:65:ALA:HB1 | 7:AG:127:ALA:HB3 | 2.02 | 0.41 |
| 10:AJ:38:ILE:HG13 | 10:AJ:71:LEU:HB3 | 2.03 | 0.41 |
| 11:AK:44:SER:O | 11:AK:48:ILE:HD13 | 2.21 | 0.41 |
| 1:AA:129:U:H5' | 17:AQ:3:LYS:HZ3 | 1.86 | 0.41 |
| 19:AS:22:LEU:O | 19:AS:27:GLU:HG3 | 2.21 | 0.41 |
| 20:AT:86:ARG:O | 20:AT:90:GLN:NE2 | 2.54 | 0.41 |
| 48:B2:65:ASN:OD1 | 48:B2:69:ARG:NH1 | 2.39 | 0.41 |
| 50:B4:40:HIS:O | 50:B4:43:TYR:N | 2.54 | 0.41 |
| 25:BA:146:G:C6 | 25:BA:147:U:C4 | 3.09 | 0.41 |
| 25:BA:215:G:H21 | 25:BA:217:A:H62 | 1.67 | 0.41 |
| 25:BA:2240:G:C5 | 25:BA:2241:C:C4 | 3.09 | 0.41 |
| 25:BA:26:G:C6 | 25:BA:27:G:N1 | 2.88 | 0.41 |
| 25:BA:441:C:O2' | 25:BA:442:A:H5' | 2.21 | 0.41 |
| 25:BA:1830:G:O2' | 27:BD:181:GLU:OE2 | 2.29 | 0.41 |
| 40:BU:19:LYS:O | 40:BU:22:LYS:HG3 | 2.21 | 0.41 |
| 41:BV:98:GLU:CD | 41:BV:100:ARG:HH11 | 2.24 | 0.41 |
| 45:BZ:119:GLU:OE2 | 45:BZ:122:ARG:NH1 | 2.54 | 0.41 |
| 1:CA:1047:G:H1 | 1:CA:1210:C:N4 | 2.16 | 0.41 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:H6 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1233:G:H2' | 1:CA:1234:C:C6 | 2.55 | 0.41 |
| 1:CA:353:A:C8 | 1:CA:353:A:H5' | 2.49 | 0.41 |
| 1:CA:410:G:OP1 | 4:CD:30:LYS:NZ | 2.22 | 0.41 |
| 1:CA:505:G:C6 | 1:CA:535:A:C2 | 3.09 | 0.41 |
| 1:CA:589:C:O2' | 1:CA:590:C:H5' | 2.21 | 0.41 |
| 3:CC:11:ARG:HD3 | 3:CC:15:THR:HB | 2.02 | 0.41 |
| 3:CC:59:ARG:HG3 | 3:CC:64:VAL:HA | 2.03 | 0.41 |
| 4:CD:196:LEU:O | 4:CD:198:VAL:N | 2.46 | 0.41 |
| 4:CD:88:VAL:HG13 | 5:CE:97:GLY:HA2 | 2.02 | 0.41 |
| 1:CA:1330:U:O3' | 13:CM:23:TYR:HE1 | 2.04 | 0.41 |
| 16:CP:58:TYR:O | 16:CP:61:SER:N | 2.52 | 0.41 |
| 52:D6:5:VAL:O | 52:D6:27:LYS:HG2 | 2.21 | 0.41 |
| 25:DA:1533:G:C2 | 25:DA:1537:G:C6 | 3.08 | 0.41 |
| 25:DA:1739:U:O2' | 25:DA:1740:G:H8 | 2.04 | 0.41 |
| 25:DA:863:A:H2' | 25:DA:864:G:H8 | 1.86 | 0.41 |
| 25:DA:878:A:C6 | 25:DA:900:A:N7 | 2.89 | 0.41 |
| 26:DB:24:G:N7 | 26:DB:56:G:H2' | 2.35 | 0.41 |
| 26:DB:43:C:C4 | 26:DB:45:A:C6 | 3.08 | 0.41 |
| 27:DD:12:SER:HB3 | 27:DD:208:LYS:HB3 | 2.03 | 0.41 |
| 29:DF:110:LEU:HD11 | 29:DF:181:LEU:HD23 | 2.03 | 0.41 |
| 30:DG:11:TYR:O | 30:DG:16:ARG:N | 2.49 | 0.41 |
| 30:DG:53:LEU:HA | 30:DG:53:LEU:HD23 | 1.84 | 0.41 |
| 37:DR:20:LEU:O | 37:DR:24:GLN:HG3 | 2.21 | 0.41 |
| 45:DZ:5:LEU:HG | 45:DZ:47:VAL:HG21 | 2.03 | 0.41 |
| 1:AA:1125:U:H2' | 1:AA:1125:U:OP2 | 2.21 | 0.41 |
| 1:AA:1216:G:N2 | 1:AA:1217:C:C2 | 2.89 | 0.41 |
| 1:AA:1371:G:C6 | 1:AA:1372:U:C4 | 3.08 | 0.41 |
| 1:AA:475:G:O2' | 1:AA:476:G:H5' | 2.19 | 0.41 |
| 1:AA:827:U:H2' | 1:AA:859:A:H61 | 1.85 | 0.41 |
| 1:AA:991:U:H1' | 1:AA:993:G:H8 | 1.86 | 0.41 |
| 2:AB:197:VAL:HB | 2:AB:200:ILE:CG2 | 2.51 | 0.41 |
| 3:AC:150:LYS:HG2 | 3:AC:151:VAL:N | 2.36 | 0.41 |
| 6:AF:19:LEU:HD11 | 6:AF:59:TYR:CE2 | 2.56 | 0.41 |
| 54:B8:50:LEU:HA | 54:B8:50:LEU:HD23 | 1.94 | 0.41 |
| 25:BA:1024:G:C2 | 25:BA:1032:C:C2 | 3.09 | 0.41 |
| 25:BA:1210:G:H2' | 25:BA:1211:U:C6 | 2.56 | 0.41 |
| 25:BA:1908:C:O5' | 25:BA:1908:C:H6 | 2.04 | 0.41 |
| 25:BA:2710:U:H2' | 25:BA:2711:C:C6 | 2.56 | 0.41 |
| 26:BB:78:A:H2' | 26:BB:79:C:O4' | 2.21 | 0.41 |
| 31:BH:117:PRO:HG3 | 31:BH:123:PHE:CD2 | 2.56 | 0.41 |
| 36:BQ:16:ARG:HG3 | 36:BQ:17:LEU:H | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:BZ:14:LYS:HA | 45:BZ:15:PRO:HD3 | 1.95 | 0.41 |
| 45:BZ:52:SER:OG | 45:BZ:53:ILE:N | 2.54 | 0.41 |
| 1:CA:20:U:H2' | 1:CA:21:G:O4' | 2.21 | 0.41 |
| 1:CA:426:G:OP1 | 4:CD:38:TYR:OH | 2.33 | 0.41 |
| 1:CA:955:U:H2' | 1:CA:956:U:O4' | 2.21 | 0.41 |
| 1:CA:991:U:H3' | 1:CA:1212:U:C4 | 2.56 | 0.41 |
| 2:CB:127:ILE:O | 2:CB:128:GLU:HB2 | 2.20 | 0.41 |
| 2:CB:137:ARG:HB3 | 2:CB:137:ARG:NH1 | 2.36 | 0.41 |
| 4:CD:50:ARG:HA | 4:CD:51:PRO:HD3 | 1.92 | 0.41 |
| 7:CG:46:ALA:O | 7:CG:50:ILE:HG23 | 2.21 | 0.41 |
| 13:CM:107:ALA:HB3 | 13:CM:111:LYS:HE3 | 2.03 | 0.41 |
| 15:CO:81:LEU:HD11 | 15:CO:85:LEU:HD12 | 2.02 | 0.41 |
| 1:CA:263:A:OP1 | 20:CT:79:ARG:NH1 | 2.54 | 0.41 |
| 25:DA:1334:G:H2' | 25:DA:1335:U:C6 | 2.56 | 0.41 |
| 1:CA:1492:A:H2' | 25:DA:1913:A:H62 | 1.84 | 0.41 |
| 25:DA:2193:G:H2' | 25:DA:2194:G:H8 | 1.87 | 0.41 |
| 25:DA:2287:A:C4 | 25:DA:2289:G:C8 | 3.09 | 0.41 |
| 25:DA:2416:C:O2' | 25:DA:2417:C:H5' | 2.21 | 0.41 |
| 25:DA:2746:U:H2' | 25:DA:2747:G:H5' | 2.01 | 0.41 |
| 25:DA:2801(A):A:N3 | 25:DA:2895:U:H1' | 2.36 | 0.41 |
| 25:DA:623:G:C6 | 25:DA:624:C:C4 | 3.09 | 0.41 |
| 25:DA:658:C:H2' | 25:DA:659:C:H6 | 1.85 | 0.41 |
| 25:DA:855:G:H2' | 25:DA:856:C:C6 | 2.56 | 0.41 |
| 25:DA:994:C:H1' | 41:DV:10:LYS:HE3 | 2.03 | 0.41 |
| 32:DI:104:GLN:O | 32:DI:105:HIS:CG | 2.73 | 0.41 |
| 26:DB:114:C:H4' | 38:DS:46:VAL:HG22 | 2.02 | 0.41 |
| 38:DS:61:ASN:O | 38:DS:65:VAL:HG23 | 2.21 | 0.41 |
| 44:DY:5:MET:HB2 | 44:DY:5:MET:HE2 | 1.91 | 0.41 |
| 1:AA:1127:G:C2' | 1:AA:1128:C:H5' | 2.50 | 0.40 |
| 1:AA:1314:C:N4 | 1:AA:1315:U:O4 | 2.54 | 0.40 |
| 1:AA:933:G:C6 | 1:AA:1385:G:C6 | 3.09 | 0.40 |
| 1:AA:266:G:C8 | 1:AA:266:G:H5' | 2.56 | 0.40 |
| 1:AA:44:G:H2' | 1:AA:45:U:O4' | 2.20 | 0.40 |
| 1:AA:584:G:O6 | 61:AA:4012:HOH:O | 2.20 | 0.40 |
| 1:AA:684:A:C6 | 1:AA:685:G:C6 | 3.09 | 0.40 |
| 2:AB:102:LEU:HB3 | 2:AB:180:LEU:HD12 | 2.02 | 0.40 |
| 2:AB:189:ASP:OD1 | 2:AB:189:ASP:N | 2.35 | 0.40 |
| 2:AB:78:GLN:NE2 | 2:AB:95:GLN:OE1 | 2.54 | 0.40 |
| 1:AA:407:G:O2' | 4:AD:116:GLN:HG3 | 2.21 | 0.40 |
| 5:AE:69:VAL:HA | 5:AE:70:PRO:HD3 | 1.72 | 0.40 |
| 6:AF:37:VAL:HG12 | 6:AF:38:GLU:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:AG:79:ARG:HB2 | 7:AG:79:ARG:HH21 | 1.85 | 0.40 |
| 18:AR:59:SER:OG | 18:AR:62:GLU:HG2 | 2.21 | 0.40 |
| 1:AA:1223:C:P | 19:AS:78:ARG:HH21 | 2.44 | 0.40 |
| 47:B1:86:SER:H | 47:B1:89:GLU:HG3 | 1.85 | 0.40 |
| 48:B2:48:HIS:CE1 | 48:B2:49:LYS:HG3 | 2.56 | 0.40 |
| 54:B8:16:ILE:HD11 | 54:B8:62:LEU:HD12 | 2.02 | 0.40 |
| 25:BA:1067:A:C3' | 25:BA:1067:A:C8 | 3.04 | 0.40 |
| 25:BA:1223:C:H2' | 25:BA:1224:C:H6 | 1.85 | 0.40 |
| 25:BA:1431:G:H4' | 25:BA:1432:C:OP1 | 2.21 | 0.40 |
| 25:BA:1541:A:H2' | 25:BA:1542:A:C8 | 2.55 | 0.40 |
| 25:BA:2564:U:C2 | 25:BA:2566:U:H5' | 2.56 | 0.40 |
| 25:BA:2718:G:C2 | 25:BA:2719:G:H1' | 2.56 | 0.40 |
| 25:BA:496:A:OP1 | 25:BA:496:A:H4' | 2.20 | 0.40 |
| 25:BA:815:G:C6 | 25:BA:816:G:C5 | 3.08 | 0.40 |
| 25:BA:857:U:O5' | 25:BA:857:U:H6 | 2.04 | 0.40 |
| 25:BA:922:G:O2' | 45:BZ:151:HIS:CE1 | 2.74 | 0.40 |
| 25:BA:639:G:N2 | 29:BF:44:ARG:O | 2.53 | 0.40 |
| 29:BF:56:GLU:OE2 | 29:BF:93:LYS:NZ | 2.47 | 0.40 |
| 28:BE:9:VAL:HB | 39:BT:3:ARG:HG2 | 2.02 | 0.40 |
| 41:BV:14:VAL:HB | 41:BV:96:ILE:HG13 | 2.03 | 0.40 |
| 45:BZ:91:LEU:HD13 | 45:BZ:91:LEU:HA | 1.88 | 0.40 |
| 1:CA:1074:G:C2 | 1:CA:1075:C:C2 | 3.09 | 0.40 |
| 1:CA:1220:G:H2' | 1:CA:1221:G:O4' | 2.20 | 0.40 |
| 1:CA:1325:C:O2' | 1:CA:1326:C:H5' | 2.22 | 0.40 |
| 1:CA:233:C:H6 | 1:CA:233:C:O5' | 2.04 | 0.40 |
| 1:CA:236:G:C6 | 1:CA:237:C:C4 | 3.09 | 0.40 |
| 1:CA:446:G:H1 | 1:CA:488:C:H42 | 1.70 | 0.40 |
| 1:CA:401:C:O2' | 1:CA:621:A:N3 | 2.47 | 0.40 |
| 2:CB:13:ALA:C | 2:CB:15:VAL:H | 2.25 | 0.40 |
| 4:CD:11:LEU:HD23 | 4:CD:66:ARG:HB3 | 2.03 | 0.40 |
| 7:CG:155:ARG:NH1 | 7:CG:155:ARG:HB3 | 2.36 | 0.40 |
| 5:CE:152:ARG:HG3 | 8:CH:43:GLY:O | 2.21 | 0.40 |
| 9:CI:116:LYS:HA | 9:CI:123:PRO:HD3 | 2.02 | 0.40 |
| 9:CI:96:LEU:O | 9:CI:100:GLY:N | 2.54 | 0.40 |
| 12:CL:28:LYS:N | 12:CL:29:GLY:HA2 | 2.36 | 0.40 |
| 12:CL:6:THR:HG23 | 12:CL:9:GLN:OE1 | 2.21 | 0.40 |
| 13:CM:92:HIS:CE1 | 13:CM:98:VAL:HG21 | 2.55 | 0.40 |
| 18:CR:51:LEU:HA | 18:CR:52:PRO:HD3 | 1.94 | 0.40 |
| 19:CS:41:VAL:CG1 | 19:CS:43:GLU:H | 2.29 | 0.40 |
| 19:CS:52:TYR:HB2 | 19:CS:57:HIS:CE1 | 2.56 | 0.40 |
| 19:CS:63:THR:OG1 | 19:CS:64:GLU:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:2361:A:P | 54:D8:27:THR:HG1 | 2.44 | 0.40 |
| 25:DA:1131:G:C2 | 25:DA:1132:A:C4 | 3.10 | 0.40 |
| 25:DA:1195:G:O2' | 25:DA:1226:A:N1 | 2.46 | 0.40 |
| 25:DA:1590:U:H2' | 25:DA:1591:G:C8 | 2.57 | 0.40 |
| 25:DA:1682:G:H1' | 25:DA:1762:A:C6 | 2.57 | 0.40 |
| 25:DA:1801:G:H3' | 25:DA:1802:A:H5' | 2.03 | 0.40 |
| 25:DA:1957:C:O2' | 25:DA:1985:G:H1' | 2.22 | 0.40 |
| 25:DA:2228:G:C5 | 25:DA:2229:C:C4 | 3.09 | 0.40 |
| 25:DA:227:A:C2 | 25:DA:2407:G:H1' | 2.56 | 0.40 |
| 25:DA:2436:G:C6 | 25:DA:2437:U:C4 | 3.10 | 0.40 |
| 25:DA:2716:U:O2' | 25:DA:2717:G:H5' | 2.20 | 0.40 |
| 25:DA:89:G:C3' | 25:DA:90:U:H5'' | 2.44 | 0.40 |
| 27:DD:164:GLN:NE2 | 27:DD:176:ARG:HH22 | 2.19 | 0.40 |
| 28:DE:2:LYS:HB2 | 28:DE:95:ILE:HD12 | 2.03 | 0.40 |
| 29:DF:101:LEU:HD12 | 29:DF:102:PRO:HD2 | 2.03 | 0.40 |
| 31:DH:9:ILE:HA | 31:DH:10:PRO:HD2 | 1.94 | 0.40 |
| 31:DH:149:ARG:HA | 31:DH:162:ILE:HG21 | 2.03 | 0.40 |
| 32:DI:60:GLU:CB | 32:DI:61:ARG:HH21 | 2.34 | 0.40 |
| 32:DI:72:LEU:HB2 | 32:DI:138:ILE:HG21 | 2.03 | 0.40 |
| 35:DP:121:LYS:HG2 | 35:DP:122:PRO:HD2 | 2.03 | 0.40 |
| 40:DU:80:ILE:HD13 | 40:DU:80:ILE:HA | 1.91 | 0.40 |
| 44:DY:40:GLU:O | 44:DY:42:VAL:HG23 | 2.21 | 0.40 |
| 45:DZ:33:LEU:HD21 | 45:DZ:90:VAL:HG21 | 2.03 | 0.40 |
| 1:AA:1110:A:OP2 | 61:AA:4115:HOH:O | 2.22 | 0.40 |
| 1:AA:1139:G:N2 | 1:AA:1143:G:C6 | 2.89 | 0.40 |
| 1:AA:1164:G:H2' | 1:AA:1165:C:C6 | 2.56 | 0.40 |
| 1:AA:1164:G:O2' | 1:AA:1165:C:H5' | 2.21 | 0.40 |
| 1:AA:237:C:OP2 | 17:AQ:40:LYS:NZ | 2.48 | 0.40 |
| 1:AA:491:G:C4 | 1:AA:492:G:C8 | 3.09 | 0.40 |
| 1:AA:670:G:C4 | 1:AA:671:G:C8 | 3.09 | 0.40 |
| 1:AA:92:C:H2' | 1:AA:93:G:C8 | 2.56 | 0.40 |
| 2:AB:55:PHE:CE1 | 2:AB:218:ALA:HA | 2.56 | 0.40 |
| 7:AG:152:ALA:HB1 | 7:AG:155:ARG:HH21 | 1.86 | 0.40 |
| 12:AL:60:LEU:HA | 12:AL:60:LEU:HD13 | 1.93 | 0.40 |
| 12:AL:88:GLY:O | 12:AL:99:HIS:HD2 | 2.04 | 0.40 |
| 17:AQ:26:GLN:HG2 | 17:AQ:37:LYS:HG2 | 2.03 | 0.40 |
| 20:AT:45:GLN:HE21 | 20:AT:45:GLN:HB3 | 1.60 | 0.40 |
| 52:B6:40:CYS:HA | 52:B6:41:PRO:HD3 | 1.85 | 0.40 |
| 25:BA:1316:C:H5'' | 25:BA:1317:G:O5' | 2.21 | 0.40 |
| 25:BA:2075:G:OP1 | 28:BE:144:ARG:HG2 | 2.20 | 0.40 |
| 25:BA:2354:C:O2' | 25:BA:2386:C:H5'' | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:505:A:N3 | 25:BA:507:G:H5'' | 2.37 | 0.40 |
| 36:BQ:108:GLY:HA3 | 45:BZ:116:VAL:HG13 | 2.03 | 0.40 |
| 1:CA:1014:A:N3 | 1:CA:1219:U:H1' | 2.36 | 0.40 |
| 1:CA:1063:C:H3' | 1:CA:1064:G:H2' | 2.04 | 0.40 |
| 1:CA:1178:G:N3 | 1:CA:1180:A:H2 | 2.19 | 0.40 |
| 1:CA:1226:C:H6 | 13:CM:103:THR:OG1 | 2.04 | 0.40 |
| 1:CA:1244:C:H42 | 1:CA:1293:G:H1 | 1.68 | 0.40 |
| 1:CA:1465:C:H2' | 1:CA:1466:C:O4' | 2.21 | 0.40 |
| 1:CA:458:C:C2 | 1:CA:460:G:C8 | 3.10 | 0.40 |
| 1:CA:489:C:H2' | 1:CA:490:G:C8 | 2.57 | 0.40 |
| 1:CA:598:U:H2' | 1:CA:599:C:H6 | 1.86 | 0.40 |
| 3:CC:113:ALA:CB | 3:CC:202:ILE:HG13 | 2.50 | 0.40 |
| 7:CG:65:ALA:HB1 | 7:CG:127:ALA:HB3 | 2.03 | 0.40 |
| 1:CA:522:C:H5'' | 12:CL:120:TYR:OH | 2.21 | 0.40 |
| 1:CA:986:A:H1' | 19:CS:54:GLY:O | 2.21 | 0.40 |
| 20:CT:10:LEU:HD12 | 20:CT:10:LEU:HA | 1.88 | 0.40 |
| 48:D2:48:HIS:O | 48:D2:52:ASP:HB2 | 2.20 | 0.40 |
| 54:D8:9:GLY:O | 54:D8:13:ARG:HG2 | 2.20 | 0.40 |
| 54:D8:38:GLY:O | 54:D8:42:ARG:HB2 | 2.20 | 0.40 |
| 25:DA:1032:A:H2 | 25:DA:1122:G:H22 | 1.70 | 0.40 |
| 25:DA:112:U:H2' | 25:DA:113:G:O4' | 2.21 | 0.40 |
| 25:DA:1022:G:C6 | 25:DA:1140:C:N3 | 2.90 | 0.40 |
| 25:DA:1971:A:C4 | 27:DD:241:PRO:HD3 | 2.57 | 0.40 |
| 25:DA:530:G:C5 | 25:DA:2022:U:H5'' | 2.56 | 0.40 |
| 25:DA:2282:G:H4' | 25:DA:2389:G:O2' | 2.21 | 0.40 |
| 25:DA:2298:A:N1 | 25:DA:2321:G:C2 | 2.88 | 0.40 |
| 25:DA:282:A:N6 | 25:DA:284:U:C2 | 2.89 | 0.40 |
| 25:DA:300:A:H1' | 25:DA:319:C:C1' | 2.51 | 0.40 |
| 25:DA:324:A:N6 | 25:DA:338:G:O2' | 2.50 | 0.40 |
| 25:DA:699:A:H4' | 25:DA:1554:A:N6 | 2.36 | 0.40 |
| 25:DA:996:A:N6 | 25:DA:1160:G:C6 | 2.90 | 0.40 |
| 26:DB:32:C:C4 | 26:DB:33:G:N7 | 2.89 | 0.40 |
| 28:DE:93:VAL:O | 28:DE:95:ILE:N | 2.54 | 0.40 |
| 30:DG:25:TYR:CD2 | 30:DG:30:GLU:HB3 | 2.57 | 0.40 |
| 34:DO:35:VAL:HG11 | 34:DO:103:ALA:CB | 2.50 | 0.40 |
| 35:DP:46:LYS:HE3 | 35:DP:46:LYS:HB3 | 1.90 | 0.40 |
| 41:DV:40:LEU:HB2 | 41:DV:46:VAL:HG22 | 2.02 | 0.40 |
| 44:DY:19:LYS:HB3 | 44:DY:19:LYS:HE2 | 1.91 | 0.40 |
| 1:AA:1127:G:H22 | 1:AA:1147:C:N4 | 2.20 | 0.40 |
| 1:AA:1277:C:H2' | 1:AA:1279:A:H8 | 1.85 | 0.40 |
| 1:AA:1321:C:H3' | 1:AA:1322:C:H6 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1343:G:H2' | 1:AA:1344:C:C6 | 2.56 | 0.40 |
| 1:AA:184:G:O4' | 1:AA:224:C:H4' | 2.21 | 0.40 |
| 1:AA:341:C:C2' | 1:AA:342:C:H5' | 2.51 | 0.40 |
| 1:AA:477:A:O2' | 1:AA:479:C:H5' | 2.22 | 0.40 |
| 1:AA:633:G:H2' | 1:AA:634:C:C6 | 2.57 | 0.40 |
| 1:AA:731:G:OP1 | 1:AA:766:A:H1' | 2.20 | 0.40 |
| 1:AA:78:G:N2 | 1:AA:91:C:N3 | 2.69 | 0.40 |
| 1:AA:864:A:H8 | 1:AA:864:A:O5' | 2.05 | 0.40 |
| 3:AC:92:ALA:HA | 3:AC:95:THR:CB | 2.51 | 0.40 |
| 4:AD:171:GLY:HA2 | 4:AD:172:PRO:HD3 | 1.95 | 0.40 |
| 4:AD:173:TRP:HA | 4:AD:186:LEU:HB2 | 2.02 | 0.40 |
| 17:AQ:60:ILE:HG12 | 17:AQ:61:GLU:N | 2.36 | 0.40 |
| 25:BA:1736:A:N6 | 25:BA:1745:A:H2 | 2.04 | 0.40 |
| 25:BA:1900:G:H2' | 25:BA:1901:C:H6 | 1.86 | 0.40 |
| 25:BA:2428:C:H6 | 25:BA:2428:C:O5' | 2.04 | 0.40 |
| 25:BA:2430:A:H2' | 25:BA:2431:U:O4' | 2.21 | 0.40 |
| 25:BA:2701:U:OP2 | 25:BA:2882:G:N2 | 2.47 | 0.40 |
| 25:BA:26:G:C6 | 25:BA:27:G:C6 | 3.09 | 0.40 |
| 25:BA:2832:G:O2' | 25:BA:2834:C:OP2 | 2.31 | 0.40 |
| 27:BD:127:VAL:HA | 27:BD:193:VAL:HG22 | 2.04 | 0.40 |
| 27:BD:275:LYS:HB3 | 27:BD:276:LYS:H | 1.36 | 0.40 |
| 35:BP:94:GLU:HG3 | 35:BP:124:LYS:HB3 | 2.03 | 0.40 |
| 39:BT:91:ARG:HH11 | 39:BT:120:ARG:HH11 | 1.68 | 0.40 |
| 1:CA:1122:U:C4 | 1:CA:1123:A:C5 | 3.09 | 0.40 |
| 1:CA:340:U:C2 | 1:CA:350:G:N2 | 2.89 | 0.40 |
| 1:CA:41:G:H2' | 1:CA:42:G:C8 | 2.56 | 0.40 |
| 1:CA:654:G:H2' | 1:CA:655:A:O4' | 2.21 | 0.40 |
| 11:CK:104:GLN:HG2 | 11:CK:106:LYS:HG2 | 2.02 | 0.40 |
| 18:CR:44:LEU:HD11 | 18:CR:79:LEU:HB3 | 2.02 | 0.40 |
| 25:DA:1753:G:H2' | 25:DA:1755:A:OP2 | 2.22 | 0.40 |
| 25:DA:2267:A:H5'' | 25:DA:2268:A:C5' | 2.47 | 0.40 |
| 25:DA:2329:G:H2' | 25:DA:2330:G:O4' | 2.22 | 0.40 |
| 25:DA:248:G:H5' | 25:DA:250:G:N7 | 2.35 | 0.40 |
| 25:DA:2536:G:C5 | 25:DA:2537:U:C5 | 3.09 | 0.40 |
| 25:DA:310:A:HO2' | 25:DA:311:A:P | 2.44 | 0.40 |
| 25:DA:392:C:H5'' | 25:DA:409:C:H5'' | 2.03 | 0.40 |
| 25:DA:45:C:H2' | 25:DA:47:C:H6 | 1.86 | 0.40 |
| 25:DA:724:U:H2' | 25:DA:725:G:O4' | 2.21 | 0.40 |
| 25:DA:870:A:C2 | 25:DA:908:C:C2 | 3.09 | 0.40 |
| 25:DA:94(A):G:H2' | 25:DA:95:G:O4' | 2.21 | 0.40 |
| 30:DG:121:ASN:HA | 30:DG:122:PRO:HD3 | 1.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DG:165:THR:HG23 | 30:DG:168:GLU:OE2 | 2.21 | 0.40 |
| 34:DO:7:TYR:CE1 | 34:DO:20:MET:HB2 | 2.57 | 0.40 |
| 36:DQ:110:THR:HG23 | 36:DQ:113:GLN:OE1 | 2.21 | 0.40 |
| 38:DS:10:ARG:O | 38:DS:14:VAL:HG13 | 2.22 | 0.40 |
| 38:DS:50:SER:O | 38:DS:76:LYS:NZ | 2.49 | 0.40 |
| 40:DU:76:TYR:CE1 | 40:DU:80:ILE:HG13 | 2.57 | 0.40 |
| 1:AA:1030:C:N4 | 1:AA:1031:G:C6 | 2.90 | 0.40 |
| 1:AA:1122:U:C4 | 1:AA:1123:A:N7 | 2.89 | 0.40 |
| 1:AA:1247:U:H2' | 1:AA:1248:A:O4' | 2.22 | 0.40 |
| 1:AA:1443:G:C2 | 1:AA:1460:A:C2 | 3.09 | 0.40 |
| 1:AA:235:C:H2' | 1:AA:236:G:H8 | 1.87 | 0.40 |
| 1:AA:256:U:H2' | 1:AA:257:G:C8 | 2.57 | 0.40 |
| 1:AA:583:A:N6 | 1:AA:758:G:O2' | 2.54 | 0.40 |
| 2:AB:215:LEU:HD23 | 2:AB:215:LEU:HA | 1.86 | 0.40 |
| 4:AD:65:ARG:HG2 | 4:AD:75:PHE:CG | 2.57 | 0.40 |
| 5:AE:27:ARG:HB2 | 5:AE:27:ARG:HE | 1.45 | 0.40 |
| 8:AH:6:ILE:O | 8:AH:10:LEU:HG | 2.21 | 0.40 |
| 8:AH:78:GLN:HE21 | 8:AH:78:GLN:HB2 | 1.65 | 0.40 |
| 46:B0:49:LYS:O | 46:B0:50:ASN:HB2 | 2.22 | 0.40 |
| 50:B4:59:PHE:CA | 50:B4:61:ARG:H | 2.34 | 0.40 |
| 53:B7:24:THR:O | 53:B7:28:ARG:HG3 | 2.22 | 0.40 |
| 25:BA:105:C:H2' | 25:BA:106:U:H6 | 1.85 | 0.40 |
| 25:BA:2528:G:C6 | 25:BA:2529:C:N4 | 2.89 | 0.40 |
| 25:BA:2650:G:P | 28:BE:82:ARG:HH22 | 2.45 | 0.40 |
| 25:BA:1686:U:H4' | 25:BA:2711:C:H4' | 2.02 | 0.40 |
| 25:BA:511:C:H2' | 25:BA:512:C:C6 | 2.56 | 0.40 |
| 25:BA:1857:G:H4' | 27:BD:242:ARG:CZ | 2.51 | 0.40 |
| 25:BA:346:A:OP2 | 29:BF:169:ASN:HB2 | 2.21 | 0.40 |
| 31:BH:11:VAL:HA | 31:BH:12:PRO:HD3 | 1.94 | 0.40 |
| 37:BR:109:ALA:O | 37:BR:111:LEU:HD22 | 2.22 | 0.40 |
| 38:BS:36:TYR:N | 38:BS:36:TYR:CD1 | 2.90 | 0.40 |
| 40:BU:98:LEU:HA | 40:BU:98:LEU:HD23 | 1.80 | 0.40 |
| 45:BZ:34:ASN:O | 45:BZ:35:ARG:HD2 | 2.21 | 0.40 |
| 1:CA:1003:G:H2' | 1:CA:1004:A:C4' | 2.52 | 0.40 |
| 1:CA:1150:U:C4 | 1:CA:1151:A:N6 | 2.89 | 0.40 |
| 1:CA:1166:G:H2' | 1:CA:1169:A:OP2 | 2.22 | 0.40 |
| 1:CA:1317:C:H42 | 14:CN:19:ARG:HH21 | 1.69 | 0.40 |
| 1:CA:194:C:H5'' | 1:CA:195:A:OP2 | 2.22 | 0.40 |
| 1:CA:363:A:C5 | 12:CL:31:PRO:HD2 | 2.57 | 0.40 |
| 1:CA:551:U:H2' | 1:CA:552:U:C6 | 2.56 | 0.40 |
| 1:CA:596:C:H2' | 1:CA:597:G:C8 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:688:G:H2' | 1:CA:689:C:H6 | 1.85 | 0.40 |
| 1:CA:708:C:H2' | 1:CA:709:G:H8 | 1.86 | 0.40 |
| 1:CA:79:G:H1 | 1:CA:90:U:H3 | 1.70 | 0.40 |
| 6:CF:82:ARG:NH1 | 6:CF:82:ARG:HB3 | 2.36 | 0.40 |
| 8:CH:20:TYR:HA | 8:CH:65:TYR:CZ | 2.56 | 0.40 |
| 8:CH:51:VAL:HG21 | 8:CH:60:ARG:HB2 | 2.04 | 0.40 |
| 1:CA:1371:G:O3' | 9:CI:69:GLY:HA3 | 2.21 | 0.40 |
| 15:CO:74:ASP:OD1 | 15:CO:76:GLU:HB2 | 2.21 | 0.40 |
| 18:CR:52:PRO:HB2 | 18:CR:54:ARG:HG2 | 2.03 | 0.40 |
| 52:D6:25:LYS:HE3 | 52:D6:27:LYS:HA | 2.04 | 0.40 |
| 25:DA:1131:G:C8 | 25:DA:2025:C:H4' | 2.56 | 0.40 |
| 25:DA:143:G:C6 | 25:DA:143(A):C:C4 | 3.10 | 0.40 |
| 25:DA:1288:U:O2' | 25:DA:1647:G:N2 | 2.55 | 0.40 |
| 25:DA:2580:U:C5 | 25:DA:2581:G:C6 | 3.09 | 0.40 |
| 25:DA:2745:C:H4' | 31:DH:142:GLY:O | 2.20 | 0.40 |
| 25:DA:2769:C:H2' | 25:DA:2770:G:O4' | 2.21 | 0.40 |
| 25:DA:30:G:H2' | 25:DA:31:C:O4' | 2.21 | 0.40 |
| 25:DA:373:U:H2' | 25:DA:374:A:H8 | 1.86 | 0.40 |
| 26:DB:98:G:C5 | 26:DB:99:G:C8 | 3.09 | 0.40 |
| 28:DE:12:THR:HG21 | 39:DT:11:GLU:OE2 | 2.21 | 0.40 |
| 28:DE:105:THR:HG21 | 28:DE:164:ARG:CZ | 2.51 | 0.40 |
| 28:DE:38:THR:O | 28:DE:42:ASP:N | 2.40 | 0.40 |
| 37:DR:70:LEU:O | 37:DR:72:ASP:N | 2.55 | 0.40 |
| 28:DE:14:ILE:HB | 39:DT:14:TYR:CZ | 2.56 | 0.40 |
| 39:DT:59:THR:HG23 | 39:DT:78:LEU:HB2 | 2.03 | 0.40 |
| 45:DZ:96:VAL:N | 45:DZ:128:VAL:O | 2.45 | 0.40 |
| 1:AA:1005:A:H5'' | 1:AA:1006:C:OP2 | 2.20 | 0.40 |
| 1:AA:1079:G:C6 | 1:AA:1080:A:N6 | 2.90 | 0.40 |
| 1:AA:1095:U:P | 1:AA:1108:G:H1 | 2.43 | 0.40 |
| 1:AA:1367:C:N3 | 1:AA:1368:G:C8 | 2.90 | 0.40 |
| 1:AA:41:G:H2' | 1:AA:42:G:H8 | 1.87 | 0.40 |
| 1:AA:676:A:H2 | 11:AK:119:CYS:SG | 2.44 | 0.40 |
| 1:AA:69:G:H2' | 1:AA:70:G:H8 | 1.82 | 0.40 |
| 1:AA:828:A:N6 | 1:AA:829:G:C2 | 2.90 | 0.40 |
| 2:AB:19:HIS:HE1 | 2:AB:189:ASP:CB | 2.35 | 0.40 |
| 2:AB:95:GLN:HB3 | 2:AB:147:LYS:NZ | 2.36 | 0.40 |
| 4:AD:107:ARG:HH22 | 4:AD:194:LEU:HD22 | 1.86 | 0.40 |
| 4:AD:61:LYS:HD2 | 4:AD:207:TYR:OH | 2.21 | 0.40 |
| 5:AE:57:LYS:HD3 | 5:AE:61:TYR:HE2 | 1.87 | 0.40 |
| 14:AN:3:ARG:HH21 | 14:AN:3:ARG:CB | 2.34 | 0.40 |
| 16:AP:59:TRP:HB3 | 16:AP:64:ALA:HB2 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:AQ:58:GLU:O | 17:AQ:74:LEU:N | 2.43 | 0.40 |
| 18:AR:40:LEU:HA | 18:AR:40:LEU:HD23 | 1.72 | 0.40 |
| 46:B0:27:GLU:HB2 | 46:B0:69:PHE:CD1 | 2.56 | 0.40 |
| 49:B3:7:LYS:HG3 | 49:B3:34:GLU:HG3 | 2.04 | 0.40 |
| 50:B4:9:LEU:HA | 50:B4:9:LEU:HD23 | 1.96 | 0.40 |
| 25:BA:1394:G:O6 | 25:BA:1395:A:N6 | 2.55 | 0.40 |
| 25:BA:1698:G:N2 | 25:BA:2029:C:C2 | 2.90 | 0.40 |
| 25:BA:218:A:H3' | 25:BA:218:A:C8 | 2.57 | 0.40 |
| 25:BA:2274:U:O2' | 25:BA:2275:C:H5' | 2.21 | 0.40 |
| 25:BA:2310:A:H2' | 25:BA:2311:G:O4' | 2.21 | 0.40 |
| 25:BA:2372:A:C2 | 25:BA:2373:A:H1' | 2.56 | 0.40 |
| 25:BA:1781:G:O2' | 25:BA:2870:A:N1 | 2.48 | 0.40 |
| 25:BA:504:A:C6 | 25:BA:506:A:C6 | 3.09 | 0.40 |
| 25:BA:938:G:C2 | 25:BA:939:C:C2 | 3.10 | 0.40 |
| 32:BI:140:LEU:HA | 32:BI:140:LEU:HD23 | 1.71 | 0.40 |
| 41:BV:18:LEU:O | 41:BV:95:LEU:HD23 | 2.22 | 0.40 |
| 45:BZ:163:LEU:HA | 45:BZ:163:LEU:HD12 | 1.87 | 0.40 |
| 1:CA:1003:G:C2' | 1:CA:1004:A:H4' | 2.52 | 0.40 |
| 1:CA:1086:U:H2' | 1:CA:1087:G:O4' | 2.21 | 0.40 |
| 1:CA:1183:A:H5' | 1:CA:1183:A:H8 | 1.85 | 0.40 |
| 1:CA:1272:G:C5 | 1:CA:1273:G:C8 | 3.10 | 0.40 |
| 3:CC:18:TRP:O | 3:CC:21:ARG:NH1 | 2.54 | 0.40 |
| 8:CH:86:ILE:HG12 | 8:CH:135:CYS:HA | 2.04 | 0.40 |
| 10:CJ:49:VAL:HG12 | 10:CJ:61:GLU:O | 2.22 | 0.40 |
| 13:CM:90:LEU:HD23 | 13:CM:93:ARG:NE | 2.37 | 0.40 |
| 19:CS:36:ARG:NH1 | 19:CS:53:ASN:HA | 2.37 | 0.40 |
| 25:DA:1171:G:H1 | 25:DA:1178:C:H42 | 1.69 | 0.40 |
| 25:DA:1301:A:C8 | 25:DA:1303:G:C8 | 3.09 | 0.40 |
| 25:DA:1416:G:HO2' | 25:DA:1417:C:H5 | 1.65 | 0.40 |
| 25:DA:1842:G:H2' | 25:DA:1843:C:O4' | 2.22 | 0.40 |
| 25:DA:2433:A:H5'' | 25:DA:2434:A:OP1 | 2.21 | 0.40 |
| 25:DA:2748:A:C6 | 25:DA:2749:A:C5 | 3.10 | 0.40 |
| 25:DA:478:A:C6 | 25:DA:480:A:C6 | 3.09 | 0.40 |
| 37:DR:37:THR:HA | 37:DR:111:LEU:HD12 | 2.02 | 0.40 |
| 39:DT:61:PHE:CZ | 39:DT:76:PHE:HB2 | 2.57 | 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 | 229/256 (90%) | 200 (87%) | 23 (10%) | 6 (3%) | 5 | 26 |
| 2 | CB | 229/256 (90%) | 201 (88%) | 18 (8%) | 10 (4%) | 2 | 15 |
| 3 | AC | 204/239 (85%) | 179 (88%) | 22 (11%) | 3 (2%) | 10 | 39 |
| 3 | CC | 204/239 (85%) | 178 (87%) | 24 (12%) | 2 (1%) | 15 | 49 |
| 4 | AD | 206/209 (99%) | 182 (88%) | 22 (11%) | 2 (1%) | 15 | 49 |
| 4 | CD | 206/209 (99%) | 185 (90%) | 18 (9%) | 3 (2%) | 10 | 39 |
| 5 | AE | 146/162 (90%) | 127 (87%) | 15 (10%) | 4 (3%) | 5 | 25 |
| 5 | CE | 146/162 (90%) | 133 (91%) | 10 (7%) | 3 (2%) | 7 | 30 |
| 6 | AF | 98/101 (97%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 6 | CF | 98/101 (97%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 7 | AG | 153/156 (98%) | 137 (90%) | 14 (9%) | 2 (1%) | 12 | 42 |
| 7 | CG | 153/156 (98%) | 137 (90%) | 15 (10%) | 1 (1%) | 22 | 57 |
| 8 | AH | 135/138 (98%) | 129 (96%) | 6 (4%) | 0 | 100 | 100 |
| 8 | CH | 135/138 (98%) | 129 (96%) | 5 (4%) | 1 (1%) | 22 | 57 |
| 9 | AI | 125/128 (98%) | 111 (89%) | 10 (8%) | 4 (3%) | 4 | 22 |
| 9 | CI | 125/128 (98%) | 112 (90%) | 11 (9%) | 2 (2%) | 9 | 37 |
| 10 | AJ | 95/105 (90%) | 85 (90%) | 7 (7%) | 3 (3%) | 4 | 22 |
| 10 | CJ | 94/105 (90%) | 86 (92%) | 7 (7%) | 1 (1%) | 14 | 46 |
| 11 | AK | 112/129 (87%) | 98 (88%) | 13 (12%) | 1 (1%) | 17 | 52 |
| 11 | CK | 112/129 (87%) | 99 (88%) | 12 (11%) | 1 (1%) | 17 | 52 |
| 12 | AL | 120/132 (91%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 12 | CL | 120/132 (91%) | 112 (93%) | 8 (7%) | 0 | 100 | 100 |
| 13 | AM | 121/126 (96%) | 106 (88%) | 15 (12%) | 0 | 100 | 100 |
| 13 | CM | 120/126 (95%) | 104 (87%) | 14 (12%) | 2 (2%) | 9 | 36 |
| 14 | AN | 58/61 (95%) | 54 (93%) | 4 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14 | CN | 58/61 (95%) | 55 (95%) | 3 (5%) | 0 | 100 | 100 |
| 15 | AO | 86/89 (97%) | 82 (95%) | 4 (5%) | 0 | 100 | 100 |
| 15 | CO | 86/89 (97%) | 80 (93%) | 5 (6%) | 1 (1%) | 13 | 44 |
| 16 | AP | 80/88 (91%) | 69 (86%) | 11 (14%) | 0 | 100 | 100 |
| 16 | CP | 80/88 (91%) | 70 (88%) | 10 (12%) | 0 | 100 | 100 |
| 17 | AQ | 97/105 (92%) | 91 (94%) | 6 (6%) | 0 | 100 | 100 |
| 17 | CQ | 97/105 (92%) | 93 (96%) | 4 (4%) | 0 | 100 | 100 |
| 18 | AR | 66/88 (75%) | 60 (91%) | 5 (8%) | 1 (2%) | 10 | 39 |
| 18 | CR | 66/88 (75%) | 60 (91%) | 5 (8%) | 1 (2%) | 10 | 39 |
| 19 | AS | 81/93 (87%) | 74 (91%) | 7 (9%) | 0 | 100 | 100 |
| 19 | CS | 81/93 (87%) | 69 (85%) | 12 (15%) | 0 | 100 | 100 |
| 20 | AT | 94/106 (89%) | 84 (89%) | 5 (5%) | 5 (5%) | 2 | 12 |
| 20 | CT | 94/106 (89%) | 85 (90%) | 3 (3%) | 6 (6%) | 1 | 8 |
| 21 | AU | 21/27 (78%) | 17 (81%) | 4 (19%) | 0 | 100 | 100 |
| 21 | CU | 21/27 (78%) | 18 (86%) | 1 (5%) | 2 (10%) | 0 | 3 |
| 24 | AW | 3/10 (30%) | 1 (33%) | 0 | 2 (67%) | 0 | 0 |
| 24 | CW | 3/10 (30%) | 1 (33%) | 1 (33%) | 1 (33%) | 0 | 0 |
| 27 | BD | 273/276 (99%) | 259 (95%) | 13 (5%) | 1 (0%) | 34 | 69 |
| 27 | DD | 273/276 (99%) | 257 (94%) | 13 (5%) | 3 (1%) | 14 | 46 |
| 28 | BE | 202/206 (98%) | 195 (96%) | 6 (3%) | 1 (0%) | 29 | 64 |
| 28 | DE | 202/206 (98%) | 194 (96%) | 6 (3%) | 2 (1%) | 15 | 49 |
| 29 | BF | 201/210 (96%) | 193 (96%) | 7 (4%) | 1 (0%) | 29 | 64 |
| 29 | DF | 201/210 (96%) | 189 (94%) | 10 (5%) | 2 (1%) | 15 | 49 |
| 30 | BG | 179/182 (98%) | 163 (91%) | 13 (7%) | 3 (2%) | 9 | 36 |
| 30 | DG | 179/182 (98%) | 160 (89%) | 13 (7%) | 6 (3%) | 3 | 21 |
| 31 | BH | 172/180 (96%) | 161 (94%) | 10 (6%) | 1 (1%) | 25 | 59 |
| 31 | DH | 172/180 (96%) | 159 (92%) | 11 (6%) | 2 (1%) | 13 | 44 |
| 32 | BI | 144/148 (97%) | 122 (85%) | 17 (12%) | 5 (4%) | 3 | 20 |
| 32 | DI | 144/148 (97%) | 123 (85%) | 17 (12%) | 4 (3%) | 5 | 25 |
| 33 | BN | 138/140 (99%) | 134 (97%) | 4 (3%) | 0 | 100 | 100 |
| 33 | DN | 138/140 (99%) | 131 (95%) | 6 (4%) | 1 (1%) | 22 | 57 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 34 | BO | 120/122 (98%) | 115 (96%) | 4 (3%) | 1 (1%) | 19 | 54 |
| 34 | DO | 120/122 (98%) | 117 (98%) | 2 (2%) | 1 (1%) | 19 | 54 |
| 35 | BP | 147/150 (98%) | 132 (90%) | 14 (10%) | 1 (1%) | 22 | 57 |
| 35 | DP | 147/150 (98%) | 133 (90%) | 12 (8%) | 2 (1%) | 11 | 40 |
| 36 | BQ | 139/141 (99%) | 130 (94%) | 8 (6%) | 1 (1%) | 22 | 57 |
| 36 | DQ | 139/141 (99%) | 129 (93%) | 8 (6%) | 2 (1%) | 11 | 40 |
| 37 | BR | 116/118 (98%) | 110 (95%) | 5 (4%) | 1 (1%) | 17 | 52 |
| 37 | DR | 116/118 (98%) | 109 (94%) | 7 (6%) | 0 | 100 | 100 |
| 38 | BS | 108/112 (96%) | 100 (93%) | 7 (6%) | 1 (1%) | 17 | 52 |
| 38 | DS | 108/112 (96%) | 102 (94%) | 5 (5%) | 1 (1%) | 17 | 52 |
| 39 | BT | 129/146 (88%) | 124 (96%) | 4 (3%) | 1 (1%) | 19 | 54 |
| 39 | DT | 129/146 (88%) | 125 (97%) | 4 (3%) | 0 | 100 | 100 |
| 40 | BU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 40 | DU | 114/118 (97%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 41 | BV | 99/101 (98%) | 91 (92%) | 7 (7%) | 1 (1%) | 15 | 49 |
| 41 | DV | 99/101 (98%) | 92 (93%) | 6 (6%) | 1 (1%) | 15 | 49 |
| 42 | BW | 110/113 (97%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 42 | DW | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 43 | BX | 93/96 (97%) | 89 (96%) | 3 (3%) | 1 (1%) | 14 | 46 |
| 43 | DX | 93/96 (97%) | 87 (94%) | 6 (6%) | 0 | 100 | 100 |
| 44 | BY | 105/110 (96%) | 95 (90%) | 10 (10%) | 0 | 100 | 100 |
| 44 | DY | 105/110 (96%) | 97 (92%) | 8 (8%) | 0 | 100 | 100 |
| 45 | BZ | 169/206 (82%) | 150 (89%) | 17 (10%) | 2 (1%) | 13 | 44 |
| 45 | DZ | 172/206 (84%) | 157 (91%) | 15 (9%) | 0 | 100 | 100 |
| 46 | B0 | 81/85 (95%) | 77 (95%) | 3 (4%) | 1 (1%) | 13 | 44 |
| 46 | D0 | 81/85 (95%) | 76 (94%) | 5 (6%) | 0 | 100 | 100 |
| 47 | B1 | 95/98 (97%) | 93 (98%) | 0 | 2 (2%) | 7 | 30 |
| 47 | D1 | 95/98 (97%) | 92 (97%) | 2 (2%) | 1 (1%) | 14 | 46 |
| 48 | B2 | 68/72 (94%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 48 | D2 | 68/72 (94%) | 65 (96%) | 3 (4%) | 0 | 100 | 100 |
| 49 | B3 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 49 | D3 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 50 | B4 | 67/71 (94%) | 50 (75%) | 9 (13%) | 8 (12%) | 0 | 1 |
| 50 | D4 | 67/71 (94%) | 50 (75%) | 8 (12%) | 9 (13%) | 0 | 1 |
| 51 | B5 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 51 | D5 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 52 | B6 | 51/54 (94%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 52 | D6 | 51/54 (94%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 53 | B7 | 46/49 (94%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | D7 | 46/49 (94%) | 44 (96%) | 1 (2%) | 1 (2%) | 6 | 29 |
| 54 | B8 | 62/65 (95%) | 60 (97%) | 2 (3%) | 0 | 100 | 100 |
| 54 | D8 | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 55 | B9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 55 | D9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| All | All | 11415/12148 (94%) | 10525 (92%) | 749 (7%) | 141 (1%) | 13 | 44 |

All (141) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 17 | PHE |
| 2 | AB | 125 | PRO |
| 3 | AC | 65 | ALA |
| 3 | AC | 107 | GLN |
| 4 | AD | 166 | LYS |
| 7 | AG | 4 | ARG |
| 9 | AI | 54 | ASP |
| 9 | AI | 56 | LEU |
| 10 | AJ | 31 | GLY |
| 10 | AJ | 79 | ARG |
| 18 | AR | 60 | ALA |
| 20 | AT | 10 | LEU |
| 27 | BD | 275 | LYS |
| 29 | BF | 130 | ALA |
| 30 | BG | 51 | ARG |
| 30 | BG | 126 | ASP |
| 31 | BH | 126 | PRO |
| 32 | BI | 73 | GLU |
| 36 | BQ | 60 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | BS | 60 | GLY |
| 47 | B1 | 3 | LYS |
| 50 | B4 | 49 | PHE |
| 50 | B4 | 55 | ARG |
| 50 | B4 | 68 | ARG |
| 2 | CB | 16 | HIS |
| 2 | CB | 126 | GLU |
| 2 | CB | 231 | GLU |
| 3 | CC | 91 | LEU |
| 3 | CC | 181 | ASN |
| 7 | CG | 7 | ALA |
| 13 | CM | 106 | ASN |
| 20 | CT | 95 | ALA |
| 20 | CT | 99 | LEU |
| 27 | DD | 239 | ARG |
| 29 | DF | 21 | ALA |
| 29 | DF | 130 | ALA |
| 30 | DG | 14 | GLU |
| 30 | DG | 47 | LYS |
| 30 | DG | 51 | ARG |
| 30 | DG | 81 | LYS |
| 30 | DG | 126 | ASP |
| 31 | DH | 126 | PRO |
| 32 | DI | 10 | GLU |
| 35 | DP | 38 | GLN |
| 36 | DQ | 28 | ALA |
| 36 | DQ | 60 | ARG |
| 47 | D1 | 3 | LYS |
| 50 | D4 | 39 | CYS |
| 50 | D4 | 45 | GLY |
| 50 | D4 | 55 | ARG |
| 50 | D4 | 63 | TYR |
| 53 | D7 | 46 | VAL |
| 2 | AB | 16 | HIS |
| 2 | AB | 19 | HIS |
| 4 | AD | 171 | GLY |
| 5 | AE | 85 | GLY |
| 5 | AE | 140 | ARG |
| 9 | AI | 95 | LYS |
| 11 | AK | 49 | GLY |
| 20 | AT | 47 | GLY |
| 32 | BI | 11 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BI | 106 | GLY |
| 34 | BO | 5 | GLN |
| 41 | BV | 79 | VAL |
| 46 | B0 | 13 | GLY |
| 50 | B4 | 47 | GLN |
| 50 | B4 | 56 | VAL |
| 50 | B4 | 66 | SER |
| 2 | CB | 8 | LYS |
| 2 | CB | 10 | LEU |
| 2 | CB | 17 | PHE |
| 2 | CB | 20 | GLU |
| 2 | CB | 121 | LEU |
| 2 | CB | 123 | ALA |
| 9 | CI | 54 | ASP |
| 9 | CI | 55 | ALA |
| 10 | CJ | 79 | ARG |
| 11 | CK | 49 | GLY |
| 31 | DH | 80 | SER |
| 33 | DN | 2 | LYS |
| 34 | DO | 5 | GLN |
| 41 | DV | 79 | VAL |
| 50 | D4 | 38 | LYS |
| 50 | D4 | 60 | GLN |
| 50 | D4 | 62 | ARG |
| 2 | AB | 128 | GLU |
| 9 | AI | 55 | ALA |
| 20 | AT | 102 | GLY |
| 35 | BP | 29 | LYS |
| 37 | BR | 45 | ARG |
| 43 | BX | 93 | GLU |
| 45 | BZ | 152 | ALA |
| 50 | B4 | 57 | GLU |
| 50 | B4 | 62 | ARG |
| 2 | CB | 21 | ARG |
| 5 | CE | 146 | ALA |
| 13 | CM | 10 | PRO |
| 20 | CT | 47 | GLY |
| 21 | CU | 3 | LYS |
| 28 | DE | 52 | LEU |
| 32 | DI | 30 | LEU |
| 32 | DI | 135 | GLU |
| 38 | DS | 84 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | D4 | 49 | PHE |
| 3 | AC | 66 | VAL |
| 20 | AT | 71 | THR |
| 24 | AW | 7 | PRO |
| 28 | BE | 52 | LEU |
| 32 | BI | 107 | VAL |
| 39 | BT | 127 | ALA |
| 4 | CD | 47 | ARG |
| 5 | CE | 37 | ARG |
| 21 | CU | 23 | PRO |
| 24 | CW | 4 | PRO |
| 27 | DD | 3 | VAL |
| 28 | DE | 73 | GLU |
| 7 | AG | 81 | GLY |
| 30 | BG | 47 | LYS |
| 32 | BI | 117 | GLU |
| 4 | CD | 136 | PRO |
| 15 | CO | 88 | ARG |
| 18 | CR | 60 | ALA |
| 20 | CT | 71 | THR |
| 20 | CT | 102 | GLY |
| 35 | DP | 45 | LEU |
| 5 | AE | 146 | ALA |
| 10 | AJ | 77 | PRO |
| 47 | B1 | 45 | ASN |
| 8 | CH | 73 | ASP |
| 30 | DG | 117 | PHE |
| 32 | DI | 85 | GLU |
| 50 | D4 | 29 | PRO |
| 2 | AB | 231 | GLU |
| 24 | AW | 4 | PRO |
| 20 | AT | 100 | ILE |
| 20 | CT | 100 | ILE |
| 27 | DD | 238 | GLY |
| 5 | AE | 69 | VAL |
| 45 | BZ | 114 | GLY |
| 5 | CE | 69 | VAL |
| 4 | CD | 7 | 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 | 192/220 (87%) | 147 (77%) | 45 (23%) | 1 | 3 |
| 2 | CB | 187/220 (85%) | 152 (81%) | 35 (19%) | 1 | 7 |
| 3 | AC | 143/188 (76%) | 125 (87%) | 18 (13%) | 4 | 18 |
| 3 | CC | 140/188 (74%) | 122 (87%) | 18 (13%) | 4 | 18 |
| 4 | AD | 170/181 (94%) | 145 (85%) | 25 (15%) | 3 | 13 |
| 4 | CD | 173/181 (96%) | 152 (88%) | 21 (12%) | 5 | 20 |
| 5 | AE | 113/123 (92%) | 104 (92%) | 9 (8%) | 12 | 40 |
| 5 | CE | 114/123 (93%) | 107 (94%) | 7 (6%) | 18 | 49 |
| 6 | AF | 83/90 (92%) | 76 (92%) | 7 (8%) | 11 | 38 |
| 6 | CF | 85/90 (94%) | 79 (93%) | 6 (7%) | 14 | 44 |
| 7 | AG | 119/127 (94%) | 100 (84%) | 19 (16%) | 2 | 11 |
| 7 | CG | 120/127 (94%) | 102 (85%) | 18 (15%) | 3 | 12 |
| 8 | AH | 114/119 (96%) | 98 (86%) | 16 (14%) | 3 | 15 |
| 8 | CH | 114/119 (96%) | 102 (90%) | 12 (10%) | 7 | 26 |
| 9 | AI | 90/99 (91%) | 76 (84%) | 14 (16%) | 2 | 11 |
| 9 | CI | 89/99 (90%) | 75 (84%) | 14 (16%) | 2 | 11 |
| 10 | AJ | 66/92 (72%) | 60 (91%) | 6 (9%) | 9 | 33 |
| 10 | CJ | 69/92 (75%) | 64 (93%) | 5 (7%) | 14 | 44 |
| 11 | AK | 82/99 (83%) | 73 (89%) | 9 (11%) | 6 | 25 |
| 11 | CK | 83/99 (84%) | 77 (93%) | 6 (7%) | 14 | 44 |
| 12 | AL | 97/109 (89%) | 90 (93%) | 7 (7%) | 14 | 44 |
| 12 | CL | 97/109 (89%) | 87 (90%) | 10 (10%) | 7 | 27 |
| 13 | AM | 93/101 (92%) | 82 (88%) | 11 (12%) | 5 | 21 |
| 13 | CM | 92/101 (91%) | 80 (87%) | 12 (13%) | 4 | 18 |
| 14 | AN | 49/50 (98%) | 41 (84%) | 8 (16%) | 2 | 10 |
| 14 | CN | 49/50 (98%) | 42 (86%) | 7 (14%) | 3 | 14 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 15 | AO | 78/80 (98%) | 69 (88%) | 9 (12%) | 5 | 22 |
| 15 | CO | 78/80 (98%) | 66 (85%) | 12 (15%) | 2 | 11 |
| 16 | AP | 69/74 (93%) | 60 (87%) | 9 (13%) | 4 | 18 |
| 16 | CP | 68/74 (92%) | 63 (93%) | 5 (7%) | 13 | 42 |
| 17 | AQ | 94/97 (97%) | 89 (95%) | 5 (5%) | 22 | 54 |
| 17 | CQ | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 42 |
| 18 | AR | 59/77 (77%) | 55 (93%) | 4 (7%) | 16 | 45 |
| 18 | CR | 59/77 (77%) | 52 (88%) | 7 (12%) | 5 | 20 |
| 19 | AS | 69/80 (86%) | 63 (91%) | 6 (9%) | 10 | 36 |
| 19 | CS | 67/80 (84%) | 57 (85%) | 10 (15%) | 3 | 13 |
| 20 | AT | 70/82 (85%) | 61 (87%) | 9 (13%) | 4 | 18 |
| 20 | CT | 70/82 (85%) | 60 (86%) | 10 (14%) | 3 | 14 |
| 21 | AU | 18/22 (82%) | 14 (78%) | 4 (22%) | 1 | 4 |
| 21 | CU | 18/22 (82%) | 16 (89%) | 2 (11%) | 6 | 24 |
| 24 | AW | 3/3 (100%) | 2 (67%) | 1 (33%) | 0 | 0 |
| 24 | CW | 3/3 (100%) | 2 (67%) | 1 (33%) | 0 | 0 |
| 27 | BD | 215/218 (99%) | 198 (92%) | 17 (8%) | 12 | 40 |
| 27 | DD | 215/218 (99%) | 190 (88%) | 25 (12%) | 5 | 22 |
| 28 | BE | 164/166 (99%) | 142 (87%) | 22 (13%) | 4 | 16 |
| 28 | DE | 164/166 (99%) | 144 (88%) | 20 (12%) | 5 | 19 |
| 29 | BF | 160/166 (96%) | 143 (89%) | 17 (11%) | 6 | 26 |
| 29 | DF | 159/166 (96%) | 145 (91%) | 14 (9%) | 10 | 36 |
| 30 | BG | 143/156 (92%) | 123 (86%) | 20 (14%) | 3 | 15 |
| 30 | DG | 142/156 (91%) | 116 (82%) | 26 (18%) | 1 | 7 |
| 31 | BH | 144/148 (97%) | 129 (90%) | 15 (10%) | 7 | 27 |
| 31 | DH | 144/148 (97%) | 131 (91%) | 13 (9%) | 9 | 34 |
| 32 | BI | 110/124 (89%) | 82 (74%) | 28 (26%) | 0 | 1 |
| 32 | DI | 104/124 (84%) | 86 (83%) | 18 (17%) | 2 | 9 |
| 33 | BN | 118/119 (99%) | 103 (87%) | 15 (13%) | 4 | 18 |
| 33 | DN | 118/119 (99%) | 102 (86%) | 16 (14%) | 3 | 16 |
| 34 | BO | 100/100 (100%) | 94 (94%) | 6 (6%) | 19 | 49 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 34 | DO | 100/100 (100%) | 91 (91%) | 9 (9%) | 9 | 34 |
| 35 | BP | 115/116 (99%) | 102 (89%) | 13 (11%) | 6 | 23 |
| 35 | DP | 115/116 (99%) | 104 (90%) | 11 (10%) | 8 | 31 |
| 36 | BQ | 111/111 (100%) | 94 (85%) | 17 (15%) | 2 | 12 |
| 36 | DQ | 111/111 (100%) | 96 (86%) | 15 (14%) | 4 | 16 |
| 37 | BR | 101/101 (100%) | 83 (82%) | 18 (18%) | 2 | 8 |
| 37 | DR | 101/101 (100%) | 85 (84%) | 16 (16%) | 2 | 11 |
| 38 | BS | 87/88 (99%) | 77 (88%) | 10 (12%) | 5 | 22 |
| 38 | DS | 85/88 (97%) | 70 (82%) | 15 (18%) | 2 | 8 |
| 39 | BT | 115/127 (91%) | 104 (90%) | 11 (10%) | 8 | 31 |
| 39 | DT | 113/127 (89%) | 105 (93%) | 8 (7%) | 14 | 44 |
| 40 | BU | 93/94 (99%) | 83 (89%) | 10 (11%) | 6 | 25 |
| 40 | DU | 93/94 (99%) | 82 (88%) | 11 (12%) | 5 | 21 |
| 41 | BV | 80/82 (98%) | 69 (86%) | 11 (14%) | 3 | 16 |
| 41 | DV | 80/82 (98%) | 71 (89%) | 9 (11%) | 6 | 23 |
| 42 | BW | 90/92 (98%) | 79 (88%) | 11 (12%) | 5 | 19 |
| 42 | DW | 90/92 (98%) | 80 (89%) | 10 (11%) | 6 | 24 |
| 43 | BX | 77/78 (99%) | 73 (95%) | 4 (5%) | 23 | 55 |
| 43 | DX | 77/78 (99%) | 74 (96%) | 3 (4%) | 32 | 65 |
| 44 | BY | 85/91 (93%) | 79 (93%) | 6 (7%) | 14 | 44 |
| 44 | DY | 85/91 (93%) | 79 (93%) | 6 (7%) | 14 | 44 |
| 45 | BZ | 145/179 (81%) | 121 (83%) | 24 (17%) | 2 | 9 |
| 45 | DZ | 145/179 (81%) | 126 (87%) | 19 (13%) | 4 | 17 |
| 46 | B0 | 65/67 (97%) | 61 (94%) | 4 (6%) | 18 | 49 |
| 46 | D0 | 65/67 (97%) | 59 (91%) | 6 (9%) | 9 | 33 |
| 47 | B1 | 80/83 (96%) | 72 (90%) | 8 (10%) | 7 | 28 |
| 47 | D1 | 80/83 (96%) | 73 (91%) | 7 (9%) | 10 | 36 |
| 48 | B2 | 65/67 (97%) | 56 (86%) | 9 (14%) | 3 | 16 |
| 48 | D2 | 65/67 (97%) | 57 (88%) | 8 (12%) | 4 | 19 |
| 49 | B3 | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 | 16 |
| 49 | D3 | 50/52 (96%) | 43 (86%) | 7 (14%) | 3 | 15 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 50 | B4 | 59/63 (94%) | 48 (81%) | 11 (19%) | 1 | 7 |
