



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:50 pm BST

PDB ID : 1VY4
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing acylated tRNA-substrates in the A and P sites.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.60 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 |

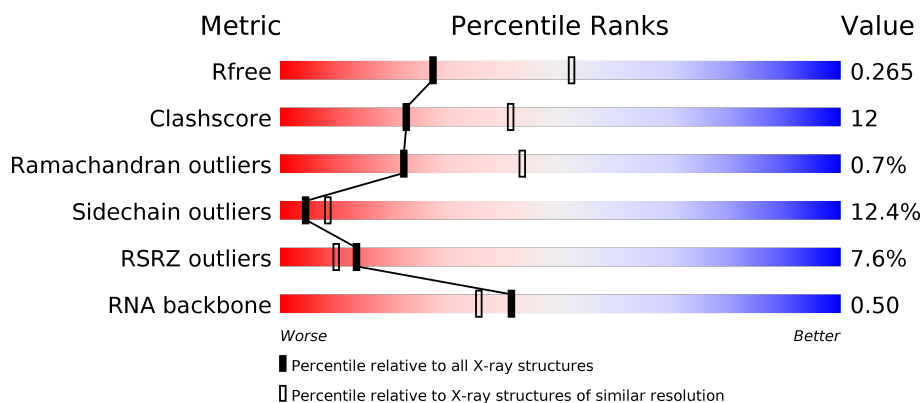
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 | 3163 (2.60-2.60) |
| Clashscore | 141614 | 3518 (2.60-2.60) |
| Ramachandran outliers | 138981 | 3455 (2.60-2.60) |
| Sidechain outliers | 138945 | 3455 (2.60-2.60) |
| RSRZ outliers | 127900 | 3104 (2.60-2.60) |
| RNA backbone | 3102 | 1040 (2.90-2.30) |

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 | 1521 | |
| 1 | CA | 1521 | |
| 2 | AB | 256 | |
| 2 | CB | 256 | |

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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 | AW | 76 | |
| 23 | CW | 76 | |
| 24 | AX | 77 | |
| 24 | CX | 77 | |
| 25 | AY | 76 | |
| 25 | CY | 76 | |
| 26 | BA | 2915 | |
| 26 | DA | 2915 | |
| 27 | BB | 121 | |
| 27 | DB | 121 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | BD | 276 | |
| 28 | DD | 276 | |
| 29 | BE | 206 | |
| 29 | DE | 206 | |
| 30 | BF | 210 | |
| 30 | DF | 210 | |
| 31 | BG | 182 | |
| 31 | DG | 182 | |
| 32 | BH | 180 | |
| 32 | DH | 180 | |
| 33 | BI | 148 | |
| 33 | DI | 148 | |
| 34 | BN | 140 | |
| 34 | DN | 140 | |
| 35 | BO | 122 | |
| 35 | DO | 122 | |
| 36 | BP | 150 | |
| 36 | DP | 150 | |
| 37 | BQ | 141 | |
| 37 | DQ | 141 | |
| 38 | BR | 118 | |
| 38 | DR | 118 | |
| 39 | BS | 112 | |
| 39 | DS | 112 | |
| 40 | BT | 146 | |




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | DT | 146 | |
| 41 | BU | 118 | |
| 41 | DU | 118 | |
| 42 | BV | 101 | |
| 42 | DV | 101 | |
| 43 | BW | 113 | |
| 43 | DW | 113 | |
| 44 | BX | 96 | |
| 44 | DX | 96 | |
| 45 | BY | 110 | |
| 45 | DY | 110 | |
| 46 | BZ | 206 | |
| 46 | DZ | 206 | |
| 47 | B0 | 85 | |
| 47 | D0 | 85 | |
| 48 | B1 | 98 | |
| 48 | D1 | 98 | |
| 49 | B2 | 72 | |
| 49 | D2 | 72 | |
| 50 | B3 | 60 | |
| 50 | D3 | 60 | |
| 51 | B4 | 71 | |
| 51 | D4 | 71 | |
| 52 | B5 | 60 | |
| 52 | D5 | 60 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 53 | B6 | 54 |  |
| 53 | D6 | 54 |  |
| 54 | B7 | 49 |  |
| 54 | D7 | 49 |  |
| 55 | B8 | 65 |  |
| 55 | D8 | 65 |  |
| 56 | B9 | 37 |  |
| 56 | 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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25 | PSU | CY | 39 | - | - | X | - |
| 25 | 5MU | CY | 54 | - | - | - | X |
| 25 | PSU | CY | 55 | - | - | - | X |
| 57 | MG | BA | 3710 | - | - | - | X |
| 57 | MG | DA | 3024 | - | - | - | X |
| 57 | MG | DA | 3033 | - | - | - | X |
| 57 | MG | DA | 3624 | - | - | - | X |
| 57 | MG | DA | 3657 | - | - | - | X |
| 57 | MG | DQ | 3003 | - | - | - | X |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297127 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 | 1497 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32185 | 14324 | 5968 | 10396 | 1497 | | | |
| 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 |
| | | | 1544 | 970 | 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 |
| | | | 1678 | 1052 | 333 | 286 | 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 |
| | | | 812 | 514 | 146 | 149 | 3 | | | |
| 6 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 820 | 518 | 147 | 152 | 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 |
| | | | 986 | 626 | 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 | | |
| | | | 833 | 519 | 156 | 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 | | |
| | | | 966 | 598 | 200 | 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 type Z.

| 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 | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 661 | 423 | 122 | 114 | 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 |
| | | | 731 | 449 | 156 | 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 | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 277 | 125 | 51 | 88 | 13 | | | |
| 22 | CV | 12 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 252 | 115 | 46 | 80 | 11 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23 | AW | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1599 | 722 | 287 | 515 | 73 | 2 | | | |
| 23 | CW | 72 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1552 | 697 | 280 | 502 | 72 | 1 | | | |

- Molecule 24 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 24 | AX | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1635 | 731 | 296 | 530 | 76 | 2 | | | |
| 24 | CX | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1635 | 731 | 296 | 530 | 76 | 2 | | | |

- Molecule 25 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 25 | AY | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1581 | 707 | 285 | 515 | 73 | 1 | | | |
| 25 | CY | 73 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1561 | 698 | 283 | 507 | 72 | 1 | | | |

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26 | BA | 2819 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60729 | 27026 | 11370 | 19515 | 2818 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26 | DA | 2800 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60311 | 26840 | 11284 | 19388 | 2799 | | | |