| 50 | D4 | 53/63 (84%) | 45 (85%) | 8 (15%) | 3 | 12 |
| 51 | B5 | 50/52 (96%) | 45 (90%) | 5 (10%) | 7 | 28 |
| 51 | D5 | 50/52 (96%) | 45 (90%) | 5 (10%) | 7 | 28 |
| 52 | B6 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 21 |
| 52 | D6 | 50/52 (96%) | 46 (92%) | 4 (8%) | 12 | 40 |
| 53 | B7 | 41/42 (98%) | 37 (90%) | 4 (10%) | 8 | 29 |
| 53 | D7 | 41/42 (98%) | 39 (95%) | 2 (5%) | 25 | 57 |
| 54 | B8 | 53/55 (96%) | 49 (92%) | 4 (8%) | 13 | 42 |
| 54 | D8 | 54/55 (98%) | 50 (93%) | 4 (7%) | 13 | 42 |
| 55 | B9 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 72 |
| 55 | D9 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 72 |
| All | All | 9325/10072 (93%) | 8209 (88%) | 1116 (12%) | 5 | 20 |

All (1116) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 7 | VAL |
| 2 | AB | 11 | LEU |
| 2 | AB | 15 | VAL |
| 2 | AB | 17 | PHE |
| 2 | AB | 19 | HIS |
| 2 | AB | 20 | GLU |
| 2 | AB | 21 | ARG |
| 2 | AB | 24 | TRP |
| 2 | AB | 49 | GLU |
| 2 | AB | 53 | ARG |
| 2 | AB | 56 | ARG |
| 2 | AB | 67 | THR |
| 2 | AB | 71 | VAL |
| 2 | AB | 80 | ILE |
| 2 | AB | 81 | VAL |
| 2 | AB | 87 | ARG |
| 2 | AB | 96 | ARG |
| 2 | AB | 109 | SER |
| 2 | AB | 112 | VAL |
| 2 | AB | 114 | ARG |
| 2 | AB | 116 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 126 | GLU |
| 2 | AB | 128 | GLU |
| 2 | AB | 142 | LEU |
| 2 | AB | 144 | ARG |
| 2 | AB | 145 | LEU |
| 2 | AB | 153 | ARG |
| 2 | AB | 155 | LEU |
| 2 | AB | 156 | LYS |
| 2 | AB | 157 | ARG |
| 2 | AB | 158 | LEU |
| 2 | AB | 170 | GLU |
| 2 | AB | 178 | ARG |
| 2 | AB | 185 | ILE |
| 2 | AB | 187 | LEU |
| 2 | AB | 190 | THR |
| 2 | AB | 196 | LEU |
| 2 | AB | 200 | ILE |
| 2 | AB | 208 | ILE |
| 2 | AB | 209 | ARG |
| 2 | AB | 217 | ARG |
| 2 | AB | 221 | LEU |
| 2 | AB | 222 | ILE |
| 2 | AB | 226 | ARG |
| 2 | AB | 233 | SER |
| 3 | AC | 3 | ASN |
| 3 | AC | 17 | ASP |
| 3 | AC | 27 | LYS |
| 3 | AC | 28 | GLN |
| 3 | AC | 29 | TYR |
| 3 | AC | 47 | LEU |
| 3 | AC | 52 | LEU |
| 3 | AC | 54 | ARG |
| 3 | AC | 77 | ILE |
| 3 | AC | 82 | GLU |
| 3 | AC | 98 | ASN |
| 3 | AC | 104 | GLN |
| 3 | AC | 118 | GLN |
| 3 | AC | 119 | ARG |
| 3 | AC | 131 | ARG |
| 3 | AC | 150 | LYS |
| 3 | AC | 154 | SER |
| 3 | AC | 165 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AD | 5 | ILE |
| 4 | AD | 19 | LEU |
| 4 | AD | 31 | CYS |
| 4 | AD | 58 | LEU |
| 4 | AD | 85 | LYS |
| 4 | AD | 86 | LYS |
| 4 | AD | 110 | PHE |
| 4 | AD | 112 | VAL |
| 4 | AD | 122 | ARG |
| 4 | AD | 126 | ILE |
| 4 | AD | 127 | THR |
| 4 | AD | 135 | LEU |
| 4 | AD | 150 | GLU |
| 4 | AD | 155 | LEU |
| 4 | AD | 158 | ILE |
| 4 | AD | 168 | ARG |
| 4 | AD | 181 | MET |
| 4 | AD | 182 | LYS |
| 4 | AD | 184 | LYS |
| 4 | AD | 187 | ARG |
| 4 | AD | 188 | LEU |
| 4 | AD | 190 | ASP |
| 4 | AD | 193 | ASP |
| 4 | AD | 196 | LEU |
| 4 | AD | 201 | GLN |
| 5 | AE | 10 | MET |
| 5 | AE | 12 | LEU |
| 5 | AE | 31 | LEU |
| 5 | AE | 40 | ARG |
| 5 | AE | 41 | VAL |
| 5 | AE | 47 | LYS |
| 5 | AE | 71 | LEU |
| 5 | AE | 78 | HIS |
| 5 | AE | 79 | GLU |
| 6 | AF | 46 | ARG |
| 6 | AF | 55 | ASP |
| 6 | AF | 63 | TYR |
| 6 | AF | 69 | GLU |
| 6 | AF | 74 | ASP |
| 6 | AF | 82 | ARG |
| 6 | AF | 94 | GLN |
| 7 | AG | 8 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AG | 9 | VAL |
| 7 | AG | 12 | LEU |
| 7 | AG | 13 | GLN |
| 7 | AG | 15 | ASP |
| 7 | AG | 21 | VAL |
| 7 | AG | 50 | ILE |
| 7 | AG | 51 | GLN |
| 7 | AG | 57 | GLU |
| 7 | AG | 75 | VAL |
| 7 | AG | 76 | ARG |
| 7 | AG | 79 | ARG |
| 7 | AG | 97 | GLN |
| 7 | AG | 104 | LEU |
| 7 | AG | 113 | GLU |
| 7 | AG | 114 | ARG |
| 7 | AG | 138 | LYS |
| 7 | AG | 140 | ASP |
| 7 | AG | 144 | MET |
| 8 | AH | 21 | LYS |
| 8 | AH | 23 | SER |
| 8 | AH | 25 | ASP |
| 8 | AH | 26 | VAL |
| 8 | AH | 37 | ARG |
| 8 | AH | 50 | ARG |
| 8 | AH | 52 | ASP |
| 8 | AH | 53 | VAL |
| 8 | AH | 63 | LEU |
| 8 | AH | 75 | ARG |
| 8 | AH | 78 | GLN |
| 8 | AH | 97 | VAL |
| 8 | AH | 98 | LYS |
| 8 | AH | 107 | LEU |
| 8 | AH | 112 | LEU |
| 8 | AH | 137 | VAL |
| 9 | AI | 23 | ASN |
| 9 | AI | 27 | THR |
| 9 | AI | 53 | VAL |
| 9 | AI | 54 | ASP |
| 9 | AI | 56 | LEU |
| 9 | AI | 60 | ASP |
| 9 | AI | 65 | VAL |
| 9 | AI | 66 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AI | 75 | ASP |
| 9 | AI | 81 | ILE |
| 9 | AI | 103 | THR |
| 9 | AI | 108 | VAL |
| 9 | AI | 127 | LYS |
| 9 | AI | 128 | ARG |
| 10 | AJ | 5 | ARG |
| 10 | AJ | 7 | LYS |
| 10 | AJ | 16 | LEU |
| 10 | AJ | 30 | SER |
| 10 | AJ | 68 | HIS |
| 10 | AJ | 96 | ILE |
| 11 | AK | 31 | THR |
| 11 | AK | 48 | ILE |
| 11 | AK | 70 | LYS |
| 11 | AK | 84 | VAL |
| 11 | AK | 95 | ILE |
| 11 | AK | 96 | ARG |
| 11 | AK | 104 | GLN |
| 11 | AK | 109 | VAL |
| 11 | AK | 120 | ARG |
| 12 | AL | 6 | THR |
| 12 | AL | 33 | ARG |
| 12 | AL | 46 | LYS |
| 12 | AL | 55 | VAL |
| 12 | AL | 67 | THR |
| 12 | AL | 70 | ILE |
| 12 | AL | 86 | ARG |
| 13 | AM | 3 | ARG |
| 13 | AM | 4 | ILE |
| 13 | AM | 8 | GLU |
| 13 | AM | 19 | LEU |
| 13 | AM | 43 | THR |
| 13 | AM | 50 | GLU |
| 13 | AM | 56 | LEU |
| 13 | AM | 70 | LEU |
| 13 | AM | 73 | GLU |
| 13 | AM | 110 | ARG |
| 13 | AM | 121 | LYS |
| 14 | AN | 3 | ARG |
| 14 | AN | 6 | LEU |
| 14 | AN | 7 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | AN | 18 | VAL |
| 14 | AN | 22 | THR |
| 14 | AN | 23 | ARG |
| 14 | AN | 32 | SER |
| 14 | AN | 33 | VAL |
| 15 | AO | 3 | ILE |
| 15 | AO | 5 | LYS |
| 15 | AO | 22 | THR |
| 15 | AO | 24 | SER |
| 15 | AO | 26 | GLU |
| 15 | AO | 39 | LEU |
| 15 | AO | 41 | GLU |
| 15 | AO | 83 | GLU |
| 15 | AO | 84 | LYS |
| 16 | AP | 2 | VAL |
| 16 | AP | 5 | ARG |
| 16 | AP | 8 | ARG |
| 16 | AP | 19 | ILE |
| 16 | AP | 20 | VAL |
| 16 | AP | 28 | ARG |
| 16 | AP | 45 | THR |
| 16 | AP | 50 | LYS |
| 16 | AP | 67 | THR |
| 17 | AQ | 14 | LYS |
| 17 | AQ | 53 | LEU |
| 17 | AQ | 60 | ILE |
| 17 | AQ | 63 | ARG |
| 17 | AQ | 74 | LEU |
| 18 | AR | 26 | LEU |
| 18 | AR | 32 | ARG |
| 18 | AR | 61 | LYS |
| 18 | AR | 82 | THR |
| 19 | AS | 5 | LEU |
| 19 | AS | 6 | LYS |
| 19 | AS | 28 | LYS |
| 19 | AS | 37 | ARG |
| 19 | AS | 63 | THR |
| 19 | AS | 65 | ASN |
| 20 | AT | 8 | ARG |
| 20 | AT | 9 | ASN |
| 20 | AT | 13 | LEU |
| 20 | AT | 31 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | AT | 45 | GLN |
| 20 | AT | 46 | GLU |
| 20 | AT | 56 | MET |
| 20 | AT | 58 | LYS |
| 20 | AT | 62 | LEU |
| 21 | AU | 7 | ARG |
| 21 | AU | 9 | ARG |
| 21 | AU | 10 | ARG |
| 21 | AU | 15 | ARG |
| 24 | AW | 2 | VAL |
| 27 | BD | 3 | VAL |
| 27 | BD | 12 | SER |
| 27 | BD | 13 | ARG |
| 27 | BD | 61 | LEU |
| 27 | BD | 71 | ASP |
| 27 | BD | 94 | LEU |
| 27 | BD | 103 | ARG |
| 27 | BD | 138 | VAL |
| 27 | BD | 142 | VAL |
| 27 | BD | 155 | LEU |
| 27 | BD | 211 | ARG |
| 27 | BD | 217 | ARG |
| 27 | BD | 221 | VAL |
| 27 | BD | 229 | VAL |
| 27 | BD | 242 | ARG |
| 27 | BD | 257 | LEU |
| 27 | BD | 260 | ARG |
| 28 | BE | 1 | MET |
| 28 | BE | 9 | VAL |
| 28 | BE | 12 | THR |
| 28 | BE | 21 | VAL |
| 28 | BE | 24 | THR |
| 28 | BE | 49 | LEU |
| 28 | BE | 73 | GLU |
| 28 | BE | 82 | ARG |
| 28 | BE | 89 | ASP |
| 28 | BE | 93 | VAL |
| 28 | BE | 97 | LYS |
| 28 | BE | 111 | ARG |
| 28 | BE | 116 | VAL |
| 28 | BE | 119 | ARG |
| 28 | BE | 144 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BE | 145 | LYS |
| 28 | BE | 154 | LYS |
| 28 | BE | 163 | GLU |
| 28 | BE | 170 | LEU |
| 28 | BE | 175 | VAL |
| 28 | BE | 181 | LEU |
| 28 | BE | 203 | LYS |
| 29 | BF | 19 | GLU |
| 29 | BF | 24 | LEU |
| 29 | BF | 33 | LEU |
| 29 | BF | 53 | THR |
| 29 | BF | 57 | VAL |
| 29 | BF | 64 | ILE |
| 29 | BF | 74 | ARG |
| 29 | BF | 78 | ILE |
| 29 | BF | 88 | VAL |
| 29 | BF | 106 | ARG |
| 29 | BF | 108 | LYS |
| 29 | BF | 110 | LEU |
| 29 | BF | 125 | LEU |
| 29 | BF | 170 | LEU |
| 29 | BF | 192 | LEU |
| 29 | BF | 197 | ASP |
| 29 | BF | 200 | GLU |
| 30 | BG | 5 | VAL |
| 30 | BG | 7 | LEU |
| 30 | BG | 28 | VAL |
| 30 | BG | 31 | VAL |
| 30 | BG | 43 | LEU |
| 30 | BG | 45 | GLU |
| 30 | BG | 78 | SER |
| 30 | BG | 81 | LYS |
| 30 | BG | 82 | LEU |
| 30 | BG | 86 | MET |
| 30 | BG | 91 | ARG |
| 30 | BG | 133 | LEU |
| 30 | BG | 135 | LEU |
| 30 | BG | 136 | ARG |
| 30 | BG | 140 | ILE |
| 30 | BG | 143 | GLU |
| 30 | BG | 148 | MET |
| 30 | BG | 159 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | BG | 170 | ARG |
| 30 | BG | 181 | ARG |
| 31 | BH | 6 | ARG |
| 31 | BH | 13 | LYS |
| 31 | BH | 15 | VAL |
| 31 | BH | 41 | MET |
| 31 | BH | 44 | VAL |
| 31 | BH | 49 | VAL |
| 31 | BH | 59 | ARG |
| 31 | BH | 69 | ARG |
| 31 | BH | 95 | ARG |
| 31 | BH | 98 | LEU |
| 31 | BH | 116 | GLU |
| 31 | BH | 122 | THR |
| 31 | BH | 129 | THR |
| 31 | BH | 172 | LYS |
| 31 | BH | 175 | LYS |
| 32 | BI | 9 | LEU |
| 32 | BI | 15 | VAL |
| 32 | BI | 19 | VAL |
| 32 | BI | 20 | ASP |
| 32 | BI | 38 | LEU |
| 32 | BI | 40 | THR |
| 32 | BI | 41 | GLU |
| 32 | BI | 43 | ASN |
| 32 | BI | 50 | ARG |
| 32 | BI | 54 | GLN |
| 32 | BI | 57 | ARG |
| 32 | BI | 60 | GLU |
| 32 | BI | 64 | GLU |
| 32 | BI | 66 | GLU |
| 32 | BI | 68 | LEU |
| 32 | BI | 74 | ASN |
| 32 | BI | 75 | LEU |
| 32 | BI | 77 | LEU |
| 32 | BI | 78 | THR |
| 32 | BI | 92 | VAL |
| 32 | BI | 96 | ASP |
| 32 | BI | 101 | LEU |
| 32 | BI | 107 | VAL |
| 32 | BI | 109 | ILE |
| 32 | BI | 114 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BI | 140 | LEU |
| 32 | BI | 142 | VAL |
| 32 | BI | 144 | VAL |
| 33 | BN | 28 | THR |
| 33 | BN | 33 | LEU |
| 33 | BN | 34 | LEU |
| 33 | BN | 46 | VAL |
| 33 | BN | 48 | MET |
| 33 | BN | 61 | ARG |
| 33 | BN | 68 | GLU |
| 33 | BN | 83 | LYS |
| 33 | BN | 87 | LEU |
| 33 | BN | 97 | ARG |
| 33 | BN | 99 | LEU |
| 33 | BN | 120 | LEU |
| 33 | BN | 121 | LYS |
| 33 | BN | 133 | GLN |
| 33 | BN | 137 | LYS |
| 34 | BO | 8 | LEU |
| 34 | BO | 23 | ARG |
| 34 | BO | 24 | VAL |
| 34 | BO | 58 | VAL |
| 34 | BO | 94 | ARG |
| 34 | BO | 98 | VAL |
| 35 | BP | 4 | SER |
| 35 | BP | 15 | ARG |
| 35 | BP | 42 | SER |
| 35 | BP | 59 | LEU |
| 35 | BP | 65 | ARG |
| 35 | BP | 83 | VAL |
| 35 | BP | 95 | VAL |
| 35 | BP | 98 | GLU |
| 35 | BP | 106 | LEU |
| 35 | BP | 112 | LEU |
| 35 | BP | 125 | VAL |
| 35 | BP | 144 | GLU |
| 35 | BP | 149 | GLU |
| 36 | BQ | 1 | MET |
| 36 | BQ | 5 | ARG |
| 36 | BQ | 7 | MET |
| 36 | BQ | 8 | LYS |
| 36 | BQ | 16 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | BQ | 21 | THR |
| 36 | BQ | 45 | GLN |
| 36 | BQ | 54 | MET |
| 36 | BQ | 56 | ARG |
| 36 | BQ | 60 | ARG |
| 36 | BQ | 75 | THR |
| 36 | BQ | 81 | VAL |
| 36 | BQ | 85 | LYS |
| 36 | BQ | 109 | VAL |
| 36 | BQ | 110 | THR |
| 36 | BQ | 129 | THR |
| 36 | BQ | 138 | ASP |
| 37 | BR | 1 | MET |
| 37 | BR | 6 | SER |
| 37 | BR | 18 | LEU |
| 37 | BR | 28 | LEU |
| 37 | BR | 29 | LEU |
| 37 | BR | 33 | ARG |
| 37 | BR | 36 | THR |
| 37 | BR | 44 | LEU |
| 37 | BR | 54 | LEU |
| 37 | BR | 60 | LEU |
| 37 | BR | 65 | LEU |
| 37 | BR | 67 | LEU |
| 37 | BR | 75 | LEU |
| 37 | BR | 79 | LEU |
| 37 | BR | 86 | ARG |
| 37 | BR | 91 | GLN |
| 37 | BR | 100 | LEU |
| 37 | BR | 111 | LEU |
| 38 | BS | 14 | VAL |
| 38 | BS | 20 | ARG |
| 38 | BS | 36 | TYR |
| 38 | BS | 43 | GLU |
| 38 | BS | 48 | LEU |
| 38 | BS | 50 | SER |
| 38 | BS | 59 | LYS |
| 38 | BS | 61 | ASN |
| 38 | BS | 78 | LEU |
| 38 | BS | 103 | GLU |
| 39 | BT | 13 | ARG |
| 39 | BT | 17 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | BT | 28 | VAL |
| 39 | BT | 39 | ARG |
| 39 | BT | 49 | VAL |
| 39 | BT | 53 | ARG |
| 39 | BT | 74 | ARG |
| 39 | BT | 78 | LEU |
| 39 | BT | 85 | LYS |
| 39 | BT | 96 | ARG |
| 39 | BT | 118 | ARG |
| 40 | BU | 8 | VAL |
| 40 | BU | 31 | SER |
| 40 | BU | 36 | ARG |
| 40 | BU | 60 | LEU |
| 40 | BU | 74 | LEU |
| 40 | BU | 83 | LEU |
| 40 | BU | 92 | ARG |
| 40 | BU | 95 | LEU |
| 40 | BU | 104 | GLN |
| 40 | BU | 117 | GLN |
| 41 | BV | 10 | LYS |
| 41 | BV | 18 | LEU |
| 41 | BV | 21 | ARG |
| 41 | BV | 51 | VAL |
| 41 | BV | 52 | VAL |
| 41 | BV | 61 | VAL |
| 41 | BV | 62 | LEU |
| 41 | BV | 72 | VAL |
| 41 | BV | 79 | VAL |
| 41 | BV | 95 | LEU |
| 41 | BV | 100 | ARG |
| 42 | BW | 11 | ARG |
| 42 | BW | 15 | ARG |
| 42 | BW | 17 | VAL |
| 42 | BW | 23 | LEU |
| 42 | BW | 27 | LYS |
| 42 | BW | 51 | LEU |
| 42 | BW | 60 | ASN |
| 42 | BW | 63 | ASP |
| 42 | BW | 67 | ASP |
| 42 | BW | 100 | THR |
| 42 | BW | 107 | LEU |
| 43 | BX | 2 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | BX | 57 | LEU |
| 43 | BX | 66 | LEU |
| 43 | BX | 70 | LEU |
| 44 | BY | 2 | ARG |
| 44 | BY | 7 | VAL |
| 44 | BY | 43 | ASN |
| 44 | BY | 72 | VAL |
| 44 | BY | 90 | LEU |
| 44 | BY | 91 | GLU |
| 45 | BZ | 5 | LEU |
| 45 | BZ | 6 | LYS |
| 45 | BZ | 11 | GLU |
| 45 | BZ | 19 | ARG |
| 45 | BZ | 31 | ARG |
| 45 | BZ | 40 | ASP |
| 45 | BZ | 41 | LEU |
| 45 | BZ | 42 | VAL |
| 45 | BZ | 61 | LEU |
| 45 | BZ | 76 | LEU |
| 45 | BZ | 82 | ARG |
| 45 | BZ | 86 | VAL |
| 45 | BZ | 87 | ASP |
| 45 | BZ | 91 | LEU |
| 45 | BZ | 107 | THR |
| 45 | BZ | 120 | ILE |
| 45 | BZ | 131 | ARG |
| 45 | BZ | 132 | ASN |
| 45 | BZ | 135 | GLU |
| 45 | BZ | 136 | PHE |
| 45 | BZ | 144 | LEU |
| 45 | BZ | 154 | ASP |
| 45 | BZ | 155 | LEU |
| 45 | BZ | 162 | GLU |
| 46 | B0 | 7 | LEU |
| 46 | B0 | 10 | THR |
| 46 | B0 | 20 | ARG |
| 46 | B0 | 55 | ARG |
| 47 | B1 | 21 | ARG |
| 47 | B1 | 26 | ARG |
| 47 | B1 | 35 | THR |
| 47 | B1 | 40 | ARG |
| 47 | B1 | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | B1 | 59 | THR |
| 47 | B1 | 89 | GLU |
| 47 | B1 | 95 | LEU |
| 48 | B2 | 28 | LYS |
| 48 | B2 | 30 | ARG |
| 48 | B2 | 41 | ILE |
| 48 | B2 | 45 | SER |
| 48 | B2 | 52 | ASP |
| 48 | B2 | 53 | LEU |
| 48 | B2 | 55 | ARG |
| 48 | B2 | 64 | LEU |
| 48 | B2 | 70 | GLN |
| 49 | B3 | 6 | VAL |
| 49 | B3 | 8 | LEU |
| 49 | B3 | 23 | LEU |
| 49 | B3 | 29 | ARG |
| 49 | B3 | 32 | GLN |
| 49 | B3 | 55 | ARG |
| 49 | B3 | 58 | VAL |
| 50 | B4 | 5 | ILE |
| 50 | B4 | 28 | LYS |
| 50 | B4 | 34 | GLU |
| 50 | B4 | 46 | GLN |
| 50 | B4 | 49 | PHE |
| 50 | B4 | 56 | VAL |
| 50 | B4 | 58 | ARG |
| 50 | B4 | 61 | ARG |
| 50 | B4 | 63 | TYR |
| 50 | B4 | 68 | ARG |
| 50 | B4 | 69 | LYS |
| 51 | B5 | 6 | VAL |
| 51 | B5 | 29 | THR |
| 51 | B5 | 40 | LYS |
| 51 | B5 | 58 | LEU |
| 51 | B5 | 60 | VAL |
| 52 | B6 | 4 | GLU |
| 52 | B6 | 6 | ARG |
| 52 | B6 | 14 | THR |
| 52 | B6 | 38 | LYS |
| 52 | B6 | 48 | VAL |
| 52 | B6 | 49 | HIS |
| 53 | B7 | 1 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 53 | B7 | 23 | ARG |
| 53 | B7 | 43 | THR |
| 53 | B7 | 47 | ARG |
| 54 | B8 | 14 | VAL |
| 54 | B8 | 29 | LYS |
| 54 | B8 | 31 | HIS |
| 54 | B8 | 32 | LEU |
| 55 | B9 | 26 | ILE |
| 2 | CB | 7 | VAL |
| 2 | CB | 11 | LEU |
| 2 | CB | 22 | LYS |
| 2 | CB | 23 | ARG |
| 2 | CB | 24 | TRP |
| 2 | CB | 44 | LEU |
| 2 | CB | 56 | ARG |
| 2 | CB | 67 | THR |
| 2 | CB | 71 | VAL |
| 2 | CB | 80 | ILE |
| 2 | CB | 108 | ILE |
| 2 | CB | 115 | LEU |
| 2 | CB | 126 | GLU |
| 2 | CB | 128 | GLU |
| 2 | CB | 140 | HIS |
| 2 | CB | 142 | LEU |
| 2 | CB | 144 | ARG |
| 2 | CB | 145 | LEU |
| 2 | CB | 153 | ARG |
| 2 | CB | 154 | LEU |
| 2 | CB | 157 | ARG |
| 2 | CB | 158 | LEU |
| 2 | CB | 160 | ASP |
| 2 | CB | 169 | LYS |
| 2 | CB | 178 | ARG |
| 2 | CB | 185 | ILE |
| 2 | CB | 187 | LEU |
| 2 | CB | 191 | ASP |
| 2 | CB | 200 | ILE |
| 2 | CB | 217 | ARG |
| 2 | CB | 221 | LEU |
| 2 | CB | 224 | GLN |
| 2 | CB | 226 | ARG |
| 2 | CB | 233 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CB | 235 | SER |
| 3 | CC | 3 | ASN |
| 3 | CC | 20 | SER |
| 3 | CC | 29 | TYR |
| 3 | CC | 47 | LEU |
| 3 | CC | 52 | LEU |
| 3 | CC | 77 | ILE |
| 3 | CC | 82 | GLU |
| 3 | CC | 98 | ASN |
| 3 | CC | 101 | LEU |
| 3 | CC | 104 | GLN |
| 3 | CC | 115 | LEU |
| 3 | CC | 118 | GLN |
| 3 | CC | 131 | ARG |
| 3 | CC | 152 | ILE |
| 3 | CC | 154 | SER |
| 3 | CC | 162 | GLN |
| 3 | CC | 164 | ARG |
| 3 | CC | 179 | ARG |
| 4 | CD | 10 | ARG |
| 4 | CD | 19 | LEU |
| 4 | CD | 31 | CYS |
| 4 | CD | 47 | ARG |
| 4 | CD | 58 | LEU |
| 4 | CD | 65 | ARG |
| 4 | CD | 96 | LEU |
| 4 | CD | 122 | ARG |
| 4 | CD | 127 | THR |
| 4 | CD | 135 | LEU |
| 4 | CD | 150 | GLU |
| 4 | CD | 155 | LEU |
| 4 | CD | 157 | LEU |
| 4 | CD | 170 | VAL |
| 4 | CD | 181 | MET |
| 4 | CD | 184 | LYS |
| 4 | CD | 187 | ARG |
| 4 | CD | 188 | LEU |
| 4 | CD | 191 | ARG |
| 4 | CD | 194 | LEU |
| 4 | CD | 201 | GLN |
| 5 | CE | 12 | LEU |
| 5 | CE | 31 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CE | 40 | ARG |
| 5 | CE | 41 | VAL |
| 5 | CE | 71 | LEU |
| 5 | CE | 79 | GLU |
| 5 | CE | 82 | VAL |
| 6 | CF | 23 | LYS |
| 6 | CF | 28 | ARG |
| 6 | CF | 41 | GLU |
| 6 | CF | 46 | ARG |
| 6 | CF | 63 | TYR |
| 6 | CF | 69 | GLU |
| 7 | CG | 9 | VAL |
| 7 | CG | 12 | LEU |
| 7 | CG | 13 | GLN |
| 7 | CG | 15 | ASP |
| 7 | CG | 16 | LEU |
| 7 | CG | 50 | ILE |
| 7 | CG | 51 | GLN |
| 7 | CG | 52 | GLU |
| 7 | CG | 58 | PRO |
| 7 | CG | 73 | MET |
| 7 | CG | 75 | VAL |
| 7 | CG | 85 | TYR |
| 7 | CG | 104 | LEU |
| 7 | CG | 113 | GLU |
| 7 | CG | 114 | ARG |
| 7 | CG | 140 | ASP |
| 7 | CG | 144 | MET |
| 7 | CG | 155 | ARG |
| 8 | CH | 21 | LYS |
| 8 | CH | 23 | SER |
| 8 | CH | 25 | ASP |
| 8 | CH | 53 | VAL |
| 8 | CH | 68 | ARG |
| 8 | CH | 78 | GLN |
| 8 | CH | 84 | ARG |
| 8 | CH | 97 | VAL |
| 8 | CH | 98 | LYS |
| 8 | CH | 99 | GLU |
| 8 | CH | 112 | LEU |
| 8 | CH | 137 | VAL |
| 9 | CI | 7 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | CI | 17 | VAL |
| 9 | CI | 23 | ASN |
| 9 | CI | 27 | THR |
| 9 | CI | 33 | PHE |
| 9 | CI | 66 | ARG |
| 9 | CI | 75 | ASP |
| 9 | CI | 81 | ILE |
| 9 | CI | 86 | VAL |
| 9 | CI | 92 | TYR |
| 9 | CI | 102 | LEU |
| 9 | CI | 124 | GLN |
| 9 | CI | 125 | TYR |
| 9 | CI | 128 | ARG |
| 10 | CJ | 6 | ILE |
| 10 | CJ | 23 | ILE |
| 10 | CJ | 29 | ARG |
| 10 | CJ | 68 | HIS |
| 10 | CJ | 96 | ILE |
| 11 | CK | 54 | ARG |
| 11 | CK | 79 | SER |
| 11 | CK | 84 | VAL |
| 11 | CK | 95 | ILE |
| 11 | CK | 96 | ARG |
| 11 | CK | 126 | ARG |
| 12 | CL | 33 | ARG |
| 12 | CL | 34 | ARG |
| 12 | CL | 52 | LEU |
| 12 | CL | 55 | VAL |
| 12 | CL | 59 | ARG |
| 12 | CL | 60 | LEU |
| 12 | CL | 70 | ILE |
| 12 | CL | 83 | VAL |
| 12 | CL | 97 | ARG |
| 12 | CL | 123 | LYS |
| 13 | CM | 3 | ARG |
| 13 | CM | 4 | ILE |
| 13 | CM | 8 | GLU |
| 13 | CM | 19 | LEU |
| 13 | CM | 27 | LYS |
| 13 | CM | 47 | ASP |
| 13 | CM | 56 | LEU |
| 13 | CM | 70 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | CM | 104 | ARG |
| 13 | CM | 106 | ASN |
| 13 | CM | 110 | ARG |
| 13 | CM | 121 | LYS |
| 14 | CN | 3 | ARG |
| 14 | CN | 7 | ILE |
| 14 | CN | 18 | VAL |
| 14 | CN | 22 | THR |
| 14 | CN | 23 | ARG |
| 14 | CN | 33 | VAL |
| 14 | CN | 50 | LYS |
| 15 | CO | 3 | ILE |
| 15 | CO | 5 | LYS |
| 15 | CO | 7 | GLU |
| 15 | CO | 10 | LYS |
| 15 | CO | 22 | THR |
| 15 | CO | 24 | SER |
| 15 | CO | 26 | GLU |
| 15 | CO | 39 | LEU |
| 15 | CO | 54 | ARG |
| 15 | CO | 76 | GLU |
| 15 | CO | 83 | GLU |
| 15 | CO | 84 | LYS |
| 16 | CP | 2 | VAL |
| 16 | CP | 5 | ARG |
| 16 | CP | 8 | ARG |
| 16 | CP | 28 | ARG |
| 16 | CP | 67 | THR |
| 17 | CQ | 6 | LEU |
| 17 | CQ | 49 | GLU |
| 17 | CQ | 60 | ILE |
| 17 | CQ | 63 | ARG |
| 17 | CQ | 66 | SER |
| 17 | CQ | 74 | LEU |
| 17 | CQ | 83 | ASP |
| 18 | CR | 26 | LEU |
| 18 | CR | 32 | ARG |
| 18 | CR | 41 | LYS |
| 18 | CR | 42 | ARG |
| 18 | CR | 54 | ARG |
| 18 | CR | 64 | ARG |
| 18 | CR | 76 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | CS | 6 | LYS |
| 19 | CS | 12 | ASP |
| 19 | CS | 28 | LYS |
| 19 | CS | 30 | LEU |
| 19 | CS | 33 | THR |
| 19 | CS | 37 | ARG |
| 19 | CS | 43 | GLU |
| 19 | CS | 56 | GLN |
| 19 | CS | 63 | THR |
| 19 | CS | 71 | LEU |
| 20 | CT | 36 | LEU |
| 20 | CT | 38 | LYS |
| 20 | CT | 45 | GLN |
| 20 | CT | 46 | GLU |
| 20 | CT | 56 | MET |
| 20 | CT | 62 | LEU |
| 20 | CT | 71 | THR |
| 20 | CT | 80 | ARG |
| 20 | CT | 90 | GLN |
| 20 | CT | 99 | LEU |
| 21 | CU | 10 | ARG |
| 21 | CU | 15 | ARG |
| 24 | CW | 2 | VAL |
| 27 | DD | 13 | ARG |
| 27 | DD | 32 | SER |
| 27 | DD | 61 | LEU |
| 27 | DD | 69 | ARG |
| 27 | DD | 88 | ARG |
| 27 | DD | 94 | LEU |
| 27 | DD | 103 | ARG |
| 27 | DD | 106 | ILE |
| 27 | DD | 113 | VAL |
| 27 | DD | 116 | GLN |
| 27 | DD | 134 | ARG |
| 27 | DD | 138 | VAL |
| 27 | DD | 142 | VAL |
| 27 | DD | 155 | LEU |
| 27 | DD | 200 | ASP |
| 27 | DD | 211 | ARG |
| 27 | DD | 217 | ARG |
| 27 | DD | 221 | VAL |
| 27 | DD | 229 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | DD | 242 | ARG |
| 27 | DD | 257 | LEU |
| 27 | DD | 259 | THR |
| 27 | DD | 260 | ARG |
| 27 | DD | 274 | ARG |
| 27 | DD | 276 | LYS |
| 28 | DE | 1 | MET |
| 28 | DE | 9 | VAL |
| 28 | DE | 12 | THR |
| 28 | DE | 21 | VAL |
| 28 | DE | 24 | THR |
| 28 | DE | 33 | VAL |
| 28 | DE | 40 | GLU |
| 28 | DE | 49 | LEU |
| 28 | DE | 52 | LEU |
| 28 | DE | 73 | GLU |
| 28 | DE | 75 | VAL |
| 28 | DE | 78 | LEU |
| 28 | DE | 82 | ARG |
| 28 | DE | 111 | ARG |
| 28 | DE | 116 | VAL |
| 28 | DE | 119 | ARG |
| 28 | DE | 144 | ARG |
| 28 | DE | 154 | LYS |
| 28 | DE | 163 | GLU |
| 28 | DE | 181 | LEU |
| 29 | DF | 12 | LEU |
| 29 | DF | 19 | GLU |
| 29 | DF | 20 | LEU |
| 29 | DF | 24 | LEU |
| 29 | DF | 33 | LEU |
| 29 | DF | 74 | ARG |
| 29 | DF | 106 | ARG |
| 29 | DF | 107 | LYS |
| 29 | DF | 108 | LYS |
| 29 | DF | 110 | LEU |
| 29 | DF | 135 | LYS |
| 29 | DF | 137 | LYS |
| 29 | DF | 192 | LEU |
| 29 | DF | 200 | GLU |
| 30 | DG | 5 | VAL |
| 30 | DG | 21 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DG | 28 | VAL |
| 30 | DG | 31 | VAL |
| 30 | DG | 35 | GLU |
| 30 | DG | 36 | LYS |
| 30 | DG | 43 | LEU |
| 30 | DG | 45 | GLU |
| 30 | DG | 49 | ASP |
| 30 | DG | 60 | LEU |
| 30 | DG | 84 | LYS |
| 30 | DG | 91 | ARG |
| 30 | DG | 98 | ARG |
| 30 | DG | 113 | ARG |
| 30 | DG | 115 | ARG |
| 30 | DG | 128 | ARG |
| 30 | DG | 133 | LEU |
| 30 | DG | 136 | ARG |
| 30 | DG | 140 | ILE |
| 30 | DG | 143 | GLU |
| 30 | DG | 145 | THR |
| 30 | DG | 148 | MET |
| 30 | DG | 153 | ARG |
| 30 | DG | 159 | VAL |
| 30 | DG | 164 | GLU |
| 30 | DG | 170 | ARG |
| 31 | DH | 3 | ARG |
| 31 | DH | 6 | ARG |
| 31 | DH | 15 | VAL |
| 31 | DH | 42 | ARG |
| 31 | DH | 69 | ARG |
| 31 | DH | 76 | VAL |
| 31 | DH | 81 | GLU |
| 31 | DH | 95 | ARG |
| 31 | DH | 98 | LEU |
| 31 | DH | 106 | THR |
| 31 | DH | 139 | GLN |
| 31 | DH | 171 | LEU |
| 31 | DH | 172 | LYS |
| 32 | DI | 15 | VAL |
| 32 | DI | 19 | VAL |
| 32 | DI | 20 | ASP |
| 32 | DI | 40 | THR |
| 32 | DI | 41 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DI | 43 | ASN |
| 32 | DI | 44 | LEU |
| 32 | DI | 57 | ARG |
| 32 | DI | 61 | ARG |
| 32 | DI | 66 | GLU |
| 32 | DI | 68 | LEU |
| 32 | DI | 75 | LEU |
| 32 | DI | 77 | LEU |
| 32 | DI | 114 | LEU |
| 32 | DI | 121 | LYS |
| 32 | DI | 140 | LEU |
| 32 | DI | 142 | VAL |
| 32 | DI | 144 | VAL |
| 33 | DN | 5 | VAL |
| 33 | DN | 12 | ARG |
| 33 | DN | 33 | LEU |
| 33 | DN | 34 | LEU |
| 33 | DN | 38 | HIS |
| 33 | DN | 46 | VAL |
| 33 | DN | 48 | MET |
| 33 | DN | 61 | ARG |
| 33 | DN | 68 | GLU |
| 33 | DN | 85 | ILE |
| 33 | DN | 87 | LEU |
| 33 | DN | 99 | LEU |
| 33 | DN | 120 | LEU |
| 33 | DN | 133 | GLN |
| 33 | DN | 137 | LYS |
| 33 | DN | 138 | LEU |
| 34 | DO | 8 | LEU |
| 34 | DO | 23 | ARG |
| 34 | DO | 24 | VAL |
| 34 | DO | 58 | VAL |
| 34 | DO | 69 | ILE |
| 34 | DO | 92 | GLU |
| 34 | DO | 94 | ARG |
| 34 | DO | 98 | VAL |
| 34 | DO | 108 | GLU |
| 35 | DP | 2 | LYS |
| 35 | DP | 29 | LYS |
| 35 | DP | 42 | SER |
| 35 | DP | 55 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | DP | 59 | LEU |
| 35 | DP | 65 | ARG |
| 35 | DP | 76 | LYS |
| 35 | DP | 77 | ARG |
| 35 | DP | 99 | LEU |
| 35 | DP | 106 | LEU |
| 35 | DP | 112 | LEU |
| 36 | DQ | 1 | MET |
| 36 | DQ | 7 | MET |
| 36 | DQ | 8 | LYS |
| 36 | DQ | 11 | LYS |
| 36 | DQ | 16 | ARG |
| 36 | DQ | 21 | THR |
| 36 | DQ | 45 | GLN |
| 36 | DQ | 55 | VAL |
| 36 | DQ | 56 | ARG |
| 36 | DQ | 60 | ARG |
| 36 | DQ | 75 | THR |
| 36 | DQ | 81 | VAL |
| 36 | DQ | 85 | LYS |
| 36 | DQ | 109 | VAL |
| 36 | DQ | 110 | THR |
| 37 | DR | 1 | MET |
| 37 | DR | 6 | SER |
| 37 | DR | 18 | LEU |
| 37 | DR | 28 | LEU |
| 37 | DR | 29 | LEU |
| 37 | DR | 33 | ARG |
| 37 | DR | 36 | THR |
| 37 | DR | 44 | LEU |
| 37 | DR | 57 | ARG |
| 37 | DR | 60 | LEU |
| 37 | DR | 65 | LEU |
| 37 | DR | 75 | LEU |
| 37 | DR | 79 | LEU |
| 37 | DR | 86 | ARG |
| 37 | DR | 100 | LEU |
| 37 | DR | 111 | LEU |
| 38 | DS | 14 | VAL |
| 38 | DS | 20 | ARG |
| 38 | DS | 35 | ILE |
| 38 | DS | 36 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | DS | 43 | GLU |
| 38 | DS | 48 | LEU |
| 38 | DS | 50 | SER |
| 38 | DS | 57 | LYS |
| 38 | DS | 58 | LEU |
| 38 | DS | 67 | ARG |
| 38 | DS | 68 | GLN |
| 38 | DS | 75 | GLU |
| 38 | DS | 78 | LEU |
| 38 | DS | 83 | LYS |
| 38 | DS | 103 | GLU |
| 39 | DT | 6 | LEU |
| 39 | DT | 13 | ARG |
| 39 | DT | 74 | ARG |
| 39 | DT | 85 | LYS |
| 39 | DT | 89 | VAL |
| 39 | DT | 96 | ARG |
| 39 | DT | 113 | LYS |
| 39 | DT | 118 | ARG |
| 40 | DU | 5 | LYS |
| 40 | DU | 31 | SER |
| 40 | DU | 59 | ARG |
| 40 | DU | 60 | LEU |
| 40 | DU | 74 | LEU |
| 40 | DU | 83 | LEU |
| 40 | DU | 89 | GLU |
| 40 | DU | 92 | ARG |
| 40 | DU | 104 | GLN |
| 40 | DU | 108 | GLU |
| 40 | DU | 114 | LYS |
| 41 | DV | 15 | GLU |
| 41 | DV | 18 | LEU |
| 41 | DV | 21 | ARG |
| 41 | DV | 52 | VAL |
| 41 | DV | 57 | VAL |
| 41 | DV | 62 | LEU |
| 41 | DV | 72 | VAL |
| 41 | DV | 79 | VAL |
| 41 | DV | 95 | LEU |
| 42 | DW | 11 | ARG |
| 42 | DW | 15 | ARG |
| 42 | DW | 17 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | DW | 23 | LEU |
| 42 | DW | 27 | LYS |
| 42 | DW | 51 | LEU |
| 42 | DW | 60 | ASN |
| 42 | DW | 63 | ASP |
| 42 | DW | 100 | THR |
| 42 | DW | 107 | LEU |
| 43 | DX | 35 | THR |
| 43 | DX | 57 | LEU |
| 43 | DX | 70 | LEU |
| 44 | DY | 2 | ARG |
| 44 | DY | 11 | ASP |
| 44 | DY | 23 | ARG |
| 44 | DY | 43 | ASN |
| 44 | DY | 72 | VAL |
| 44 | DY | 99 | CYS |
| 45 | DZ | 5 | LEU |
| 45 | DZ | 11 | GLU |
| 45 | DZ | 19 | ARG |
| 45 | DZ | 31 | ARG |
| 45 | DZ | 33 | LEU |
| 45 | DZ | 40 | ASP |
| 45 | DZ | 41 | LEU |
| 45 | DZ | 50 | GLN |
| 45 | DZ | 61 | LEU |
| 45 | DZ | 72 | ARG |
| 45 | DZ | 76 | LEU |
| 45 | DZ | 86 | VAL |
| 45 | DZ | 87 | ASP |
| 45 | DZ | 91 | LEU |
| 45 | DZ | 107 | THR |
| 45 | DZ | 154 | ASP |
| 45 | DZ | 155 | LEU |
| 45 | DZ | 162 | GLU |
| 45 | DZ | 165 | VAL |
| 46 | D0 | 7 | LEU |
| 46 | D0 | 10 | THR |
| 46 | D0 | 19 | LYS |
| 46 | D0 | 20 | ARG |
| 46 | D0 | 24 | LYS |
| 46 | D0 | 55 | ARG |
| 47 | D1 | 21 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | D1 | 26 | ARG |
| 47 | D1 | 35 | THR |
| 47 | D1 | 40 | ARG |
| 47 | D1 | 52 | ARG |
| 47 | D1 | 59 | THR |
| 47 | D1 | 78 | LYS |
| 48 | D2 | 28 | LYS |
| 48 | D2 | 30 | ARG |
| 48 | D2 | 40 | SER |
| 48 | D2 | 45 | SER |
| 48 | D2 | 52 | ASP |
| 48 | D2 | 53 | LEU |
| 48 | D2 | 55 | ARG |
| 48 | D2 | 70 | GLN |
| 49 | D3 | 6 | VAL |
| 49 | D3 | 8 | LEU |
| 49 | D3 | 23 | LEU |
| 49 | D3 | 24 | LYS |
| 49 | D3 | 30 | ARG |
| 49 | D3 | 32 | GLN |
| 49 | D3 | 44 | ARG |
| 50 | D4 | 5 | ILE |
| 50 | D4 | 44 | THR |
| 50 | D4 | 56 | VAL |
| 50 | D4 | 58 | ARG |
| 50 | D4 | 61 | ARG |
| 50 | D4 | 63 | TYR |
| 50 | D4 | 68 | ARG |
| 50 | D4 | 69 | LYS |
| 51 | D5 | 29 | THR |
| 51 | D5 | 33 | CYS |
| 51 | D5 | 40 | LYS |
| 51 | D5 | 48 | GLU |
| 51 | D5 | 58 | LEU |
| 52 | D6 | 6 | ARG |
| 52 | D6 | 9 | LEU |
| 52 | D6 | 38 | LYS |
| 52 | D6 | 48 | VAL |
| 53 | D7 | 1 | MET |
| 53 | D7 | 48 | LYS |
| 54 | D8 | 14 | VAL |
| 54 | D8 | 26 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | D8 | 29 | LYS |
| 54 | D8 | 31 | HIS |
| 55 | D9 | 26 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 40 | HIS |
| 3 | AC | 6 | HIS |
| 3 | AC | 28 | GLN |
| 3 | AC | 104 | GLN |
| 3 | AC | 118 | GLN |
| 3 | AC | 136 | GLN |
| 3 | AC | 181 | ASN |
| 4 | AD | 45 | GLN |
| 5 | AE | 20 | GLN |
| 5 | AE | 56 | GLN |
| 5 | AE | 141 | GLN |
| 6 | AF | 94 | GLN |
| 6 | AF | 100 | ASN |
| 7 | AG | 28 | ASN |
| 7 | AG | 148 | ASN |
| 9 | AI | 23 | ASN |
| 9 | AI | 31 | GLN |
| 9 | AI | 34 | ASN |
| 9 | AI | 89 | ASN |
| 10 | AJ | 13 | HIS |
| 10 | AJ | 56 | HIS |
| 11 | AK | 93 | GLN |
| 12 | AL | 78 | GLN |
| 12 | AL | 99 | HIS |
| 13 | AM | 92 | HIS |
| 15 | AO | 28 | GLN |
| 15 | AO | 62 | GLN |
| 16 | AP | 13 | HIS |
| 17 | AQ | 16 | GLN |
| 17 | AQ | 26 | GLN |
| 19 | AS | 23 | ASN |
| 19 | AS | 47 | HIS |
| 19 | AS | 65 | ASN |
| 19 | AS | 69 | HIS |
| 20 | AT | 9 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | AT | 45 | GLN |
| 20 | AT | 90 | GLN |
| 27 | BD | 253 | GLN |
| 29 | BF | 69 | HIS |
| 29 | BF | 169 | ASN |
| 29 | BF | 203 | GLN |
| 31 | BH | 158 | HIS |
| 32 | BI | 43 | ASN |
| 32 | BI | 139 | GLN |
| 35 | BP | 38 | GLN |
| 36 | BQ | 45 | GLN |
| 39 | BT | 123 | GLN |
| 40 | BU | 117 | GLN |
| 41 | BV | 80 | GLN |
| 43 | BX | 31 | HIS |
| 44 | BY | 6 | HIS |
| 44 | BY | 43 | ASN |
| 45 | BZ | 32 | HIS |
| 45 | BZ | 151 | HIS |
| 46 | B0 | 3 | HIS |
| 48 | B2 | 38 | GLN |
| 48 | B2 | 70 | GLN |
| 49 | B3 | 32 | GLN |
| 55 | B9 | 36 | GLN |
| 2 | CB | 19 | HIS |
| 2 | CB | 40 | HIS |
| 2 | CB | 224 | GLN |
| 3 | CC | 6 | HIS |
| 3 | CC | 28 | GLN |
| 3 | CC | 37 | GLN |
| 3 | CC | 104 | GLN |
| 3 | CC | 118 | GLN |
| 3 | CC | 123 | GLN |
| 3 | CC | 136 | GLN |
| 4 | CD | 45 | GLN |
| 4 | CD | 74 | GLN |
| 4 | CD | 125 | HIS |
| 5 | CE | 20 | GLN |
| 5 | CE | 78 | HIS |
| 5 | CE | 141 | GLN |
| 7 | CG | 51 | GLN |
| 8 | CH | 78 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | CI | 31 | GLN |
| 9 | CI | 58 | HIS |
| 10 | CJ | 68 | HIS |
| 11 | CK | 22 | HIS |
| 11 | CK | 93 | GLN |
| 12 | CL | 78 | GLN |
| 13 | CM | 77 | ASN |
| 15 | CO | 28 | GLN |
| 16 | CP | 16 | HIS |
| 19 | CS | 65 | ASN |
| 19 | CS | 69 | HIS |
| 20 | CT | 16 | HIS |
| 27 | DD | 87 | ASN |
| 27 | DD | 164 | GLN |
| 27 | DD | 253 | GLN |
| 28 | DE | 85 | ASN |
| 29 | DF | 69 | HIS |
| 29 | DF | 169 | ASN |
| 29 | DF | 203 | GLN |
| 30 | DG | 40 | ASN |
| 30 | DG | 79 | ASN |
| 31 | DH | 139 | GLN |
| 31 | DH | 158 | HIS |
| 32 | DI | 43 | ASN |
| 35 | DP | 38 | GLN |
| 36 | DQ | 45 | GLN |
| 37 | DR | 13 | HIS |
| 37 | DR | 71 | GLN |
| 38 | DS | 68 | GLN |
| 39 | DT | 123 | GLN |
| 41 | DV | 64 | HIS |
| 43 | DX | 31 | HIS |
| 44 | DY | 43 | ASN |
| 46 | D0 | 3 | HIS |
| 48 | D2 | 38 | GLN |
| 55 | D9 | 36 | GLN |

5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1495/1522 (98%) | 393 (26%) | 25 (1%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | CA | 1502/1522 (98%) | 388 (25%) | 31 (2%) |
| 22 | AV | 4/24 (16%) | 1 (25%) | 0 |
| 22 | CV | 4/24 (16%) | 1 (25%) | 0 |
| 23 | AX | 75/77 (97%) | 16 (21%) | 0 |
| 23 | CX | 75/77 (97%) | 16 (21%) | 0 |
| 25 | BA | 2722/2915 (93%) | 508 (18%) | 40 (1%) |
| 25 | DA | 2704/2915 (92%) | 535 (19%) | 37 (1%) |
| 26 | BB | 119/122 (97%) | 18 (15%) | 0 |
| 26 | DB | 119/122 (97%) | 24 (20%) | 1 (0%) |
| All | All | 8819/9320 (94%) | 1900 (21%) | 134 (1%) |

All (1900) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 7 | G |
| 1 | AA | 9 | G |
| 1 | AA | 15 | G |
| 1 | AA | 22 | G |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 44 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |
| 1 | AA | 50 | A |
| 1 | AA | 51 | A |
| 1 | AA | 59 | A |
| 1 | AA | 61 | G |
| 1 | AA | 63 | C |
| 1 | AA | 69 | G |
| 1 | AA | 77 | G |
| 1 | AA | 78 | G |
| 1 | AA | 79 | G |
| 1 | AA | 96 | U |
| 1 | AA | 97 | G |
| 1 | AA | 98 | G |
| 1 | AA | 101 | A |
| 1 | AA | 102 | G |
| 1 | AA | 112 | G |
| 1 | AA | 115 | G |
| 1 | AA | 116 | A |
| 1 | AA | 121 | C |
| 1 | AA | 129(A) | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 131 | C |
| 1 | AA | 138 | G |
| 1 | AA | 141 | A |
| 1 | AA | 142 | G |
| 1 | AA | 143 | A |
| 1 | AA | 144 | G |
| 1 | AA | 149 | A |
| 1 | AA | 163 | C |
| 1 | AA | 165 | C |
| 1 | AA | 166 | G |
| 1 | AA | 171 | A |
| 1 | AA | 173 | U |
| 1 | AA | 174 | C |
| 1 | AA | 180 | U |
| 1 | AA | 181 | G |
| 1 | AA | 182 | U |
| 1 | AA | 189(D) | C |
| 1 | AA | 189(F) | U |
| 1 | AA | 190 | U |
| 1 | AA | 193 | C |
| 1 | AA | 194 | C |
| 1 | AA | 195 | A |
| 1 | AA | 197 | A |
| 1 | AA | 199 | G |
| 1 | AA | 201 | C |
| 1 | AA | 203 | U |
| 1 | AA | 204 | U |
| 1 | AA | 216 | G |
| 1 | AA | 220 | G |
| 1 | AA | 247 | G |
| 1 | AA | 251 | G |
| 1 | AA | 258 | G |
| 1 | AA | 266 | G |
| 1 | AA | 267 | C |
| 1 | AA | 269 | C |
| 1 | AA | 277 | C |
| 1 | AA | 281 | G |
| 1 | AA | 289 | G |
| 1 | AA | 298 | A |
| 1 | AA | 301 | G |
| 1 | AA | 321 | A |
| 1 | AA | 328 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 332 | G |
| 1 | AA | 342 | C |
| 1 | AA | 346 | G |
| 1 | AA | 347 | G |
| 1 | AA | 348 | G |
| 1 | AA | 349 | A |
| 1 | AA | 351 | G |
| 1 | AA | 352 | C |
| 1 | AA | 353 | A |
| 1 | AA | 354 | G |
| 1 | AA | 355 | C |
| 1 | AA | 367 | U |
| 1 | AA | 372 | C |
| 1 | AA | 373 | A |
| 1 | AA | 383 | A |
| 1 | AA | 388 | G |
| 1 | AA | 396 | G |
| 1 | AA | 397 | A |
| 1 | AA | 398 | C |
| 1 | AA | 403 | C |
| 1 | AA | 406 | G |
| 1 | AA | 409 | G |
| 1 | AA | 411 | A |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 414 | A |
| 1 | AA | 415 | A |
| 1 | AA | 422 | C |
| 1 | AA | 424 | G |
| 1 | AA | 429 | U |
| 1 | AA | 430 | A |
| 1 | AA | 439 | A |
| 1 | AA | 442 | C |
| 1 | AA | 443 | C |
| 1 | AA | 452 | A |
| 1 | AA | 461 | A |
| 1 | AA | 471 | G |
| 1 | AA | 474 | G |
| 1 | AA | 484 | G |
| 1 | AA | 485 | G |
| 1 | AA | 492 | G |
| 1 | AA | 496 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 498 | U |
| 1 | AA | 505 | G |
| 1 | AA | 509 | A |
| 1 | AA | 510 | A |
| 1 | AA | 511 | C |
| 1 | AA | 513 | C |
| 1 | AA | 518 | C |
| 1 | AA | 521 | G |
| 1 | AA | 527 | G |
| 1 | AA | 531 | U |
| 1 | AA | 532 | A |
| 1 | AA | 533 | A |
| 1 | AA | 536 | C |
| 1 | AA | 544 | G |
| 1 | AA | 547 | A |
| 1 | AA | 553 | A |
| 1 | AA | 559 | A |
| 1 | AA | 561 | U |
| 1 | AA | 571 | U |
| 1 | AA | 572 | A |
| 1 | AA | 573 | A |
| 1 | AA | 576 | G |
| 1 | AA | 592 | G |
| 1 | AA | 596 | C |
| 1 | AA | 597 | G |
| 1 | AA | 606 | G |
| 1 | AA | 626 | U |
| 1 | AA | 630 | G |
| 1 | AA | 631 | G |
| 1 | AA | 633 | G |
| 1 | AA | 639 | G |
| 1 | AA | 641 | U |
| 1 | AA | 649 | G |
| 1 | AA | 650 | G |
| 1 | AA | 651 | C |
| 1 | AA | 653 | A |
| 1 | AA | 665 | A |
| 1 | AA | 673 | G |
| 1 | AA | 680 | C |
| 1 | AA | 687 | A |
| 1 | AA | 688 | G |
| 1 | AA | 693 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 704 | A |
| 1 | AA | 711 | G |
| 1 | AA | 721 | G |
| 1 | AA | 723 | U |
| 1 | AA | 724 | G |
| 1 | AA | 731 | G |
| 1 | AA | 749 | C |
| 1 | AA | 752 | G |
| 1 | AA | 755 | G |
| 1 | AA | 760 | G |
| 1 | AA | 774 | G |
| 1 | AA | 777 | A |
| 1 | AA | 786 | G |
| 1 | AA | 792 | A |
| 1 | AA | 793 | U |
| 1 | AA | 794 | A |
| 1 | AA | 802 | A |
| 1 | AA | 806 | C |
| 1 | AA | 812 | C |
| 1 | AA | 815 | A |
| 1 | AA | 816 | A |
| 1 | AA | 817 | C |
| 1 | AA | 818 | G |
| 1 | AA | 821 | G |
| 1 | AA | 827 | U |
| 1 | AA | 828 | A |
| 1 | AA | 829 | G |
| 1 | AA | 836 | G |
| 1 | AA | 839 | U |
| 1 | AA | 840 | C |
| 1 | AA | 841 | U |
| 1 | AA | 851 | G |
| 1 | AA | 855 | G |
| 1 | AA | 858 | G |
| 1 | AA | 859 | A |
| 1 | AA | 870 | U |
| 1 | AA | 873 | A |
| 1 | AA | 876 | G |
| 1 | AA | 902 | G |
| 1 | AA | 914 | A |
| 1 | AA | 916 | G |
| 1 | AA | 922 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 926 | G |
| 1 | AA | 927 | G |
| 1 | AA | 934 | C |
| 1 | AA | 935 | A |
| 1 | AA | 942 | G |
| 1 | AA | 958 | A |
| 1 | AA | 960 | U |
| 1 | AA | 961 | U |
| 1 | AA | 967 | C |
| 1 | AA | 968 | A |
| 1 | AA | 969 | A |
| 1 | AA | 971 | G |
| 1 | AA | 972 | C |
| 1 | AA | 974 | A |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 982 | U |
| 1 | AA | 983 | A |
| 1 | AA | 991 | U |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 999 | C |
| 1 | AA | 1000 | U |
| 1 | AA | 1001 | A |
| 1 | AA | 1001(A) | G |
| 1 | AA | 1002 | G |
| 1 | AA | 1003 | G |
| 1 | AA | 1004 | A |
| 1 | AA | 1005 | A |
| 1 | AA | 1006 | C |
| 1 | AA | 1007 | C |
| 1 | AA | 1009 | G |
| 1 | AA | 1011 | G |
| 1 | AA | 1013 | G |
| 1 | AA | 1014 | A |
| 1 | AA | 1019 | C |
| 1 | AA | 1020 | U |
| 1 | AA | 1022 | G |
| 1 | AA | 1024 | G |
| 1 | AA | 1025 | U |
| 1 | AA | 1026 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1027 | C |
| 1 | AA | 1028 | C |
| 1 | AA | 1029 | C |
| 1 | AA | 1030 | C |
| 1 | AA | 1030(A) | G |
| 1 | AA | 1030(C) | G |
| 1 | AA | 1031 | G |
| 1 | AA | 1033 | G |
| 1 | AA | 1035 | A |
| 1 | AA | 1036 | G |
| 1 | AA | 1037 | C |
| 1 | AA | 1039 | C |
| 1 | AA | 1042 | G |
| 1 | AA | 1043 | C |
| 1 | AA | 1052 | U |
| 1 | AA | 1053 | G |
| 1 | AA | 1054 | C |
| 1 | AA | 1055 | A |
| 1 | AA | 1065 | U |
| 1 | AA | 1066 | C |
| 1 | AA | 1068 | G |
| 1 | AA | 1070 | U |
| 1 | AA | 1076 | C |
| 1 | AA | 1081 | G |
| 1 | AA | 1087 | G |
| 1 | AA | 1091 | U |
| 1 | AA | 1092 | A |
| 1 | AA | 1093 | A |
| 1 | AA | 1094 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1101 | A |
| 1 | AA | 1104 | G |
| 1 | AA | 1108 | G |
| 1 | AA | 1109 | C |
| 1 | AA | 1119 | C |
| 1 | AA | 1124 | G |
| 1 | AA | 1125 | U |
| 1 | AA | 1126 | U |
| 1 | AA | 1128 | C |
| 1 | AA | 1130 | A |
| 1 | AA | 1132 | C |
| 1 | AA | 1134 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1135 | U |
| 1 | AA | 1136 | U |
| 1 | AA | 1137 | C |
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1141 | C |
| 1 | AA | 1145 | C |
| 1 | AA | 1146 | A |
| 1 | AA | 1151 | A |
| 1 | AA | 1152 | A |
| 1 | AA | 1154 | G |
| 1 | AA | 1157 | A |
| 1 | AA | 1159 | U |
| 1 | AA | 1160 | G |
| 1 | AA | 1161 | C |
| 1 | AA | 1166 | G |
| 1 | AA | 1173 | G |
| 1 | AA | 1176 | A |
| 1 | AA | 1181 | G |
| 1 | AA | 1183 | A |
| 1 | AA | 1184 | G |
| 1 | AA | 1189 | C |
| 1 | AA | 1193 | G |
| 1 | AA | 1196 | U |
| 1 | AA | 1197 | G |
| 1 | AA | 1200 | C |
| 1 | AA | 1202 | G |
| 1 | AA | 1204 | A |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1214 | C |
| 1 | AA | 1223 | C |
| 1 | AA | 1224 | G |
| 1 | AA | 1227 | A |
| 1 | AA | 1235 | U |
| 1 | AA | 1236 | A |
| 1 | AA | 1238 | A |
| 1 | AA | 1250 | A |
| 1 | AA | 1256 | A |
| 1 | AA | 1257 | U |
| 1 | AA | 1258 | G |
| 1 | AA | 1259 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 1260 | C |
| 1 | AA | 1262 | C |
| 1 | AA | 1270 | C |
| 1 | AA | 1271 | G |
| 1 | AA | 1273 | G |
| 1 | AA | 1278 | U |
| 1 | AA | 1279 | A |
| 1 | AA | 1280 | A |
| 1 | AA | 1281 | U |
| 1 | AA | 1282 | C |
| 1 | AA | 1283 | G |
| 1 | AA | 1284 | C |
| 1 | AA | 1286 | A |
| 1 | AA | 1287 | A |
| 1 | AA | 1294 | G |
| 1 | AA | 1296 | C |
| 1 | AA | 1297 | C |
| 1 | AA | 1299 | A |
| 1 | AA | 1300 | G |
| 1 | AA | 1302 | U |
| 1 | AA | 1305 | G |
| 1 | AA | 1311 | G |
| 1 | AA | 1314 | C |
| 1 | AA | 1317 | C |
| 1 | AA | 1320 | C |
| 1 | AA | 1322 | C |
| 1 | AA | 1323 | G |
| 1 | AA | 1338 | G |
| 1 | AA | 1340 | A |
| 1 | AA | 1343 | G |
| 1 | AA | 1346 | A |
| 1 | AA | 1347 | G |
| 1 | AA | 1353 | G |
| 1 | AA | 1354 | C |
| 1 | AA | 1358 | U |
| 1 | AA | 1360 | A |
| 1 | AA | 1361 | G |
| 1 | AA | 1363 | C |
| 1 | AA | 1370 | G |
| 1 | AA | 1377 | A |
| 1 | AA | 1379 | G |
| 1 | AA | 1393 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1396 | A |
| 1 | AA | 1397 | C |
| 1 | AA | 1402 | C |
| 1 | AA | 1419 | G |
| 1 | AA | 1422 | G |
| 1 | AA | 1442 | G |
| 1 | AA | 1442(A) | G |
| 1 | AA | 1442(B) | A |
| 1 | AA | 1446 | U |
| 1 | AA | 1447 | A |
| 1 | AA | 1452 | C |
| 1 | AA | 1456 | G |
| 1 | AA | 1457 | G |
| 1 | AA | 1469 | G |
| 1 | AA | 1487 | G |
| 1 | AA | 1489 | G |
| 1 | AA | 1493 | A |
| 1 | AA | 1494 | G |
| 1 | AA | 1497 | G |
| 1 | AA | 1502 | A |
| 1 | AA | 1503 | A |
| 1 | AA | 1504 | G |
| 1 | AA | 1506 | U |
| 1 | AA | 1517 | G |
| 1 | AA | 1520 | G |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 1 | AA | 1531 | A |
| 1 | AA | 1532 | U |
| 22 | AV | 15 | A |
| 23 | AX | 6 | G |
| 23 | AX | 9 | G |
| 23 | AX | 13 | C |
| 23 | AX | 19 | G |
| 23 | AX | 21 | A |
| 23 | AX | 26 | G |
| 23 | AX | 28 | C |
| 23 | AX | 31 | G |
| 23 | AX | 42 | G |
| 23 | AX | 47 | U |
| 23 | AX | 60 | U |
| 23 | AX | 61 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | AX | 67 | C |
| 23 | AX | 68 | C |
| 23 | AX | 70 | G |
| 23 | AX | 76 | A |
| 25 | BA | 9 | U |
| 25 | BA | 11 | G |
| 25 | BA | 12 | U |
| 25 | BA | 14 | A |
| 25 | BA | 34 | C |
| 25 | BA | 36 | G |
| 25 | BA | 45 | C |
| 25 | BA | 54 | G |
| 25 | BA | 62 | U |
| 25 | BA | 63 | A |
| 25 | BA | 70 | A |
| 25 | BA | 71 | U |
| 25 | BA | 73 | A |
| 25 | BA | 74 | G |
| 25 | BA | 83 | A |
| 25 | BA | 90 | A |
| 25 | BA | 99 | G |
| 25 | BA | 116 | A |
| 25 | BA | 118 | U |
| 25 | BA | 120 | G |
| 25 | BA | 125 | A |
| 25 | BA | 155 | C |
| 25 | BA | 161 | C |
| 25 | BA | 185 | A |
| 25 | BA | 187 | C |
| 25 | BA | 188 | A |
| 25 | BA | 194 | G |
| 25 | BA | 203 | G |
| 25 | BA | 204 | G |
| 25 | BA | 205 | A |
| 25 | BA | 206 | G |
| 25 | BA | 210 | A |
| 25 | BA | 211 | A |
| 25 | BA | 217 | A |
| 25 | BA | 218 | A |
| 25 | BA | 222 | A |
| 25 | BA | 237 | G |
| 25 | BA | 250 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BA | 263 | C |
| 25 | BA | 265 | U |
| 25 | BA | 269 | G |
| 25 | BA | 271 | U |
| 25 | BA | 272 | U |
| 25 | BA | 273 | G |
| 25 | BA | 274 | U |
| 25 | BA | 275 | C |
| 25 | BA | 276 | C |
| 25 | BA | 279 | G |
| 25 | BA | 288 | U |
| 25 | BA | 289 | G |
| 25 | BA | 294 | C |
| 25 | BA | 296 | U |
| 25 | BA | 303 | C |
| 25 | BA | 306 | A |
| 25 | BA | 307 | A |
| 25 | BA | 332 | G |
| 25 | BA | 335 | A |
| 25 | BA | 353 | G |
| 25 | BA | 354 | A |
| 25 | BA | 360 | C |
| 25 | BA | 376 | G |
| 25 | BA | 381 | A |
| 25 | BA | 387 | G |
| 25 | BA | 391 | G |
| 25 | BA | 399 | G |
| 25 | BA | 407 | U |
| 25 | BA | 413 | G |
| 25 | BA | 432 | U |
| 25 | BA | 434 | G |
| 25 | BA | 438 | G |
| 25 | BA | 439 | A |
| 25 | BA | 448 | U |
| 25 | BA | 455 | A |
| 25 | BA | 469 | A |
| 25 | BA | 470 | C |
| 25 | BA | 474 | U |
| 25 | BA | 478 | G |
| 25 | BA | 482 | C |
| 25 | BA | 483 | A |
| 25 | BA | 496 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BA | 505 | A |
| 25 | BA | 506 | A |
| 25 | BA | 507 | G |
| 25 | BA | 508 | A |
| 25 | BA | 515 | G |
| 25 | BA | 519 | G |
| 25 | BA | 522 | A |
| 25 | BA | 526 | A |
| 25 | BA | 529 | U |
| 25 | BA | 530 | A |
| 25 | BA | 534 | C |
| 25 | BA | 543 | G |
| 25 | BA | 549 | U |
| 25 | BA | 554 | A |
| 25 | BA | 555 | G |
| 25 | BA | 556 | C |
| 25 | BA | 557 | A |
| 25 | BA | 558 | G |
| 25 | BA | 569 | G |
| 25 | BA | 573 | G |
| 25 | BA | 586 | G |
| 25 | BA | 596 | G |
| 25 | BA | 598 | A |
| 25 | BA | 609 | A |
| 25 | BA | 610 | C |
| 25 | BA | 616 | G |
| 25 | BA | 625 | G |
| 25 | BA | 626 | A |
| 25 | BA | 627 | G |
| 25 | BA | 630 | U |
| 25 | BA | 633 | G |
| 25 | BA | 638 | U |
| 25 | BA | 639 | G |
| 25 | BA | 641 | G |
| 25 | BA | 659 | C |
| 25 | BA | 662 | A |
| 25 | BA | 670 | C |
| 25 | BA | 671 | A |
| 25 | BA | 692 | C |
| 25 | BA | 693 | G |
| 25 | BA | 697 | C |
| 25 | BA | 698 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | BA | 701 | A |
| 25 | BA | 712 | C |
| 25 | BA | 716 | G |
| 25 | BA | 724 | A |
| 25 | BA | 733 | G |
| 25 | BA | 745 | C |
| 25 | BA | 749 | G |
| 25 | BA | 764 | G |
| 25 | BA | 777 | C |
| 25 | BA | 811 | A |
| 25 | BA | 822 | G |
| 25 | BA | 823 | G |
| 25 | BA | 826 | U |
| 25 | BA | 829 | A |
| 25 | BA | 831 | A |
| 25 | BA | 832 | G |
| 25 | BA | 839 | G |
| 25 | BA | 852 | G |
| 25 | BA | 858 | U |
| 25 | BA | 859 | C |
| 25 | BA | 866 | A |
| 25 | BA | 874 | U |
| 25 | BA | 875 | U |
| 25 | BA | 877 | G |
| 25 | BA | 902 | G |
| 25 | BA | 906 | G |
| 25 | BA | 926 | G |
| 25 | BA | 927 | G |
| 25 | BA | 928 | G |
| 25 | BA | 929 | G |
| 25 | BA | 930 | G |
| 25 | BA | 931 | C |
| 25 | BA | 932 | C |
| 25 | BA | 933 | C |
| 25 | BA | 934 | A |
| 25 | BA | 935 | C |
| 25 | BA | 937 | A |
| 25 | BA | 938 | G |
| 25 | BA | 940 | C |
| 25 | BA | 942 | A |
| 25 | BA | 944 | C |
| 25 | BA | 945 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | BA | 946 | A |
| 25 | BA | 956 | A |
| 25 | BA | 965 | G |
| 25 | BA | 977 | G |
| 25 | BA | 983 | G |
| 25 | BA | 986 | A |
| 25 | BA | 989 | G |
| 25 | BA | 990 | A |
| 25 | BA | 991 | G |
| 25 | BA | 998 | A |
| 25 | BA | 1003 | U |
| 25 | BA | 1004 | A |
| 25 | BA | 1006 | C |
| 25 | BA | 1015 | C |
| 25 | BA | 1019 | G |
| 25 | BA | 1020 | C |
| 25 | BA | 1029 | A |
| 25 | BA | 1036 | A |
| 25 | BA | 1042 | A |
| 25 | BA | 1051 | C |
| 25 | BA | 1058 | U |
| 25 | BA | 1059 | C |
| 25 | BA | 1066 | A |
| 25 | BA | 1067 | A |
| 25 | BA | 1068 | G |
| 25 | BA | 1069 | U |
| 25 | BA | 1072 | U |
| 25 | BA | 1076 | G |
| 25 | BA | 1079 | U |
| 25 | BA | 1080 | G |
| 25 | BA | 1085 | G |
| 25 | BA | 1087 | C |
| 25 | BA | 1088 | G |
| 25 | BA | 1089 | C |
| 25 | BA | 1091 | A |
| 25 | BA | 1092 | A |
| 25 | BA | 1093 | G |
| 25 | BA | 1153 | G |
| 25 | BA | 1154 | U |
| 25 | BA | 1156 | G |
| 25 | BA | 1158 | G |
| 25 | BA | 1168 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 1174 | A |
| 25 | BA | 1175 | A |
| 25 | BA | 1176 | U |
| 25 | BA | 1180 | C |
| 25 | BA | 1181 | G |
| 25 | BA | 1184 | G |
| 25 | BA | 1186 | U |
| 25 | BA | 1187 | U |
| 25 | BA | 1188 | A |
| 25 | BA | 1189 | A |
| 25 | BA | 1195 | G |
| 25 | BA | 1202 | A |
| 25 | BA | 1210 | G |
| 25 | BA | 1216 | G |
| 25 | BA | 1217 | G |
| 25 | BA | 1218 | G |
| 25 | BA | 1219 | A |
| 25 | BA | 1220 | U |
| 25 | BA | 1221 | G |
| 25 | BA | 1222 | A |
| 25 | BA | 1223 | C |
| 25 | BA | 1225 | C |
| 25 | BA | 1229 | G |
| 25 | BA | 1255 | A |
| 25 | BA | 1256 | U |
| 25 | BA | 1263 | C |
| 25 | BA | 1266 | C |
| 25 | BA | 1296 | G |
| 25 | BA | 1298 | G |
| 25 | BA | 1299 | A |
| 25 | BA | 1302 | G |
| 25 | BA | 1311 | A |
| 25 | BA | 1317 | G |
| 25 | BA | 1318 | A |
| 25 | BA | 1319 | U |
| 25 | BA | 1321 | A |
| 25 | BA | 1346 | U |
| 25 | BA | 1347 | A |
| 25 | BA | 1359 | U |
| 25 | BA | 1360 | C |
| 25 | BA | 1367 | A |
| 25 | BA | 1384 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | BA | 1398 | U |
| 25 | BA | 1405 | A |
| 25 | BA | 1406 | A |
| 25 | BA | 1411 | A |
| 25 | BA | 1416 | C |
| 25 | BA | 1417 | G |
| 25 | BA | 1418 | U |
| 25 | BA | 1426 | G |
| 25 | BA | 1430 | A |
| 25 | BA | 1431 | G |
| 25 | BA | 1432 | C |
| 25 | BA | 1462 | G |
| 25 | BA | 1463 | C |
| 25 | BA | 1466 | U |
| 25 | BA | 1467 | G |
| 25 | BA | 1468 | G |
| 25 | BA | 1474 | C |
| 25 | BA | 1487 | G |
| 25 | BA | 1491 | A |
| 25 | BA | 1496 | A |
| 25 | BA | 1507 | A |
| 25 | BA | 1514 | C |
| 25 | BA | 1518 | A |
| 25 | BA | 1519 | A |
| 25 | BA | 1525 | G |
| 25 | BA | 1529 | G |
| 25 | BA | 1536 | A |
| 25 | BA | 1539 | C |
| 25 | BA | 1554 | A |
| 25 | BA | 1555 | C |
| 25 | BA | 1556 | A |
| 25 | BA | 1569 | U |
| 25 | BA | 1574 | A |
| 25 | BA | 1578 | C |
| 25 | BA | 1579 | C |
| 25 | BA | 1589 | A |
| 25 | BA | 1590 | C |
| 25 | BA | 1592 | A |
| 25 | BA | 1605 | A |
| 25 | BA | 1613 | A |
| 25 | BA | 1616 | A |
| 25 | BA | 1625 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 1628 | G |
| 25 | BA | 1631 | C |
| 25 | BA | 1632 | A |
| 25 | BA | 1654 | A |
| 25 | BA | 1655 | A |
| 25 | BA | 1656 | A |
| 25 | BA | 1660 | A |
| 25 | BA | 1686 | U |
| 25 | BA | 1694 | G |
| 25 | BA | 1695 | C |
| 25 | BA | 1696 | G |
| 25 | BA | 1701 | A |
| 25 | BA | 1711 | A |
| 25 | BA | 1721 | G |
| 25 | BA | 1722 | C |
| 25 | BA | 1735 | U |
| 25 | BA | 1742 | G |
| 25 | BA | 1743 | G |
| 25 | BA | 1747 | A |
| 25 | BA | 1748 | A |
| 25 | BA | 1766 | G |
| 25 | BA | 1767 | A |
| 25 | BA | 1768 | U |
| 25 | BA | 1769 | G |
| 25 | BA | 1776 | G |
| 25 | BA | 1777 | G |
| 25 | BA | 1779 | G |
| 25 | BA | 1787 | G |
| 25 | BA | 1791 | A |
| 25 | BA | 1794 | G |
| 25 | BA | 1795 | G |
| 25 | BA | 1804 | A |
| 25 | BA | 1811 | A |
| 25 | BA | 1813 | C |
| 25 | BA | 1822 | A |
| 25 | BA | 1831 | C |
| 25 | BA | 1832 | G |
| 25 | BA | 1843 | A |
| 25 | BA | 1847 | G |
| 25 | BA | 1860 | A |
| 25 | BA | 1870 | G |
| 25 | BA | 1878 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | BA | 1879 | A |
| 25 | BA | 1899 | A |
| 25 | BA | 1900 | G |
| 25 | BA | 1911 | A |
| 25 | BA | 1922 | A |
| 25 | BA | 1928 | G |
| 25 | BA | 1935 | A |
| 25 | BA | 1936 | C |
| 25 | BA | 1941 | A |
| 25 | BA | 1951 | G |
| 25 | BA | 1952 | G |
| 25 | BA | 1953 | U |
| 25 | BA | 1954 | A |
| 25 | BA | 1958 | A |
| 25 | BA | 1960 | A |
| 25 | BA | 1963 | C |
| 25 | BA | 1977 | U |
| 25 | BA | 1985 | U |
| 25 | BA | 1987 | C |
| 25 | BA | 1989 | C |
| 25 | BA | 1992 | A |
| 25 | BA | 1993 | A |
| 25 | BA | 1994 | A |
| 25 | BA | 2014 | G |
| 25 | BA | 2015 | U |
| 25 | BA | 2019 | G |
| 25 | BA | 2042 | A |
| 25 | BA | 2045 | G |
| 25 | BA | 2053 | A |
| 25 | BA | 2054 | G |
| 25 | BA | 2055 | A |
| 25 | BA | 2065 | C |
| 25 | BA | 2071 | G |
| 25 | BA | 2074 | G |
| 25 | BA | 2077 | C |
| 25 | BA | 2078 | G |
| 25 | BA | 2082 | A |
| 25 | BA | 2083 | G |
| 25 | BA | 2084 | A |
| 25 | BA | 2091 | G |
| 25 | BA | 2115 | G |
| 25 | BA | 2121 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2122 | G |
| 25 | BA | 2212 | G |
| 25 | BA | 2214 | G |
| 25 | BA | 2217 | C |
| 25 | BA | 2220 | A |
| 25 | BA | 2227 | G |
| 25 | BA | 2228 | G |
| 25 | BA | 2229 | A |
| 25 | BA | 2230 | U |
| 25 | BA | 2237 | A |
| 25 | BA | 2246 | G |
| 25 | BA | 2250 | G |
| 25 | BA | 2251 | G |
| 25 | BA | 2260 | C |
| 25 | BA | 2264 | G |
| 25 | BA | 2280 | A |
| 25 | BA | 2281 | A |
| 25 | BA | 2285 | A |
| 25 | BA | 2287 | C |
| 25 | BA | 2295 | C |
| 25 | BA | 2299 | A |
| 25 | BA | 2301 | G |
| 25 | BA | 2306 | C |
| 25 | BA | 2308 | U |
| 25 | BA | 2317 | A |
| 25 | BA | 2320 | G |
| 25 | BA | 2326 | C |
| 25 | BA | 2332 | A |
| 25 | BA | 2337 | G |
| 25 | BA | 2339 | A |
| 25 | BA | 2346 | G |
| 25 | BA | 2347 | A |
| 25 | BA | 2348 | A |
| 25 | BA | 2353 | G |
| 25 | BA | 2355 | C |
| 25 | BA | 2359 | C |
| 25 | BA | 2362 | C |
| 25 | BA | 2366 | G |
| 25 | BA | 2373 | A |
| 25 | BA | 2384 | G |
| 25 | BA | 2388 | A |
| 25 | BA | 2391 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | BA | 2395 | G |
| 25 | BA | 2397 | C |
| 25 | BA | 2401 | G |
| 25 | BA | 2412 | G |
| 25 | BA | 2418 | U |
| 25 | BA | 2422 | G |
| 25 | BA | 2430 | A |
| 25 | BA | 2434 | A |
| 25 | BA | 2435 | U |
| 25 | BA | 2436 | C |
| 25 | BA | 2437 | A |
| 25 | BA | 2441 | G |
| 25 | BA | 2442 | A |
| 25 | BA | 2443 | U |
| 25 | BA | 2447 | A |
| 25 | BA | 2451 | A |
| 25 | BA | 2453 | C |
| 25 | BA | 2459 | G |
| 25 | BA | 2460 | A |
| 25 | BA | 2480 | G |
| 25 | BA | 2481 | A |
| 25 | BA | 2486 | C |
| 25 | BA | 2488 | A |
| 25 | BA | 2490 | A |
| 25 | BA | 2510 | C |
| 25 | BA | 2514 | G |
| 25 | BA | 2517 | G |
| 25 | BA | 2518 | U |
| 25 | BA | 2530 | A |
| 25 | BA | 2532 | C |
| 25 | BA | 2537 | G |
| 25 | BA | 2541 | G |
| 25 | BA | 2547 | G |
| 25 | BA | 2566 | U |
| 25 | BA | 2578 | A |
| 25 | BA | 2579 | G |
| 25 | BA | 2594 | G |
| 25 | BA | 2614 | A |
| 25 | BA | 2615 | G |
| 25 | BA | 2621 | U |
| 25 | BA | 2622 | C |
| 25 | BA | 2623 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2624 | C |
| 25 | BA | 2632 | C |
| 25 | BA | 2641 | A |
| 25 | BA | 2642 | G |
| 25 | BA | 2653 | G |
| 25 | BA | 2666 | A |
| 25 | BA | 2674 | A |
| 25 | BA | 2690 | C |
| 25 | BA | 2691 | A |
| 25 | BA | 2701 | U |
| 25 | BA | 2702 | C |
| 25 | BA | 2703 | C |
| 25 | BA | 2714 | U |
| 25 | BA | 2715 | C |
| 25 | BA | 2719 | G |
| 25 | BA | 2725 | A |
| 25 | BA | 2726 | A |
| 25 | BA | 2727 | G |
| 25 | BA | 2739 | U |
| 25 | BA | 2746 | A |
| 25 | BA | 2764 | G |
| 25 | BA | 2770 | A |
| 25 | BA | 2771 | A |
| 25 | BA | 2777 | A |
| 25 | BA | 2778 | A |
| 25 | BA | 2779 | G |
| 25 | BA | 2782 | C |
| 25 | BA | 2788 | A |
| 25 | BA | 2791 | A |
| 25 | BA | 2803 | A |
| 25 | BA | 2804 | C |
| 25 | BA | 2807 | C |
| 25 | BA | 2813 | G |
| 25 | BA | 2816 | G |
| 25 | BA | 2828 | G |
| 25 | BA | 2830 | A |
| 25 | BA | 2831 | A |
| 25 | BA | 2843 | G |
| 25 | BA | 2845 | A |
| 25 | BA | 2849 | G |
| 25 | BA | 2876 | U |
| 25 | BA | 2882 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2883 | A |
| 25 | BA | 2884 | C |
| 25 | BA | 2890 | C |
| 25 | BA | 2893 | A |
| 25 | BA | 2899 | C |
| 25 | BA | 2901 | A |
| 25 | BA | 2903 | G |
| 25 | BA | 2906 | U |
| 26 | BB | 2 | C |
| 26 | BB | 7 | G |
| 26 | BB | 12 | C |
| 26 | BB | 13 | A |
| 26 | BB | 34 | U |
| 26 | BB | 42 | C |
| 26 | BB | 56 | G |
| 26 | BB | 59 | A |
| 26 | BB | 73 | A |
| 26 | BB | 75 | G |
| 26 | BB | 85 | G |
| 26 | BB | 88 | C |
| 26 | BB | 89 | G |
| 26 | BB | 93 | G |
| 26 | BB | 106 | G |
| 26 | BB | 110 | G |
| 26 | BB | 112 | U |
| 26 | BB | 119 | G |
| 1 | CA | 7 | G |
| 1 | CA | 9 | G |
| 1 | CA | 15 | G |
| 1 | CA | 22 | G |
| 1 | CA | 32 | A |
| 1 | CA | 39 | G |
| 1 | CA | 44 | G |
| 1 | CA | 47 | C |
| 1 | CA | 48 | C |
| 1 | CA | 50 | A |
| 1 | CA | 51 | A |
| 1 | CA | 59 | A |
| 1 | CA | 63 | C |
| 1 | CA | 65 | U |
| 1 | CA | 66 | G |
| 1 | CA | 69 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 77 | G |
| 1 | CA | 78 | G |
| 1 | CA | 79 | G |
| 1 | CA | 80 | G |
| 1 | CA | 88 | A |
| 1 | CA | 89 | C |
| 1 | CA | 96 | U |
| 1 | CA | 97 | G |
| 1 | CA | 98 | G |
| 1 | CA | 101 | A |
| 1 | CA | 102 | G |
| 1 | CA | 112 | G |
| 1 | CA | 115 | G |
| 1 | CA | 116 | A |
| 1 | CA | 121 | C |
| 1 | CA | 129(A) | G |
| 1 | CA | 131 | C |
| 1 | CA | 138 | G |
| 1 | CA | 142 | G |
| 1 | CA | 144 | G |
| 1 | CA | 163 | C |
| 1 | CA | 165 | C |
| 1 | CA | 166 | G |
| 1 | CA | 171 | A |
| 1 | CA | 173 | U |
| 1 | CA | 174 | C |
| 1 | CA | 180 | U |
| 1 | CA | 181 | G |
| 1 | CA | 182 | U |
| 1 | CA | 189(D) | C |
| 1 | CA | 189(F) | U |
| 1 | CA | 190 | U |
| 1 | CA | 193 | C |
| 1 | CA | 194 | C |
| 1 | CA | 195 | A |
| 1 | CA | 197 | A |
| 1 | CA | 199 | G |
| 1 | CA | 201 | C |
| 1 | CA | 203 | U |
| 1 | CA | 204 | U |
| 1 | CA | 216 | G |
| 1 | CA | 220 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 247 | G |
| 1 | CA | 251 | G |
| 1 | CA | 258 | G |
| 1 | CA | 265 | G |
| 1 | CA | 266 | G |
| 1 | CA | 267 | C |
| 1 | CA | 269 | C |
| 1 | CA | 277 | C |
| 1 | CA | 281 | G |
| 1 | CA | 289 | G |
| 1 | CA | 298 | A |
| 1 | CA | 321 | A |
| 1 | CA | 328 | C |
| 1 | CA | 332 | G |
| 1 | CA | 342 | C |
| 1 | CA | 344 | A |
| 1 | CA | 346 | G |
| 1 | CA | 351 | G |
| 1 | CA | 352 | C |
| 1 | CA | 353 | A |
| 1 | CA | 354 | G |
| 1 | CA | 355 | C |
| 1 | CA | 367 | U |
| 1 | CA | 372 | C |
| 1 | CA | 373 | A |
| 1 | CA | 383 | A |
| 1 | CA | 388 | G |
| 1 | CA | 396 | G |
| 1 | CA | 397 | A |
| 1 | CA | 398 | C |
| 1 | CA | 403 | C |
| 1 | CA | 406 | G |
| 1 | CA | 409 | G |
| 1 | CA | 411 | A |
| 1 | CA | 412 | A |
| 1 | CA | 413 | G |
| 1 | CA | 414 | A |
| 1 | CA | 415 | A |
| 1 | CA | 422 | C |
| 1 | CA | 424 | G |
| 1 | CA | 427 | U |
| 1 | CA | 429 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 430 | A |
| 1 | CA | 439 | A |
| 1 | CA | 442 | C |
| 1 | CA | 452 | A |
| 1 | CA | 461 | A |
| 1 | CA | 471 | G |
| 1 | CA | 474 | G |
| 1 | CA | 484 | G |
| 1 | CA | 485 | G |
| 1 | CA | 492 | G |
| 1 | CA | 496 | A |
| 1 | CA | 498 | U |
| 1 | CA | 505 | G |
| 1 | CA | 509 | A |
| 1 | CA | 510 | A |
| 1 | CA | 511 | C |
| 1 | CA | 513 | C |
| 1 | CA | 518 | C |
| 1 | CA | 521 | G |
| 1 | CA | 527 | G |
| 1 | CA | 531 | U |
| 1 | CA | 532 | A |
| 1 | CA | 533 | A |
| 1 | CA | 536 | C |
| 1 | CA | 544 | G |
| 1 | CA | 547 | A |
| 1 | CA | 553 | A |
| 1 | CA | 559 | A |
| 1 | CA | 561 | U |
| 1 | CA | 571 | U |
| 1 | CA | 572 | A |
| 1 | CA | 573 | A |
| 1 | CA | 576 | G |
| 1 | CA | 592 | G |
| 1 | CA | 596 | C |
| 1 | CA | 597 | G |
| 1 | CA | 600 | C |
| 1 | CA | 606 | G |
| 1 | CA | 626 | U |
| 1 | CA | 630 | G |
| 1 | CA | 631 | G |
| 1 | CA | 633 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 639 | G |
| 1 | CA | 641 | U |
| 1 | CA | 650 | G |
| 1 | CA | 651 | C |
| 1 | CA | 653 | A |
| 1 | CA | 665 | A |
| 1 | CA | 673 | G |
| 1 | CA | 680 | C |
| 1 | CA | 687 | A |
| 1 | CA | 688 | G |
| 1 | CA | 693 | G |
| 1 | CA | 711 | G |
| 1 | CA | 721 | G |
| 1 | CA | 723 | U |
| 1 | CA | 724 | G |
| 1 | CA | 731 | G |
| 1 | CA | 752 | G |
| 1 | CA | 755 | G |
| 1 | CA | 760 | G |
| 1 | CA | 774 | G |
| 1 | CA | 777 | A |
| 1 | CA | 786 | G |
| 1 | CA | 792 | A |
| 1 | CA | 793 | U |
| 1 | CA | 794 | A |
| 1 | CA | 802 | A |
| 1 | CA | 806 | C |
| 1 | CA | 812 | C |
| 1 | CA | 815 | A |
| 1 | CA | 816 | A |
| 1 | CA | 817 | C |
| 1 | CA | 818 | G |
| 1 | CA | 821 | G |
| 1 | CA | 827 | U |
| 1 | CA | 828 | A |
| 1 | CA | 829 | G |
| 1 | CA | 836 | G |
| 1 | CA | 839 | U |
| 1 | CA | 840 | C |
| 1 | CA | 841 | U |
| 1 | CA | 851 | G |
| 1 | CA | 855 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 858 | G |
| 1 | CA | 859 | A |
| 1 | CA | 873 | A |
| 1 | CA | 876 | G |
| 1 | CA | 902 | G |
| 1 | CA | 914 | A |
| 1 | CA | 916 | G |
| 1 | CA | 922 | G |
| 1 | CA | 926 | G |
| 1 | CA | 927 | G |
| 1 | CA | 934 | C |
| 1 | CA | 935 | A |
| 1 | CA | 942 | G |
| 1 | CA | 958 | A |
| 1 | CA | 960 | U |
| 1 | CA | 961 | U |
| 1 | CA | 967 | C |
| 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 | 982 | U |
| 1 | CA | 983 | A |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |
| 1 | CA | 993 | G |
| 1 | CA | 995 | C |
| 1 | CA | 1001 | A |
| 1 | CA | 1001(A) | G |
| 1 | CA | 1002 | G |
| 1 | CA | 1003 | G |
| 1 | CA | 1004 | A |
| 1 | CA | 1005 | A |
| 1 | CA | 1006 | C |
| 1 | CA | 1007 | C |
| 1 | CA | 1011 | G |
| 1 | CA | 1013 | G |
| 1 | CA | 1014 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 1019 | C |
| 1 | CA | 1020 | U |
| 1 | CA | 1022 | G |
| 1 | CA | 1025 | U |
| 1 | CA | 1026 | G |
| 1 | CA | 1027 | C |
| 1 | CA | 1028 | C |
| 1 | CA | 1030 | C |
| 1 | CA | 1030(A) | G |
| 1 | CA | 1030(C) | G |
| 1 | CA | 1031 | G |
| 1 | CA | 1033 | G |
| 1 | CA | 1035 | A |
| 1 | CA | 1036 | G |
| 1 | CA | 1037 | C |
| 1 | CA | 1039 | C |
| 1 | CA | 1041 | A |
| 1 | CA | 1042 | G |
| 1 | CA | 1043 | C |
| 1 | CA | 1052 | U |
| 1 | CA | 1053 | G |
| 1 | CA | 1054 | C |
| 1 | CA | 1055 | A |
| 1 | CA | 1063 | C |
| 1 | CA | 1065 | U |
| 1 | CA | 1066 | C |
| 1 | CA | 1068 | G |
| 1 | CA | 1070 | U |
| 1 | CA | 1076 | C |
| 1 | CA | 1081 | G |
| 1 | CA | 1087 | G |
| 1 | CA | 1089 | G |
| 1 | CA | 1091 | U |
| 1 | CA | 1092 | A |
| 1 | CA | 1093 | A |
| 1 | CA | 1094 | G |
| 1 | CA | 1095 | U |
| 1 | CA | 1101 | A |
| 1 | CA | 1104 | G |
| 1 | CA | 1108 | G |
| 1 | CA | 1109 | C |
| 1 | CA | 1117 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1119 | C |
| 1 | CA | 1120 | G |
| 1 | CA | 1122 | U |
| 1 | CA | 1124 | G |
| 1 | CA | 1125 | U |
| 1 | CA | 1128 | C |
| 1 | CA | 1129 | C |
| 1 | CA | 1130 | A |
| 1 | CA | 1132 | C |
| 1 | CA | 1134 | G |
| 1 | CA | 1135 | U |
| 1 | CA | 1136 | U |
| 1 | CA | 1137 | C |
| 1 | CA | 1138 | G |
| 1 | CA | 1139 | G |
| 1 | CA | 1141 | C |
| 1 | CA | 1145 | C |
| 1 | CA | 1146 | A |
| 1 | CA | 1147 | C |
| 1 | CA | 1151 | A |
| 1 | CA | 1152 | A |
| 1 | CA | 1154 | G |
| 1 | CA | 1157 | A |
| 1 | CA | 1159 | U |
| 1 | CA | 1160 | G |
| 1 | CA | 1161 | C |
| 1 | CA | 1163 | C |
| 1 | CA | 1171 | G |
| 1 | CA | 1173 | G |
| 1 | CA | 1176 | A |
| 1 | CA | 1181 | G |
| 1 | CA | 1183 | A |
| 1 | CA | 1184 | G |
| 1 | CA | 1189 | C |
| 1 | CA | 1193 | G |
| 1 | CA | 1196 | U |
| 1 | CA | 1197 | G |
| 1 | CA | 1200 | C |
| 1 | CA | 1202 | G |
| 1 | CA | 1204 | A |
| 1 | CA | 1211 | U |
| 1 | CA | 1212 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1213 | A |
| 1 | CA | 1214 | C |
| 1 | CA | 1223 | C |
| 1 | CA | 1224 | G |
| 1 | CA | 1227 | A |
| 1 | CA | 1235 | U |
| 1 | CA | 1236 | A |
| 1 | CA | 1238 | A |
| 1 | CA | 1250 | A |
| 1 | CA | 1256 | A |
| 1 | CA | 1257 | U |
| 1 | CA | 1258 | G |
| 1 | CA | 1259 | C |
| 1 | CA | 1260 | C |
| 1 | CA | 1262 | C |
| 1 | CA | 1270 | C |
| 1 | CA | 1271 | G |
| 1 | CA | 1273 | G |
| 1 | CA | 1278 | U |
| 1 | CA | 1279 | A |
| 1 | CA | 1280 | A |
| 1 | CA | 1281 | U |
| 1 | CA | 1282 | C |
| 1 | CA | 1283 | G |
| 1 | CA | 1284 | C |
| 1 | CA | 1287 | A |
| 1 | CA | 1297 | C |
| 1 | CA | 1299 | A |
| 1 | CA | 1300 | G |
| 1 | CA | 1305 | G |
| 1 | CA | 1311 | G |
| 1 | CA | 1314 | C |
| 1 | CA | 1317 | C |
| 1 | CA | 1320 | C |
| 1 | CA | 1322 | C |
| 1 | CA | 1323 | G |
| 1 | CA | 1338 | G |
| 1 | CA | 1340 | A |
| 1 | CA | 1343 | G |
| 1 | CA | 1346 | A |
| 1 | CA | 1347 | G |
| 1 | CA | 1353 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 1354 | C |
| 1 | CA | 1358 | U |
| 1 | CA | 1360 | A |
| 1 | CA | 1361 | G |
| 1 | CA | 1363 | C |
| 1 | CA | 1370 | G |
| 1 | CA | 1377 | A |
| 1 | CA | 1379 | G |
| 1 | CA | 1393 | U |
| 1 | CA | 1396 | A |
| 1 | CA | 1397 | C |
| 1 | CA | 1402 | C |
| 1 | CA | 1419 | G |
| 1 | CA | 1422 | G |
| 1 | CA | 1442 | G |
| 1 | CA | 1442(A) | G |
| 1 | CA | 1442(B) | A |
| 1 | CA | 1447 | A |
| 1 | CA | 1456 | G |
| 1 | CA | 1457 | G |
| 1 | CA | 1469 | G |
| 1 | CA | 1487 | G |
| 1 | CA | 1489 | G |
| 1 | CA | 1493 | A |
| 1 | CA | 1497 | G |
| 1 | CA | 1502 | A |
| 1 | CA | 1503 | A |
| 1 | CA | 1504 | G |
| 1 | CA | 1506 | U |
| 1 | CA | 1517 | G |
| 1 | CA | 1519 | A |
| 1 | CA | 1520 | G |
| 1 | CA | 1529 | G |
| 1 | CA | 1530 | G |
| 1 | CA | 1531 | A |
| 1 | CA | 1532 | U |
| 22 | CV | 15 | A |
| 23 | CX | 6 | G |
| 23 | CX | 9 | G |
| 23 | CX | 13 | C |
| 23 | CX | 19 | G |
| 23 | CX | 20 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | CX | 21 | A |
| 23 | CX | 28 | C |
| 23 | CX | 31 | G |
| 23 | CX | 42 | G |
| 23 | CX | 47 | U |
| 23 | CX | 48 | C |
| 23 | CX | 60 | U |
| 23 | CX | 61 | C |
| 23 | CX | 68 | C |
| 23 | CX | 70 | G |
| 23 | CX | 76 | A |
| 25 | DA | 8 | A |
| 25 | DA | 10 | G |
| 25 | DA | 12 | U |
| 25 | DA | 15 | G |
| 25 | DA | 32 | C |
| 25 | DA | 34 | C |
| 25 | DA | 35 | G |
| 25 | DA | 36 | G |
| 25 | DA | 41 | C |
| 25 | DA | 45 | C |
| 25 | DA | 55 | G |
| 25 | DA | 61 | G |
| 25 | DA | 71 | A |
| 25 | DA | 74 | A |
| 25 | DA | 75 | G |
| 25 | DA | 83 | G |
| 25 | DA | 84 | A |
| 25 | DA | 90 | U |
| 25 | DA | 95 | G |
| 25 | DA | 100 | G |
| 25 | DA | 102 | G |
| 25 | DA | 118 | A |
| 25 | DA | 119 | A |
| 25 | DA | 120 | U |
| 25 | DA | 125 | G |
| 25 | DA | 133 | C |
| 25 | DA | 141 | A |
| 25 | DA | 149 | A |
| 25 | DA | 154(A) | C |
| 25 | DA | 157 | U |
| 25 | DA | 173 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DA | 180 | G |
| 25 | DA | 181 | A |
| 25 | DA | 182 | A |
| 25 | DA | 188 | G |
| 25 | DA | 196 | A |
| 25 | DA | 199 | A |
| 25 | DA | 205 | G |
| 25 | DA | 214 | G |
| 25 | DA | 215 | G |
| 25 | DA | 216 | A |
| 25 | DA | 221 | A |
| 25 | DA | 222 | A |
| 25 | DA | 225 | A |
| 25 | DA | 229 | A |
| 25 | DA | 233 | A |
| 25 | DA | 248 | G |
| 25 | DA | 250 | G |
| 25 | DA | 266 | G |
| 25 | DA | 267 | C |
| 25 | DA | 271(E) | U |
| 25 | DA | 271(H) | G |
| 25 | DA | 271(J) | C |
| 25 | DA | 271(K) | U |
| 25 | DA | 271(L) | U |
| 25 | DA | 271(M) | G |
| 25 | DA | 271(N) | U |
| 25 | DA | 271(T) | C |
| 25 | DA | 272(A) | U |
| 25 | DA | 272(B) | G |
| 25 | DA | 277 | C |
| 25 | DA | 278 | A |
| 25 | DA | 292 | C |
| 25 | DA | 304 | G |
| 25 | DA | 311 | A |
| 25 | DA | 312 | G |
| 25 | DA | 324 | A |
| 25 | DA | 327 | G |
| 25 | DA | 329 | G |
| 25 | DA | 330 | A |
| 25 | DA | 333 | G |
| 25 | DA | 338 | G |
| 25 | DA | 339 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | DA | 342 | G |
| 25 | DA | 348 | G |
| 25 | DA | 351 | G |
| 25 | DA | 352 | G |
| 25 | DA | 363 | G |
| 25 | DA | 363(C) | G |
| 25 | DA | 386 | G |
| 25 | DA | 396 | G |
| 25 | DA | 399 | G |
| 25 | DA | 405 | U |
| 25 | DA | 407 | G |
| 25 | DA | 411 | G |
| 25 | DA | 412 | A |
| 25 | DA | 415 | A |
| 25 | DA | 428 | A |
| 25 | DA | 437 | G |
| 25 | DA | 438 | G |
| 25 | DA | 443 | A |
| 25 | DA | 444 | C |
| 25 | DA | 454 | A |
| 25 | DA | 455 | C |
| 25 | DA | 456 | C |
| 25 | DA | 457 | A |
| 25 | DA | 470 | A |
| 25 | DA | 480 | A |
| 25 | DA | 481 | G |
| 25 | DA | 504 | U |
| 25 | DA | 505 | A |
| 25 | DA | 509 | C |
| 25 | DA | 524 | U |
| 25 | DA | 527 | C |
| 25 | DA | 528 | A |
| 25 | DA | 529 | A |
| 25 | DA | 530 | G |
| 25 | DA | 531 | C |
| 25 | DA | 532 | A |
| 25 | DA | 533 | G |
| 25 | DA | 545 | G |
| 25 | DA | 563 | G |
| 25 | DA | 568 | U |
| 25 | DA | 573 | G |
| 25 | DA | 575 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | DA | 586 | A |
| 25 | DA | 587 | C |
| 25 | DA | 592 | G |
| 25 | DA | 603 | A |
| 25 | DA | 604 | G |
| 25 | DA | 606 | U |
| 25 | DA | 607 | U |
| 25 | DA | 610 | G |
| 25 | DA | 614(B) | G |
| 25 | DA | 614(C) | A |
| 25 | DA | 615 | G |
| 25 | DA | 631 | A |
| 25 | DA | 634 | C |
| 25 | DA | 637 | A |
| 25 | DA | 645 | C |
| 25 | DA | 646 | A |
| 25 | DA | 652(B) | A |
| 25 | DA | 652(C) | G |
| 25 | DA | 652(E) | G |
| 25 | DA | 652(U) | G |
| 25 | DA | 669 | G |
| 25 | DA | 670 | A |
| 25 | DA | 686 | G |
| 25 | DA | 717 | G |
| 25 | DA | 726 | G |
| 25 | DA | 730 | C |
| 25 | DA | 747 | U |
| 25 | DA | 749 | C |
| 25 | DA | 752 | A |
| 25 | DA | 753 | C |
| 25 | DA | 765 | G |
| 25 | DA | 771 | G |
| 25 | DA | 775 | G |
| 25 | DA | 776 | G |
| 25 | DA | 782 | A |
| 25 | DA | 784 | A |
| 25 | DA | 785 | G |
| 25 | DA | 790 | C |
| 25 | DA | 792 | G |
| 25 | DA | 805 | G |
| 25 | DA | 812 | C |
| 25 | DA | 819 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DA | 827 | U |
| 25 | DA | 854 | G |
| 25 | DA | 857 | C |
| 25 | DA | 859 | G |
| 25 | DA | 866 | A |
| 25 | DA | 867 | C |
| 25 | DA | 869 | G |
| 25 | DA | 871 | U |
| 25 | DA | 874 | G |
| 25 | DA | 878 | A |
| 25 | DA | 879 | G |
| 25 | DA | 880 | G |
| 25 | DA | 884 | C |
| 25 | DA | 886 | C |
| 25 | DA | 887 | A |
| 25 | DA | 888 | C |
| 25 | DA | 889 | C |
| 25 | DA | 890 | A |
| 25 | DA | 895 | U |
| 25 | DA | 896 | A |
| 25 | DA | 897 | C |
| 25 | DA | 898 | C |
| 25 | DA | 899 | A |
| 25 | DA | 900 | A |
| 25 | DA | 901 | A |
| 25 | DA | 910 | A |
| 25 | DA | 911 | A |
| 25 | DA | 913 | U |
| 25 | DA | 914 | C |
| 25 | DA | 917 | A |
| 25 | DA | 923 | C |
| 25 | DA | 926 | A |
| 25 | DA | 932 | G |
| 25 | DA | 938 | G |
| 25 | DA | 941 | A |
| 25 | DA | 945 | A |
| 25 | DA | 946 | G |
| 25 | DA | 953 | A |
| 25 | DA | 957 | A |
| 25 | DA | 958 | U |
| 25 | DA | 959 | A |
| 25 | DA | 961 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DA | 974 | G |
| 25 | DA | 975 | C |
| 25 | DA | 983 | A |
| 25 | DA | 996 | A |
| 25 | DA | 1010 | A |
| 25 | DA | 1012 | U |
| 25 | DA | 1013 | C |
| 25 | DA | 1020 | A |
| 25 | DA | 1022 | G |
| 25 | DA | 1023 | U |
| 25 | DA | 1025 | G |
| 25 | DA | 1027 | A |
| 25 | DA | 1033 | U |
| 25 | DA | 1034 | G |
| 25 | DA | 1038 | C |
| 25 | DA | 1039 | G |
| 25 | DA | 1040 | C |
| 25 | DA | 1041 | C |
| 25 | DA | 1043 | C |
| 25 | DA | 1114 | G |
| 25 | DA | 1115 | G |
| 25 | DA | 1118 | C |
| 25 | DA | 1119 | C |
| 25 | DA | 1130 | U |
| 25 | DA | 1135 | C |
| 25 | DA | 1136 | G |
| 25 | DA | 1139 | G |
| 25 | DA | 1142(A) | A |
| 25 | DA | 1155 | A |
| 25 | DA | 1170 | G |
| 25 | DA | 1171 | G |
| 25 | DA | 1186 | G |
| 25 | DA | 1204 | A |
| 25 | DA | 1205 | U |
| 25 | DA | 1210 | A |
| 25 | DA | 1211 | U |
| 25 | DA | 1219 | G |
| 25 | DA | 1220 | A |
| 25 | DA | 1230 | C |
| 25 | DA | 1249 | U |
| 25 | DA | 1253 | A |
| 25 | DA | 1256 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | DA | 1271 | G |
| 25 | DA | 1272 | A |
| 25 | DA | 1273 | U |
| 25 | DA | 1284 | A |
| 25 | DA | 1287 | A |
| 25 | DA | 1300 | U |
| 25 | DA | 1301 | A |
| 25 | DA | 1313 | U |
| 25 | DA | 1314 | C |
| 25 | DA | 1315 | C |
| 25 | DA | 1321 | A |
| 25 | DA | 1332 | G |
| 25 | DA | 1345 | C |
| 25 | DA | 1359 | A |
| 25 | DA | 1360 | A |
| 25 | DA | 1365 | A |
| 25 | DA | 1366 | A |
| 25 | DA | 1368 | G |
| 25 | DA | 1370 | C |
| 25 | DA | 1380 | G |
| 25 | DA | 1384 | A |
| 25 | DA | 1385 | G |
| 25 | DA | 1386 | C |
| 25 | DA | 1395 | A |
| 25 | DA | 1403 | C |
| 25 | DA | 1410 | G |
| 25 | DA | 1411 | C |
| 25 | DA | 1416 | G |
| 25 | DA | 1417 | C |
| 25 | DA | 1419 | A |
| 25 | DA | 1420 | U |
| 25 | DA | 1421 | G |
| 25 | DA | 1427 | A |
| 25 | DA | 1428 | C |
| 25 | DA | 1437 | C |
| 25 | DA | 1445 | A |
| 25 | DA | 1445(A) | C |
| 25 | DA | 1449 | A |
| 25 | DA | 1450 | G |
| 25 | DA | 1455 | G |
| 25 | DA | 1459 | G |
| 25 | DA | 1466 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | DA | 1467 | C |
| 25 | DA | 1471 | A |
| 25 | DA | 1482 | G |
| 25 | DA | 1490 | A |
| 25 | DA | 1492 | G |
| 25 | DA | 1493 | C |
| 25 | DA | 1495 | A |
| 25 | DA | 1496 | A |
| 25 | DA | 1497 | U |
| 25 | DA | 1504 | C |
| 25 | DA | 1508 | A |
| 25 | DA | 1509 | C |
| 25 | DA | 1509(A) | A |
| 25 | DA | 1531 | C |
| 25 | DA | 1541 | G |
| 25 | DA | 1542 | A |
| 25 | DA | 1543 | C |
| 25 | DA | 1547 | C |
| 25 | DA | 1554 | A |
| 25 | DA | 1558 | A |
| 25 | DA | 1559 | G |
| 25 | DA | 1566 | A |
| 25 | DA | 1569 | A |
| 25 | DA | 1578 | U |
| 25 | DA | 1580 | A |
| 25 | DA | 1586 | A |
| 25 | DA | 1588 | C |
| 25 | DA | 1595 | G |
| 25 | DA | 1598 | C |
| 25 | DA | 1603 | A |
| 25 | DA | 1608 | A |
| 25 | DA | 1609 | A |
| 25 | DA | 1610 | A |
| 25 | DA | 1613 | G |
| 25 | DA | 1618 | A |
| 25 | DA | 1625 | C |
| 25 | DA | 1631(A) | A |
| 25 | DA | 1632 | A |
| 25 | DA | 1640 | C |
| 25 | DA | 1648 | C |
| 25 | DA | 1654 | A |
| 25 | DA | 1674 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DA | 1676 | A |
| 25 | DA | 1682 | G |
| 25 | DA | 1696 | G |
| 25 | DA | 1700 | A |
| 25 | DA | 1701 | A |
| 25 | DA | 1703 | G |
| 25 | DA | 1718 | G |
| 25 | DA | 1721 | G |
| 25 | DA | 1722 | A |
| 25 | DA | 1740 | G |
| 25 | DA | 1746 | G |
| 25 | DA | 1756 | G |
| 25 | DA | 1762 | A |
| 25 | DA | 1763 | G |
| 25 | DA | 1764 | G |
| 25 | DA | 1773 | A |
| 25 | DA | 1780 | A |
| 25 | DA | 1782 | C |
| 25 | DA | 1786 | A |
| 25 | DA | 1791 | A |
| 25 | DA | 1800 | C |
| 25 | DA | 1801 | G |
| 25 | DA | 1812 | A |
| 25 | DA | 1816 | G |
| 25 | DA | 1823 | G |
| 25 | DA | 1829 | A |
| 25 | DA | 1835 | G |
| 25 | DA | 1836 | C |
| 25 | DA | 1847 | A |
| 25 | DA | 1848 | A |
| 25 | DA | 1860 | G |
| 25 | DA | 1877 | A |
| 25 | DA | 1878 | G |
| 25 | DA | 1881 | C |
| 25 | DA | 1900 | A |
| 25 | DA | 1906 | G |
| 25 | DA | 1913 | A |
| 25 | DA | 1914 | C |
| 25 | DA | 1926 | U |
| 25 | DA | 1929 | G |
| 25 | DA | 1930 | G |
| 25 | DA | 1931 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DA | 1936 | A |
| 25 | DA | 1938 | A |
| 25 | DA | 1955 | U |
| 25 | DA | 1960 | A |
| 25 | DA | 1963 | U |
| 25 | DA | 1966 | A |
| 25 | DA | 1967 | C |
| 25 | DA | 1970 | A |
| 25 | DA | 1971 | A |
| 25 | DA | 1972 | A |
| 25 | DA | 1984 | G |
| 25 | DA | 1993 | U |
| 25 | DA | 1997 | G |
| 25 | DA | 2005 | A |
| 25 | DA | 2020 | A |
| 25 | DA | 2021 | C |
| 25 | DA | 2023 | G |
| 25 | DA | 2031 | A |
| 25 | DA | 2032 | G |
| 25 | DA | 2033 | A |
| 25 | DA | 2034 | U |
| 25 | DA | 2039 | C |
| 25 | DA | 2043 | C |
| 25 | DA | 2049 | G |
| 25 | DA | 2055 | C |
| 25 | DA | 2056 | G |
| 25 | DA | 2060 | A |
| 25 | DA | 2061 | G |
| 25 | DA | 2062 | A |
| 25 | DA | 2069 | G |
| 25 | DA | 2076 | U |
| 25 | DA | 2082 | A |
| 25 | DA | 2093 | G |
| 25 | DA | 2097 | C |
| 25 | DA | 2099 | U |
| 25 | DA | 2101 | G |
| 25 | DA | 2189 | U |
| 25 | DA | 2192 | G |
| 25 | DA | 2193 | G |
| 25 | DA | 2198 | A |
| 25 | DA | 2206 | G |
| 25 | DA | 2207 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 2208 | A |
| 25 | DA | 2218 | U |
| 25 | DA | 2219 | G |
| 25 | DA | 2225 | A |
| 25 | DA | 2235 | G |
| 25 | DA | 2238 | G |
| 25 | DA | 2239 | G |
| 25 | DA | 2243 | U |
| 25 | DA | 2251 | G |
| 25 | DA | 2267 | A |
| 25 | DA | 2268 | A |
| 25 | DA | 2269 | A |
| 25 | DA | 2275 | C |
| 25 | DA | 2278 | A |
| 25 | DA | 2279 | G |
| 25 | DA | 2283 | C |
| 25 | DA | 2286 | A |
| 25 | DA | 2287 | A |
| 25 | DA | 2289 | G |