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 27 | BB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |
| 27 | DB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 28 | BD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |
| 28 | DD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2142 | 1352 | 426 | 361 | 3 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 985 | 298 | 270 | 6 | | | |
| 29 | DE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 985 | 298 | 270 | 6 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 30 | BF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1584 | 1009 | 298 | 275 | 2 | | | |
| 30 | DF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1580 | 1007 | 297 | 274 | 2 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1425 | 914 | 256 | 251 | 4 | | | |
| 31 | DG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1424 | 911 | 258 | 251 | 4 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |
| 32 | DH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1085 | 693 | 189 | 202 | 1 | | | |
| 33 | DI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1073 | 688 | 188 | 196 | 1 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | BN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |
| 34 | DN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 35 | DO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | BP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1139 | 709 | 231 | 196 | 3 | | | |
| 36 | DP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1135 | 706 | 230 | 196 | 3 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 37 | DQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 38 | DR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 39 | BS | 110 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 877 | 553 | 175 | 149 | | | | |
| 39 | DS | 110 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 870 | 549 | 173 | 148 | | | | |

- Molecule 40 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1091 | 680 | 225 | 185 | 1 | | | |
| 40 | DT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1083 | 675 | 224 | 183 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |
| 41 | DU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | DV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 557 | 174 | 153 | 2 | | | |
| 43 | DW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 557 | 174 | 153 | 2 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |
| 44 | DX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |
| 45 | DY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BZ | 171 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1349 | 862 | 243 | 242 | 2 | | | |
| 46 | DZ | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1360 | 870 | 243 | 245 | 2 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | B0 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 404 | 139 | 109 | 1 | | | |
| 47 | D0 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 404 | 139 | 109 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | B1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |
| 48 | D1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | B2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |
| 49 | D2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 50 | B3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 50 | D3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 464 | 296 | 90 | 78 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51 | B4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 558 | 352 | 102 | 99 | 5 | | | |
| 51 | D4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 532 | 339 | 97 | 91 | 5 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |
| 52 | D5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L33.

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

- Molecule 54 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54 | B7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 54 | D7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 55 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 56 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 56 | B9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 56 | D9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57 | B4 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | BA | 814 | Total | Mg | 0 | 0 |
| | | | 814 | 814 | | |
| 57 | AK | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | DQ | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | D3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | AB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DF | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | B8 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BE | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | AW | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | AN | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BP | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | AX | 15 | Total 15 | Mg 15 | 0 | 0 |
| 57 | DN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CA | 169 | Total 169 | Mg 169 | 0 | 0 |
| 57 | B5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | BB | 23 | Total 23 | Mg 23 | 0 | 0 |
| 57 | D8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | AE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DB | 13 | Total 13 | Mg 13 | 0 | 0 |
| 57 | CF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BF | 11 | Total 11 | Mg 11 | 0 | 0 |
| 57 | BX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B2 | 1 | Total 1 | Mg 1 | 0 | 0 |

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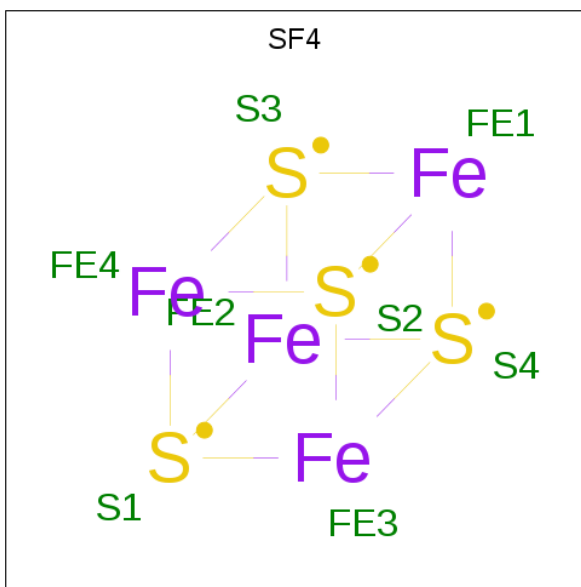
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | AA | 216 | Total 216 | Mg 216 | 0 | 0 |
| 57 | BQ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | CX | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B6 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | AM | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BU | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | DR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BN | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | CT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | D0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DE | 7 | Total 7 | Mg 7 | 0 | 0 |
| 57 | CJ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BR | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DA | 664 | Total 664 | Mg 664 | 0 | 0 |
| 57 | AU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DW | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B7 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | AL | 2 | Total 2 | Mg 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 57 | BV | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | DP | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BZ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CW | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BD | 10 | Total 10 | Mg 10 | 0 | 0 |
| 57 | AT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | CE | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BW | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | AY | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | DD | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | CK | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | AF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BH | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 58 | AD | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 58 | CD | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59 | B5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | CN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | BY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | B9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | DY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | D5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | AN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | D6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | B6 | 1 | Total 1 | Zn 1 | 0 | 0 |

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

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

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61 | AA | 210 | Total 210 | O 210 | 0 | 0 |
| 61 | AD | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | AE | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AJ | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | AL | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AM | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AV | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AW | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | AX | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | AY | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BA | 1405 | Total 1406 | O 1406 | 0 | 1 |
| 61 | BB | 37 | Total 37 | O 37 | 0 | 0 |
| 61 | BD | 15 | Total 15 | O 15 | 0 | 0 |
| 61 | BE | 17 | Total 17 | O 17 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 61 | BF | 11 | Total 11 | O 11 | 0 | 0 |
| 61 | BG | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BH | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BI | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BN | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BO | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BP | 13 | Total 13 | O 13 | 0 | 0 |
| 61 | BQ | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | BR | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BS | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BT | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BU | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | BV | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BW | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BX | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BZ | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | B0 | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | B1 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | B3 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | B5 | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | B6 | 2 | Total 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | B7 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | B8 | 13 | Total 13 | O 13 | 0 | 0 |
| 61 | B9 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CA | 156 | Total 156 | O 156 | 0 | 0 |
| 61 | CE | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | CH | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CJ | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CK | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CL | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CT | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CW | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | CX | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | CY | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DA | 989 | Total 989 | O 989 | 0 | 0 |
| 61 | DB | 9 | Total 9 | O 9 | 0 | 0 |
| 61 | DD | 18 | Total 18 | O 18 | 0 | 0 |
| 61 | DE | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | DF | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | DN | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DP | 12 | Total 12 | O 12 | 0 | 0 |
| 61 | DQ | 1 | Total 1 | O 1 | 0 | 0 |