| 25 | DA | 2291 | U |
| 25 | DA | 2298 | A |
| 25 | DA | 2303 | G |
| 25 | DA | 2305 | A |
| 25 | DA | 2308 | G |
| 25 | DA | 2312 | U |
| 25 | DA | 2318 | G |
| 25 | DA | 2319 | G |
| 25 | DA | 2320 | A |
| 25 | DA | 2321 | G |
| 25 | DA | 2325 | G |
| 25 | DA | 2327 | A |
| 25 | DA | 2334 | G |
| 25 | DA | 2335 | A |
| 25 | DA | 2336 | A |
| 25 | DA | 2343 | C |
| 25 | DA | 2347 | C |
| 25 | DA | 2348 | U |
| 25 | DA | 2359 | C |
| 25 | DA | 2376 | A |
| 25 | DA | 2383 | G |
| 25 | DA | 2384 | G |
| 25 | DA | 2385 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 2388 | A |
| 25 | DA | 2391 | G |
| 25 | DA | 2401 | U |
| 25 | DA | 2402 | C |
| 25 | DA | 2406 | U |
| 25 | DA | 2410 | G |
| 25 | DA | 2413 | G |
| 25 | DA | 2414 | G |
| 25 | DA | 2422 | A |
| 25 | DA | 2425 | A |
| 25 | DA | 2429 | G |
| 25 | DA | 2430 | A |
| 25 | DA | 2434 | A |
| 25 | DA | 2435 | A |
| 25 | DA | 2439 | A |
| 25 | DA | 2441 | C |
| 25 | DA | 2448 | A |
| 25 | DA | 2465 | C |
| 25 | DA | 2468 | G |
| 25 | DA | 2469 | A |
| 25 | DA | 2474 | C |
| 25 | DA | 2476 | A |
| 25 | DA | 2487 | G |
| 25 | DA | 2492 | U |
| 25 | DA | 2497 | A |
| 25 | DA | 2502 | G |
| 25 | DA | 2505 | G |
| 25 | DA | 2518 | A |
| 25 | DA | 2520 | C |
| 25 | DA | 2525 | G |
| 25 | DA | 2529 | G |
| 25 | DA | 2549 | G |
| 25 | DA | 2554 | U |
| 25 | DA | 2566 | A |
| 25 | DA | 2567 | G |
| 25 | DA | 2586 | C |
| 25 | DA | 2602 | A |
| 25 | DA | 2609 | U |
| 25 | DA | 2611 | U |
| 25 | DA | 2612 | C |
| 25 | DA | 2615 | U |
| 25 | DA | 2629 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | DA | 2630 | G |
| 25 | DA | 2632 | A |
| 25 | DA | 2654 | A |
| 25 | DA | 2663 | G |
| 25 | DA | 2689 | U |
| 25 | DA | 2690 | C |
| 25 | DA | 2691 | C |
| 25 | DA | 2703 | C |
| 25 | DA | 2712(A) | A |
| 25 | DA | 2713 | A |
| 25 | DA | 2717 | G |
| 25 | DA | 2726 | U |
| 25 | DA | 2733 | A |
| 25 | DA | 2751 | G |
| 25 | DA | 2752 | C |
| 25 | DA | 2757 | A |
| 25 | DA | 2758 | A |
| 25 | DA | 2761 | G |
| 25 | DA | 2764 | A |
| 25 | DA | 2765 | A |
| 25 | DA | 2766 | G |
| 25 | DA | 2778 | A |
| 25 | DA | 2779 | U |
| 25 | DA | 2780 | G |
| 25 | DA | 2789 | C |
| 25 | DA | 2793 | G |
| 25 | DA | 2802 | G |
| 25 | DA | 2803 | C |
| 25 | DA | 2804 | C |
| 25 | DA | 2818 | G |
| 25 | DA | 2820 | A |
| 25 | DA | 2821 | A |
| 25 | DA | 2833 | G |
| 25 | DA | 2835 | A |
| 25 | DA | 2872 | G |
| 25 | DA | 2879 | C |
| 25 | DA | 2880 | C |
| 25 | DA | 2892 | A |
| 25 | DA | 2893 | G |
| 25 | DA | 2894 | G |
| 25 | DA | 2895 | U |
| 25 | DA | 2897 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | DB | 2 | C |
| 26 | DB | 7 | G |
| 26 | DB | 8 | U |
| 26 | DB | 12 | C |
| 26 | DB | 13 | A |
| 26 | DB | 34 | U |
| 26 | DB | 42 | C |
| 26 | DB | 45 | A |
| 26 | DB | 46 | A |
| 26 | DB | 56 | G |
| 26 | DB | 59 | A |
| 26 | DB | 72 | G |
| 26 | DB | 73 | A |
| 26 | DB | 75 | G |
| 26 | DB | 85 | G |
| 26 | DB | 88 | C |
| 26 | DB | 89 | G |
| 26 | DB | 90 | A |
| 26 | DB | 93 | G |
| 26 | DB | 106 | G |
| 26 | DB | 110 | G |
| 26 | DB | 112 | U |
| 26 | DB | 116 | G |
| 26 | DB | 119 | G |

All (134) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 97 | G |
| 1 | AA | 115 | G |
| 1 | AA | 148 | G |
| 1 | AA | 266 | G |
| 1 | AA | 429 | U |
| 1 | AA | 509 | A |
| 1 | AA | 532 | A |
| 1 | AA | 560 | U |
| 1 | AA | 687 | A |
| 1 | AA | 793 | U |
| 1 | AA | 913 | A |
| 1 | AA | 991 | U |
| 1 | AA | 1027 | C |
| 1 | AA | 1042 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 1054 | C |
| 1 | AA | 1064 | G |
| 1 | AA | 1065 | U |
| 1 | AA | 1067 | A |
| 1 | AA | 1125 | U |
| 1 | AA | 1165 | C |
| 1 | AA | 1201 | A |
| 1 | AA | 1256 | A |
| 1 | AA | 1285 | A |
| 1 | AA | 1299 | A |
| 1 | AA | 1442 | G |
| 25 | BA | 70 | A |
| 25 | BA | 99 | G |
| 25 | BA | 184 | A |
| 25 | BA | 185 | A |
| 25 | BA | 273 | G |
| 25 | BA | 302 | A |
| 25 | BA | 553 | A |
| 25 | BA | 716 | G |
| 25 | BA | 732 | A |
| 25 | BA | 793 | A |
| 25 | BA | 811 | A |
| 25 | BA | 821 | A |
| 25 | BA | 874 | U |
| 25 | BA | 945 | A |
| 25 | BA | 990 | A |
| 25 | BA | 1003 | U |
| 25 | BA | 1019 | G |
| 25 | BA | 1219 | A |
| 25 | BA | 1220 | U |
| 25 | BA | 1221 | G |
| 25 | BA | 1255 | A |
| 25 | BA | 1425 | A |
| 25 | BA | 1466 | U |
| 25 | BA | 1507 | A |
| 25 | BA | 1577 | C |
| 25 | BA | 1654 | A |
| 25 | BA | 1655 | A |
| 25 | BA | 1700 | G |
| 25 | BA | 1793 | A |
| 25 | BA | 2014 | G |
| 25 | BA | 2228 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2347 | A |
| 25 | BA | 2418 | U |
| 25 | BA | 2434 | A |
| 25 | BA | 2442 | A |
| 25 | BA | 2623 | U |
| 25 | BA | 2701 | U |
| 25 | BA | 2763 | A |
| 25 | BA | 2769 | U |
| 25 | BA | 2902 | G |
| 1 | CA | 4 | U |
| 1 | CA | 5 | U |
| 1 | CA | 65 | U |
| 1 | CA | 97 | G |
| 1 | CA | 115 | G |
| 1 | CA | 204 | U |
| 1 | CA | 266 | G |
| 1 | CA | 429 | U |
| 1 | CA | 509 | A |
| 1 | CA | 532 | A |
| 1 | CA | 560 | U |
| 1 | CA | 687 | A |
| 1 | CA | 793 | U |
| 1 | CA | 913 | A |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |
| 1 | CA | 1005 | A |
| 1 | CA | 1027 | C |
| 1 | CA | 1054 | C |
| 1 | CA | 1064 | G |
| 1 | CA | 1065 | U |
| 1 | CA | 1067 | A |
| 1 | CA | 1128 | C |
| 1 | CA | 1137 | C |
| 1 | CA | 1183 | A |
| 1 | CA | 1201 | A |
| 1 | CA | 1212 | U |
| 1 | CA | 1256 | A |
| 1 | CA | 1299 | A |
| 1 | CA | 1442 | G |
| 1 | CA | 1531 | A |
| 25 | DA | 195 | A |
| 25 | DA | 249 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | DA | 271(M) | G |
| 25 | DA | 277 | C |
| 25 | DA | 310 | A |
| 25 | DA | 503 | A |
| 25 | DA | 528 | A |
| 25 | DA | 620 | G |
| 25 | DA | 669 | G |
| 25 | DA | 685 | A |
| 25 | DA | 752 | A |
| 25 | DA | 827 | U |
| 25 | DA | 856 | C |
| 25 | DA | 900 | A |
| 25 | DA | 1026 | U |
| 25 | DA | 1210 | A |
| 25 | DA | 1378 | A |
| 25 | DA | 1379 | A |
| 25 | DA | 1395 | A |
| 25 | DA | 1420 | U |
| 25 | DA | 1427 | A |
| 25 | DA | 1530 | C |
| 25 | DA | 1543 | C |
| 25 | DA | 1558 | A |
| 25 | DA | 1559 | G |
| 25 | DA | 1608 | A |
| 25 | DA | 1653 | G |
| 25 | DA | 1790 | C |
| 25 | DA | 1992 | G |
| 25 | DA | 2318 | G |
| 25 | DA | 2335 | A |
| 25 | DA | 2406 | U |
| 25 | DA | 2439 | A |
| 25 | DA | 2611 | U |
| 25 | DA | 2689 | U |
| 25 | DA | 2750 | A |
| 25 | DA | 2756 | U |
| 26 | DB | 45 | A |

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | 2R3 | CW | 8 | 24 | 12,14,15 | 0.66 | 0 | 16,18,20 | 1.63 | 5 (31%) |
| 24 | MVA | CW | 5 | 24 | 6,7,8 | 0.70 | 0 | 7,8,10 | 1.42 | 1 (14%) |
| 24 | MVA | AW | 9 | 24 | 6,7,8 | 0.46 | 0 | 7,8,10 | 0.95 | 1 (14%) |
| 24 | 2QZ | AW | 1 | 24 | 7,8,9 | 0.38 | 0 | 8,10,12 | 4.18 | 1 (12%) |
| 24 | MVA | CW | 9 | 24 | 6,7,8 | 0.97 | 1 (16%) | 7,8,10 | 1.53 | 1 (14%) |
| 24 | 2QY | AW | 10 | 24 | 12,13,14 | 2.00 | 1 (8%) | 13,16,18 | 3.53 | 4 (30%) |
| 24 | 2R1 | AW | 6 | 24 | 10,10,11 | 1.78 | 3 (30%) | 6,13,15 | 5.49 | 2 (33%) |
| 24 | 2R3 | AW | 8 | 24 | 12,14,15 | 0.80 | 0 | 16,18,20 | 1.73 | 5 (31%) |
| 24 | MVA | AW | 5 | 24 | 6,7,8 | 0.37 | 0 | 7,8,10 | 1.11 | 0 |
| 24 | 2QZ | CW | 1 | 24 | 7,8,9 | 0.61 | 0 | 8,10,12 | 3.72 | 2 (25%) |
| 24 | 004 | CW | 3 | 24 | 9,10,11 | 1.22 | 1 (11%) | 9,12,14 | 0.97 | 0 |
| 24 | 2R1 | CW | 6 | 24 | 10,10,11 | 1.86 | 2 (20%) | 6,13,15 | 4.48 | 2 (33%) |
| 24 | 2QY | CW | 10 | 24 | 12,13,14 | 2.25 | 2 (16%) | 13,16,18 | 2.99 | 2 (15%) |
| 24 | 004 | AW | 3 | 24 | 9,10,11 | 0.97 | 1 (11%) | 9,12,14 | 1.20 | 2 (22%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 24 | 2R3 | CW | 8 | 24 | - | 7/11/12/14 | 0/1/1/1 |
| 24 | MVA | CW | 5 | 24 | - | 6/6/8/10 | - |
| 24 | MVA | AW | 9 | 24 | - | 5/6/8/10 | - |
| 24 | 2QZ | AW | 1 | 24 | - | 3/6/10/12 | - |
| 24 | MVA | CW | 9 | 24 | - | 5/6/8/10 | - |
| 24 | 2QY | AW | 10 | 24 | - | 3/4/8/10 | 0/1/1/1 |
| 24 | 2R1 | AW | 6 | 24 | - | 1/2/14/16 | 0/1/1/1 |
| 24 | 2R3 | AW | 8 | 24 | - | 4/11/12/14 | 0/1/1/1 |
| 24 | MVA | AW | 5 | 24 | - | 3/6/8/10 | - |
| 24 | 2QZ | CW | 1 | 24 | - | 2/6/10/12 | - |
| 24 | 004 | CW | 3 | 24 | - | 0/4/6/8 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 24 | 2R1 | CW | 6 | 24 | - | 0/2/14/16 | 0/1/1/1 |
| 24 | 2QY | CW | 10 | 24 | - | 2/4/8/10 | 0/1/1/1 |
| 24 | 004 | AW | 3 | 24 | - | 0/4/6/8 | 0/1/1/1 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | CW | 10 | 2QY | C-CA | 6.88 | 1.53 | 1.43 |
| 24 | AW | 10 | 2QY | C-CA | 6.24 | 1.52 | 1.43 |
| 24 | CW | 6 | 2R1 | CA-N | 3.90 | 1.46 | 1.36 |
| 24 | AW | 6 | 2R1 | CA-N | 3.57 | 1.45 | 1.36 |
| 24 | CW | 6 | 2R1 | C-CA | 3.43 | 1.50 | 1.45 |
| 24 | CW | 10 | 2QY | CG-CB | 3.19 | 1.53 | 1.46 |
| 24 | CW | 3 | 004 | CB-CA | -3.04 | 1.49 | 1.52 |
| 24 | AW | 6 | 2R1 | OD1-CG1 | 2.31 | 1.55 | 1.43 |
| 24 | CW | 9 | MVA | CB-CA | 2.26 | 1.58 | 1.54 |
| 24 | AW | 6 | 2R1 | C-CA | 2.19 | 1.48 | 1.45 |
| 24 | AW | 3 | 004 | CA-C | 2.12 | 1.55 | 1.51 |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 24 | AW | 6 | 2R1 | OD2-CG2-CB | -12.79 | 88.98 | 112.24 |
| 24 | AW | 1 | 2QZ | OG1-CB-CG2 | 11.22 | 142.97 | 109.74 |
| 24 | CW | 6 | 2R1 | OD2-CG2-CB | -10.33 | 93.46 | 112.24 |
| 24 | AW | 10 | 2QY | CN-N-CA | -10.27 | 107.83 | 123.45 |
| 24 | CW | 1 | 2QZ | OG1-CB-CG2 | 9.77 | 138.68 | 109.74 |
| 24 | CW | 10 | 2QY | CN-N-CA | -9.36 | 109.22 | 123.45 |
| 24 | AW | 10 | 2QY | O-C-CA | -5.65 | 118.21 | 125.39 |
| 24 | CW | 10 | 2QY | O-C-CA | -4.86 | 119.21 | 125.39 |
| 24 | AW | 6 | 2R1 | O-C-CA | -3.42 | 119.16 | 125.54 |
| 24 | AW | 8 | 2R3 | OB-CB-CA | 3.41 | 114.47 | 107.28 |
| 24 | AW | 10 | 2QY | CG-CB-CA | -3.40 | 123.86 | 130.62 |
| 24 | CW | 6 | 2R1 | O-C-CA | -3.17 | 119.62 | 125.54 |
| 24 | CW | 8 | 2R3 | CO-OH-CZ | -3.10 | 110.78 | 117.51 |
| 24 | AW | 8 | 2R3 | CE2-CD2-CG | 3.01 | 124.22 | 121.20 |
| 24 | CW | 5 | MVA | CB-CA-N | 2.95 | 115.01 | 111.17 |
| 24 | CW | 8 | 2R3 | CD2-CE2-CZ | -2.70 | 116.43 | 119.73 |
| 24 | CW | 8 | 2R3 | CE2-CD2-CG | 2.50 | 123.71 | 121.20 |
| 24 | CW | 1 | 2QZ | CB-CA-C | -2.35 | 108.03 | 111.77 |
| 24 | CW | 8 | 2R3 | O-C-CA | -2.28 | 118.81 | 124.78 |
| 24 | AW | 8 | 2R3 | CD2-CE2-CZ | -2.27 | 116.95 | 119.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 24 | AW | 8 | 2R3 | CO-OH-CZ | -2.26 | 112.62 | 117.51 |
| 24 | AW | 10 | 2QY | CD1-CG-CD2 | 2.24 | 120.96 | 117.64 |
| 24 | AW | 8 | 2R3 | CD1-CE1-CZ | 2.21 | 122.43 | 119.73 |
| 24 | AW | 9 | MVA | O-C-CA | -2.13 | 118.89 | 124.83 |
| 24 | CW | 9 | MVA | CB-CA-N | 2.10 | 113.91 | 111.17 |
| 24 | CW | 8 | 2R3 | OB-CB-CA | 2.07 | 111.64 | 107.28 |
| 24 | AW | 3 | 004 | CG1-CB-CA | -2.05 | 117.35 | 120.65 |
| 24 | AW | 3 | 004 | CG2-CB-CA | 2.03 | 123.92 | 120.65 |

There are no chirality outliers.

All (41) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 24 | CW | 8 | 2R3 | N-CA-CB-OB |
| 24 | CW | 8 | 2R3 | N-CA-CB-CG |
| 24 | CW | 8 | 2R3 | C-CA-CB-OB |
| 24 | CW | 8 | 2R3 | C-CA-CB-CG |
| 24 | CW | 5 | MVA | N-CA-CB-CG1 |
| 24 | CW | 5 | MVA | N-CA-CB-CG2 |
| 24 | CW | 5 | MVA | C-CA-CB-CG1 |
| 24 | CW | 5 | MVA | C-CA-CB-CG2 |
| 24 | AW | 9 | MVA | N-CA-CB-CG1 |
| 24 | AW | 9 | MVA | N-CA-CB-CG2 |
| 24 | AW | 9 | MVA | C-CA-CB-CG1 |
| 24 | AW | 9 | MVA | C-CA-CB-CG2 |
| 24 | AW | 1 | 2QZ | N-CA-CB-OG1 |
| 24 | AW | 1 | 2QZ | N-CA-CB-CG2 |
| 24 | AW | 1 | 2QZ | C-CA-CB-OG1 |
| 24 | CW | 9 | MVA | N-CA-CB-CG1 |
| 24 | CW | 9 | MVA | N-CA-CB-CG2 |
| 24 | CW | 9 | MVA | C-CA-CB-CG1 |
| 24 | CW | 9 | MVA | C-CA-CB-CG2 |
| 24 | AW | 10 | 2QY | O-C-CA-CB |
| 24 | AW | 8 | 2R3 | N-CA-CB-OB |
| 24 | AW | 8 | 2R3 | N-CA-CB-CG |
| 24 | AW | 8 | 2R3 | C-CA-CB-OB |
| 24 | AW | 8 | 2R3 | C-CA-CB-CG |
| 24 | AW | 5 | MVA | CB-CA-N-CN |
| 24 | AW | 5 | MVA | C-CA-CB-CG1 |
| 24 | AW | 5 | MVA | C-CA-CB-CG2 |
| 24 | CW | 1 | 2QZ | N-CA-CB-OG1 |
| 24 | CW | 10 | 2QY | O-C-CA-CB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 24 | AW | 10 | 2QY | CA-CB-CG-CD2 |
| 24 | AW | 10 | 2QY | CA-CB-CG-CD1 |
| 24 | CW | 8 | 2R3 | CE2-CZ-OH-CO |
| 24 | CW | 8 | 2R3 | CE1-CZ-OH-CO |
| 24 | AW | 6 | 2R1 | CG1-CB-CG2-OD2 |
| 24 | CW | 5 | MVA | CB-CA-N-CN |
| 24 | AW | 9 | MVA | CB-CA-N-CN |
| 24 | CW | 9 | MVA | CB-CA-N-CN |
| 24 | CW | 5 | MVA | O-C-CA-CB |
| 24 | CW | 10 | 2QY | CA-CB-CG-CD1 |
| 24 | CW | 1 | 2QZ | C-CA-CB-OG1 |
| 24 | CW | 8 | 2R3 | O-C-CA-CB |

There are no ring outliers.

13 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | CW | 8 | 2R3 | 2 | 0 |
| 24 | CW | 5 | MVA | 2 | 0 |
| 24 | AW | 9 | MVA | 3 | 0 |
| 24 | AW | 1 | 2QZ | 2 | 0 |
| 24 | CW | 9 | MVA | 6 | 0 |
| 24 | AW | 10 | 2QY | 5 | 0 |
| 24 | AW | 6 | 2R1 | 1 | 0 |
| 24 | AW | 8 | 2R3 | 1 | 0 |
| 24 | CW | 1 | 2QZ | 2 | 0 |
| 24 | CW | 3 | 004 | 1 | 0 |
| 24 | CW | 6 | 2R1 | 1 | 0 |
| 24 | CW | 10 | 2QY | 9 | 0 |
| 24 | AW | 3 | 004 | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1991 ligands modelled in this entry, 1987 are monoatomic - leaving 4 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 | $\# Z > 2$ |
| 57 | SF4 | CD | 501 | 4 | 0,12,12 | 0.00 | - | - | | |
| 59 | FME | CX | 101 | 23 | 8,9,10 | 1.05 | 1 (12%) | 7,9,11 | 1.32 | 2 (28%) |
| 57 | SF4 | AD | 501 | 4 | 0,12,12 | 0.00 | - | - | | |
| 59 | FME | AX | 101 | 23 | 8,9,10 | 0.93 | 0 | 7,9,11 | 1.49 | 1 (14%) |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 57 | SF4 | CD | 501 | 4 | - | - | 0/6/5/5 |
| 59 | FME | CX | 101 | 23 | - | 3/7/9/11 | - |
| 57 | SF4 | AD | 501 | 4 | - | - | 0/6/5/5 |
| 59 | FME | AX | 101 | 23 | - | 3/7/9/11 | - |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 59 | CX | 101 | FME | CA-N | 2.14 | 1.49 | 1.46 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 59 | AX | 101 | FME | CA-N-CN | -2.85 | 118.44 | 122.82 |
| 59 | CX | 101 | FME | CA-N-CN | -2.17 | 119.49 | 122.82 |
| 59 | CX | 101 | FME | C-CA-N | 2.10 | 113.52 | 109.73 |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 59 | CX | 101 | FME | O1-CN-N-CA |
| 59 | CX | 101 | FME | O-C-CA-CB |
| 59 | AX | 101 | FME | O1-CN-N-CA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 59 | AX | 101 | FME | O-C-CA-CB |
| 59 | CX | 101 | FME | CA-CB-CG-SD |
| 59 | AX | 101 | FME | CB-CA-N-CN |

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 57 | CD | 501 | SF4 | 1 | 0 |
| 59 | CX | 101 | FME | 2 | 0 |
| 57 | AD | 501 | SF4 | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1498/1522 (98%) | -0.17 | 32 (2%) 63 43 | 36, 80, 103, 123 | 0 |
| 1 | CA | 1503/1522 (98%) | -0.18 | 34 (2%) 60 39 | 38, 80, 103, 122 | 0 |
| 2 | AB | 231/256 (90%) | -0.07 | 8 (3%) 44 23 | 71, 88, 98, 107 | 0 |
| 2 | CB | 231/256 (90%) | 0.20 | 12 (5%) 27 12 | 71, 89, 99, 108 | 0 |
| 3 | AC | 206/239 (86%) | 0.18 | 6 (2%) 51 28 | 74, 87, 96, 108 | 0 |
| 3 | CC | 206/239 (86%) | 0.33 | 13 (6%) 20 8 | 75, 89, 98, 106 | 0 |
| 4 | AD | 208/209 (99%) | 0.06 | 4 (1%) 66 46 | 62, 80, 92, 99 | 0 |
| 4 | CD | 208/209 (99%) | -0.15 | 0 100 100 | 61, 79, 92, 99 | 0 |
| 5 | AE | 148/162 (91%) | -0.25 | 0 100 100 | 53, 73, 83, 96 | 0 |
| 5 | CE | 148/162 (91%) | -0.22 | 0 100 100 | 54, 74, 85, 98 | 0 |
| 6 | AF | 100/101 (99%) | -0.22 | 0 100 100 | 60, 78, 89, 92 | 0 |
| 6 | CF | 100/101 (99%) | -0.32 | 0 100 100 | 62, 79, 89, 94 | 0 |
| 7 | AG | 155/156 (99%) | 0.29 | 11 (7%) 16 6 | 74, 85, 97, 104 | 0 |
| 7 | CG | 155/156 (99%) | 0.36 | 10 (6%) 18 8 | 76, 86, 99, 105 | 0 |
| 8 | AH | 137/138 (99%) | -0.08 | 0 100 100 | 60, 75, 83, 90 | 0 |
| 8 | CH | 137/138 (99%) | -0.15 | 0 100 100 | 61, 76, 83, 90 | 0 |
| 9 | AI | 127/128 (99%) | 0.44 | 8 (6%) 20 8 | 70, 92, 99, 103 | 0 |
| 9 | CI | 127/128 (99%) | 0.98 | 22 (17%) 1 0 | 69, 93, 100, 105 | 0 |
| 10 | AJ | 97/105 (92%) | 0.66 | 12 (12%) 4 1 | 71, 93, 101, 106 | 0 |
| 10 | CJ | 96/105 (91%) | 0.68 | 12 (12%) 3 1 | 75, 95, 102, 107 | 0 |
| 11 | AK | 114/129 (88%) | -0.24 | 0 100 100 | 53, 74, 88, 93 | 0 |
| 11 | CK | 114/129 (88%) | -0.02 | 3 (2%) 56 33 | 54, 76, 88, 93 | 0 |
| 12 | AL | 122/132 (92%) | -0.18 | 1 (0%) 86 72 | 56, 68, 80, 86 | 0 |
| 12 | CL | 122/132 (92%) | -0.19 | 0 100 100 | 55, 68, 79, 87 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AM | 123/126 (97%) | 0.29 | 9 (7%) 15 6 | 67, 83, 95, 104 | 0 |
| 13 | CM | 122/126 (96%) | 0.58 | 11 (9%) 9 3 | 77, 91, 101, 105 | 0 |
| 14 | AN | 60/61 (98%) | 0.17 | 2 (3%) 46 24 | 74, 85, 95, 97 | 0 |
| 14 | CN | 60/61 (98%) | 0.56 | 4 (6%) 17 7 | 77, 88, 95, 100 | 0 |
| 15 | AO | 88/89 (98%) | -0.23 | 0 100 100 | 59, 73, 87, 94 | 0 |
| 15 | CO | 88/89 (98%) | 0.04 | 1 (1%) 80 64 | 58, 73, 87, 95 | 0 |
| 16 | AP | 82/88 (93%) | 0.41 | 2 (2%) 59 37 | 66, 77, 88, 95 | 0 |
| 16 | CP | 82/88 (93%) | -0.01 | 0 100 100 | 66, 76, 89, 93 | 0 |
| 17 | AQ | 99/105 (94%) | 0.02 | 0 100 100 | 59, 73, 84, 87 | 0 |
| 17 | CQ | 99/105 (94%) | -0.07 | 1 (1%) 82 67 | 60, 73, 84, 85 | 0 |
| 18 | AR | 68/88 (77%) | 0.16 | 1 (1%) 73 54 | 66, 76, 86, 90 | 0 |
| 18 | CR | 68/88 (77%) | 0.39 | 0 100 100 | 67, 77, 87, 89 | 0 |
| 19 | AS | 83/93 (89%) | 0.79 | 11 (13%) 3 1 | 79, 91, 100, 105 | 0 |
| 19 | CS | 83/93 (89%) | 1.23 | 16 (19%) 1 0 | 82, 92, 102, 106 | 0 |
| 20 | AT | 96/106 (90%) | 0.07 | 0 100 100 | 62, 75, 88, 91 | 0 |
| 20 | CT | 96/106 (90%) | 0.09 | 1 (1%) 82 67 | 62, 75, 86, 94 | 0 |
| 21 | AU | 23/27 (85%) | 1.22 | 5 (21%) 0 0 | 76, 87, 90, 91 | 0 |
| 21 | CU | 23/27 (85%) | 1.16 | 5 (21%) 0 0 | 77, 87, 91, 92 | 0 |
| 22 | AV | 7/24 (29%) | 0.02 | 0 100 100 | 61, 73, 97, 100 | 0 |
| 22 | CV | 6/24 (25%) | 0.36 | 0 100 100 | 64, 75, 94, 103 | 0 |
| 23 | AX | 76/77 (98%) | 0.02 | 0 100 100 | 48, 79, 96, 101 | 0 |
| 23 | CX | 76/77 (98%) | 0.02 | 0 100 100 | 47, 81, 98, 101 | 0 |
| 24 | AW | 3/10 (30%) | -0.00 | 0 100 100 | 78, 78, 93, 96 | 0 |
| 24 | CW | 3/10 (30%) | 0.56 | 1 (33%) 0 0 | 67, 67, 87, 96 | 0 |
| 25 | BA | 2731/2915 (93%) | -0.28 | 11 (0%) 92 84 | 24, 44, 86, 114 | 0 |
| 25 | DA | 2714/2915 (93%) | -0.49 | 18 (0%) 87 75 | 27, 48, 87, 118 | 0 |
| 26 | BB | 120/122 (98%) | -0.40 | 0 100 100 | 41, 68, 81, 96 | 0 |
| 26 | DB | 120/122 (98%) | -0.33 | 0 100 100 | 47, 73, 86, 98 | 0 |
| 27 | BD | 275/276 (99%) | -0.47 | 1 (0%) 92 84 | 24, 41, 62, 85 | 0 |
| 27 | DD | 275/276 (99%) | -0.47 | 0 100 100 | 25, 44, 63, 86 | 0 |
| 28 | BE | 204/206 (99%) | -0.35 | 0 100 100 | 22, 45, 68, 90 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28 | DE | 204/206 (99%) | -0.45 | 0 100 100 | 24, 47, 70, 90 | 0 |
| 29 | BF | 203/210 (96%) | -0.33 | 0 100 100 | 24, 53, 77, 97 | 0 |
| 29 | DF | 203/210 (96%) | -0.45 | 0 100 100 | 25, 56, 79, 96 | 0 |
| 30 | BG | 181/182 (99%) | -0.30 | 2 (1%) 80 64 | 61, 76, 89, 100 | 0 |
| 30 | DG | 181/182 (99%) | 0.09 | 5 (2%) 53 30 | 65, 79, 91, 100 | 0 |
| 31 | BH | 174/180 (96%) | -0.32 | 0 100 100 | 49, 67, 81, 85 | 0 |
| 31 | DH | 174/180 (96%) | 0.52 | 17 (9%) 7 2 | 54, 72, 85, 89 | 0 |
| 32 | BI | 146/148 (98%) | -0.16 | 0 100 100 | 49, 77, 88, 94 | 0 |
| 32 | DI | 146/148 (98%) | 0.14 | 5 (3%) 45 24 | 49, 78, 88, 94 | 0 |
| 33 | BN | 140/140 (100%) | -0.37 | 0 100 100 | 33, 48, 71, 78 | 0 |
| 33 | DN | 140/140 (100%) | -0.42 | 0 100 100 | 35, 52, 73, 81 | 0 |
| 34 | BO | 122/122 (100%) | -0.50 | 0 100 100 | 23, 40, 61, 76 | 0 |
| 34 | DO | 122/122 (100%) | -0.47 | 0 100 100 | 37, 53, 71, 80 | 0 |
| 35 | BP | 149/150 (99%) | -0.32 | 0 100 100 | 25, 54, 77, 83 | 0 |
| 35 | DP | 149/150 (99%) | -0.07 | 1 (0%) 87 75 | 27, 57, 81, 87 | 0 |
| 36 | BQ | 141/141 (100%) | -0.33 | 0 100 100 | 36, 52, 68, 79 | 0 |
| 36 | DQ | 141/141 (100%) | -0.45 | 0 100 100 | 38, 55, 71, 81 | 0 |
| 37 | BR | 118/118 (100%) | -0.50 | 0 100 100 | 20, 35, 52, 64 | 0 |
| 37 | DR | 118/118 (100%) | -0.40 | 0 100 100 | 36, 52, 68, 84 | 0 |
| 38 | BS | 110/112 (98%) | -0.43 | 0 100 100 | 35, 54, 71, 85 | 0 |
| 38 | DS | 110/112 (98%) | 0.27 | 5 (4%) 33 16 | 65, 81, 92, 95 | 0 |
| 39 | BT | 131/146 (89%) | -0.48 | 0 100 100 | 31, 45, 75, 92 | 0 |
| 39 | DT | 131/146 (89%) | -0.45 | 0 100 100 | 45, 59, 80, 90 | 0 |
| 40 | BU | 116/118 (98%) | -0.64 | 0 100 100 | 21, 31, 52, 63 | 0 |
| 40 | DU | 116/118 (98%) | -0.34 | 1 (0%) 84 69 | 36, 61, 78, 92 | 0 |
| 41 | BV | 101/101 (100%) | -0.42 | 0 100 100 | 27, 53, 73, 80 | 0 |
| 41 | DV | 101/101 (100%) | -0.19 | 0 100 100 | 29, 58, 78, 80 | 0 |
| 42 | BW | 112/113 (99%) | -0.43 | 0 100 100 | 27, 38, 62, 92 | 0 |
| 42 | DW | 112/113 (99%) | -0.25 | 0 100 100 | 30, 42, 64, 94 | 0 |
| 43 | BX | 95/96 (98%) | -0.37 | 0 100 100 | 29, 47, 72, 81 | 0 |
| 43 | DX | 95/96 (98%) | -0.29 | 2 (2%) 63 43 | 33, 51, 73, 82 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | BY | 107/110 (97%) | -0.19 | 2 (1%) 66 46 | 39, 61, 80, 89 | 0 |
| 44 | DY | 107/110 (97%) | 0.29 | 4 (3%) 41 21 | 43, 65, 82, 92 | 0 |
| 45 | BZ | 171/206 (83%) | -0.39 | 0 100 100 | 53, 71, 85, 96 | 0 |
| 45 | DZ | 174/206 (84%) | -0.07 | 0 100 100 | 58, 74, 87, 95 | 0 |
| 46 | B0 | 83/85 (97%) | -0.08 | 7 (8%) 11 4 | 25, 39, 80, 108 | 0 |
| 46 | D0 | 83/85 (97%) | 0.42 | 10 (12%) 4 2 | 42, 66, 86, 104 | 0 |
| 47 | B1 | 97/98 (98%) | -0.27 | 1 (1%) 82 67 | 27, 44, 74, 83 | 0 |
| 47 | D1 | 97/98 (98%) | -0.23 | 1 (1%) 82 67 | 35, 58, 79, 86 | 0 |
| 48 | B2 | 70/72 (97%) | -0.54 | 0 100 100 | 35, 48, 64, 90 | 0 |
| 48 | D2 | 70/72 (97%) | -0.26 | 0 100 100 | 59, 74, 83, 92 | 0 |
| 49 | B3 | 59/60 (98%) | -0.36 | 0 100 100 | 24, 38, 63, 85 | 0 |
| 49 | D3 | 59/60 (98%) | 0.19 | 1 (1%) 70 49 | 45, 62, 80, 90 | 0 |
| 50 | B4 | 69/71 (97%) | -0.18 | 1 (1%) 75 56 | 60, 85, 103, 105 | 0 |
| 50 | D4 | 69/71 (97%) | 0.38 | 5 (7%) 15 6 | 82, 96, 106, 112 | 0 |
| 51 | B5 | 59/60 (98%) | -0.61 | 0 100 100 | 14, 36, 59, 74 | 0 |
| 51 | D5 | 59/60 (98%) | -0.54 | 0 100 100 | 31, 50, 72, 82 | 0 |
| 52 | B6 | 53/54 (98%) | -0.27 | 0 100 100 | 43, 53, 68, 75 | 0 |
| 52 | D6 | 53/54 (98%) | -0.25 | 0 100 100 | 45, 56, 69, 73 | 0 |
| 53 | B7 | 48/49 (97%) | -0.30 | 0 100 100 | 24, 32, 62, 84 | 0 |
| 53 | D7 | 48/49 (97%) | -0.15 | 1 (2%) 63 43 | 26, 35, 63, 86 | 0 |
| 54 | B8 | 64/65 (98%) | -0.30 | 0 100 100 | 31, 42, 51, 64 | 0 |
| 54 | D8 | 64/65 (98%) | -0.30 | 0 100 100 | 34, 46, 56, 66 | 0 |
| 55 | B9 | 37/37 (100%) | 0.06 | 0 100 100 | 43, 53, 71, 77 | 0 |
| 55 | D9 | 37/37 (100%) | 0.62 | 3 (8%) 12 5 | 46, 58, 73, 78 | 0 |
| All | All | 20462/21468 (95%) | -0.18 | 362 (1%) 68 47 | 14, 65, 95, 123 | 0 |

All (362) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13 | CM | 124 | PRO | 15.2 |
| 13 | CM | 123 | ALA | 12.7 |
| 13 | AM | 124 | PRO | 9.7 |
| 13 | AM | 123 | ALA | 9.5 |
| 46 | B0 | 3 | HIS | 8.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | CM | 122 | LYS | 7.7 |
| 7 | CG | 78 | ARG | 6.6 |
| 1 | CA | 1030(B) | C | 6.5 |
| 46 | D0 | 3 | HIS | 5.9 |
| 3 | CC | 159 | GLY | 5.9 |
| 19 | CS | 49 | ILE | 5.8 |
| 9 | CI | 30 | GLY | 5.4 |
| 9 | CI | 36 | TYR | 5.4 |
| 13 | CM | 121 | LYS | 5.3 |
| 1 | AA | 1000 | U | 5.3 |
| 13 | AM | 122 | LYS | 5.2 |
| 3 | CC | 155 | GLY | 5.2 |
| 46 | B0 | 7 | LEU | 5.1 |
| 7 | AG | 78 | ARG | 4.9 |
| 1 | AA | 1030(B) | C | 4.8 |
| 7 | CG | 79 | ARG | 4.8 |
| 7 | AG | 79 | ARG | 4.7 |
| 1 | CA | 1001(A) | G | 4.7 |
| 25 | DA | 229 | A | 4.7 |
| 46 | B0 | 6 | GLY | 4.6 |
| 1 | CA | 1532 | U | 4.6 |
| 7 | AG | 156 | TRP | 4.6 |
| 1 | AA | 1036 | G | 4.5 |
| 40 | DU | 117 | GLN | 4.5 |
| 7 | CG | 156 | TRP | 4.5 |
| 13 | CM | 120 | LYS | 4.5 |
| 1 | AA | 1001 | A | 4.5 |
| 10 | CJ | 6 | ILE | 4.3 |
| 1 | CA | 1026 | G | 4.3 |
| 46 | D0 | 8 | GLY | 4.2 |
| 7 | AG | 153 | HIS | 4.1 |
| 1 | AA | 202 | U | 4.1 |
| 2 | CB | 232 | PRO | 4.1 |
| 1 | AA | 1001(A) | G | 4.1 |
| 9 | CI | 7 | THR | 4.0 |
| 19 | CS | 38 | SER | 4.0 |
| 46 | B0 | 5 | LYS | 4.0 |
| 25 | DA | 2802 | G | 4.0 |
| 3 | CC | 160 | ALA | 4.0 |
| 50 | D4 | 68 | ARG | 4.0 |
| 1 | AA | 1030(C) | G | 3.9 |
| 13 | AM | 121 | LYS | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 46 | D0 | 2 | ALA | 3.9 |
| 9 | CI | 62 | TYR | 3.8 |
| 46 | D0 | 6 | GLY | 3.8 |
| 31 | DH | 112 | PRO | 3.8 |
| 1 | AA | 1028 | C | 3.8 |
| 3 | AC | 206 | GLU | 3.8 |
| 7 | CG | 2 | ALA | 3.8 |
| 1 | CA | 1002 | G | 3.8 |
| 1 | CA | 1030(C) | G | 3.8 |
| 31 | DH | 2 | SER | 3.8 |
| 10 | AJ | 35 | SER | 3.8 |
| 19 | AS | 39 | THR | 3.7 |
| 9 | CI | 9 | ARG | 3.7 |
| 13 | CM | 119 | GLY | 3.7 |
| 25 | BA | 1555 | C | 3.7 |
| 46 | D0 | 76 | GLY | 3.6 |
| 1 | AA | 1002 | G | 3.6 |
| 46 | B0 | 8 | GLY | 3.6 |
| 1 | CA | 1001 | A | 3.6 |
| 19 | CS | 48 | THR | 3.6 |
| 1 | CA | 1034 | G | 3.6 |
| 7 | AG | 85 | TYR | 3.6 |
| 25 | DA | 2793 | G | 3.6 |
| 7 | CG | 84 | ASN | 3.5 |
| 1 | CA | 1036 | G | 3.5 |
| 10 | CJ | 20 | ALA | 3.5 |
| 7 | AG | 77 | SER | 3.5 |
| 31 | DH | 103 | LEU | 3.5 |
| 1 | CA | 1035 | A | 3.5 |
| 46 | D0 | 5 | LYS | 3.5 |
| 55 | D9 | 12 | ASP | 3.5 |
| 10 | AJ | 6 | ILE | 3.4 |
| 47 | D1 | 2 | SER | 3.4 |
| 31 | DH | 111 | HIS | 3.4 |
| 1 | CA | 1030(A) | G | 3.4 |
| 1 | AA | 1026 | G | 3.4 |
| 2 | AB | 228 | GLY | 3.4 |
| 2 | CB | 135 | GLN | 3.4 |
| 7 | CG | 82 | GLY | 3.4 |
| 19 | AS | 38 | SER | 3.3 |
| 1 | AA | 1037 | C | 3.3 |
| 10 | AJ | 5 | ARG | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | AA | 1044 | A | 3.3 |
| 21 | AU | 18 | TYR | 3.3 |
| 25 | DA | 652(B) | A | 3.2 |
| 7 | CG | 4 | ARG | 3.2 |
| 43 | DX | 68 | ARG | 3.2 |
| 10 | CJ | 85 | LEU | 3.2 |
| 7 | CG | 77 | SER | 3.2 |
| 31 | DH | 102 | ALA | 3.2 |
| 2 | AB | 133 | LYS | 3.2 |
| 31 | DH | 115 | VAL | 3.2 |
| 25 | BA | 2815 | C | 3.2 |
| 4 | AD | 179 | GLU | 3.1 |
| 3 | AC | 87 | LEU | 3.1 |
| 10 | CJ | 89 | ASP | 3.1 |
| 9 | CI | 66 | ARG | 3.1 |
| 1 | CA | 1531 | A | 3.1 |
| 46 | D0 | 7 | LEU | 3.1 |
| 1 | AA | 1030 | C | 3.1 |
| 10 | AJ | 98 | ILE | 3.1 |
| 3 | AC | 193 | TYR | 3.1 |
| 30 | DG | 2 | PRO | 3.1 |
| 9 | AI | 33 | PHE | 3.1 |
| 53 | D7 | 48 | LYS | 3.1 |
| 11 | CK | 13 | GLN | 3.0 |
| 55 | D9 | 13 | LYS | 3.0 |
| 31 | DH | 82 | GLY | 3.0 |
| 31 | DH | 43 | VAL | 3.0 |
| 19 | AS | 72 | GLY | 3.0 |
| 25 | DA | 2803 | C | 3.0 |
| 9 | AI | 15 | ALA | 3.0 |
| 1 | AA | 204 | U | 3.0 |
| 38 | DS | 35 | ILE | 3.0 |
| 1 | AA | 1029 | C | 3.0 |
| 25 | BA | 935 | C | 3.0 |
| 10 | AJ | 7 | LYS | 3.0 |
| 14 | AN | 17 | LYS | 2.9 |
| 1 | AA | 999 | C | 2.9 |
| 25 | BA | 2814 | C | 2.9 |
| 25 | DA | 1509 | C | 2.9 |
| 19 | AS | 50 | ALA | 2.9 |
| 1 | AA | 201 | C | 2.9 |
| 3 | AC | 160 | ALA | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 20 | CT | 9 | ASN | 2.9 |
| 44 | BY | 1 | MET | 2.9 |
| 25 | BA | 2816 | G | 2.9 |
| 19 | CS | 47 | HIS | 2.9 |
| 7 | AG | 80 | VAL | 2.8 |
| 21 | CU | 24 | ARG | 2.8 |
| 3 | CC | 154 | SER | 2.8 |
| 25 | BA | 2807 | C | 2.8 |
| 4 | AD | 180 | GLY | 2.8 |
| 25 | BA | 1221 | G | 2.8 |
| 46 | B0 | 4 | LYS | 2.8 |
| 31 | DH | 113 | VAL | 2.8 |
| 7 | AG | 84 | ASN | 2.8 |
| 19 | CS | 12 | ASP | 2.8 |
| 21 | CU | 14 | TRP | 2.7 |
| 9 | CI | 37 | PHE | 2.7 |
| 31 | DH | 105 | LEU | 2.7 |
| 1 | CA | 1037 | C | 2.7 |
| 3 | CC | 193 | TYR | 2.7 |
| 13 | CM | 102 | ARG | 2.7 |
| 9 | CI | 15 | ALA | 2.7 |
| 1 | CA | 1040 | U | 2.7 |
| 19 | CS | 69 | HIS | 2.7 |
| 1 | CA | 1286 | A | 2.7 |
| 1 | AA | 1030(A) | G | 2.7 |
| 7 | CG | 154 | TYR | 2.7 |
| 19 | AS | 59 | PRO | 2.7 |
| 21 | AU | 11 | GLY | 2.7 |
| 44 | DY | 58 | GLY | 2.7 |
| 2 | CB | 132 | LYS | 2.6 |
| 46 | B0 | 2 | ALA | 2.7 |
| 10 | AJ | 73 | ASP | 2.6 |
| 3 | AC | 192 | THR | 2.6 |
| 30 | BG | 75 | LYS | 2.6 |
| 19 | AS | 71 | LEU | 2.6 |
| 1 | CA | 1023 | G | 2.6 |
| 50 | D4 | 52 | THR | 2.6 |
| 9 | CI | 21 | PRO | 2.6 |
| 14 | CN | 17 | LYS | 2.6 |
| 43 | DX | 92 | LEU | 2.6 |
| 14 | CN | 8 | GLU | 2.6 |
| 1 | AA | 1007 | C | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 1 | CA | 1041 | A | 2.6 |
| 25 | BA | 2806 | G | 2.6 |
| 10 | CJ | 21 | GLN | 2.6 |
| 25 | DA | 2801(A) | A | 2.6 |
| 1 | CA | 1027 | C | 2.6 |
| 1 | CA | 1042 | G | 2.5 |
| 9 | CI | 128 | ARG | 2.5 |
| 30 | DG | 75 | LYS | 2.5 |
| 7 | AG | 16 | LEU | 2.5 |
| 2 | CB | 133 | LYS | 2.5 |
| 3 | CC | 190 | ARG | 2.5 |
| 32 | DI | 12 | LEU | 2.5 |
| 19 | CS | 75 | ALA | 2.5 |
| 13 | AM | 97 | PRO | 2.5 |
| 49 | D3 | 60 | GLU | 2.5 |
| 10 | CJ | 26 | ALA | 2.5 |
| 25 | DA | 2792 | G | 2.5 |
| 50 | B4 | 66 | SER | 2.5 |
| 50 | D4 | 69 | LYS | 2.5 |
| 9 | AI | 62 | TYR | 2.5 |
| 44 | DY | 59 | GLY | 2.5 |
| 1 | CA | 1257 | U | 2.5 |
| 9 | AI | 47 | LEU | 2.5 |
| 25 | DA | 888 | C | 2.5 |
| 1 | CA | 1003 | G | 2.5 |
| 14 | CN | 2 | ALA | 2.5 |
| 31 | DH | 107 | VAL | 2.5 |
| 9 | CI | 29 | ASN | 2.5 |
| 13 | CM | 110 | ARG | 2.5 |
| 1 | AA | 1027 | C | 2.5 |
| 10 | AJ | 71 | LEU | 2.5 |
| 44 | DY | 88 | LYS | 2.5 |
| 1 | CA | 1024 | G | 2.5 |
| 10 | AJ | 34 | VAL | 2.4 |
| 31 | DH | 169 | VAL | 2.4 |
| 9 | CI | 35 | GLU | 2.4 |
| 1 | AA | 1023 | G | 2.4 |
| 10 | AJ | 36 | GLY | 2.4 |
| 25 | DA | 2805 | G | 2.4 |
| 32 | DI | 13 | GLY | 2.4 |
| 25 | DA | 2188 | C | 2.4 |
| 1 | CA | 1030(D) | A | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | AI | 37 | PHE | 2.4 |
| 10 | AJ | 72 | VAL | 2.4 |
| 10 | CJ | 40 | LEU | 2.4 |
| 1 | CA | 80 | G | 2.4 |
| 1 | AA | 1041 | A | 2.4 |
| 9 | CI | 10 | ARG | 2.4 |
| 55 | D9 | 16 | VAL | 2.4 |
| 19 | AS | 40 | ILE | 2.4 |
| 25 | BA | 696 | C | 2.4 |
| 7 | AG | 154 | TYR | 2.4 |
| 1 | AA | 1024 | G | 2.4 |
| 31 | DH | 116 | GLU | 2.4 |
| 2 | CB | 115 | LEU | 2.4 |
| 10 | AJ | 8 | LEU | 2.4 |
| 13 | AM | 119 | GLY | 2.4 |
| 31 | DH | 94 | TYR | 2.4 |
| 19 | CS | 9 | VAL | 2.4 |
| 2 | AB | 122 | PHE | 2.4 |
| 10 | CJ | 65 | LEU | 2.4 |
| 44 | DY | 5 | MET | 2.4 |
| 3 | CC | 191 | THR | 2.4 |
| 32 | DI | 11 | ASN | 2.4 |
| 1 | AA | 1031 | G | 2.4 |
| 3 | CC | 177 | THR | 2.4 |
| 2 | CB | 134 | GLU | 2.3 |
| 17 | CQ | 100 | LYS | 2.3 |
| 10 | CJ | 5 | ARG | 2.3 |
| 2 | CB | 137 | ARG | 2.3 |
| 25 | DA | 2807 | G | 2.3 |
| 10 | CJ | 27 | ALA | 2.3 |
| 1 | CA | 1029 | C | 2.3 |
| 19 | AS | 60 | VAL | 2.3 |
| 4 | AD | 152 | SER | 2.3 |
| 19 | CS | 35 | SER | 2.3 |
| 25 | DA | 2794 | C | 2.3 |
| 19 | CS | 13 | ASP | 2.3 |
| 30 | BG | 49 | ASP | 2.3 |
| 15 | CO | 6 | GLU | 2.3 |
| 21 | CU | 6 | ARG | 2.3 |
| 25 | DA | 2896 | C | 2.3 |
| 9 | CI | 28 | VAL | 2.3 |
| 9 | CI | 33 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | CC | 206 | GLU | 2.3 |
| 19 | CS | 43 | GLU | 2.3 |
| 2 | CB | 48 | MET | 2.3 |
| 38 | DS | 33 | LYS | 2.3 |
| 1 | CA | 1030 | C | 2.3 |
| 2 | CB | 122 | PHE | 2.3 |
| 3 | CC | 189 | ALA | 2.3 |
| 9 | AI | 36 | TYR | 2.3 |
| 25 | DA | 2897 | U | 2.3 |
| 21 | AU | 17 | THR | 2.3 |
| 30 | DG | 76 | SER | 2.3 |
| 12 | AL | 99 | HIS | 2.3 |
| 19 | AS | 56 | GLN | 2.3 |
| 3 | CC | 64 | VAL | 2.3 |
| 1 | CA | 1031 | G | 2.3 |
| 10 | CJ | 38 | ILE | 2.3 |
| 13 | AM | 120 | LYS | 2.3 |
| 2 | AB | 227 | GLY | 2.3 |
| 9 | CI | 27 | THR | 2.3 |
| 30 | DG | 136 | ARG | 2.3 |
| 1 | AA | 1531 | A | 2.3 |
| 9 | CI | 5 | TYR | 2.3 |
| 11 | CK | 31 | THR | 2.2 |
| 1 | AA | 1137 | C | 2.2 |
| 25 | DA | 2894 | G | 2.2 |
| 16 | AP | 7 | ALA | 2.2 |
| 16 | AP | 19 | ILE | 2.2 |
| 32 | DI | 86 | THR | 2.2 |
| 1 | AA | 1034 | G | 2.2 |
| 1 | CA | 1033 | G | 2.2 |
| 38 | DS | 52 | SER | 2.2 |
| 19 | CS | 44 | MET | 2.2 |
| 3 | AC | 100 | ALA | 2.2 |
| 31 | DH | 106 | THR | 2.2 |
| 38 | DS | 58 | LEU | 2.2 |
| 14 | CN | 25 | VAL | 2.2 |
| 9 | CI | 127 | LYS | 2.2 |
| 1 | AA | 1257 | U | 2.2 |
| 10 | CJ | 72 | VAL | 2.2 |
| 1 | AA | 1039 | C | 2.2 |
| 3 | CC | 158 | GLY | 2.2 |
| 19 | AS | 30 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 19 | CS | 53 | ASN | 2.2 |
| 32 | DI | 77 | LEU | 2.2 |
| 11 | CK | 42 | TRP | 2.2 |
| 50 | D4 | 49 | PHE | 2.2 |
| 10 | AJ | 75 | ILE | 2.2 |
| 31 | DH | 110 | SER | 2.2 |
| 21 | AU | 5 | ASP | 2.2 |
| 21 | CU | 8 | THR | 2.2 |
| 1 | CA | 1000 | U | 2.2 |
| 9 | CI | 88 | TYR | 2.2 |
| 13 | AM | 2 | ALA | 2.2 |
| 50 | D4 | 67 | TYR | 2.2 |
| 2 | AB | 135 | GLN | 2.2 |
| 2 | CB | 131 | PRO | 2.2 |
| 19 | CS | 28 | LYS | 2.2 |
| 1 | AA | 1003 | G | 2.2 |
| 25 | DA | 879 | G | 2.2 |
| 7 | AG | 82 | GLY | 2.2 |
| 14 | AN | 15 | LYS | 2.1 |
| 3 | CC | 102 | ASN | 2.1 |
| 27 | BD | 276 | LYS | 2.1 |
| 44 | BY | 63 | LYS | 2.1 |
| 19 | CS | 16 | LEU | 2.1 |
| 2 | AB | 129 | GLU | 2.1 |
| 13 | AM | 96 | LEU | 2.1 |
| 9 | AI | 46 | ALA | 2.1 |
| 9 | AI | 26 | VAL | 2.1 |
| 9 | CI | 6 | GLY | 2.1 |
| 21 | CU | 12 | LYS | 2.1 |
| 9 | CI | 98 | PRO | 2.1 |
| 4 | AD | 175 | SER | 2.1 |
| 31 | DH | 159 | GLU | 2.1 |
| 2 | CB | 113 | HIS | 2.1 |
| 13 | CM | 78 | ILE | 2.1 |
| 1 | CA | 1283 | G | 2.1 |
| 46 | D0 | 9 | SER | 2.1 |
| 1 | AA | 1286 | A | 2.1 |
| 2 | AB | 63 | MET | 2.1 |
| 1 | CA | 1149 | C | 2.1 |
| 38 | DS | 57 | LYS | 2.1 |
| 46 | D0 | 4 | LYS | 2.1 |
| 13 | CM | 6 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | CA | 1493 | A | 2.1 |
| 47 | B1 | 2 | SER | 2.1 |
| 2 | CB | 165 | VAL | 2.1 |
| 24 | CW | 2 | VAL | 2.1 |
| 1 | CA | 1004 | A | 2.1 |
| 18 | AR | 31 | LEU | 2.1 |
| 13 | CM | 92 | HIS | 2.1 |
| 46 | D0 | 77 | ARG | 2.0 |
| 1 | CA | 1038 | C | 2.0 |
| 9 | CI | 123 | PRO | 2.0 |
| 19 | CS | 79 | THR | 2.0 |
| 30 | DG | 122 | PRO | 2.0 |
| 35 | DP | 78 | PRO | 2.0 |
| 19 | AS | 4 | SER | 2.0 |
| 1 | AA | 1038 | C | 2.0 |
| 25 | BA | 2813 | G | 2.0 |
| 2 | AB | 214 | ILE | 2.0 |
| 21 | AU | 2 | GLY | 2.0 |
| 25 | BA | 2805 | G | 2.0 |
| 25 | DA | 652(U) | G | 2.0 |
| 7 | CG | 16 | LEU | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 24 | 004 | AW | 3 | 10/11 | 0.83 | 0.13 | 71,89,99,106 | 0 |
| 24 | 2R1 | AW | 6 | 10/11 | 0.90 | 0.12 | 68,82,98,104 | 0 |
| 24 | 2QY | CW | 10 | 13/14 | 0.91 | 0.14 | 55,69,84,94 | 0 |
| 24 | MVA | CW | 9 | 8/9 | 0.92 | 0.21 | 61,72,80,84 | 0 |
| 24 | MVA | AW | 9 | 8/9 | 0.93 | 0.24 | 65,78,87,91 | 0 |
| 24 | MVA | AW | 5 | 8/9 | 0.93 | 0.19 | 66,87,90,90 | 0 |
| 24 | 2R1 | CW | 6 | 10/11 | 0.94 | 0.11 | 79,86,90,94 | 0 |
| 24 | MVA | CW | 5 | 8/9 | 0.94 | 0.20 | 51,78,86,88 | 0 |
| 24 | 004 | CW | 3 | 10/11 | 0.94 | 0.15 | 60,76,84,86 | 0 |
| 24 | 2QZ | AW | 1 | 9/10 | 0.95 | 0.22 | 58,64,81,82 | 0 |
| 24 | 2QZ | CW | 1 | 9/10 | 0.95 | 0.24 | 57,72,81,93 | 0 |
| 24 | 2R3 | AW | 8 | 14/15 | 0.95 | 0.15 | 54,79,87,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 24 | 2R3 | CW | 8 | 14/15 | 0.96 | 0.11 | 47,70,74,79 | 0 |
| 24 | 2QY | AW | 10 | 13/14 | 0.97 | 0.14 | 55,67,75,79 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3093 | 1/1 | 0.37 | 0.58 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3295 | 1/1 | 0.40 | 0.57 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3094 | 1/1 | 0.40 | 0.86 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3043 | 1/1 | 0.50 | 0.50 | 74,74,74,74 | 0 |
| 56 | MG | CA | 3041 | 1/1 | 0.50 | 0.69 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3247 | 1/1 | 0.51 | 0.96 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3427 | 1/1 | 0.58 | 0.54 | 60,60,60,60 | 0 |
| 56 | MG | CA | 3042 | 1/1 | 0.58 | 0.56 | 85,85,85,85 | 0 |
| 56 | MG | DA | 3464 | 1/1 | 0.60 | 0.56 | 50,50,50,50 | 0 |
| 56 | MG | AA | 3114 | 1/1 | 0.60 | 0.51 | 66,66,66,66 | 0 |
| 56 | MG | AA | 3079 | 1/1 | 0.60 | 1.07 | 74,74,74,74 | 0 |
| 56 | MG | B4 | 3001 | 1/1 | 0.61 | 0.27 | 100,100,100,100 | 0 |
| 56 | MG | AA | 3116 | 1/1 | 0.61 | 0.53 | 52,52,52,52 | 0 |
| 56 | MG | CA | 3053 | 1/1 | 0.62 | 1.19 | 73,73,73,73 | 0 |
| 56 | MG | AA | 3147 | 1/1 | 0.63 | 0.49 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3613 | 1/1 | 0.64 | 0.29 | 76,76,76,76 | 0 |
| 56 | MG | AA | 3087 | 1/1 | 0.64 | 0.36 | 72,72,72,72 | 0 |
| 56 | MG | CA | 3016 | 1/1 | 0.64 | 0.48 | 76,76,76,76 | 0 |
| 56 | MG | AA | 3045 | 1/1 | 0.64 | 0.31 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3028 | 1/1 | 0.65 | 0.46 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3622 | 1/1 | 0.65 | 0.52 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3135 | 1/1 | 0.65 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | AA | 3129 | 1/1 | 0.65 | 0.30 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3162 | 1/1 | 0.66 | 0.13 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3691 | 1/1 | 0.67 | 0.38 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3545 | 1/1 | 0.67 | 0.62 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3068 | 1/1 | 0.67 | 0.33 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3131 | 1/1 | 0.68 | 0.23 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3186 | 1/1 | 0.68 | 0.51 | 53,53,53,53 | 0 |
| 56 | MG | CA | 3025 | 1/1 | 0.69 | 0.18 | 94,94,94,94 | 0 |
| 56 | MG | AA | 3023 | 1/1 | 0.69 | 0.17 | 65,65,65,65 | 0 |
| 56 | MG | DB | 3003 | 1/1 | 0.69 | 0.12 | 63,63,63,63 | 0 |
| 56 | MG | AX | 102 | 1/1 | 0.69 | 0.25 | 74,74,74,74 | 0 |
| 56 | MG | CA | 3038 | 1/1 | 0.69 | 0.46 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3125 | 1/1 | 0.69 | 0.55 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3211 | 1/1 | 0.69 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | CA | 3135 | 1/1 | 0.70 | 0.56 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3103 | 1/1 | 0.70 | 0.78 | 48,48,48,48 | 0 |
| 59 | FME | CX | 101 | 10/11 | 0.70 | 0.57 | 71,82,97,105 | 0 |
| 56 | MG | BA | 3579 | 1/1 | 0.70 | 0.24 | 63,63,63,63 | 0 |
| 56 | MG | AA | 3084 | 1/1 | 0.70 | 0.36 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3235 | 1/1 | 0.71 | 0.28 | 47,47,47,47 | 0 |
| 56 | MG | AA | 3048 | 1/1 | 0.71 | 0.25 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3270 | 1/1 | 0.71 | 0.31 | 50,50,50,50 | 0 |
| 56 | MG | AA | 3044 | 1/1 | 0.71 | 0.22 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3581 | 1/1 | 0.71 | 0.86 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3117 | 1/1 | 0.71 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | AA | 3128 | 1/1 | 0.71 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3223 | 1/1 | 0.71 | 0.26 | 66,66,66,66 | 0 |
| 56 | MG | CA | 3030 | 1/1 | 0.71 | 0.45 | 73,73,73,73 | 0 |
| 56 | MG | CA | 3024 | 1/1 | 0.72 | 0.44 | 65,65,65,65 | 0 |
| 58 | ZN | B4 | 3002 | 1/1 | 0.72 | 0.07 | 165,165,165,165 | 0 |
| 56 | MG | AA | 3037 | 1/1 | 0.72 | 0.41 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3703 | 1/1 | 0.72 | 0.22 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3263 | 1/1 | 0.72 | 0.23 | 79,79,79,79 | 0 |
| 56 | MG | CA | 3067 | 1/1 | 0.73 | 0.30 | 80,80,80,80 | 0 |
| 56 | MG | BF | 307 | 1/1 | 0.73 | 0.40 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3085 | 1/1 | 0.73 | 0.46 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3297 | 1/1 | 0.73 | 1.46 | 53,53,53,53 | 0 |
| 56 | MG | DW | 202 | 1/1 | 0.73 | 0.42 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3065 | 1/1 | 0.73 | 0.44 | 50,50,50,50 | 0 |
| 56 | MG | CA | 3055 | 1/1 | 0.73 | 0.28 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3632 | 1/1 | 0.73 | 0.30 | 57,57,57,57 | 0 |
| 56 | MG | AA | 3065 | 1/1 | 0.73 | 0.27 | 60,60,60,60 | 0 |
| 56 | MG | AA | 3020 | 1/1 | 0.73 | 0.10 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3289 | 1/1 | 0.73 | 0.34 | 60,60,60,60 | 0 |
| 56 | MG | B1 | 3001 | 1/1 | 0.74 | 0.86 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3086 | 1/1 | 0.74 | 0.30 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3287 | 1/1 | 0.74 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3699 | 1/1 | 0.74 | 0.52 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3438 | 1/1 | 0.74 | 0.51 | 70,70,70,70 | 0 |
| 56 | MG | AA | 3006 | 1/1 | 0.74 | 0.08 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3089 | 1/1 | 0.74 | 0.57 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3117 | 1/1 | 0.75 | 0.26 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3011 | 1/1 | 0.75 | 0.38 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3049 | 1/1 | 0.75 | 0.30 | 58,58,58,58 | 0 |
| 56 | MG | CA | 3127 | 1/1 | 0.76 | 0.25 | 79,79,79,79 | 0 |
| 56 | MG | CA | 3033 | 1/1 | 0.76 | 0.19 | 68,68,68,68 | 0 |
| 56 | MG | CX | 103 | 1/1 | 0.76 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3064 | 1/1 | 0.76 | 0.41 | 50,50,50,50 | 0 |
| 56 | MG | AA | 3035 | 1/1 | 0.76 | 0.42 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3410 | 1/1 | 0.76 | 0.22 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3056 | 1/1 | 0.76 | 0.37 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3231 | 1/1 | 0.76 | 0.55 | 38,38,38,38 | 0 |
| 56 | MG | BU | 206 | 1/1 | 0.76 | 0.38 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3228 | 1/1 | 0.76 | 0.25 | 45,45,45,45 | 0 |
| 56 | MG | CA | 3018 | 1/1 | 0.76 | 0.31 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3075 | 1/1 | 0.76 | 0.26 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3123 | 1/1 | 0.76 | 0.23 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3206 | 1/1 | 0.76 | 0.35 | 57,57,57,57 | 0 |
| 56 | MG | AA | 3090 | 1/1 | 0.77 | 0.17 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3587 | 1/1 | 0.77 | 0.14 | 64,64,64,64 | 0 |
| 56 | MG | AX | 108 | 1/1 | 0.77 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3051 | 1/1 | 0.77 | 0.50 | 73,73,73,73 | 0 |
| 56 | MG | AA | 3120 | 1/1 | 0.77 | 0.63 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3098 | 1/1 | 0.78 | 1.25 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3087 | 1/1 | 0.78 | 0.45 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3063 | 1/1 | 0.78 | 0.30 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3241 | 1/1 | 0.78 | 0.38 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3615 | 1/1 | 0.78 | 0.40 | 60,60,60,60 | 0 |
| 56 | MG | AA | 3100 | 1/1 | 0.78 | 0.67 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3096 | 1/1 | 0.78 | 0.28 | 44,44,44,44 | 0 |
| 56 | MG | AA | 3127 | 1/1 | 0.78 | 0.18 | 62,62,62,62 | 0 |
| 56 | MG | AA | 3088 | 1/1 | 0.78 | 0.33 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3160 | 1/1 | 0.78 | 0.65 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3718 | 1/1 | 0.78 | 0.37 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3275 | 1/1 | 0.78 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3071 | 1/1 | 0.79 | 0.29 | 60,60,60,60 | 0 |
| 56 | MG | BB | 3005 | 1/1 | 0.79 | 0.28 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3209 | 1/1 | 0.79 | 0.38 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3113 | 1/1 | 0.79 | 0.28 | 68,68,68,68 | 0 |
| 56 | MG | AA | 3076 | 1/1 | 0.79 | 0.29 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3352 | 1/1 | 0.79 | 0.38 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3089 | 1/1 | 0.79 | 0.39 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3022 | 1/1 | 0.79 | 0.34 | 52,52,52,52 | 0 |
| 56 | MG | CA | 3021 | 1/1 | 0.79 | 0.22 | 53,53,53,53 | 0 |
| 56 | MG | DG | 3001 | 1/1 | 0.79 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | AA | 3089 | 1/1 | 0.80 | 0.43 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3069 | 1/1 | 0.80 | 0.44 | 41,41,41,41 | 0 |
| 56 | MG | DB | 3007 | 1/1 | 0.80 | 0.27 | 45,45,45,45 | 0 |
| 56 | MG | AA | 3118 | 1/1 | 0.80 | 0.32 | 52,52,52,52 | 0 |
| 56 | MG | AA | 3061 | 1/1 | 0.80 | 0.19 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3731 | 1/1 | 0.80 | 0.36 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3454 | 1/1 | 0.80 | 0.31 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3062 | 1/1 | 0.80 | 0.26 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3658 | 1/1 | 0.80 | 0.27 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3314 | 1/1 | 0.80 | 0.19 | 64,64,64,64 | 0 |
| 56 | MG | B0 | 103 | 1/1 | 0.80 | 0.84 | 59,59,59,59 | 0 |
| 56 | MG | CA | 3147 | 1/1 | 0.80 | 0.26 | 66,66,66,66 | 0 |
| 56 | MG | CA | 3138 | 1/1 | 0.80 | 0.24 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3158 | 1/1 | 0.80 | 0.54 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3525 | 1/1 | 0.80 | 0.70 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3293 | 1/1 | 0.80 | 0.27 | 53,53,53,53 | 0 |
| 56 | MG | AA | 3110 | 1/1 | 0.80 | 0.24 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3029 | 1/1 | 0.80 | 0.38 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3113 | 1/1 | 0.80 | 0.57 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3402 | 1/1 | 0.80 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3499 | 1/1 | 0.80 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | CA | 3144 | 1/1 | 0.81 | 0.59 | 63,63,63,63 | 0 |
| 56 | MG | DB | 3001 | 1/1 | 0.81 | 0.25 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3146 | 1/1 | 0.81 | 0.29 | 52,52,52,52 | 0 |
| 56 | MG | AA | 3012 | 1/1 | 0.81 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | AX | 103 | 1/1 | 0.81 | 0.08 | 66,66,66,66 | 0 |
| 56 | MG | BB | 3003 | 1/1 | 0.81 | 0.25 | 43,43,43,43 | 0 |
| 56 | MG | BB | 3004 | 1/1 | 0.81 | 0.26 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3180 | 1/1 | 0.81 | 0.99 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3155 | 1/1 | 0.81 | 0.38 | 57,57,57,57 | 0 |
| 56 | MG | BW | 201 | 1/1 | 0.81 | 0.88 | 53,53,53,53 | 0 |
| 56 | MG | CA | 3172 | 1/1 | 0.81 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3003 | 1/1 | 0.81 | 0.35 | 56,56,56,56 | 0 |
| 56 | MG | CA | 3073 | 1/1 | 0.81 | 0.39 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3370 | 1/1 | 0.81 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | DE | 302 | 1/1 | 0.81 | 0.38 | 44,44,44,44 | 0 |
| 56 | MG | CA | 3123 | 1/1 | 0.81 | 0.14 | 77,77,77,77 | 0 |
| 56 | MG | AA | 3085 | 1/1 | 0.81 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | CE | 3001 | 1/1 | 0.81 | 0.32 | 68,68,68,68 | 0 |
| 56 | MG | AA | 3030 | 1/1 | 0.81 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3492 | 1/1 | 0.81 | 0.37 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3647 | 1/1 | 0.81 | 0.37 | 66,66,66,66 | 0 |
| 56 | MG | CA | 3057 | 1/1 | 0.81 | 0.26 | 49,49,49,49 | 0 |
| 56 | MG | CA | 3060 | 1/1 | 0.81 | 0.37 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3187 | 1/1 | 0.82 | 0.44 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3444 | 1/1 | 0.82 | 0.15 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3677 | 1/1 | 0.82 | 0.27 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3719 | 1/1 | 0.82 | 0.25 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3739 | 1/1 | 0.82 | 0.76 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3157 | 1/1 | 0.82 | 0.39 | 63,63,63,63 | 0 |
| 56 | MG | CA | 3007 | 1/1 | 0.82 | 0.56 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3290 | 1/1 | 0.82 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | AA | 3038 | 1/1 | 0.82 | 0.35 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3452 | 1/1 | 0.82 | 0.26 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3497 | 1/1 | 0.82 | 0.23 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3562 | 1/1 | 0.82 | 0.10 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3024 | 1/1 | 0.82 | 0.36 | 65,65,65,65 | 0 |
| 56 | MG | BD | 311 | 1/1 | 0.82 | 0.54 | 45,45,45,45 | 0 |
| 56 | MG | CA | 3161 | 1/1 | 0.82 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3706 | 1/1 | 0.82 | 0.46 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3244 | 1/1 | 0.82 | 0.47 | 65,65,65,65 | 0 |
| 56 | MG | CA | 3114 | 1/1 | 0.82 | 0.27 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3611 | 1/1 | 0.82 | 0.28 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3402 | 1/1 | 0.82 | 0.25 | 71,71,71,71 | 0 |
| 56 | MG | B2 | 101 | 1/1 | 0.82 | 0.36 | 40,40,40,40 | 0 |
| 56 | MG | CA | 3015 | 1/1 | 0.82 | 0.34 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3189 | 1/1 | 0.82 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3083 | 1/1 | 0.82 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3123 | 1/1 | 0.82 | 0.33 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3736 | 1/1 | 0.82 | 0.24 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3134 | 1/1 | 0.82 | 0.31 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3279 | 1/1 | 0.82 | 0.31 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3242 | 1/1 | 0.82 | 0.36 | 48,48,48,48 | 0 |
| 56 | MG | DQ | 205 | 1/1 | 0.82 | 0.40 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3388 | 1/1 | 0.82 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3367 | 1/1 | 0.83 | 0.26 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3071 | 1/1 | 0.83 | 0.52 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3087 | 1/1 | 0.83 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3140 | 1/1 | 0.83 | 0.34 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3515 | 1/1 | 0.83 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3166 | 1/1 | 0.83 | 0.53 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3318 | 1/1 | 0.83 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3071 | 1/1 | 0.83 | 0.30 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3048 | 1/1 | 0.83 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3279 | 1/1 | 0.83 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3631 | 1/1 | 0.83 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3068 | 1/1 | 0.83 | 0.45 | 54,54,54,54 | 0 |
| 56 | MG | BZ | 3001 | 1/1 | 0.83 | 0.28 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3163 | 1/1 | 0.83 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | AA | 3022 | 1/1 | 0.83 | 0.27 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3496 | 1/1 | 0.83 | 0.40 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3152 | 1/1 | 0.83 | 0.33 | 46,46,46,46 | 0 |
| 56 | MG | CA | 3003 | 1/1 | 0.83 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3334 | 1/1 | 0.83 | 0.30 | 73,73,73,73 | 0 |
| 56 | MG | CA | 3032 | 1/1 | 0.83 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3598 | 1/1 | 0.83 | 0.30 | 66,66,66,66 | 0 |
| 56 | MG | CA | 3139 | 1/1 | 0.83 | 0.27 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3164 | 1/1 | 0.83 | 0.72 | 56,56,56,56 | 0 |
| 56 | MG | CA | 3035 | 1/1 | 0.83 | 0.23 | 52,52,52,52 | 0 |
| 56 | MG | B0 | 102 | 1/1 | 0.83 | 0.61 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3673 | 1/1 | 0.83 | 0.20 | 53,53,53,53 | 0 |
| 56 | MG | AA | 3014 | 1/1 | 0.83 | 0.19 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3256 | 1/1 | 0.84 | 0.18 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3084 | 1/1 | 0.84 | 0.32 | 70,70,70,70 | 0 |
| 56 | MG | CA | 3031 | 1/1 | 0.84 | 0.39 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3423 | 1/1 | 0.84 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | CA | 3023 | 1/1 | 0.84 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3198 | 1/1 | 0.84 | 0.29 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3598 | 1/1 | 0.84 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3609 | 1/1 | 0.84 | 0.35 | 64,64,64,64 | 0 |
| 56 | MG | AA | 3077 | 1/1 | 0.84 | 0.41 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3458 | 1/1 | 0.84 | 0.15 | 71,71,71,71 | 0 |
| 56 | MG | CA | 3070 | 1/1 | 0.84 | 0.34 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3102 | 1/1 | 0.84 | 0.32 | 52,52,52,52 | 0 |
| 56 | MG | AA | 3029 | 1/1 | 0.84 | 0.69 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3165 | 1/1 | 0.84 | 0.31 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3483 | 1/1 | 0.84 | 0.19 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3240 | 1/1 | 0.84 | 0.17 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3059 | 1/1 | 0.84 | 1.19 | 54,54,54,54 | 0 |
| 56 | MG | AA | 3140 | 1/1 | 0.84 | 0.12 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3104 | 1/1 | 0.84 | 0.28 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3008 | 1/1 | 0.84 | 0.78 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3288 | 1/1 | 0.84 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | CA | 3081 | 1/1 | 0.84 | 0.10 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3285 | 1/1 | 0.85 | 0.14 | 32,32,32,32 | 0 |
| 56 | MG | DD | 307 | 1/1 | 0.85 | 0.61 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3613 | 1/1 | 0.85 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3357 | 1/1 | 0.85 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3136 | 1/1 | 0.85 | 0.23 | 58,58,58,58 | 0 |
| 56 | MG | CA | 3109 | 1/1 | 0.85 | 0.11 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3061 | 1/1 | 0.85 | 0.45 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3099 | 1/1 | 0.85 | 0.27 | 44,44,44,44 | 0 |
| 56 | MG | AA | 3094 | 1/1 | 0.85 | 0.21 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3157 | 1/1 | 0.85 | 0.99 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3088 | 1/1 | 0.85 | 0.36 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3111 | 1/1 | 0.85 | 0.40 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3238 | 1/1 | 0.85 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3222 | 1/1 | 0.85 | 0.13 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3040 | 1/1 | 0.85 | 0.35 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3140 | 1/1 | 0.85 | 0.19 | 64,64,64,64 | 0 |
| 56 | MG | B7 | 104 | 1/1 | 0.85 | 0.13 | 51,51,51,51 | 0 |
| 58 | ZN | D4 | 501 | 1/1 | 0.85 | 0.09 | 153,153,153,153 | 0 |
| 56 | MG | DF | 302 | 1/1 | 0.85 | 0.27 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3484 | 1/1 | 0.85 | 0.25 | 51,51,51,51 | 0 |
| 56 | MG | CA | 3005 | 1/1 | 0.85 | 0.32 | 54,54,54,54 | 0 |
| 56 | MG | CA | 3039 | 1/1 | 0.85 | 0.36 | 72,72,72,72 | 0 |
| 56 | MG | AA | 3212 | 1/1 | 0.85 | 0.15 | 79,79,79,79 | 0 |
| 56 | MG | DV | 202 | 1/1 | 0.85 | 0.84 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3135 | 1/1 | 0.85 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | BB | 3017 | 1/1 | 0.85 | 0.20 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3065 | 1/1 | 0.85 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3624 | 1/1 | 0.85 | 0.25 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3669 | 1/1 | 0.85 | 0.24 | 75,75,75,75 | 0 |
| 56 | MG | CA | 3158 | 1/1 | 0.85 | 0.22 | 76,76,76,76 | 0 |
| 56 | MG | DR | 201 | 1/1 | 0.85 | 0.62 | 65,65,65,65 | 0 |
| 56 | MG | AA | 3164 | 1/1 | 0.85 | 0.38 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3531 | 1/1 | 0.85 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3009 | 1/1 | 0.85 | 0.17 | 25,25,25,25 | 0 |
| 56 | MG | CA | 3103 | 1/1 | 0.85 | 0.19 | 83,83,83,83 | 0 |
| 56 | MG | CA | 3163 | 1/1 | 0.85 | 0.24 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3456 | 1/1 | 0.85 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3124 | 1/1 | 0.85 | 0.13 | 67,67,67,67 | 0 |
| 56 | MG | BD | 301 | 1/1 | 0.85 | 0.27 | 28,28,28,28 | 0 |
| 56 | MG | AA | 3218 | 1/1 | 0.85 | 0.54 | 65,65,65,65 | 0 |
| 56 | MG | BU | 205 | 1/1 | 0.85 | 0.33 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3626 | 1/1 | 0.85 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | AA | 3015 | 1/1 | 0.85 | 0.16 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3175 | 1/1 | 0.85 | 0.25 | 48,48,48,48 | 0 |
| 56 | MG | BF | 308 | 1/1 | 0.86 | 0.25 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3590 | 1/1 | 0.86 | 0.13 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3198 | 1/1 | 0.86 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | B9 | 502 | 1/1 | 0.86 | 0.27 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3632 | 1/1 | 0.86 | 0.19 | 71,71,71,71 | 0 |
| 56 | MG | CA | 3063 | 1/1 | 0.86 | 0.09 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3282 | 1/1 | 0.86 | 0.37 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3249 | 1/1 | 0.86 | 0.24 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3004 | 1/1 | 0.86 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3253 | 1/1 | 0.86 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3168 | 1/1 | 0.86 | 0.39 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3641 | 1/1 | 0.86 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3070 | 1/1 | 0.86 | 0.27 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3093 | 1/1 | 0.86 | 0.20 | 53,53,53,53 | 0 |
| 56 | MG | CA | 3131 | 1/1 | 0.86 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3027 | 1/1 | 0.86 | 0.23 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3277 | 1/1 | 0.86 | 0.37 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3712 | 1/1 | 0.86 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3022 | 1/1 | 0.86 | 0.25 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3112 | 1/1 | 0.86 | 0.43 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3482 | 1/1 | 0.86 | 0.13 | 55,55,55,55 | 0 |
| 56 | MG | BE | 303 | 1/1 | 0.86 | 0.17 | 29,29,29,29 | 0 |
| 56 | MG | D5 | 101 | 1/1 | 0.86 | 0.48 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3462 | 1/1 | 0.86 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3553 | 1/1 | 0.86 | 0.36 | 70,70,70,70 | 0 |
| 56 | MG | AA | 3013 | 1/1 | 0.86 | 0.23 | 78,78,78,78 | 0 |
| 56 | MG | AX | 106 | 1/1 | 0.86 | 0.17 | 73,73,73,73 | 0 |
| 56 | MG | CQ | 201 | 1/1 | 0.86 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3110 | 1/1 | 0.86 | 0.34 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3474 | 1/1 | 0.86 | 0.21 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3592 | 1/1 | 0.86 | 0.15 | 65,65,65,65 | 0 |
| 56 | MG | DV | 203 | 1/1 | 0.86 | 0.74 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3062 | 1/1 | 0.86 | 0.34 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3054 | 1/1 | 0.86 | 0.39 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3036 | 1/1 | 0.86 | 0.29 | 35,35,35,35 | 0 |
| 56 | MG | CA | 3110 | 1/1 | 0.86 | 0.21 | 97,97,97,97 | 0 |
| 59 | FME | AX | 101 | 10/11 | 0.86 | 0.44 | 48,75,97,113 | 0 |
| 56 | MG | CA | 3068 | 1/1 | 0.86 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3095 | 1/1 | 0.86 | 0.23 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3001 | 1/1 | 0.86 | 0.18 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3495 | 1/1 | 0.87 | 0.34 | 84,84,84,84 | 0 |
| 56 | MG | AA | 3042 | 1/1 | 0.87 | 0.33 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3079 | 1/1 | 0.87 | 0.27 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3221 | 1/1 | 0.87 | 0.27 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3081 | 1/1 | 0.87 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3252 | 1/1 | 0.87 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3268 | 1/1 | 0.87 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3058 | 1/1 | 0.87 | 0.34 | 47,47,47,47 | 0 |
| 56 | MG | DD | 302 | 1/1 | 0.87 | 0.23 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3260 | 1/1 | 0.87 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | CA | 3155 | 1/1 | 0.87 | 0.16 | 71,71,71,71 | 0 |
| 56 | MG | AA | 3074 | 1/1 | 0.87 | 0.44 | 47,47,47,47 | 0 |
| 56 | MG | AA | 3075 | 1/1 | 0.87 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3053 | 1/1 | 0.87 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3108 | 1/1 | 0.87 | 0.46 | 37,37,37,37 | 0 |
| 60 | K | BA | 3300 | 1/1 | 0.87 | 0.28 | 100,100,100,100 | 0 |
| 56 | MG | BA | 3156 | 1/1 | 0.87 | 0.40 | 56,56,56,56 | 0 |
| 56 | MG | BB | 3008 | 1/1 | 0.87 | 0.21 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3171 | 1/1 | 0.87 | 0.25 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3236 | 1/1 | 0.87 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3032 | 1/1 | 0.87 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3137 | 1/1 | 0.87 | 0.21 | 42,42,42,42 | 0 |
| 56 | MG | CA | 3146 | 1/1 | 0.87 | 0.20 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3115 | 1/1 | 0.87 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3292 | 1/1 | 0.87 | 0.22 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3501 | 1/1 | 0.87 | 0.25 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3591 | 1/1 | 0.87 | 0.26 | 58,58,58,58 | 0 |
| 56 | MG | AA | 3166 | 1/1 | 0.87 | 0.18 | 48,48,48,48 | 0 |
| 56 | MG | CA | 3142 | 1/1 | 0.87 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3727 | 1/1 | 0.87 | 0.66 | 68,68,68,68 | 0 |
| 56 | MG | CA | 3091 | 1/1 | 0.87 | 0.17 | 72,72,72,72 | 0 |
| 56 | MG | AA | 3067 | 1/1 | 0.87 | 0.37 | 87,87,87,87 | 0 |
| 56 | MG | BW | 203 | 1/1 | 0.87 | 0.32 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3481 | 1/1 | 0.87 | 0.27 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3060 | 1/1 | 0.87 | 0.25 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3125 | 1/1 | 0.87 | 0.13 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3080 | 1/1 | 0.87 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3643 | 1/1 | 0.87 | 0.28 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3009 | 1/1 | 0.87 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3214 | 1/1 | 0.87 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3161 | 1/1 | 0.87 | 0.30 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3006 | 1/1 | 0.87 | 0.27 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3500 | 1/1 | 0.87 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3102 | 1/1 | 0.88 | 0.25 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3208 | 1/1 | 0.88 | 0.94 | 43,43,43,43 | 0 |
| 56 | MG | BN | 3002 | 1/1 | 0.88 | 0.30 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3240 | 1/1 | 0.88 | 0.26 | 51,51,51,51 | 0 |
| 56 | MG | AA | 3019 | 1/1 | 0.88 | 0.39 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3100 | 1/1 | 0.88 | 0.25 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3398 | 1/1 | 0.88 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3214 | 1/1 | 0.88 | 0.27 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3217 | 1/1 | 0.88 | 0.57 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3192 | 1/1 | 0.88 | 0.48 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3185 | 1/1 | 0.88 | 0.58 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3310 | 1/1 | 0.88 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | AA | 3050 | 1/1 | 0.88 | 0.50 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3210 | 1/1 | 0.88 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3138 | 1/1 | 0.88 | 0.54 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3147 | 1/1 | 0.88 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3514 | 1/1 | 0.88 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3320 | 1/1 | 0.88 | 0.29 | 57,57,57,57 | 0 |
| 56 | MG | CA | 3040 | 1/1 | 0.88 | 0.35 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3343 | 1/1 | 0.88 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3252 | 1/1 | 0.88 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | AA | 3131 | 1/1 | 0.88 | 0.50 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3205 | 1/1 | 0.88 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | CA | 3034 | 1/1 | 0.88 | 0.26 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3216 | 1/1 | 0.88 | 0.22 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3134 | 1/1 | 0.88 | 0.23 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3150 | 1/1 | 0.88 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3168 | 1/1 | 0.88 | 0.28 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3280 | 1/1 | 0.88 | 0.69 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3599 | 1/1 | 0.88 | 0.23 | 72,72,72,72 | 0 |
| 56 | MG | CA | 3164 | 1/1 | 0.88 | 0.39 | 49,49,49,49 | 0 |
| 56 | MG | AA | 3033 | 1/1 | 0.88 | 0.38 | 64,64,64,64 | 0 |
| 56 | MG | CA | 3071 | 1/1 | 0.88 | 0.08 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3062 | 1/1 | 0.88 | 0.34 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3298 | 1/1 | 0.88 | 0.33 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3092 | 1/1 | 0.88 | 0.60 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3119 | 1/1 | 0.88 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3354 | 1/1 | 0.88 | 0.15 | 74,74,74,74 | 0 |
| 56 | MG | BG | 3002 | 1/1 | 0.88 | 0.11 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3122 | 1/1 | 0.88 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3078 | 1/1 | 0.88 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | DB | 3011 | 1/1 | 0.88 | 0.34 | 55,55,55,55 | 0 |
| 56 | MG | AN | 103 | 1/1 | 0.88 | 0.38 | 60,60,60,60 | 0 |
| 56 | MG | CA | 3126 | 1/1 | 0.88 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3163 | 1/1 | 0.88 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3045 | 1/1 | 0.88 | 0.29 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3373 | 1/1 | 0.88 | 0.28 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3058 | 1/1 | 0.88 | 0.45 | 38,38,38,38 | 0 |
| 56 | MG | CA | 3027 | 1/1 | 0.88 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3005 | 1/1 | 0.88 | 0.21 | 42,42,42,42 | 0 |
| 56 | MG | AA | 3046 | 1/1 | 0.88 | 0.12 | 73,73,73,73 | 0 |
| 56 | MG | AA | 3132 | 1/1 | 0.88 | 0.36 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3346 | 1/1 | 0.88 | 0.23 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3604 | 1/1 | 0.88 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3224 | 1/1 | 0.88 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3110 | 1/1 | 0.88 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3086 | 1/1 | 0.88 | 0.30 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3693 | 1/1 | 0.88 | 0.14 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3067 | 1/1 | 0.88 | 0.54 | 43,43,43,43 | 0 |
| 56 | MG | DQ | 201 | 1/1 | 0.88 | 0.43 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3009 | 1/1 | 0.88 | 0.23 | 79,79,79,79 | 0 |
| 56 | MG | CA | 3143 | 1/1 | 0.88 | 0.07 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3524 | 1/1 | 0.88 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | AA | 3032 | 1/1 | 0.88 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | CA | 3157 | 1/1 | 0.88 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | CA | 3002 | 1/1 | 0.88 | 0.07 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3023 | 1/1 | 0.88 | 0.13 | 66,66,66,66 | 0 |
| 56 | MG | AA | 3133 | 1/1 | 0.88 | 0.35 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3092 | 1/1 | 0.88 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | CA | 3159 | 1/1 | 0.88 | 0.61 | 91,91,91,91 | 0 |
| 56 | MG | DA | 3460 | 1/1 | 0.89 | 0.36 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3405 | 1/1 | 0.89 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3336 | 1/1 | 0.89 | 0.21 | 54,54,54,54 | 0 |
| 56 | MG | CA | 3029 | 1/1 | 0.89 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3509 | 1/1 | 0.89 | 0.16 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3638 | 1/1 | 0.89 | 0.30 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3487 | 1/1 | 0.89 | 0.19 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3018 | 1/1 | 0.89 | 0.47 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3132 | 1/1 | 0.89 | 0.71 | 54,54,54,54 | 0 |
| 56 | MG | AA | 3002 | 1/1 | 0.89 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3191 | 1/1 | 0.89 | 0.44 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3365 | 1/1 | 0.89 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3218 | 1/1 | 0.89 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3585 | 1/1 | 0.89 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3145 | 1/1 | 0.89 | 0.46 | 65,65,65,65 | 0 |
| 56 | MG | AA | 3031 | 1/1 | 0.89 | 0.22 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3590 | 1/1 | 0.89 | 0.17 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3104 | 1/1 | 0.89 | 0.28 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3167 | 1/1 | 0.89 | 0.23 | 48,48,48,48 | 0 |
| 56 | MG | CA | 3160 | 1/1 | 0.89 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3523 | 1/1 | 0.89 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3286 | 1/1 | 0.89 | 0.17 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3237 | 1/1 | 0.89 | 0.55 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3149 | 1/1 | 0.89 | 0.55 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3005 | 1/1 | 0.89 | 0.18 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3127 | 1/1 | 0.89 | 0.38 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3355 | 1/1 | 0.89 | 0.23 | 64,64,64,64 | 0 |
| 56 | MG | AA | 3047 | 1/1 | 0.89 | 0.31 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3039 | 1/1 | 0.89 | 0.24 | 60,60,60,60 | 0 |
| 56 | MG | BN | 3003 | 1/1 | 0.89 | 0.39 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3195 | 1/1 | 0.89 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3197 | 1/1 | 0.89 | 0.30 | 39,39,39,39 | 0 |
| 56 | MG | CA | 3079 | 1/1 | 0.89 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3200 | 1/1 | 0.89 | 0.21 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3017 | 1/1 | 0.89 | 0.54 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3103 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | AA | 3181 | 1/1 | 0.89 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3292 | 1/1 | 0.89 | 0.21 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3169 | 1/1 | 0.89 | 0.38 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3253 | 1/1 | 0.89 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3560 | 1/1 | 0.89 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | CA | 3037 | 1/1 | 0.89 | 0.31 | 67,67,67,67 | 0 |
| 56 | MG | DV | 204 | 1/1 | 0.89 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3251 | 1/1 | 0.89 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3623 | 1/1 | 0.89 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3061 | 1/1 | 0.89 | 0.49 | 51,51,51,51 | 0 |
| 56 | MG | CA | 3086 | 1/1 | 0.89 | 0.20 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3441 | 1/1 | 0.89 | 0.30 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3243 | 1/1 | 0.89 | 0.21 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3147 | 1/1 | 0.89 | 0.24 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3048 | 1/1 | 0.89 | 0.37 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3309 | 1/1 | 0.89 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3194 | 1/1 | 0.89 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3139 | 1/1 | 0.89 | 0.34 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3356 | 1/1 | 0.89 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3558 | 1/1 | 0.89 | 0.22 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3159 | 1/1 | 0.89 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3387 | 1/1 | 0.89 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | AA | 3134 | 1/1 | 0.89 | 0.43 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3177 | 1/1 | 0.89 | 0.21 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3664 | 1/1 | 0.89 | 0.26 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3215 | 1/1 | 0.89 | 0.14 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3361 | 1/1 | 0.89 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3230 | 1/1 | 0.89 | 0.47 | 46,46,46,46 | 0 |
| 56 | MG | CA | 3036 | 1/1 | 0.89 | 0.52 | 68,68,68,68 | 0 |
| 56 | MG | CA | 3170 | 1/1 | 0.89 | 0.48 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3503 | 1/1 | 0.90 | 0.17 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3213 | 1/1 | 0.90 | 0.21 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3463 | 1/1 | 0.90 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3219 | 1/1 | 0.90 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | B7 | 101 | 1/1 | 0.90 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3596 | 1/1 | 0.90 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | AA | 3115 | 1/1 | 0.90 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3119 | 1/1 | 0.90 | 0.37 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3075 | 1/1 | 0.90 | 0.33 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3457 | 1/1 | 0.90 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3181 | 1/1 | 0.90 | 0.34 | 38,38,38,38 | 0 |
| 56 | MG | AA | 3184 | 1/1 | 0.90 | 0.10 | 72,72,72,72 | 0 |
| 56 | MG | BQ | 203 | 1/1 | 0.90 | 0.22 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3391 | 1/1 | 0.90 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3066 | 1/1 | 0.90 | 0.37 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3548 | 1/1 | 0.90 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3255 | 1/1 | 0.90 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3042 | 1/1 | 0.90 | 0.25 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3144 | 1/1 | 0.90 | 0.27 | 74,74,74,74 | 0 |