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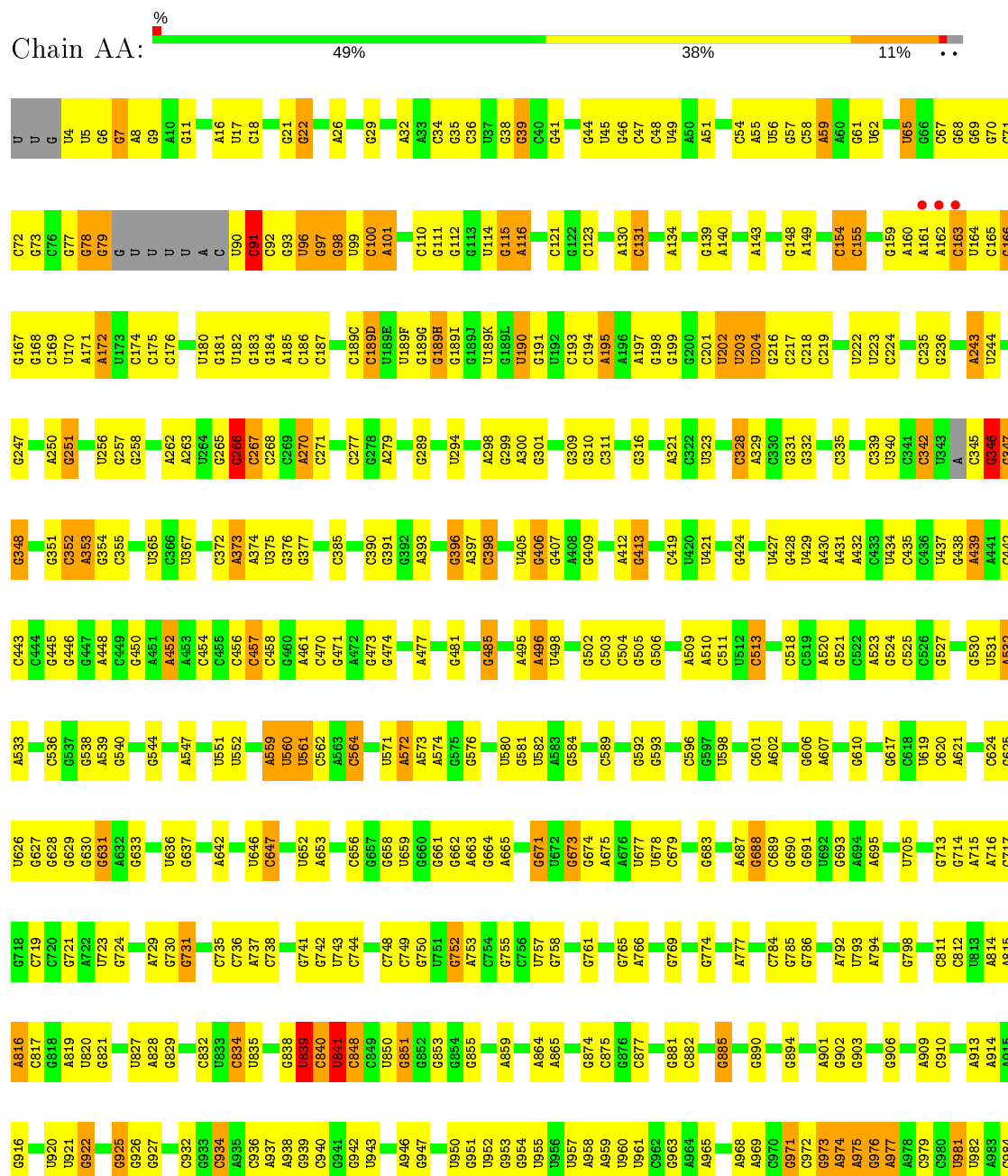
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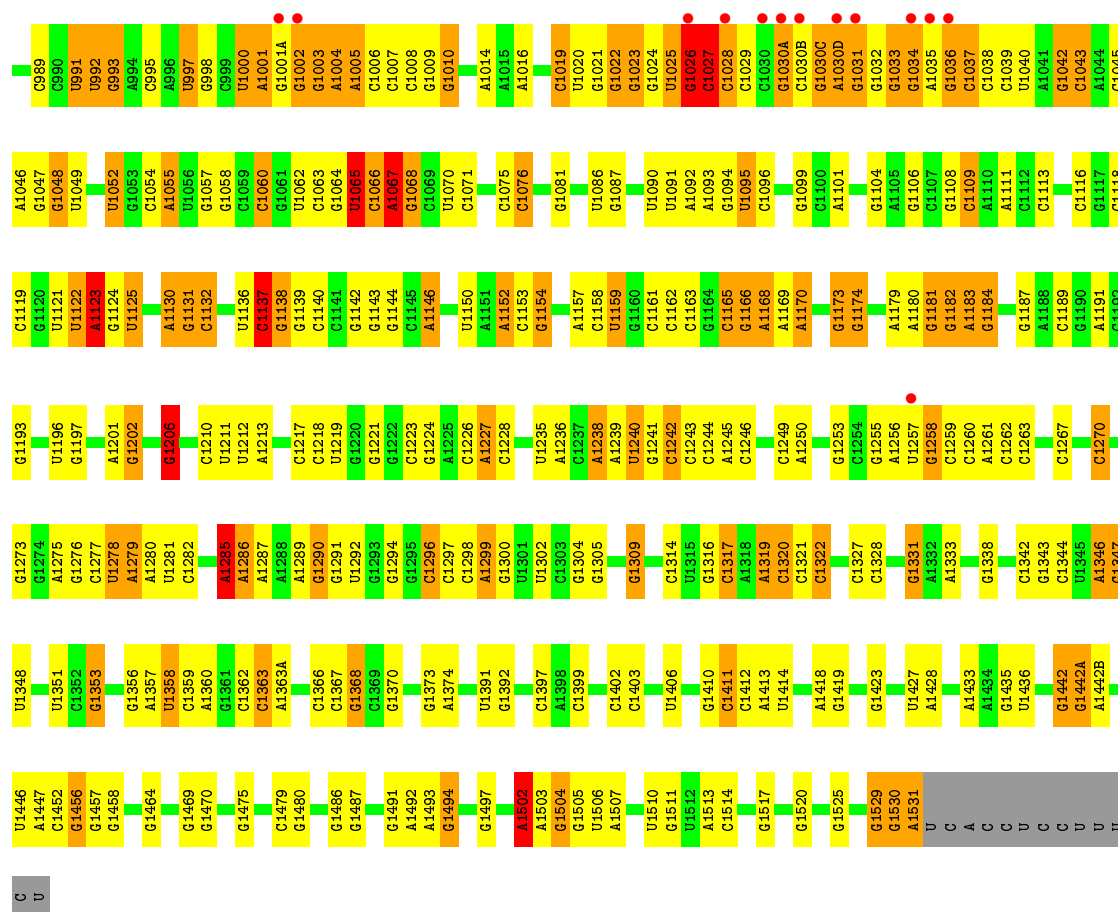
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 61 | DT | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | DU | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DV | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DW | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DX | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DY | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D0 | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | D1 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D3 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | D5 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D6 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D8 | 3 | Total 3 | O 3 | 0 | 0 |

3 Residue-property plots

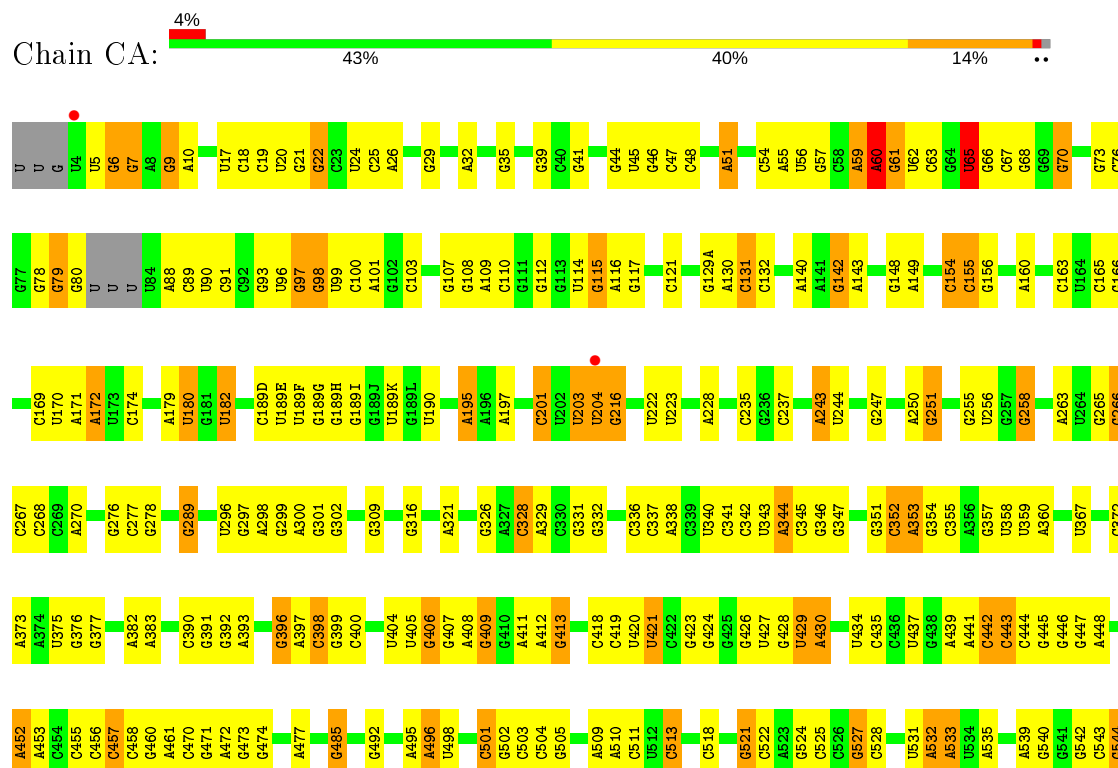
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