| 56 | MG | CT | 3001 | 1/1 | 0.90 | 0.43 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3105 | 1/1 | 0.90 | 0.44 | 34,34,34,34 | 0 |
| 56 | MG | AA | 3123 | 1/1 | 0.90 | 0.43 | 39,39,39,39 | 0 |
| 56 | MG | BE | 305 | 1/1 | 0.90 | 0.70 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3096 | 1/1 | 0.90 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3159 | 1/1 | 0.90 | 0.30 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3602 | 1/1 | 0.90 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3671 | 1/1 | 0.90 | 0.33 | 57,57,57,57 | 0 |
| 56 | MG | AA | 3052 | 1/1 | 0.90 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3125 | 1/1 | 0.90 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3708 | 1/1 | 0.90 | 0.23 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3359 | 1/1 | 0.90 | 0.23 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3011 | 1/1 | 0.90 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3350 | 1/1 | 0.90 | 0.24 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3620 | 1/1 | 0.90 | 0.19 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3126 | 1/1 | 0.90 | 0.34 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3284 | 1/1 | 0.90 | 0.14 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3440 | 1/1 | 0.90 | 0.32 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3139 | 1/1 | 0.90 | 0.25 | 51,51,51,51 | 0 |
| 56 | MG | AA | 3080 | 1/1 | 0.90 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3517 | 1/1 | 0.90 | 0.19 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3194 | 1/1 | 0.90 | 0.18 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3150 | 1/1 | 0.90 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3369 | 1/1 | 0.90 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3193 | 1/1 | 0.90 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | AK | 3001 | 1/1 | 0.90 | 0.18 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3640 | 1/1 | 0.90 | 0.68 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3128 | 1/1 | 0.90 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3007 | 1/1 | 0.90 | 0.23 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3593 | 1/1 | 0.90 | 0.23 | 73,73,73,73 | 0 |
| 56 | MG | CA | 3046 | 1/1 | 0.90 | 0.38 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3183 | 1/1 | 0.90 | 0.24 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3047 | 1/1 | 0.90 | 0.42 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3129 | 1/1 | 0.90 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3582 | 1/1 | 0.90 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3077 | 1/1 | 0.90 | 0.28 | 50,50,50,50 | 0 |
| 56 | MG | AA | 3092 | 1/1 | 0.90 | 0.51 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3538 | 1/1 | 0.90 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3683 | 1/1 | 0.90 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3730 | 1/1 | 0.90 | 0.64 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3461 | 1/1 | 0.90 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3609 | 1/1 | 0.90 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3578 | 1/1 | 0.90 | 0.32 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3243 | 1/1 | 0.90 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3624 | 1/1 | 0.90 | 0.40 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3264 | 1/1 | 0.90 | 0.32 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3714 | 1/1 | 0.90 | 0.21 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3218 | 1/1 | 0.90 | 0.25 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3465 | 1/1 | 0.90 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3174 | 1/1 | 0.90 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | B7 | 103 | 1/1 | 0.90 | 0.85 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3019 | 1/1 | 0.90 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | AA | 3005 | 1/1 | 0.90 | 0.20 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3560 | 1/1 | 0.90 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3462 | 1/1 | 0.90 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3610 | 1/1 | 0.90 | 0.28 | 54,54,54,54 | 0 |
| 56 | MG | AA | 3003 | 1/1 | 0.90 | 0.24 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3577 | 1/1 | 0.90 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3048 | 1/1 | 0.90 | 0.23 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3363 | 1/1 | 0.90 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3044 | 1/1 | 0.90 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | DF | 303 | 1/1 | 0.90 | 0.33 | 43,43,43,43 | 0 |
| 56 | MG | DB | 3005 | 1/1 | 0.90 | 0.26 | 43,43,43,43 | 0 |
| 56 | MG | AA | 3124 | 1/1 | 0.90 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3738 | 1/1 | 0.90 | 0.35 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3254 | 1/1 | 0.90 | 0.22 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3046 | 1/1 | 0.90 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | AA | 3217 | 1/1 | 0.90 | 0.65 | 67,67,67,67 | 0 |
| 56 | MG | AA | 3215 | 1/1 | 0.90 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | CA | 3153 | 1/1 | 0.90 | 0.10 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3105 | 1/1 | 0.90 | 0.38 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3180 | 1/1 | 0.90 | 0.38 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3114 | 1/1 | 0.90 | 0.36 | 51,51,51,51 | 0 |
| 56 | MG | CA | 3162 | 1/1 | 0.91 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3653 | 1/1 | 0.91 | 0.35 | 60,60,60,60 | 0 |
| 56 | MG | CA | 3119 | 1/1 | 0.91 | 0.24 | 64,64,64,64 | 0 |
| 56 | MG | AN | 101 | 1/1 | 0.91 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3049 | 1/1 | 0.91 | 0.38 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3248 | 1/1 | 0.91 | 0.24 | 43,43,43,43 | 0 |
| 56 | MG | BF | 302 | 1/1 | 0.91 | 0.31 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3568 | 1/1 | 0.91 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | CA | 3151 | 1/1 | 0.91 | 0.25 | 80,80,80,80 | 0 |
| 56 | MG | AA | 3142 | 1/1 | 0.91 | 0.26 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3419 | 1/1 | 0.91 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3172 | 1/1 | 0.91 | 0.43 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3594 | 1/1 | 0.91 | 0.30 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3666 | 1/1 | 0.91 | 0.32 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3507 | 1/1 | 0.91 | 0.10 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3055 | 1/1 | 0.91 | 0.23 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3226 | 1/1 | 0.91 | 0.21 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3621 | 1/1 | 0.91 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3262 | 1/1 | 0.91 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3335 | 1/1 | 0.91 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3567 | 1/1 | 0.91 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | BB | 3009 | 1/1 | 0.91 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3051 | 1/1 | 0.91 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3464 | 1/1 | 0.91 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3342 | 1/1 | 0.91 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3466 | 1/1 | 0.91 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3496 | 1/1 | 0.91 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3187 | 1/1 | 0.91 | 0.64 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3689 | 1/1 | 0.91 | 0.23 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3481 | 1/1 | 0.91 | 0.23 | 38,38,38,38 | 0 |
| 56 | MG | AX | 105 | 1/1 | 0.91 | 0.69 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3391 | 1/1 | 0.91 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3020 | 1/1 | 0.91 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3638 | 1/1 | 0.91 | 0.21 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3505 | 1/1 | 0.91 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | BN | 3001 | 1/1 | 0.91 | 0.76 | 54,54,54,54 | 0 |
| 56 | MG | DF | 301 | 1/1 | 0.91 | 0.51 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3132 | 1/1 | 0.91 | 0.25 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3526 | 1/1 | 0.91 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3512 | 1/1 | 0.91 | 0.25 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3372 | 1/1 | 0.91 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | AA | 3219 | 1/1 | 0.91 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3619 | 1/1 | 0.91 | 0.27 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3466 | 1/1 | 0.91 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3183 | 1/1 | 0.91 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3635 | 1/1 | 0.91 | 0.32 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3401 | 1/1 | 0.91 | 0.29 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3303 | 1/1 | 0.91 | 0.16 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3443 | 1/1 | 0.91 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3360 | 1/1 | 0.91 | 0.25 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3106 | 1/1 | 0.91 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3226 | 1/1 | 0.91 | 0.30 | 32,32,32,32 | 0 |
| 56 | MG | BD | 312 | 1/1 | 0.91 | 0.85 | 80,80,80,80 | 0 |
| 56 | MG | CA | 3106 | 1/1 | 0.91 | 0.34 | 64,64,64,64 | 0 |
| 56 | MG | AA | 3011 | 1/1 | 0.91 | 1.19 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3056 | 1/1 | 0.91 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3269 | 1/1 | 0.91 | 0.65 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3041 | 1/1 | 0.91 | 0.45 | 57,57,57,57 | 0 |
| 56 | MG | DF | 304 | 1/1 | 0.91 | 0.28 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3121 | 1/1 | 0.91 | 0.53 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3024 | 1/1 | 0.91 | 0.40 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3056 | 1/1 | 0.91 | 0.42 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3676 | 1/1 | 0.91 | 0.22 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3172 | 1/1 | 0.91 | 0.98 | 48,48,48,48 | 0 |
| 56 | MG | AX | 107 | 1/1 | 0.91 | 0.25 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3315 | 1/1 | 0.91 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | CA | 3010 | 1/1 | 0.91 | 0.11 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3376 | 1/1 | 0.91 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3653 | 1/1 | 0.91 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3149 | 1/1 | 0.91 | 0.06 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3143 | 1/1 | 0.91 | 0.31 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3169 | 1/1 | 0.91 | 0.16 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3430 | 1/1 | 0.91 | 0.28 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3339 | 1/1 | 0.91 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3038 | 1/1 | 0.91 | 0.60 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3137 | 1/1 | 0.91 | 0.29 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3331 | 1/1 | 0.91 | 0.19 | 47,47,47,47 | 0 |
| 56 | MG | AA | 3081 | 1/1 | 0.91 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3069 | 1/1 | 0.91 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3148 | 1/1 | 0.91 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3033 | 1/1 | 0.91 | 0.25 | 39,39,39,39 | 0 |
| 56 | MG | CA | 3006 | 1/1 | 0.91 | 0.17 | 77,77,77,77 | 0 |
| 56 | MG | AA | 3101 | 1/1 | 0.91 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3143 | 1/1 | 0.91 | 0.22 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3125 | 1/1 | 0.91 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | AA | 3136 | 1/1 | 0.91 | 0.08 | 62,62,62,62 | 0 |
| 56 | MG | D8 | 5001 | 1/1 | 0.91 | 0.41 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3073 | 1/1 | 0.91 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | CA | 3047 | 1/1 | 0.91 | 0.16 | 63,63,63,63 | 0 |
| 56 | MG | CA | 3152 | 1/1 | 0.92 | 0.38 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3040 | 1/1 | 0.92 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3221 | 1/1 | 0.92 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3617 | 1/1 | 0.92 | 0.24 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3170 | 1/1 | 0.92 | 0.80 | 57,57,57,57 | 0 |
| 56 | MG | AA | 3105 | 1/1 | 0.92 | 0.22 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3179 | 1/1 | 0.92 | 0.22 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3190 | 1/1 | 0.92 | 0.32 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3295 | 1/1 | 0.92 | 0.24 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3536 | 1/1 | 0.92 | 0.16 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3029 | 1/1 | 0.92 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3505 | 1/1 | 0.92 | 0.06 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3258 | 1/1 | 0.92 | 0.23 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3016 | 1/1 | 0.92 | 0.24 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3151 | 1/1 | 0.92 | 0.29 | 60,60,60,60 | 0 |
| 56 | MG | AA | 3211 | 1/1 | 0.92 | 0.20 | 36,36,36,36 | 0 |
| 56 | MG | AA | 3162 | 1/1 | 0.92 | 0.23 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3532 | 1/1 | 0.92 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | AA | 3194 | 1/1 | 0.92 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3225 | 1/1 | 0.92 | 0.33 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3502 | 1/1 | 0.92 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3246 | 1/1 | 0.92 | 0.17 | 24,24,24,24 | 0 |
| 56 | MG | CA | 3111 | 1/1 | 0.92 | 0.12 | 64,64,64,64 | 0 |
| 56 | MG | CA | 3104 | 1/1 | 0.92 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3140 | 1/1 | 0.92 | 0.16 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3502 | 1/1 | 0.92 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3698 | 1/1 | 0.92 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3188 | 1/1 | 0.92 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3097 | 1/1 | 0.92 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3459 | 1/1 | 0.92 | 0.11 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3651 | 1/1 | 0.92 | 0.60 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3111 | 1/1 | 0.92 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3735 | 1/1 | 0.92 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3325 | 1/1 | 0.92 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3453 | 1/1 | 0.92 | 0.36 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3254 | 1/1 | 0.92 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | CA | 3136 | 1/1 | 0.92 | 0.18 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3109 | 1/1 | 0.92 | 0.55 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3139 | 1/1 | 0.92 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3014 | 1/1 | 0.92 | 0.21 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3597 | 1/1 | 0.92 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3006 | 1/1 | 0.92 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | BU | 201 | 1/1 | 0.92 | 0.75 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3141 | 1/1 | 0.92 | 0.30 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3636 | 1/1 | 0.92 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3050 | 1/1 | 0.92 | 0.57 | 31,31,31,31 | 0 |
| 56 | MG | AA | 3191 | 1/1 | 0.92 | 0.13 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3401 | 1/1 | 0.92 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3562 | 1/1 | 0.92 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3468 | 1/1 | 0.92 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | AA | 3082 | 1/1 | 0.92 | 0.24 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3196 | 1/1 | 0.92 | 0.76 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3296 | 1/1 | 0.92 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3633 | 1/1 | 0.92 | 0.13 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3099 | 1/1 | 0.92 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3074 | 1/1 | 0.92 | 0.21 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3543 | 1/1 | 0.92 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3188 | 1/1 | 0.92 | 0.33 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3225 | 1/1 | 0.92 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | AA | 3041 | 1/1 | 0.92 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3340 | 1/1 | 0.92 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3406 | 1/1 | 0.92 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | BR | 204 | 1/1 | 0.92 | 0.61 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3489 | 1/1 | 0.92 | 0.16 | 36,36,36,36 | 0 |
| 56 | MG | AA | 3072 | 1/1 | 0.92 | 0.26 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3256 | 1/1 | 0.92 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3652 | 1/1 | 0.92 | 0.20 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3328 | 1/1 | 0.92 | 0.21 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3108 | 1/1 | 0.92 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3554 | 1/1 | 0.92 | 0.18 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3478 | 1/1 | 0.92 | 0.25 | 46,46,46,46 | 0 |
| 56 | MG | BB | 3014 | 1/1 | 0.92 | 0.13 | 69,69,69,69 | 0 |
| 56 | MG | BG | 3001 | 1/1 | 0.92 | 0.13 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3090 | 1/1 | 0.92 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3122 | 1/1 | 0.92 | 0.27 | 52,52,52,52 | 0 |
| 56 | MG | AA | 3200 | 1/1 | 0.92 | 0.24 | 68,68,68,68 | 0 |
| 56 | MG | AA | 3069 | 1/1 | 0.92 | 0.14 | 84,84,84,84 | 0 |
| 56 | MG | BD | 304 | 1/1 | 0.92 | 0.51 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3202 | 1/1 | 0.92 | 0.33 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3432 | 1/1 | 0.92 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3601 | 1/1 | 0.92 | 0.28 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3509 | 1/1 | 0.92 | 0.13 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3611 | 1/1 | 0.92 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | AA | 3034 | 1/1 | 0.92 | 0.18 | 48,48,48,48 | 0 |
| 56 | MG | CA | 3105 | 1/1 | 0.92 | 0.09 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3116 | 1/1 | 0.92 | 0.31 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3039 | 1/1 | 0.92 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | AA | 3024 | 1/1 | 0.92 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3107 | 1/1 | 0.92 | 0.30 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3117 | 1/1 | 0.92 | 0.15 | 68,68,68,68 | 0 |
| 56 | MG | AA | 3098 | 1/1 | 0.92 | 0.35 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3013 | 1/1 | 0.92 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3052 | 1/1 | 0.92 | 0.25 | 29,29,29,29 | 0 |
| 56 | MG | AA | 3154 | 1/1 | 0.92 | 0.08 | 63,63,63,63 | 0 |
| 56 | MG | AA | 3025 | 1/1 | 0.92 | 0.14 | 69,69,69,69 | 0 |
| 56 | MG | CA | 3065 | 1/1 | 0.92 | 0.23 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3374 | 1/1 | 0.92 | 0.19 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3245 | 1/1 | 0.92 | 0.30 | 47,47,47,47 | 0 |
| 56 | MG | BF | 304 | 1/1 | 0.92 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | AA | 3036 | 1/1 | 0.92 | 0.23 | 71,71,71,71 | 0 |
| 56 | MG | AA | 3198 | 1/1 | 0.92 | 0.11 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3430 | 1/1 | 0.92 | 0.32 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3537 | 1/1 | 0.93 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3470 | 1/1 | 0.93 | 0.28 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3326 | 1/1 | 0.93 | 0.20 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3515 | 1/1 | 0.93 | 0.05 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3133 | 1/1 | 0.93 | 0.27 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3072 | 1/1 | 0.93 | 0.28 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3366 | 1/1 | 0.93 | 0.35 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3246 | 1/1 | 0.93 | 0.24 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3599 | 1/1 | 0.93 | 0.31 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3135 | 1/1 | 0.93 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | CA | 3134 | 1/1 | 0.93 | 0.17 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3549 | 1/1 | 0.93 | 0.22 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3414 | 1/1 | 0.93 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3597 | 1/1 | 0.93 | 0.35 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3603 | 1/1 | 0.93 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3054 | 1/1 | 0.93 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3387 | 1/1 | 0.93 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3066 | 1/1 | 0.93 | 0.31 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3273 | 1/1 | 0.93 | 0.39 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3336 | 1/1 | 0.93 | 0.12 | 27,27,27,27 | 0 |
| 56 | MG | B0 | 101 | 1/1 | 0.93 | 0.20 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3690 | 1/1 | 0.93 | 0.17 | 53,53,53,53 | 0 |
| 58 | ZN | AN | 102 | 1/1 | 0.93 | 0.12 | 90,90,90,90 | 0 |
| 56 | MG | BD | 306 | 1/1 | 0.93 | 0.45 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3687 | 1/1 | 0.93 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3424 | 1/1 | 0.93 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | DB | 3012 | 1/1 | 0.93 | 0.27 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3238 | 1/1 | 0.93 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3403 | 1/1 | 0.93 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3008 | 1/1 | 0.93 | 0.23 | 51,51,51,51 | 0 |
| 56 | MG | DW | 201 | 1/1 | 0.93 | 0.31 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3206 | 1/1 | 0.93 | 0.07 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3519 | 1/1 | 0.93 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | CA | 3107 | 1/1 | 0.93 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3273 | 1/1 | 0.93 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3521 | 1/1 | 0.93 | 0.12 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3098 | 1/1 | 0.93 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3394 | 1/1 | 0.93 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | CA | 3019 | 1/1 | 0.93 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3199 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | B8 | 101 | 1/1 | 0.93 | 0.47 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3020 | 1/1 | 0.93 | 0.30 | 52,52,52,52 | 0 |
| 56 | MG | AA | 3058 | 1/1 | 0.93 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3589 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3257 | 1/1 | 0.93 | 0.30 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3182 | 1/1 | 0.93 | 0.31 | 51,51,51,51 | 0 |
| 60 | K | DA | 3231 | 1/1 | 0.93 | 0.22 | 96,96,96,96 | 0 |
| 56 | MG | DA | 3305 | 1/1 | 0.93 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3400 | 1/1 | 0.93 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3067 | 1/1 | 0.93 | 0.33 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3072 | 1/1 | 0.93 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3579 | 1/1 | 0.93 | 0.17 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3233 | 1/1 | 0.93 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3281 | 1/1 | 0.93 | 0.21 | 42,42,42,42 | 0 |
| 56 | MG | CA | 3074 | 1/1 | 0.93 | 0.18 | 54,54,54,54 | 0 |
| 56 | MG | AA | 3008 | 1/1 | 0.93 | 0.41 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3280 | 1/1 | 0.93 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3474 | 1/1 | 0.93 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3144 | 1/1 | 0.93 | 0.39 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3684 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3415 | 1/1 | 0.93 | 0.25 | 56,56,56,56 | 0 |
| 56 | MG | CA | 3099 | 1/1 | 0.93 | 0.33 | 65,65,65,65 | 0 |
| 56 | MG | CA | 3087 | 1/1 | 0.93 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3050 | 1/1 | 0.93 | 0.15 | 21,21,21,21 | 0 |
| 56 | MG | AA | 3026 | 1/1 | 0.93 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3556 | 1/1 | 0.93 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3446 | 1/1 | 0.93 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3303 | 1/1 | 0.93 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | BX | 3001 | 1/1 | 0.93 | 0.29 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3141 | 1/1 | 0.93 | 0.25 | 70,70,70,70 | 0 |
| 56 | MG | AA | 3189 | 1/1 | 0.93 | 0.10 | 77,77,77,77 | 0 |
| 56 | MG | AA | 3202 | 1/1 | 0.93 | 0.23 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3443 | 1/1 | 0.93 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3640 | 1/1 | 0.93 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3212 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3728 | 1/1 | 0.93 | 0.52 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3373 | 1/1 | 0.93 | 0.23 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3408 | 1/1 | 0.93 | 0.15 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3146 | 1/1 | 0.93 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3002 | 1/1 | 0.93 | 0.19 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3643 | 1/1 | 0.93 | 0.72 | 53,53,53,53 | 0 |
| 56 | MG | AA | 3173 | 1/1 | 0.93 | 0.24 | 32,32,32,32 | 0 |
| 56 | MG | BW | 205 | 1/1 | 0.93 | 0.46 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3028 | 1/1 | 0.93 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3030 | 1/1 | 0.93 | 0.43 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3527 | 1/1 | 0.93 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3437 | 1/1 | 0.93 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | AV | 101 | 1/1 | 0.93 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3722 | 1/1 | 0.93 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3060 | 1/1 | 0.93 | 0.40 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3153 | 1/1 | 0.93 | 0.32 | 35,35,35,35 | 0 |
| 56 | MG | AA | 3049 | 1/1 | 0.93 | 0.50 | 51,51,51,51 | 0 |
| 58 | ZN | CN | 501 | 1/1 | 0.93 | 0.12 | 108,108,108,108 | 0 |
| 56 | MG | DA | 3155 | 1/1 | 0.93 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3559 | 1/1 | 0.93 | 0.19 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3045 | 1/1 | 0.93 | 0.37 | 41,41,41,41 | 0 |
| 56 | MG | BE | 306 | 1/1 | 0.93 | 0.44 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3152 | 1/1 | 0.93 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3580 | 1/1 | 0.93 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3555 | 1/1 | 0.93 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3704 | 1/1 | 0.93 | 0.19 | 85,85,85,85 | 0 |
| 56 | MG | DD | 308 | 1/1 | 0.93 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3608 | 1/1 | 0.93 | 0.13 | 68,68,68,68 | 0 |
| 56 | MG | AA | 3201 | 1/1 | 0.93 | 0.12 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3015 | 1/1 | 0.93 | 0.26 | 49,49,49,49 | 0 |
| 56 | MG | B3 | 103 | 1/1 | 0.93 | 0.62 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3450 | 1/1 | 0.93 | 0.16 | 43,43,43,43 | 0 |
| 56 | MG | AA | 3167 | 1/1 | 0.93 | 0.19 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3278 | 1/1 | 0.93 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3724 | 1/1 | 0.93 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3012 | 1/1 | 0.93 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | AA | 3177 | 1/1 | 0.93 | 0.14 | 80,80,80,80 | 0 |
| 56 | MG | BB | 3006 | 1/1 | 0.93 | 0.24 | 39,39,39,39 | 0 |
| 56 | MG | AA | 3068 | 1/1 | 0.93 | 0.08 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3012 | 1/1 | 0.93 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | CA | 3089 | 1/1 | 0.93 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3647 | 1/1 | 0.93 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3250 | 1/1 | 0.93 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3711 | 1/1 | 0.93 | 0.17 | 86,86,86,86 | 0 |
| 56 | MG | BA | 3716 | 1/1 | 0.93 | 0.11 | 27,27,27,27 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3199 | 1/1 | 0.93 | 0.17 | 88,88,88,88 | 0 |
| 56 | MG | BU | 204 | 1/1 | 0.93 | 0.39 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3255 | 1/1 | 0.93 | 0.20 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3299 | 1/1 | 0.93 | 0.23 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3592 | 1/1 | 0.93 | 0.17 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3447 | 1/1 | 0.93 | 0.05 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3193 | 1/1 | 0.93 | 0.57 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3357 | 1/1 | 0.93 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3190 | 1/1 | 0.93 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | CA | 3097 | 1/1 | 0.93 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3472 | 1/1 | 0.93 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3334 | 1/1 | 0.93 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3076 | 1/1 | 0.93 | 0.56 | 44,44,44,44 | 0 |
| 56 | MG | AA | 3060 | 1/1 | 0.93 | 0.53 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3627 | 1/1 | 0.93 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | AA | 3018 | 1/1 | 0.94 | 0.27 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3535 | 1/1 | 0.94 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3052 | 1/1 | 0.94 | 0.20 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3207 | 1/1 | 0.94 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | AA | 3210 | 1/1 | 0.94 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3646 | 1/1 | 0.94 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | AA | 3016 | 1/1 | 0.94 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3091 | 1/1 | 0.94 | 0.60 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3211 | 1/1 | 0.94 | 0.29 | 38,38,38,38 | 0 |
| 56 | MG | AA | 3112 | 1/1 | 0.94 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3074 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3237 | 1/1 | 0.94 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3362 | 1/1 | 0.94 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3101 | 1/1 | 0.94 | 0.33 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3293 | 1/1 | 0.94 | 0.18 | 45,45,45,45 | 0 |
| 56 | MG | BD | 305 | 1/1 | 0.94 | 0.23 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3364 | 1/1 | 0.94 | 0.19 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3196 | 1/1 | 0.94 | 0.34 | 44,44,44,44 | 0 |
| 56 | MG | DF | 305 | 1/1 | 0.94 | 0.73 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3661 | 1/1 | 0.94 | 0.15 | 68,68,68,68 | 0 |
| 56 | MG | BQ | 202 | 1/1 | 0.94 | 0.30 | 28,28,28,28 | 0 |
| 56 | MG | DY | 502 | 1/1 | 0.94 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | CA | 3014 | 1/1 | 0.94 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3635 | 1/1 | 0.94 | 0.10 | 78,78,78,78 | 0 |
| 56 | MG | CA | 3061 | 1/1 | 0.94 | 0.30 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3053 | 1/1 | 0.94 | 0.33 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3631 | 1/1 | 0.94 | 0.14 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3574 | 1/1 | 0.94 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | DE | 305 | 1/1 | 0.94 | 0.64 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3578 | 1/1 | 0.94 | 0.38 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3185 | 1/1 | 0.94 | 0.20 | 47,47,47,47 | 0 |
| 56 | MG | DQ | 202 | 1/1 | 0.94 | 0.22 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3393 | 1/1 | 0.94 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3650 | 1/1 | 0.94 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3344 | 1/1 | 0.94 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3148 | 1/1 | 0.94 | 0.35 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3419 | 1/1 | 0.94 | 0.14 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3082 | 1/1 | 0.94 | 0.29 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3137 | 1/1 | 0.94 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | CA | 3076 | 1/1 | 0.94 | 0.33 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3057 | 1/1 | 0.94 | 0.27 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3386 | 1/1 | 0.94 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3285 | 1/1 | 0.94 | 0.26 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3027 | 1/1 | 0.94 | 0.43 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3377 | 1/1 | 0.94 | 0.14 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3209 | 1/1 | 0.94 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3086 | 1/1 | 0.94 | 0.33 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3433 | 1/1 | 0.94 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3546 | 1/1 | 0.94 | 0.31 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3095 | 1/1 | 0.94 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | CA | 3058 | 1/1 | 0.94 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | AM | 3001 | 1/1 | 0.94 | 0.06 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3476 | 1/1 | 0.94 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3511 | 1/1 | 0.94 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3358 | 1/1 | 0.94 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | CA | 3116 | 1/1 | 0.94 | 0.17 | 76,76,76,76 | 0 |
| 56 | MG | DD | 305 | 1/1 | 0.94 | 0.64 | 49,49,49,49 | 0 |
| 56 | MG | CA | 3149 | 1/1 | 0.94 | 0.18 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3573 | 1/1 | 0.94 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | AA | 3145 | 1/1 | 0.94 | 0.25 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3161 | 1/1 | 0.94 | 0.65 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3439 | 1/1 | 0.94 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3229 | 1/1 | 0.94 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3124 | 1/1 | 0.94 | 0.23 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3304 | 1/1 | 0.94 | 0.19 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3499 | 1/1 | 0.94 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3084 | 1/1 | 0.94 | 0.14 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3659 | 1/1 | 0.94 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | AF | 3001 | 1/1 | 0.94 | 0.17 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3288 | 1/1 | 0.94 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3539 | 1/1 | 0.94 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3686 | 1/1 | 0.94 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3100 | 1/1 | 0.94 | 0.50 | 56,56,56,56 | 0 |
| 56 | MG | AA | 3017 | 1/1 | 0.94 | 0.27 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3079 | 1/1 | 0.94 | 0.28 | 42,42,42,42 | 0 |
| 56 | MG | DB | 3009 | 1/1 | 0.94 | 0.37 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3038 | 1/1 | 0.94 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3692 | 1/1 | 0.94 | 0.40 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3435 | 1/1 | 0.94 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3660 | 1/1 | 0.94 | 0.27 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3378 | 1/1 | 0.94 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | CA | 3137 | 1/1 | 0.94 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3510 | 1/1 | 0.94 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3634 | 1/1 | 0.94 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3164 | 1/1 | 0.94 | 0.26 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3570 | 1/1 | 0.94 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3063 | 1/1 | 0.94 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3469 | 1/1 | 0.94 | 0.21 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3106 | 1/1 | 0.94 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3107 | 1/1 | 0.94 | 0.23 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3392 | 1/1 | 0.94 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | CA | 3167 | 1/1 | 0.94 | 0.09 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3610 | 1/1 | 0.94 | 0.21 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3528 | 1/1 | 0.94 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3449 | 1/1 | 0.94 | 0.12 | 21,21,21,21 | 0 |