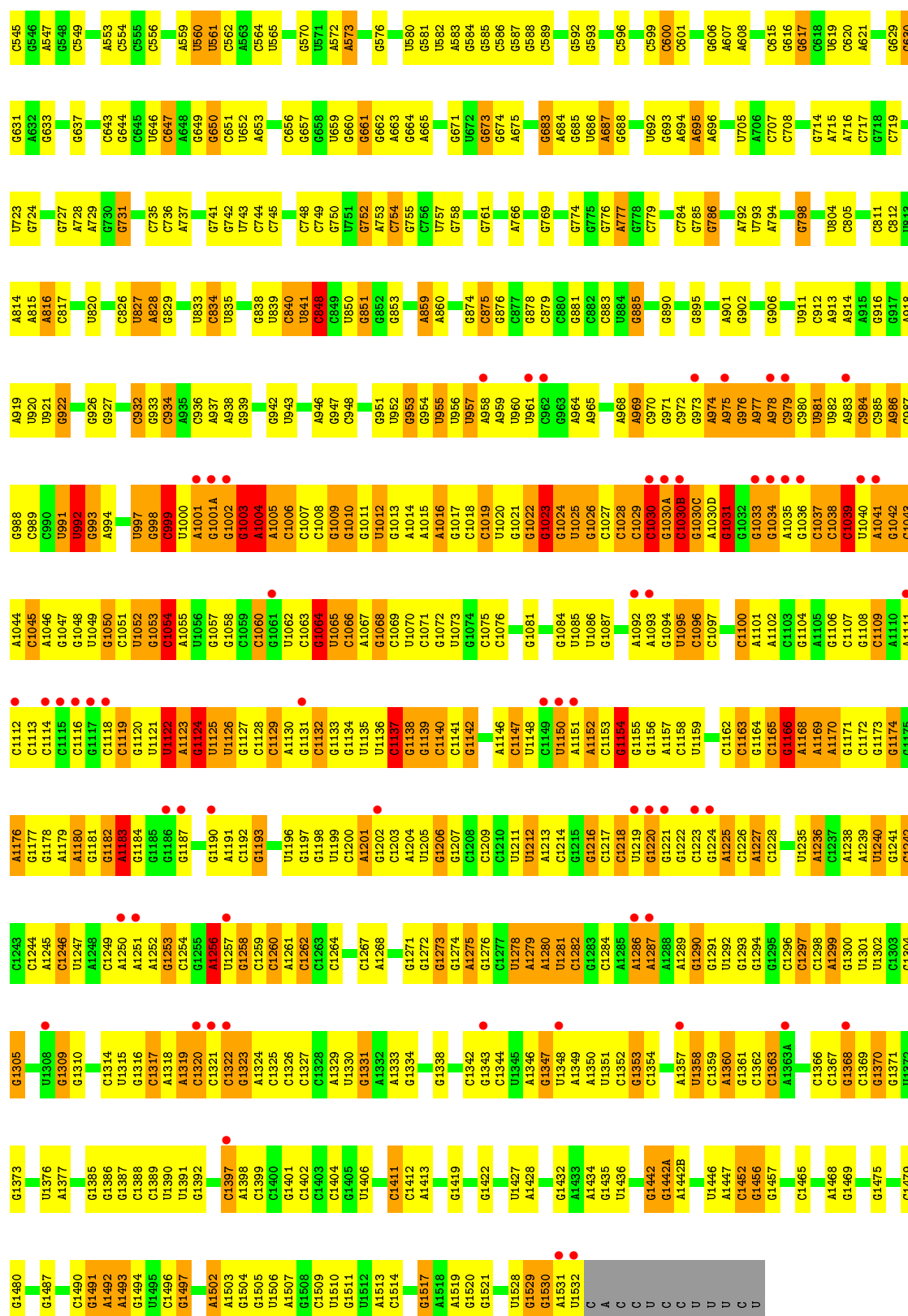
• Molecule 1: 16S Ribosomal RNA



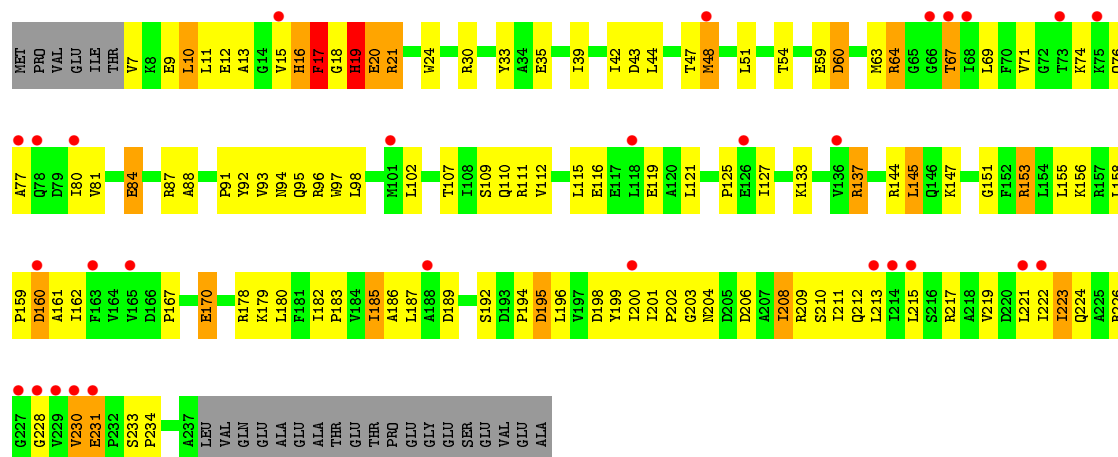


- Molecule 1: 16S Ribosomal RNA

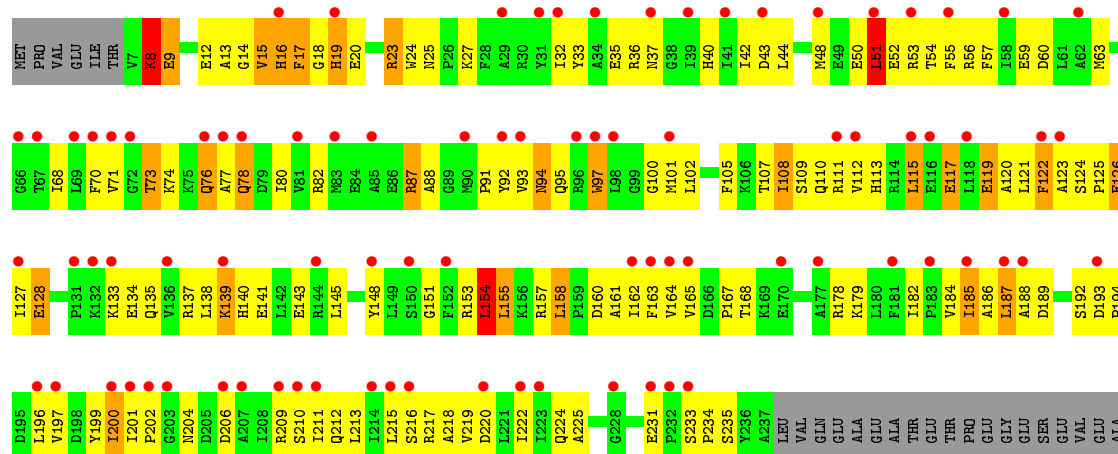




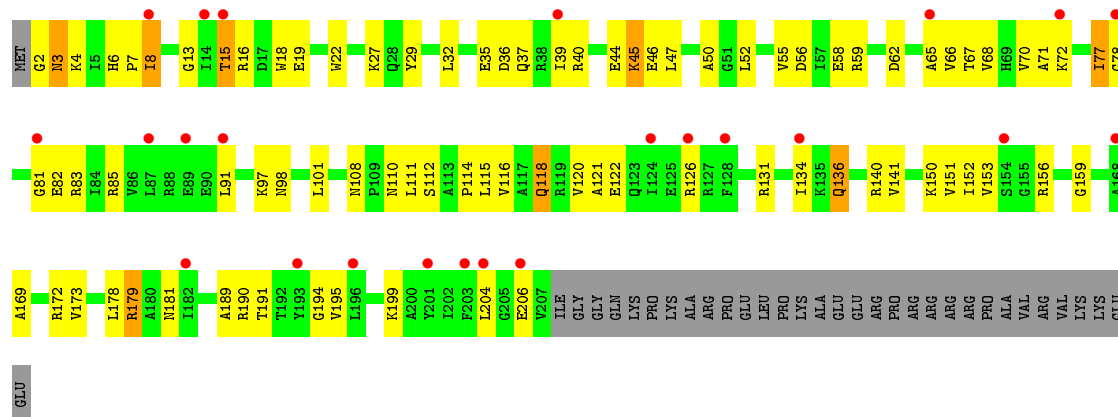
• Molecule 2: 30S ribosomal protein S2



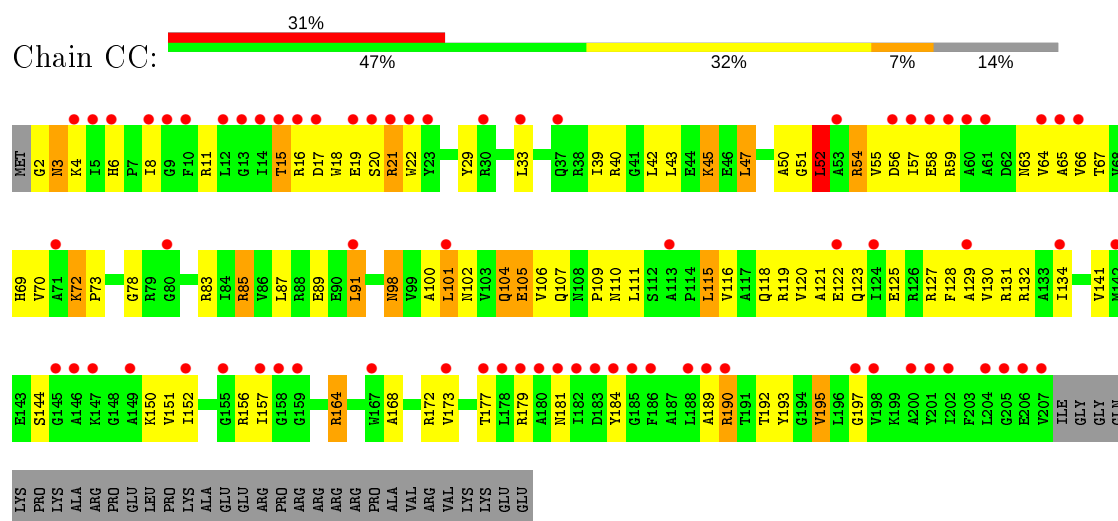
• Molecule 2: 30S ribosomal protein S2



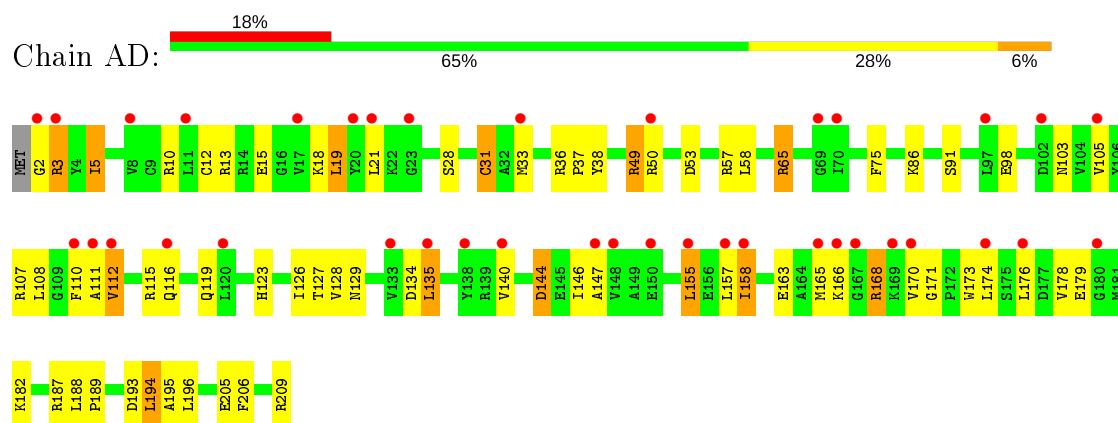
• Molecule 3: 30S ribosomal protein S3



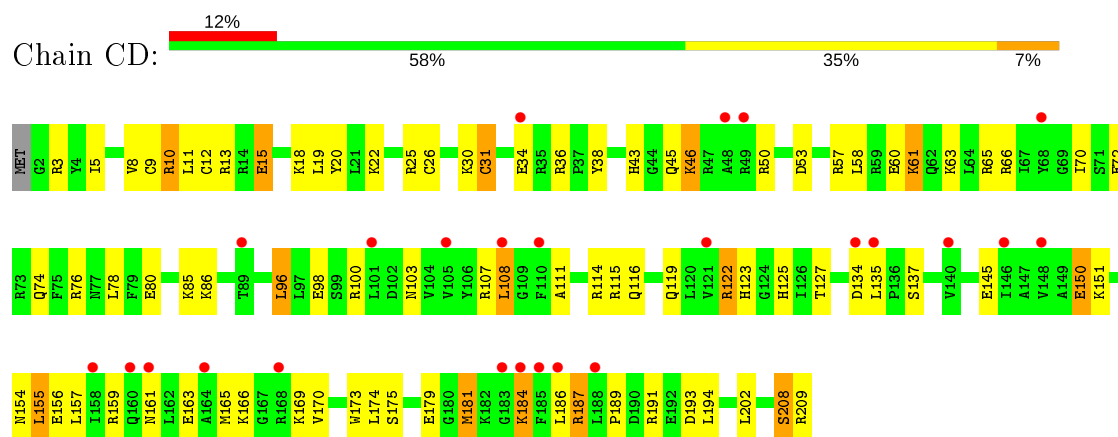
• Molecule 3: 30S ribosomal protein S3



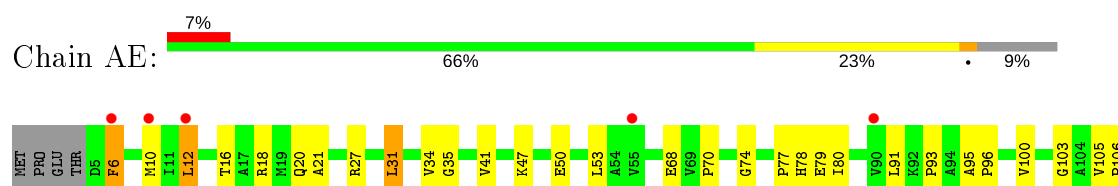
• Molecule 4: 30S ribosomal protein S4

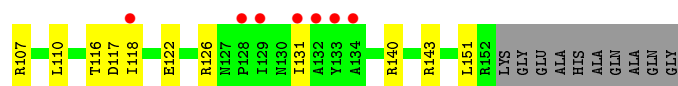


• Molecule 4: 30S ribosomal protein S4

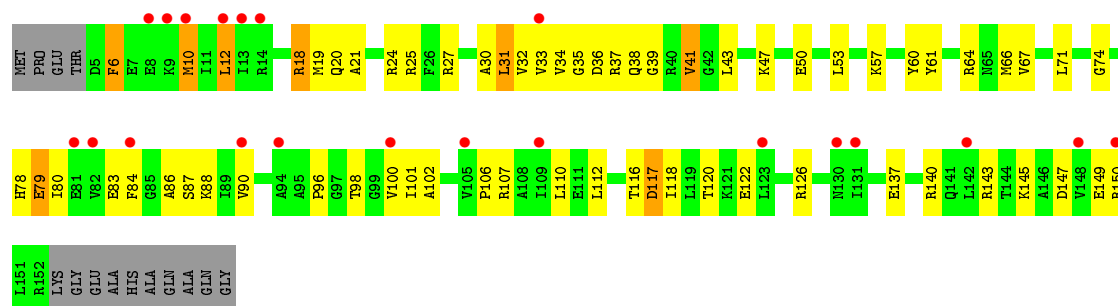


• Molecule 5: 30S ribosomal protein S5

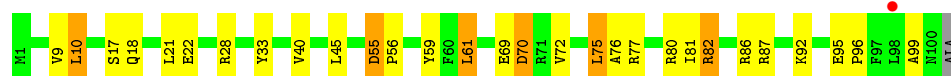




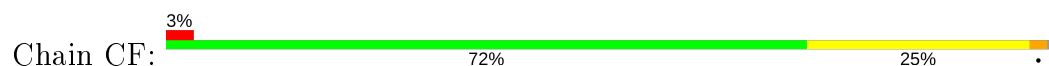
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6