| 56 | MG | DR | 202 | 1/1 | 0.94 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3453 | 1/1 | 0.94 | 0.19 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3442 | 1/1 | 0.94 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3197 | 1/1 | 0.94 | 0.30 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3127 | 1/1 | 0.94 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3142 | 1/1 | 0.94 | 0.71 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3090 | 1/1 | 0.94 | 0.34 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3452 | 1/1 | 0.94 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | AA | 3010 | 1/1 | 0.94 | 0.37 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3057 | 1/1 | 0.94 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3114 | 1/1 | 0.94 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3066 | 1/1 | 0.94 | 0.26 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3156 | 1/1 | 0.94 | 0.56 | 29,29,29,29 | 0 |
| 56 | MG | B0 | 104 | 1/1 | 0.94 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | BB | 3018 | 1/1 | 0.94 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3175 | 1/1 | 0.94 | 0.17 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3124 | 1/1 | 0.94 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | BQ | 205 | 1/1 | 0.94 | 0.42 | 49,49,49,49 | 0 |
| 56 | MG | CA | 3044 | 1/1 | 0.94 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3178 | 1/1 | 0.94 | 0.28 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3261 | 1/1 | 0.94 | 0.26 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3306 | 1/1 | 0.94 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3565 | 1/1 | 0.94 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3572 | 1/1 | 0.94 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3465 | 1/1 | 0.94 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3146 | 1/1 | 0.94 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | BD | 307 | 1/1 | 0.94 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3417 | 1/1 | 0.94 | 0.18 | 18,18,18,18 | 0 |
| 56 | MG | BA | 3412 | 1/1 | 0.94 | 0.18 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3383 | 1/1 | 0.94 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3278 | 1/1 | 0.94 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3552 | 1/1 | 0.94 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3564 | 1/1 | 0.94 | 0.77 | 61,61,61,61 | 0 |
| 56 | MG | BR | 202 | 1/1 | 0.94 | 0.29 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3347 | 1/1 | 0.94 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3501 | 1/1 | 0.94 | 0.20 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3259 | 1/1 | 0.94 | 0.49 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3016 | 1/1 | 0.94 | 0.27 | 37,37,37,37 | 0 |
| 56 | MG | BY | 201 | 1/1 | 0.94 | 0.43 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3431 | 1/1 | 0.94 | 0.23 | 17,17,17,17 | 0 |
| 56 | MG | AA | 3109 | 1/1 | 0.94 | 0.33 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3018 | 1/1 | 0.94 | 0.34 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3209 | 1/1 | 0.94 | 0.40 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3482 | 1/1 | 0.94 | 0.17 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3717 | 1/1 | 0.94 | 0.22 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3204 | 1/1 | 0.94 | 0.41 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3044 | 1/1 | 0.94 | 0.30 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3688 | 1/1 | 0.94 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | DB | 3008 | 1/1 | 0.94 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3617 | 1/1 | 0.94 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | AA | 3054 | 1/1 | 0.94 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | CA | 3084 | 1/1 | 0.94 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3301 | 1/1 | 0.94 | 0.13 | 56,56,56,56 | 0 |
| 56 | MG | CF | 3001 | 1/1 | 0.94 | 0.22 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3494 | 1/1 | 0.95 | 0.09 | 78,78,78,78 | 0 |
| 56 | MG | CA | 3013 | 1/1 | 0.95 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3325 | 1/1 | 0.95 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3014 | 1/1 | 0.95 | 0.77 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3358 | 1/1 | 0.95 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3534 | 1/1 | 0.95 | 0.19 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3138 | 1/1 | 0.95 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3220 | 1/1 | 0.95 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3145 | 1/1 | 0.95 | 0.40 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3422 | 1/1 | 0.95 | 0.23 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3639 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3421 | 1/1 | 0.95 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | DB | 3010 | 1/1 | 0.95 | 0.18 | 73,73,73,73 | 0 |
| 56 | MG | CA | 3102 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | DD | 301 | 1/1 | 0.95 | 0.32 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3507 | 1/1 | 0.95 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3297 | 1/1 | 0.95 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3017 | 1/1 | 0.95 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3511 | 1/1 | 0.95 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3490 | 1/1 | 0.95 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3353 | 1/1 | 0.95 | 0.24 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3353 | 1/1 | 0.95 | 0.10 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3319 | 1/1 | 0.95 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | AA | 3196 | 1/1 | 0.95 | 0.31 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3053 | 1/1 | 0.95 | 0.35 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3382 | 1/1 | 0.95 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3645 | 1/1 | 0.95 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3329 | 1/1 | 0.95 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3047 | 1/1 | 0.95 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | BG | 3004 | 1/1 | 0.95 | 0.04 | 62,62,62,62 | 0 |
| 56 | MG | AA | 3130 | 1/1 | 0.95 | 0.23 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3197 | 1/1 | 0.95 | 0.45 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3510 | 1/1 | 0.95 | 0.24 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3594 | 1/1 | 0.95 | 0.31 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3326 | 1/1 | 0.95 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | AA | 3155 | 1/1 | 0.95 | 0.16 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3595 | 1/1 | 0.95 | 0.16 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3498 | 1/1 | 0.95 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3516 | 1/1 | 0.95 | 0.17 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3055 | 1/1 | 0.95 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3520 | 1/1 | 0.95 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3672 | 1/1 | 0.95 | 0.30 | 48,48,48,48 | 0 |
| 56 | MG | B5 | 502 | 1/1 | 0.95 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3397 | 1/1 | 0.95 | 0.19 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3233 | 1/1 | 0.95 | 0.18 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3479 | 1/1 | 0.95 | 0.19 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3121 | 1/1 | 0.95 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3461 | 1/1 | 0.95 | 0.24 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3312 | 1/1 | 0.95 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3283 | 1/1 | 0.95 | 0.21 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3330 | 1/1 | 0.95 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | AA | 3007 | 1/1 | 0.95 | 0.19 | 82,82,82,82 | 0 |
| 56 | MG | AA | 3187 | 1/1 | 0.95 | 0.04 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3078 | 1/1 | 0.95 | 0.26 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3545 | 1/1 | 0.95 | 0.24 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3267 | 1/1 | 0.95 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3001 | 1/1 | 0.95 | 0.30 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3004 | 1/1 | 0.95 | 0.19 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3348 | 1/1 | 0.95 | 0.20 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3605 | 1/1 | 0.95 | 0.30 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3580 | 1/1 | 0.95 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3588 | 1/1 | 0.95 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3576 | 1/1 | 0.95 | 0.26 | 23,23,23,23 | 0 |
| 56 | MG | CA | 3082 | 1/1 | 0.95 | 0.08 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3697 | 1/1 | 0.95 | 0.14 | 78,78,78,78 | 0 |
| 56 | MG | BV | 202 | 1/1 | 0.95 | 0.44 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3245 | 1/1 | 0.95 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3261 | 1/1 | 0.95 | 0.22 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3406 | 1/1 | 0.95 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3138 | 1/1 | 0.95 | 0.22 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3563 | 1/1 | 0.95 | 0.21 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3042 | 1/1 | 0.95 | 0.76 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3548 | 1/1 | 0.95 | 0.22 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3547 | 1/1 | 0.95 | 0.18 | 31,31,31,31 | 0 |
| 56 | MG | BU | 208 | 1/1 | 0.95 | 0.88 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3550 | 1/1 | 0.95 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3407 | 1/1 | 0.95 | 0.24 | 21,21,21,21 | 0 |
| 56 | MG | CA | 3156 | 1/1 | 0.95 | 0.15 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3216 | 1/1 | 0.95 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3700 | 1/1 | 0.95 | 0.12 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3470 | 1/1 | 0.95 | 0.24 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3306 | 1/1 | 0.95 | 0.21 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3202 | 1/1 | 0.95 | 0.24 | 41,41,41,41 | 0 |
| 56 | MG | DD | 306 | 1/1 | 0.95 | 1.14 | 44,44,44,44 | 0 |
| 56 | MG | AX | 104 | 1/1 | 0.95 | 0.14 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3627 | 1/1 | 0.95 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3271 | 1/1 | 0.95 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3614 | 1/1 | 0.95 | 0.20 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3010 | 1/1 | 0.95 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | AA | 3070 | 1/1 | 0.95 | 0.10 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3484 | 1/1 | 0.95 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3628 | 1/1 | 0.95 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3141 | 1/1 | 0.95 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3451 | 1/1 | 0.95 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | AA | 3195 | 1/1 | 0.95 | 0.16 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3339 | 1/1 | 0.95 | 0.22 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3118 | 1/1 | 0.95 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | AA | 3056 | 1/1 | 0.95 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | CA | 3020 | 1/1 | 0.95 | 0.18 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3201 | 1/1 | 0.95 | 0.29 | 36,36,36,36 | 0 |
| 56 | MG | AA | 3168 | 1/1 | 0.95 | 0.31 | 68,68,68,68 | 0 |
| 56 | MG | AA | 3083 | 1/1 | 0.95 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3555 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | DB | 3006 | 1/1 | 0.95 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3286 | 1/1 | 0.95 | 0.26 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3129 | 1/1 | 0.95 | 0.25 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3648 | 1/1 | 0.95 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3284 | 1/1 | 0.95 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | BV | 203 | 1/1 | 0.95 | 1.03 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3037 | 1/1 | 0.95 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | DE | 306 | 1/1 | 0.95 | 0.14 | 32,32,32,32 | 0 |
| 56 | MG | AA | 3213 | 1/1 | 0.95 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | CA | 3011 | 1/1 | 0.95 | 0.28 | 42,42,42,42 | 0 |
| 56 | MG | AA | 3040 | 1/1 | 0.95 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3332 | 1/1 | 0.95 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | AA | 3078 | 1/1 | 0.95 | 0.27 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3229 | 1/1 | 0.95 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3030 | 1/1 | 0.95 | 0.28 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3322 | 1/1 | 0.95 | 0.13 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3506 | 1/1 | 0.95 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | CA | 3090 | 1/1 | 0.95 | 0.18 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3298 | 1/1 | 0.95 | 0.32 | 37,37,37,37 | 0 |
| 56 | MG | D5 | 102 | 1/1 | 0.95 | 0.58 | 55,55,55,55 | 0 |
| 56 | MG | AA | 3064 | 1/1 | 0.95 | 0.30 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3441 | 1/1 | 0.95 | 0.25 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3620 | 1/1 | 0.95 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | AA | 3111 | 1/1 | 0.95 | 0.17 | 95,95,95,95 | 0 |
| 56 | MG | DA | 3396 | 1/1 | 0.95 | 0.19 | 35,35,35,35 | 0 |
| 56 | MG | CA | 3108 | 1/1 | 0.95 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3506 | 1/1 | 0.95 | 0.07 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3154 | 1/1 | 0.95 | 0.61 | 45,45,45,45 | 0 |
| 56 | MG | AA | 3126 | 1/1 | 0.95 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3169 | 1/1 | 0.95 | 0.70 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3224 | 1/1 | 0.95 | 0.73 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3535 | 1/1 | 0.95 | 0.19 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3601 | 1/1 | 0.95 | 0.12 | 77,77,77,77 | 0 |
| 56 | MG | AA | 3216 | 1/1 | 0.95 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3189 | 1/1 | 0.95 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3540 | 1/1 | 0.95 | 0.27 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3097 | 1/1 | 0.95 | 0.19 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3619 | 1/1 | 0.95 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3522 | 1/1 | 0.95 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3041 | 1/1 | 0.95 | 0.38 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3083 | 1/1 | 0.95 | 0.25 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3350 | 1/1 | 0.95 | 0.04 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3232 | 1/1 | 0.95 | 0.25 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3260 | 1/1 | 0.95 | 0.17 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3541 | 1/1 | 0.95 | 0.23 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3384 | 1/1 | 0.95 | 0.11 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3654 | 1/1 | 0.95 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | CA | 3094 | 1/1 | 0.95 | 0.18 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3276 | 1/1 | 0.95 | 0.32 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3034 | 1/1 | 0.95 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | DB | 3002 | 1/1 | 0.95 | 0.25 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3120 | 1/1 | 0.95 | 0.76 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3299 | 1/1 | 0.95 | 0.22 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3444 | 1/1 | 0.95 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3004 | 1/1 | 0.95 | 0.12 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3558 | 1/1 | 0.95 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3570 | 1/1 | 0.95 | 0.22 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3566 | 1/1 | 0.95 | 0.14 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3616 | 1/1 | 0.95 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3263 | 1/1 | 0.95 | 0.19 | 31,31,31,31 | 0 |
| 56 | MG | CA | 3075 | 1/1 | 0.95 | 0.17 | 76,76,76,76 | 0 |
| 56 | MG | BE | 307 | 1/1 | 0.95 | 0.24 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3618 | 1/1 | 0.95 | 0.27 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3585 | 1/1 | 0.95 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3589 | 1/1 | 0.95 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | AA | 3170 | 1/1 | 0.95 | 0.16 | 101,101,101,101 | 0 |
| 56 | MG | DA | 3130 | 1/1 | 0.95 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | BN | 3005 | 1/1 | 0.95 | 0.85 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3434 | 1/1 | 0.95 | 0.26 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3565 | 1/1 | 0.95 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3500 | 1/1 | 0.95 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3603 | 1/1 | 0.95 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3059 | 1/1 | 0.95 | 0.60 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3626 | 1/1 | 0.95 | 0.07 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3411 | 1/1 | 0.95 | 0.17 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3043 | 1/1 | 0.95 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3101 | 1/1 | 0.95 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3031 | 1/1 | 0.95 | 0.29 | 55,55,55,55 | 0 |
| 56 | MG | AA | 3148 | 1/1 | 0.95 | 0.21 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3307 | 1/1 | 0.95 | 0.30 | 37,37,37,37 | 0 |
| 56 | MG | BU | 202 | 1/1 | 0.95 | 0.36 | 32,32,32,32 | 0 |
| 56 | MG | BP | 201 | 1/1 | 0.95 | 0.66 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3576 | 1/1 | 0.95 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | CA | 3066 | 1/1 | 0.95 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3595 | 1/1 | 0.95 | 0.18 | 72,72,72,72 | 0 |
| 56 | MG | AA | 3122 | 1/1 | 0.95 | 0.54 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3073 | 1/1 | 0.95 | 0.85 | 41,41,41,41 | 0 |
| 56 | MG | CA | 3009 | 1/1 | 0.95 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3674 | 1/1 | 0.95 | 0.18 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3654 | 1/1 | 0.95 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3021 | 1/1 | 0.95 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3426 | 1/1 | 0.96 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3709 | 1/1 | 0.96 | 0.12 | 86,86,86,86 | 0 |
| 56 | MG | BA | 3324 | 1/1 | 0.96 | 0.18 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3422 | 1/1 | 0.96 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3007 | 1/1 | 0.96 | 0.23 | 30,30,30,30 | 0 |
| 56 | MG | D3 | 101 | 1/1 | 0.96 | 0.45 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3276 | 1/1 | 0.96 | 0.22 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3630 | 1/1 | 0.96 | 0.25 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3417 | 1/1 | 0.96 | 0.15 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3385 | 1/1 | 0.96 | 0.24 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3270 | 1/1 | 0.96 | 0.20 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3199 | 1/1 | 0.96 | 0.46 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3259 | 1/1 | 0.96 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | CA | 3028 | 1/1 | 0.96 | 0.44 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3413 | 1/1 | 0.96 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3405 | 1/1 | 0.96 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | AA | 3178 | 1/1 | 0.96 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | AA | 3157 | 1/1 | 0.96 | 0.08 | 35,35,35,35 | 0 |
| 56 | MG | CA | 3132 | 1/1 | 0.96 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3082 | 1/1 | 0.96 | 0.10 | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3606 | 1/1 | 0.96 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3182 | 1/1 | 0.96 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3440 | 1/1 | 0.96 | 0.40 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3512 | 1/1 | 0.96 | 0.23 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3348 | 1/1 | 0.96 | 0.32 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3395 | 1/1 | 0.96 | 0.20 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3366 | 1/1 | 0.96 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3416 | 1/1 | 0.96 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3524 | 1/1 | 0.96 | 0.25 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3223 | 1/1 | 0.96 | 0.68 | 47,47,47,47 | 0 |
| 56 | MG | CA | 3113 | 1/1 | 0.96 | 0.23 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3367 | 1/1 | 0.96 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3615 | 1/1 | 0.96 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3537 | 1/1 | 0.96 | 0.38 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3217 | 1/1 | 0.96 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3486 | 1/1 | 0.96 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3321 | 1/1 | 0.96 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3409 | 1/1 | 0.96 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3035 | 1/1 | 0.96 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3651 | 1/1 | 0.96 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | DE | 301 | 1/1 | 0.96 | 0.61 | 51,51,51,51 | 0 |
| 56 | MG | BV | 204 | 1/1 | 0.96 | 0.20 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3607 | 1/1 | 0.96 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3463 | 1/1 | 0.96 | 0.37 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3538 | 1/1 | 0.96 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3368 | 1/1 | 0.96 | 0.20 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3568 | 1/1 | 0.96 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | DB | 3004 | 1/1 | 0.96 | 0.14 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3380 | 1/1 | 0.96 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | CA | 3145 | 1/1 | 0.96 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3191 | 1/1 | 0.96 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3076 | 1/1 | 0.96 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3584 | 1/1 | 0.96 | 0.18 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3649 | 1/1 | 0.96 | 0.17 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3121 | 1/1 | 0.96 | 0.27 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3118 | 1/1 | 0.96 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | AA | 3175 | 1/1 | 0.96 | 0.14 | 76,76,76,76 | 0 |
| 56 | MG | CA | 3026 | 1/1 | 0.96 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3420 | 1/1 | 0.96 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3234 | 1/1 | 0.96 | 0.30 | 55,55,55,55 | 0 |
| 56 | MG | BB | 3002 | 1/1 | 0.96 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3130 | 1/1 | 0.96 | 0.58 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3176 | 1/1 | 0.96 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3117 | 1/1 | 0.96 | 0.24 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3403 | 1/1 | 0.96 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | CA | 3096 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3485 | 1/1 | 0.96 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3266 | 1/1 | 0.96 | 0.33 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3341 | 1/1 | 0.96 | 0.19 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3151 | 1/1 | 0.96 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3665 | 1/1 | 0.96 | 0.21 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3021 | 1/1 | 0.96 | 0.27 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3359 | 1/1 | 0.96 | 0.20 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3345 | 1/1 | 0.96 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3542 | 1/1 | 0.96 | 0.23 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3429 | 1/1 | 0.96 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3203 | 1/1 | 0.96 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3247 | 1/1 | 0.96 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3642 | 1/1 | 0.96 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3477 | 1/1 | 0.96 | 0.11 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3340 | 1/1 | 0.96 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | AA | 3055 | 1/1 | 0.96 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3551 | 1/1 | 0.96 | 0.22 | 25,25,25,25 | 0 |
| 56 | MG | BE | 301 | 1/1 | 0.96 | 0.56 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3488 | 1/1 | 0.96 | 0.35 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3637 | 1/1 | 0.96 | 0.28 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3685 | 1/1 | 0.96 | 0.09 | 67,67,67,67 | 0 |
| 56 | MG | AA | 3108 | 1/1 | 0.96 | 0.47 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3054 | 1/1 | 0.96 | 0.29 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3606 | 1/1 | 0.96 | 0.23 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3622 | 1/1 | 0.96 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3153 | 1/1 | 0.96 | 0.20 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3201 | 1/1 | 0.96 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3472 | 1/1 | 0.96 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3641 | 1/1 | 0.96 | 0.43 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3737 | 1/1 | 0.96 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | DV | 201 | 1/1 | 0.96 | 0.38 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3248 | 1/1 | 0.96 | 0.29 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3715 | 1/1 | 0.96 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | DN | 5001 | 1/1 | 0.96 | 0.12 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3289 | 1/1 | 0.96 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3491 | 1/1 | 0.96 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | BD | 309 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3605 | 1/1 | 0.96 | 0.15 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3166 | 1/1 | 0.96 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3361 | 1/1 | 0.96 | 0.26 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3381 | 1/1 | 0.96 | 0.27 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3571 | 1/1 | 0.96 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | DF | 306 | 1/1 | 0.96 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3013 | 1/1 | 0.96 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3158 | 1/1 | 0.96 | 0.34 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3386 | 1/1 | 0.96 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3439 | 1/1 | 0.96 | 0.19 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3629 | 1/1 | 0.96 | 0.17 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3399 | 1/1 | 0.96 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | BG | 3003 | 1/1 | 0.96 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3503 | 1/1 | 0.96 | 0.28 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3213 | 1/1 | 0.96 | 0.05 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3109 | 1/1 | 0.96 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3557 | 1/1 | 0.96 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3485 | 1/1 | 0.96 | 0.29 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3257 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3513 | 1/1 | 0.96 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3432 | 1/1 | 0.96 | 0.27 | 66,66,66,66 | 0 |
| 56 | MG | DE | 304 | 1/1 | 0.96 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3091 | 1/1 | 0.96 | 0.38 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3311 | 1/1 | 0.96 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3219 | 1/1 | 0.96 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3397 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3291 | 1/1 | 0.96 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3001 | 1/1 | 0.96 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3642 | 1/1 | 0.96 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | AD | 502 | 1/1 | 0.96 | 0.46 | 43,43,43,43 | 0 |
| 56 | MG | AA | 3104 | 1/1 | 0.96 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3015 | 1/1 | 0.96 | 0.34 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3384 | 1/1 | 0.96 | 0.39 | 60,60,60,60 | 0 |
| 56 | MG | CA | 3095 | 1/1 | 0.96 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3112 | 1/1 | 0.96 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3561 | 1/1 | 0.96 | 0.19 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3648 | 1/1 | 0.96 | 0.30 | 49,49,49,49 | 0 |
| 56 | MG | AA | 3099 | 1/1 | 0.96 | 0.42 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3457 | 1/1 | 0.96 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3333 | 1/1 | 0.96 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | BD | 302 | 1/1 | 0.96 | 0.36 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3726 | 1/1 | 0.96 | 0.55 | 47,47,47,47 | 0 |
| 56 | MG | AA | 3021 | 1/1 | 0.96 | 0.20 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3530 | 1/1 | 0.96 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | AA | 3183 | 1/1 | 0.96 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3497 | 1/1 | 0.96 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3115 | 1/1 | 0.96 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | AA | 3107 | 1/1 | 0.96 | 0.31 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3707 | 1/1 | 0.96 | 0.20 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3639 | 1/1 | 0.96 | 0.30 | 15,15,15,15 | 0 |
| 56 | MG | DA | 3513 | 1/1 | 0.96 | 0.22 | 49,49,49,49 | 0 |
| 56 | MG | BB | 3007 | 1/1 | 0.96 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | AA | 3161 | 1/1 | 0.96 | 0.12 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3265 | 1/1 | 0.96 | 0.11 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3468 | 1/1 | 0.96 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3389 | 1/1 | 0.96 | 0.28 | 27,27,27,27 | 0 |
| 56 | MG | BP | 204 | 1/1 | 0.96 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3039 | 1/1 | 0.96 | 0.40 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3094 | 1/1 | 0.96 | 0.18 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3625 | 1/1 | 0.96 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3543 | 1/1 | 0.96 | 0.29 | 52,52,52,52 | 0 |
| 56 | MG | AA | 3174 | 1/1 | 0.96 | 0.22 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3152 | 1/1 | 0.96 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3607 | 1/1 | 0.96 | 0.43 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3266 | 1/1 | 0.96 | 0.23 | 43,43,43,43 | 0 |
| 56 | MG | CA | 3072 | 1/1 | 0.96 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | BW | 202 | 1/1 | 0.96 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3249 | 1/1 | 0.96 | 0.21 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3575 | 1/1 | 0.96 | 0.19 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3663 | 1/1 | 0.96 | 0.23 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3178 | 1/1 | 0.96 | 0.37 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3235 | 1/1 | 0.96 | 0.19 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3206 | 1/1 | 0.96 | 0.26 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3498 | 1/1 | 0.96 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3577 | 1/1 | 0.96 | 0.25 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3343 | 1/1 | 0.96 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3153 | 1/1 | 0.96 | 0.13 | 45,45,45,45 | 0 |
| 58 | ZN | D9 | 501 | 1/1 | 0.96 | 0.05 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3633 | 1/1 | 0.96 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3025 | 1/1 | 0.96 | 0.25 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3483 | 1/1 | 0.96 | 0.26 | 53,53,53,53 | 0 |
| 56 | MG | BW | 204 | 1/1 | 0.96 | 0.35 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3575 | 1/1 | 0.96 | 0.19 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3425 | 1/1 | 0.96 | 0.11 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3566 | 1/1 | 0.96 | 0.09 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3518 | 1/1 | 0.96 | 0.20 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3426 | 1/1 | 0.96 | 0.15 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3287 | 1/1 | 0.96 | 0.27 | 53,53,53,53 | 0 |
| 56 | MG | CA | 3012 | 1/1 | 0.96 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3345 | 1/1 | 0.96 | 0.21 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3458 | 1/1 | 0.96 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3425 | 1/1 | 0.96 | 0.36 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3265 | 1/1 | 0.96 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3657 | 1/1 | 0.96 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3536 | 1/1 | 0.96 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3504 | 1/1 | 0.96 | 0.29 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3628 | 1/1 | 0.96 | 0.22 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3362 | 1/1 | 0.96 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3133 | 1/1 | 0.96 | 0.15 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3637 | 1/1 | 0.96 | 0.35 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3328 | 1/1 | 0.96 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3142 | 1/1 | 0.96 | 0.24 | 33,33,33,33 | 0 |
| 56 | MG | BD | 303 | 1/1 | 0.96 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3427 | 1/1 | 0.96 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | BV | 201 | 1/1 | 0.96 | 0.40 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3667 | 1/1 | 0.96 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3434 | 1/1 | 0.96 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3294 | 1/1 | 0.96 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3376 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3106 | 1/1 | 0.96 | 0.25 | 56,56,56,56 | 0 |
| 56 | MG | AA | 3149 | 1/1 | 0.96 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3093 | 1/1 | 0.96 | 0.22 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3319 | 1/1 | 0.96 | 0.17 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3544 | 1/1 | 0.96 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3604 | 1/1 | 0.96 | 0.11 | 72,72,72,72 | 0 |
| 56 | MG | CA | 3004 | 1/1 | 0.96 | 0.21 | 96,96,96,96 | 0 |
| 56 | MG | CA | 3078 | 1/1 | 0.96 | 0.29 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3220 | 1/1 | 0.97 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3374 | 1/1 | 0.97 | 0.05 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3317 | 1/1 | 0.97 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3057 | 1/1 | 0.97 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3563 | 1/1 | 0.97 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3587 | 1/1 | 0.97 | 0.18 | 23,23,23,23 | 0 |
| 56 | MG | BD | 308 | 1/1 | 0.97 | 0.33 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3701 | 1/1 | 0.97 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3077 | 1/1 | 0.97 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3445 | 1/1 | 0.97 | 0.23 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3119 | 1/1 | 0.97 | 0.25 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3323 | 1/1 | 0.97 | 0.15 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3456 | 1/1 | 0.97 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3309 | 1/1 | 0.97 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3296 | 1/1 | 0.97 | 0.25 | 46,46,46,46 | 0 |
| 56 | MG | D0 | 101 | 1/1 | 0.97 | 0.12 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3115 | 1/1 | 0.97 | 0.26 | 36,36,36,36 | 0 |