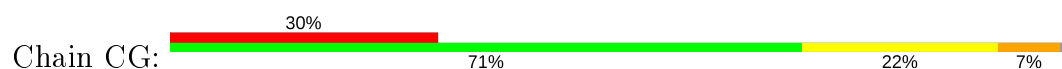
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

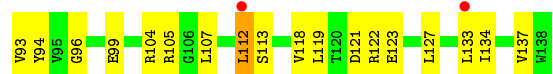
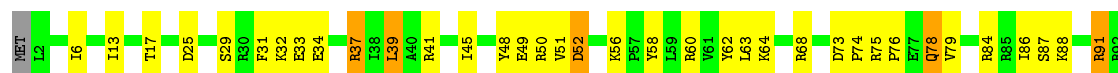


- Molecule 7: 30S ribosomal protein S7

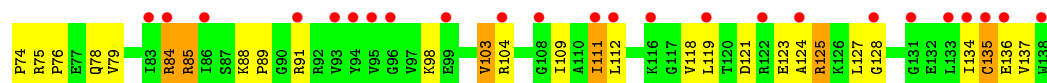
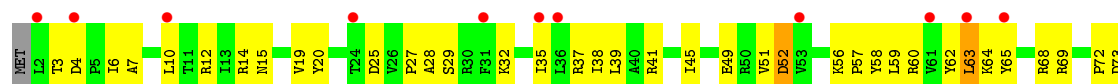




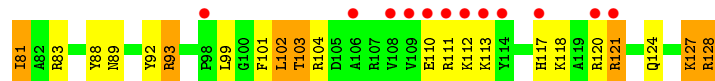
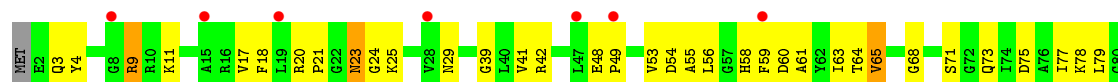
- Molecule 8: 30S ribosomal protein S8



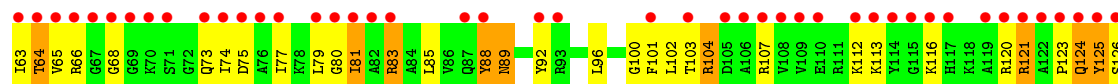
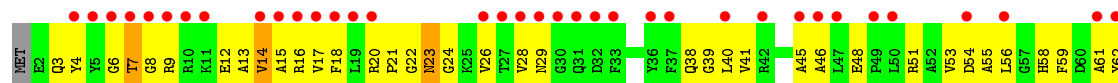
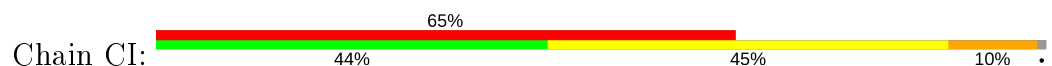
- Molecule 8: 30S ribosomal protein S8



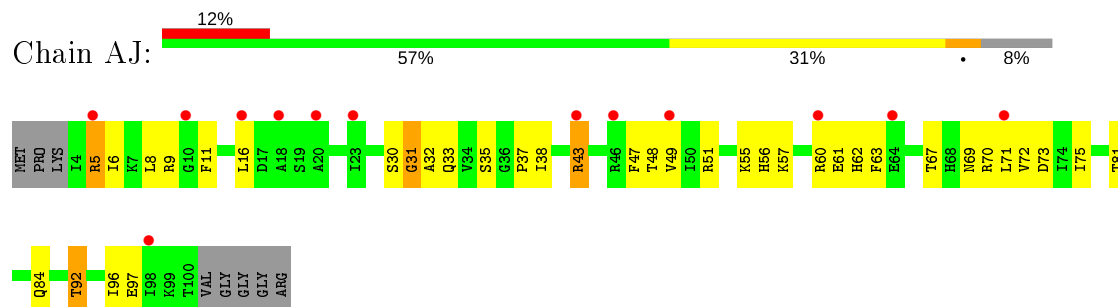
- Molecule 9: 30S ribosomal protein S9



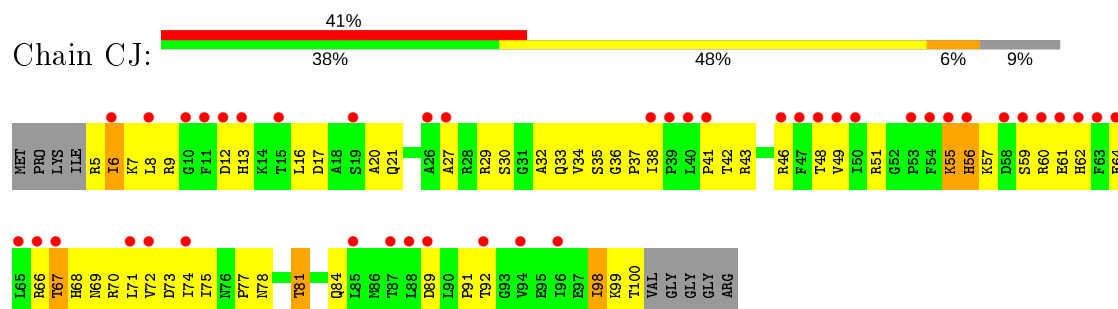
- Molecule 9: 30S ribosomal protein S9



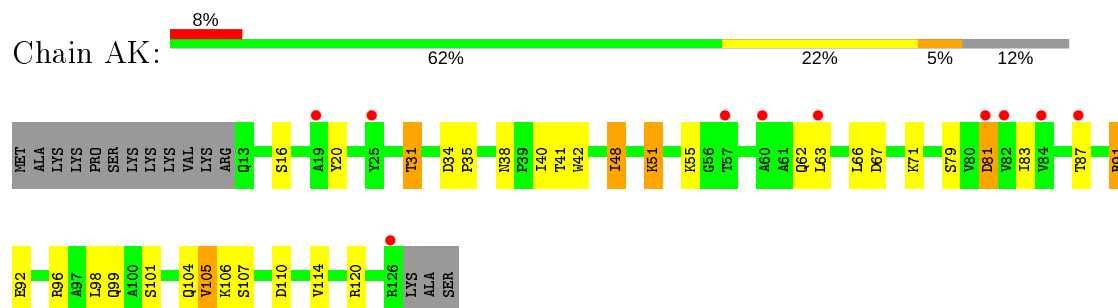
• Molecule 10: 30S ribosomal protein S10