| 56 | MG | DD | 304 | 1/1 | 0.97 | 0.23 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3450 | 1/1 | 0.97 | 0.27 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3360 | 1/1 | 0.97 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3349 | 1/1 | 0.97 | 0.26 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3437 | 1/1 | 0.97 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3184 | 1/1 | 0.97 | 0.38 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3032 | 1/1 | 0.97 | 0.19 | 49,49,49,49 | 0 |
| 56 | MG | BF | 301 | 1/1 | 0.97 | 0.52 | 45,45,45,45 | 0 |
| 56 | MG | CX | 104 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3621 | 1/1 | 0.97 | 0.36 | 74,74,74,74 | 0 |
| 56 | MG | BB | 3015 | 1/1 | 0.97 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | CA | 3121 | 1/1 | 0.97 | 0.27 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3242 | 1/1 | 0.97 | 0.23 | 35,35,35,35 | 0 |
| 56 | MG | BQ | 204 | 1/1 | 0.97 | 0.18 | 12,12,12,12 | 0 |
| 56 | MG | CA | 3118 | 1/1 | 0.97 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3564 | 1/1 | 0.97 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3037 | 1/1 | 0.97 | 0.30 | 35,35,35,35 | 0 |
| 56 | MG | CA | 3120 | 1/1 | 0.97 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3251 | 1/1 | 0.97 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3596 | 1/1 | 0.97 | 0.10 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3063 | 1/1 | 0.97 | 0.28 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3530 | 1/1 | 0.97 | 0.28 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3034 | 1/1 | 0.97 | 0.41 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3203 | 1/1 | 0.97 | 0.26 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3471 | 1/1 | 0.97 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3272 | 1/1 | 0.97 | 0.34 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3171 | 1/1 | 0.97 | 0.41 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3232 | 1/1 | 0.97 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | AA | 3221 | 1/1 | 0.97 | 0.10 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3455 | 1/1 | 0.97 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | CA | 3130 | 1/1 | 0.97 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3636 | 1/1 | 0.97 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | AA | 3186 | 1/1 | 0.97 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3446 | 1/1 | 0.97 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3085 | 1/1 | 0.97 | 0.12 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3156 | 1/1 | 0.97 | 0.17 | 62,62,62,62 | 0 |
| 56 | MG | CX | 102 | 1/1 | 0.97 | 0.06 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3495 | 1/1 | 0.97 | 0.22 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3539 | 1/1 | 0.97 | 0.16 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3335 | 1/1 | 0.97 | 0.26 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3176 | 1/1 | 0.97 | 0.27 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3436 | 1/1 | 0.97 | 0.07 | 62,62,62,62 | 0 |
| 58 | ZN | D6 | 501 | 1/1 | 0.97 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3586 | 1/1 | 0.97 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3267 | 1/1 | 0.97 | 0.16 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3338 | 1/1 | 0.97 | 0.21 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3344 | 1/1 | 0.97 | 0.11 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3258 | 1/1 | 0.97 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | AA | 3158 | 1/1 | 0.97 | 0.20 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3490 | 1/1 | 0.97 | 0.26 | 38,38,38,38 | 0 |
| 58 | ZN | DY | 501 | 1/1 | 0.97 | 0.05 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3431 | 1/1 | 0.97 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3486 | 1/1 | 0.97 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3584 | 1/1 | 0.97 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3160 | 1/1 | 0.97 | 0.30 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3322 | 1/1 | 0.97 | 0.23 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3239 | 1/1 | 0.97 | 0.21 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3274 | 1/1 | 0.97 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3720 | 1/1 | 0.97 | 0.20 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3521 | 1/1 | 0.97 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3518 | 1/1 | 0.97 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3573 | 1/1 | 0.97 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3160 | 1/1 | 0.97 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3162 | 1/1 | 0.97 | 0.19 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3428 | 1/1 | 0.97 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3302 | 1/1 | 0.97 | 0.18 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3327 | 1/1 | 0.97 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | BE | 304 | 1/1 | 0.97 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | CA | 3043 | 1/1 | 0.97 | 0.34 | 49,49,49,49 | 0 |
| 56 | MG | CA | 3083 | 1/1 | 0.97 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3369 | 1/1 | 0.97 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | AA | 3208 | 1/1 | 0.97 | 0.34 | 46,46,46,46 | 0 |
| 56 | MG | CA | 3050 | 1/1 | 0.97 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3449 | 1/1 | 0.97 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3173 | 1/1 | 0.97 | 0.41 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3583 | 1/1 | 0.97 | 0.28 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3170 | 1/1 | 0.97 | 0.66 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DQ | 203 | 1/1 | 0.97 | 0.32 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3630 | 1/1 | 0.97 | 0.20 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3710 | 1/1 | 0.97 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3176 | 1/1 | 0.97 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3600 | 1/1 | 0.97 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3210 | 1/1 | 0.97 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3282 | 1/1 | 0.97 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3302 | 1/1 | 0.97 | 0.13 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3547 | 1/1 | 0.97 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3002 | 1/1 | 0.97 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3694 | 1/1 | 0.97 | 0.37 | 56,56,56,56 | 0 |
| 56 | MG | AX | 110 | 1/1 | 0.97 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3623 | 1/1 | 0.97 | 0.21 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3489 | 1/1 | 0.97 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3241 | 1/1 | 0.97 | 0.21 | 15,15,15,15 | 0 |
| 56 | MG | DA | 3023 | 1/1 | 0.97 | 0.28 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3212 | 1/1 | 0.97 | 0.28 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3088 | 1/1 | 0.97 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3300 | 1/1 | 0.97 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3682 | 1/1 | 0.97 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3180 | 1/1 | 0.97 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3559 | 1/1 | 0.97 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3182 | 1/1 | 0.97 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3493 | 1/1 | 0.97 | 0.37 | 15,15,15,15 | 0 |
| 56 | MG | DA | 3421 | 1/1 | 0.97 | 0.19 | 34,34,34,34 | 0 |
| 56 | MG | DO | 5001 | 1/1 | 0.97 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3412 | 1/1 | 0.97 | 0.28 | 30,30,30,30 | 0 |
| 56 | MG | AA | 3204 | 1/1 | 0.97 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | CA | 3166 | 1/1 | 0.97 | 0.23 | 59,59,59,59 | 0 |
| 56 | MG | AA | 3102 | 1/1 | 0.97 | 0.06 | 64,64,64,64 | 0 |
| 56 | MG | BP | 202 | 1/1 | 0.97 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3552 | 1/1 | 0.97 | 0.23 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3120 | 1/1 | 0.97 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3364 | 1/1 | 0.97 | 0.24 | 29,29,29,29 | 0 |
| 56 | MG | AA | 3185 | 1/1 | 0.97 | 0.28 | 46,46,46,46 | 0 |
| 56 | MG | DQ | 204 | 1/1 | 0.97 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3644 | 1/1 | 0.97 | 0.16 | 43,43,43,43 | 0 |
| 56 | MG | DD | 303 | 1/1 | 0.97 | 0.20 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3680 | 1/1 | 0.97 | 0.35 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3508 | 1/1 | 0.97 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3116 | 1/1 | 0.97 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3311 | 1/1 | 0.97 | 0.23 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3371 | 1/1 | 0.97 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3554 | 1/1 | 0.97 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3096 | 1/1 | 0.97 | 0.35 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3275 | 1/1 | 0.97 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3455 | 1/1 | 0.97 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3572 | 1/1 | 0.97 | 0.20 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3616 | 1/1 | 0.97 | 0.23 | 62,62,62,62 | 0 |
| 56 | MG | BF | 305 | 1/1 | 0.97 | 0.32 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3550 | 1/1 | 0.97 | 0.24 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3404 | 1/1 | 0.97 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3428 | 1/1 | 0.97 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3294 | 1/1 | 0.97 | 0.28 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3167 | 1/1 | 0.97 | 0.39 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3734 | 1/1 | 0.97 | 0.26 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3514 | 1/1 | 0.97 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3479 | 1/1 | 0.97 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3351 | 1/1 | 0.97 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3291 | 1/1 | 0.97 | 0.24 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3396 | 1/1 | 0.97 | 0.18 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3504 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3593 | 1/1 | 0.97 | 0.14 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3438 | 1/1 | 0.97 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3315 | 1/1 | 0.97 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3571 | 1/1 | 0.97 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | BE | 310 | 1/1 | 0.97 | 0.24 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3705 | 1/1 | 0.97 | 0.05 | 39,39,39,39 | 0 |
| 56 | MG | CA | 3088 | 1/1 | 0.97 | 0.26 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3026 | 1/1 | 0.97 | 0.47 | 36,36,36,36 | 0 |
| 56 | MG | CA | 3171 | 1/1 | 0.97 | 0.32 | 67,67,67,67 | 0 |
| 56 | MG | CA | 3049 | 1/1 | 0.97 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3375 | 1/1 | 0.97 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3582 | 1/1 | 0.97 | 0.22 | 25,25,25,25 | 0 |
| 56 | MG | BB | 3001 | 1/1 | 0.97 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | BF | 306 | 1/1 | 0.97 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3517 | 1/1 | 0.97 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3262 | 1/1 | 0.97 | 0.22 | 44,44,44,44 | 0 |
| 56 | MG | AA | 3207 | 1/1 | 0.97 | 0.28 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3064 | 1/1 | 0.97 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3349 | 1/1 | 0.97 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3379 | 1/1 | 0.97 | 0.22 | 22,22,22,22 | 0 |
| 56 | MG | BO | 201 | 1/1 | 0.97 | 0.14 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3136 | 1/1 | 0.97 | 0.11 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3329 | 1/1 | 0.97 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | CA | 3169 | 1/1 | 0.97 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3695 | 1/1 | 0.97 | 0.17 | 15,15,15,15 | 0 |
| 56 | MG | DA | 3184 | 1/1 | 0.97 | 0.32 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3003 | 1/1 | 0.97 | 0.16 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3269 | 1/1 | 0.97 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3473 | 1/1 | 0.97 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | AA | 3150 | 1/1 | 0.97 | 0.27 | 46,46,46,46 | 0 |
| 56 | MG | AA | 3203 | 1/1 | 0.97 | 0.12 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3650 | 1/1 | 0.97 | 0.58 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3721 | 1/1 | 0.97 | 0.08 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3646 | 1/1 | 0.97 | 0.23 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3204 | 1/1 | 0.97 | 0.40 | 25,25,25,25 | 0 |
| 56 | MG | B8 | 103 | 1/1 | 0.97 | 0.19 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3392 | 1/1 | 0.97 | 0.26 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3363 | 1/1 | 0.97 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3031 | 1/1 | 0.97 | 0.79 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3527 | 1/1 | 0.97 | 0.18 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3274 | 1/1 | 0.97 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3475 | 1/1 | 0.97 | 0.21 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3696 | 1/1 | 0.97 | 0.26 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3729 | 1/1 | 0.97 | 0.40 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3451 | 1/1 | 0.97 | 0.30 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3493 | 1/1 | 0.97 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | AA | 3171 | 1/1 | 0.97 | 0.25 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3629 | 1/1 | 0.97 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3239 | 1/1 | 0.97 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3314 | 1/1 | 0.97 | 0.17 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3534 | 1/1 | 0.97 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3368 | 1/1 | 0.97 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3400 | 1/1 | 0.97 | 0.19 | 24,24,24,24 | 0 |
| 56 | MG | BP | 203 | 1/1 | 0.97 | 0.69 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3668 | 1/1 | 0.97 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3546 | 1/1 | 0.97 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3333 | 1/1 | 0.97 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3033 | 1/1 | 0.97 | 0.37 | 35,35,35,35 | 0 |
| 56 | MG | CA | 3101 | 1/1 | 0.97 | 0.18 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3713 | 1/1 | 0.97 | 0.10 | 66,66,66,66 | 0 |
| 56 | MG | CA | 3052 | 1/1 | 0.97 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3469 | 1/1 | 0.97 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3043 | 1/1 | 0.97 | 0.45 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3435 | 1/1 | 0.97 | 0.23 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3192 | 1/1 | 0.97 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3173 | 1/1 | 0.97 | 0.58 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3488 | 1/1 | 0.97 | 0.04 | 46,46,46,46 | 0 |
| 56 | MG | BR | 203 | 1/1 | 0.97 | 0.18 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3532 | 1/1 | 0.97 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3352 | 1/1 | 0.97 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3080 | 1/1 | 0.97 | 0.52 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3390 | 1/1 | 0.97 | 0.25 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3447 | 1/1 | 0.97 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | CA | 3112 | 1/1 | 0.97 | 0.23 | 59,59,59,59 | 0 |
| 56 | MG | CA | 3059 | 1/1 | 0.97 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | CA | 3045 | 1/1 | 0.97 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3356 | 1/1 | 0.97 | 0.11 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3556 | 1/1 | 0.98 | 0.31 | 27,27,27,27 | 0 |
| 56 | MG | AA | 3193 | 1/1 | 0.98 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3602 | 1/1 | 0.98 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3433 | 1/1 | 0.98 | 0.24 | 39,39,39,39 | 0 |
| 58 | ZN | BY | 202 | 1/1 | 0.98 | 0.09 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3215 | 1/1 | 0.98 | 0.30 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3475 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3436 | 1/1 | 0.98 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3411 | 1/1 | 0.98 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | CA | 3051 | 1/1 | 0.98 | 0.10 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3393 | 1/1 | 0.98 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3551 | 1/1 | 0.98 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3723 | 1/1 | 0.98 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3150 | 1/1 | 0.98 | 0.45 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3177 | 1/1 | 0.98 | 0.08 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3313 | 1/1 | 0.98 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3445 | 1/1 | 0.98 | 0.20 | 25,25,25,25 | 0 |
| 56 | MG | BB | 3016 | 1/1 | 0.98 | 0.12 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3491 | 1/1 | 0.98 | 0.19 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3404 | 1/1 | 0.98 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | AA | 3179 | 1/1 | 0.98 | 0.26 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3290 | 1/1 | 0.98 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3347 | 1/1 | 0.98 | 0.27 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3733 | 1/1 | 0.98 | 0.11 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3310 | 1/1 | 0.98 | 0.17 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3308 | 1/1 | 0.98 | 0.32 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3591 | 1/1 | 0.98 | 0.32 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3424 | 1/1 | 0.98 | 0.17 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3569 | 1/1 | 0.98 | 0.18 | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CE | 3002 | 1/1 | 0.98 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3337 | 1/1 | 0.98 | 0.17 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3480 | 1/1 | 0.98 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3341 | 1/1 | 0.98 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3268 | 1/1 | 0.98 | 0.17 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3679 | 1/1 | 0.98 | 0.40 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3448 | 1/1 | 0.98 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3207 | 1/1 | 0.98 | 0.23 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3681 | 1/1 | 0.98 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3165 | 1/1 | 0.98 | 0.15 | 23,23,23,23 | 0 |
| 56 | MG | CA | 3128 | 1/1 | 0.98 | 0.26 | 41,41,41,41 | 0 |
| 56 | MG | AA | 3220 | 1/1 | 0.98 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3010 | 1/1 | 0.98 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3586 | 1/1 | 0.98 | 0.19 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3354 | 1/1 | 0.98 | 0.15 | 27,27,27,27 | 0 |
| 56 | MG | CA | 3098 | 1/1 | 0.98 | 0.23 | 46,46,46,46 | 0 |
| 56 | MG | BN | 3004 | 1/1 | 0.98 | 0.40 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3081 | 1/1 | 0.98 | 0.08 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3380 | 1/1 | 0.98 | 0.16 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3525 | 1/1 | 0.98 | 0.23 | 43,43,43,43 | 0 |
| 56 | MG | CA | 3064 | 1/1 | 0.98 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3569 | 1/1 | 0.98 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3487 | 1/1 | 0.98 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3236 | 1/1 | 0.98 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3283 | 1/1 | 0.98 | 0.15 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3372 | 1/1 | 0.98 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3420 | 1/1 | 0.98 | 0.30 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3418 | 1/1 | 0.98 | 0.15 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3035 | 1/1 | 0.98 | 0.23 | 56,56,56,56 | 0 |
| 56 | MG | BB | 3013 | 1/1 | 0.98 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3059 | 1/1 | 0.98 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | B8 | 102 | 1/1 | 0.98 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3174 | 1/1 | 0.98 | 0.26 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3523 | 1/1 | 0.98 | 0.06 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3370 | 1/1 | 0.98 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3418 | 1/1 | 0.98 | 0.17 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3026 | 1/1 | 0.98 | 0.21 | 37,37,37,37 | 0 |
| 56 | MG | BU | 207 | 1/1 | 0.98 | 0.21 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3316 | 1/1 | 0.98 | 0.16 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3264 | 1/1 | 0.98 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3454 | 1/1 | 0.98 | 0.09 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3561 | 1/1 | 0.98 | 0.19 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3448 | 1/1 | 0.98 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3600 | 1/1 | 0.98 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3228 | 1/1 | 0.98 | 0.27 | 63,63,63,63 | 0 |
| 56 | MG | BB | 3012 | 1/1 | 0.98 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3557 | 1/1 | 0.98 | 0.23 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3522 | 1/1 | 0.98 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3477 | 1/1 | 0.98 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | B3 | 101 | 1/1 | 0.98 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3394 | 1/1 | 0.98 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3113 | 1/1 | 0.98 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | CA | 3022 | 1/1 | 0.98 | 0.04 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3588 | 1/1 | 0.98 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3389 | 1/1 | 0.98 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3277 | 1/1 | 0.98 | 0.25 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3244 | 1/1 | 0.98 | 0.31 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3337 | 1/1 | 0.98 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | CA | 3168 | 1/1 | 0.98 | 0.39 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3670 | 1/1 | 0.98 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | CA | 3148 | 1/1 | 0.98 | 0.19 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3408 | 1/1 | 0.98 | 0.22 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3544 | 1/1 | 0.98 | 0.23 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3036 | 1/1 | 0.98 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | BU | 203 | 1/1 | 0.98 | 0.35 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3317 | 1/1 | 0.98 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | BE | 308 | 1/1 | 0.98 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3008 | 1/1 | 0.98 | 0.13 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3316 | 1/1 | 0.98 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3165 | 1/1 | 0.98 | 0.24 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3222 | 1/1 | 0.98 | 0.29 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3649 | 1/1 | 0.98 | 0.24 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3529 | 1/1 | 0.98 | 0.10 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3574 | 1/1 | 0.98 | 0.08 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3467 | 1/1 | 0.98 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3027 | 1/1 | 0.98 | 0.06 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3305 | 1/1 | 0.98 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3205 | 1/1 | 0.98 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3541 | 1/1 | 0.98 | 0.28 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3581 | 1/1 | 0.98 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3382 | 1/1 | 0.98 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3365 | 1/1 | 0.98 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | BD | 310 | 1/1 | 0.98 | 0.31 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3533 | 1/1 | 0.98 | 0.18 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3062 | 1/1 | 0.98 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3250 | 1/1 | 0.98 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3377 | 1/1 | 0.98 | 0.24 | 59,59,59,59 | 0 |
| 56 | MG | AA | 3091 | 1/1 | 0.98 | 0.15 | 75,75,75,75 | 0 |
| 56 | MG | CA | 3133 | 1/1 | 0.98 | 0.05 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3702 | 1/1 | 0.98 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | BR | 201 | 1/1 | 0.98 | 0.60 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3046 | 1/1 | 0.98 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | CA | 3129 | 1/1 | 0.98 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3095 | 1/1 | 0.98 | 0.47 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3131 | 1/1 | 0.98 | 0.72 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3208 | 1/1 | 0.98 | 0.28 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3473 | 1/1 | 0.98 | 0.31 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3227 | 1/1 | 0.98 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3308 | 1/1 | 0.98 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | BE | 302 | 1/1 | 0.98 | 0.22 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3330 | 1/1 | 0.98 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3070 | 1/1 | 0.98 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | CA | 3165 | 1/1 | 0.98 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3644 | 1/1 | 0.98 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3678 | 1/1 | 0.98 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3327 | 1/1 | 0.98 | 0.18 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3025 | 1/1 | 0.98 | 0.38 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3478 | 1/1 | 0.98 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3381 | 1/1 | 0.98 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3675 | 1/1 | 0.98 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | AA | 3097 | 1/1 | 0.98 | 0.25 | 43,43,43,43 | 0 |
| 56 | MG | CA | 3100 | 1/1 | 0.98 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3385 | 1/1 | 0.98 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3655 | 1/1 | 0.98 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3019 | 1/1 | 0.98 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3519 | 1/1 | 0.98 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3281 | 1/1 | 0.98 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3526 | 1/1 | 0.98 | 0.19 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3476 | 1/1 | 0.98 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | AA | 3143 | 1/1 | 0.98 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3227 | 1/1 | 0.98 | 0.30 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3725 | 1/1 | 0.98 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3612 | 1/1 | 0.98 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3480 | 1/1 | 0.98 | 0.20 | 17,17,17,17 | 0 |
| 56 | MG | AA | 3205 | 1/1 | 0.98 | 0.19 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3652 | 1/1 | 0.98 | 0.60 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DE | 303 | 1/1 | 0.98 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3179 | 1/1 | 0.98 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | AA | 3192 | 1/1 | 0.98 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3388 | 1/1 | 0.98 | 0.15 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3390 | 1/1 | 0.98 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3313 | 1/1 | 0.98 | 0.27 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3375 | 1/1 | 0.98 | 0.24 | 31,31,31,31 | 0 |
| 56 | MG | CA | 3092 | 1/1 | 0.98 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3395 | 1/1 | 0.98 | 0.21 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3533 | 1/1 | 0.98 | 0.08 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3429 | 1/1 | 0.98 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3467 | 1/1 | 0.98 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3307 | 1/1 | 0.98 | 0.20 | 33,33,33,33 | 0 |
| 56 | MG | AA | 3103 | 1/1 | 0.98 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | CA | 3085 | 1/1 | 0.98 | 0.30 | 43,43,43,43 | 0 |
| 56 | MG | BE | 309 | 1/1 | 0.98 | 0.27 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3398 | 1/1 | 0.98 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3656 | 1/1 | 0.98 | 0.11 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3634 | 1/1 | 0.98 | 0.70 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3567 | 1/1 | 0.98 | 0.22 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3583 | 1/1 | 0.98 | 0.20 | 27,27,27,27 | 0 |
| 56 | MG | AA | 3163 | 1/1 | 0.98 | 0.17 | 28,28,28,28 | 0 |
| 56 | MG | AA | 3172 | 1/1 | 0.98 | 0.05 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3320 | 1/1 | 0.98 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3351 | 1/1 | 0.98 | 0.38 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3323 | 1/1 | 0.98 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | CA | 3093 | 1/1 | 0.98 | 0.06 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3645 | 1/1 | 0.98 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3186 | 1/1 | 0.98 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3459 | 1/1 | 0.98 | 0.22 | 31,31,31,31 | 0 |
| 56 | MG | B3 | 102 | 1/1 | 0.98 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3195 | 1/1 | 0.98 | 0.33 | 47,47,47,47 | 0 |
| 56 | MG | BQ | 201 | 1/1 | 0.98 | 0.43 | 61,61,61,61 | 0 |
| 56 | MG | AA | 3141 | 1/1 | 0.98 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3529 | 1/1 | 0.98 | 0.21 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3234 | 1/1 | 0.98 | 0.23 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3608 | 1/1 | 0.98 | 0.27 | 57,57,57,57 | 0 |
| 56 | MG | CA | 3017 | 1/1 | 0.98 | 0.24 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3528 | 1/1 | 0.99 | 0.22 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3154 | 1/1 | 0.99 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3332 | 1/1 | 0.99 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3324 | 1/1 | 0.99 | 0.23 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3460 | 1/1 | 0.99 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | CA | 3122 | 1/1 | 0.99 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3051 | 1/1 | 0.99 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | B7 | 102 | 1/1 | 0.99 | 0.25 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3128 | 1/1 | 0.99 | 0.27 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3423 | 1/1 | 0.99 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3416 | 1/1 | 0.99 | 0.25 | 42,42,42,42 | 0 |
| 56 | MG | BF | 303 | 1/1 | 0.99 | 0.27 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3028 | 1/1 | 0.99 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3230 | 1/1 | 0.99 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3181 | 1/1 | 0.99 | 0.30 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3516 | 1/1 | 0.99 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3355 | 1/1 | 0.99 | 0.26 | 18,18,18,18 | 0 |
| 56 | MG | CA | 3069 | 1/1 | 0.99 | 0.11 | 69,69,69,69 | 0 |
| 56 | MG | CA | 3001 | 1/1 | 0.99 | 0.21 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3540 | 1/1 | 0.99 | 0.23 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3383 | 1/1 | 0.99 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | CA | 3080 | 1/1 | 0.99 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3338 | 1/1 | 0.99 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3531 | 1/1 | 0.99 | 0.29 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3508 | 1/1 | 0.99 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | AX | 109 | 1/1 | 0.99 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3399 | 1/1 | 0.99 | 0.19 | 18,18,18,18 | 0 |
| 56 | MG | AA | 3188 | 1/1 | 0.99 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3407 | 1/1 | 0.99 | 0.19 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3410 | 1/1 | 0.99 | 0.15 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3520 | 1/1 | 0.99 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3346 | 1/1 | 0.99 | 0.23 | 29,29,29,29 | 0 |
| 58 | ZN | D5 | 103 | 1/1 | 0.99 | 0.07 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3312 | 1/1 | 0.99 | 0.27 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3494 | 1/1 | 0.99 | 0.34 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3612 | 1/1 | 0.99 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3342 | 1/1 | 0.99 | 0.19 | 31,31,31,31 | 0 |
| 57 | SF4 | AD | 501 | 8/8 | 0.99 | 0.14 | 59,72,92,96 | 0 |
| 56 | MG | DA | 3190 | 1/1 | 0.99 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | BB | 3011 | 1/1 | 0.99 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3318 | 1/1 | 0.99 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3471 | 1/1 | 0.99 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3442 | 1/1 | 0.99 | 0.15 | 12,12,12,12 | 0 |
| 56 | MG | AA | 3151 | 1/1 | 0.99 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3200 | 1/1 | 0.99 | 0.27 | 25,25,25,25 | 0 |
| 56 | MG | CA | 3154 | 1/1 | 0.99 | 0.13 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3272 | 1/1 | 0.99 | 0.28 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3492 | 1/1 | 0.99 | 0.25 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3301 | 1/1 | 0.99 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3415 | 1/1 | 0.99 | 0.24 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3126 | 1/1 | 0.99 | 0.22 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3553 | 1/1 | 0.99 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3371 | 1/1 | 0.99 | 0.18 | 15,15,15,15 | 0 |
| 56 | MG | DA | 3379 | 1/1 | 0.99 | 0.22 | 28,28,28,28 | 0 |
| 56 | MG | AA | 3214 | 1/1 | 0.99 | 0.27 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3549 | 1/1 | 0.99 | 0.24 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3378 | 1/1 | 0.99 | 0.12 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3618 | 1/1 | 0.99 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | BB | 3010 | 1/1 | 0.99 | 0.26 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3542 | 1/1 | 0.99 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | CA | 3077 | 1/1 | 0.99 | 0.22 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3409 | 1/1 | 0.99 | 0.23 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3271 | 1/1 | 0.99 | 0.20 | 37,37,37,37 | 0 |
| 57 | SF4 | CD | 501 | 8/8 | 0.99 | 0.14 | 64,75,91,95 | 0 |
| 56 | MG | BA | 3732 | 1/1 | 0.99 | 0.52 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3414 | 1/1 | 0.99 | 0.21 | 19,19,19,19 | 0 |
| 56 | MG | AA | 3159 | 1/1 | 0.99 | 0.32 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3614 | 1/1 | 0.99 | 0.42 | 30,30,30,30 | 0 |
| 56 | MG | AA | 3073 | 1/1 | 0.99 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | BN | 3006 | 1/1 | 0.99 | 0.12 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3662 | 1/1 | 0.99 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3413 | 1/1 | 0.99 | 0.20 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3331 | 1/1 | 0.99 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3321 | 1/1 | 0.99 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | AA | 3144 | 1/1 | 0.99 | 0.08 | 48,48,48,48 | 0 |
| 58 | ZN | B5 | 501 | 1/1 | 0.99 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3625 | 1/1 | 0.99 | 0.10 | 35,35,35,35 | 0 |
| 58 | ZN | B6 | 501 | 1/1 | 1.00 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3304 | 1/1 | 1.00 | 0.11 | 35,35,35,35 | 0 |
| 58 | ZN | B9 | 501 | 1/1 | 1.00 | 0.12 | 48,48,48,48 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.