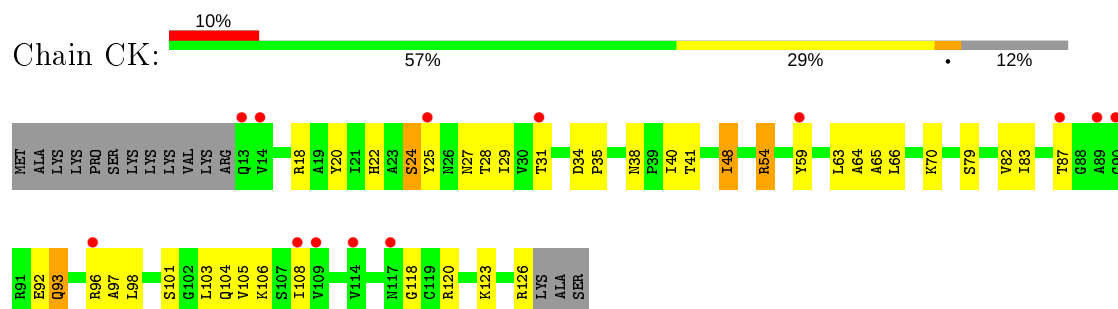
• Molecule 10: 30S ribosomal protein S10



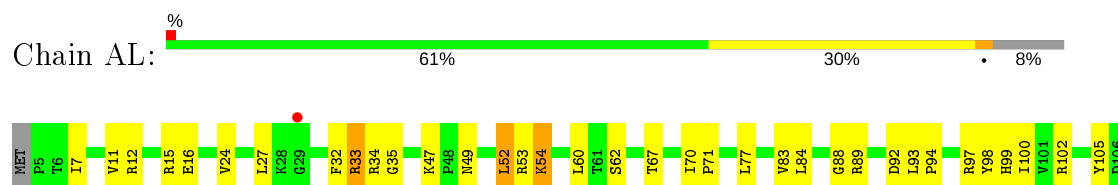
• Molecule 11: 30S ribosomal protein S11

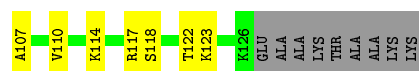


• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

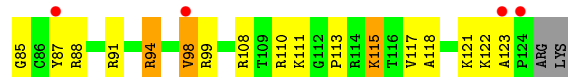
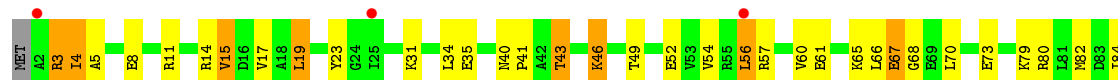




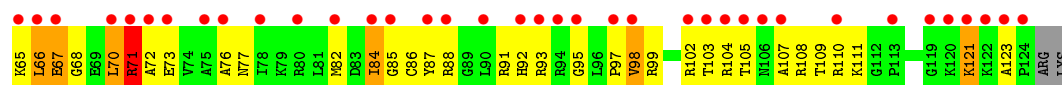
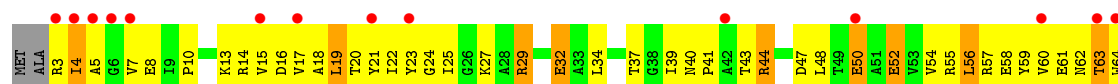
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



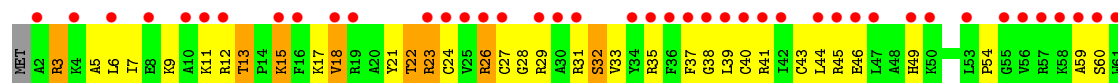
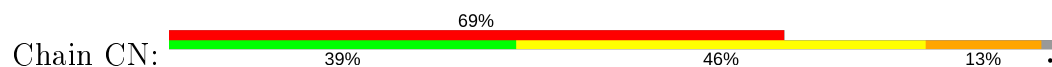
- Molecule 13: 30S ribosomal protein S13



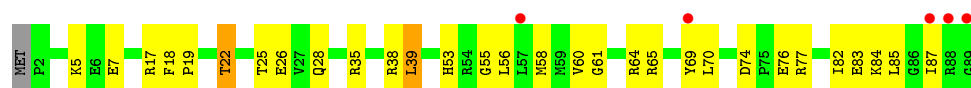
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



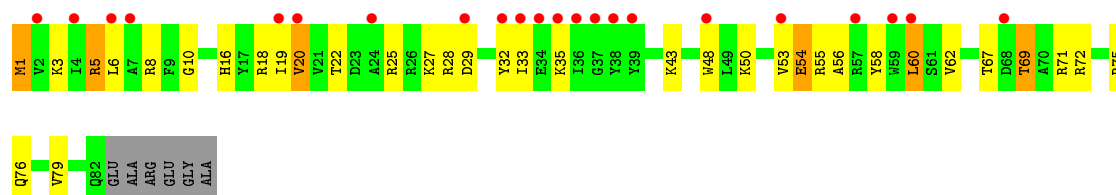
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



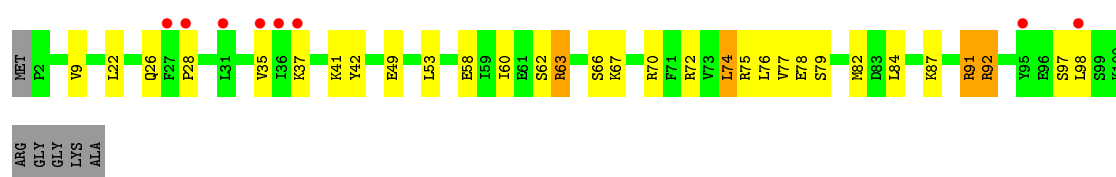
- Molecule 16: 30S ribosomal protein S16



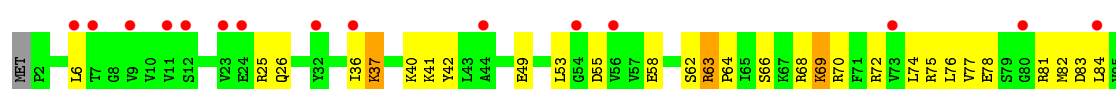
- Molecule 16: 30S ribosomal protein S16

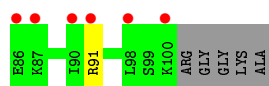


- Molecule 17: 30S ribosomal protein S17

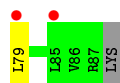
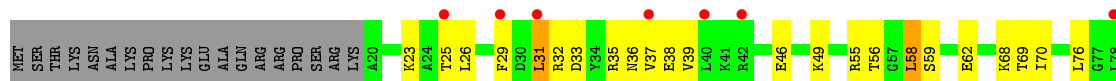


- Molecule 17: 30S ribosomal protein S17

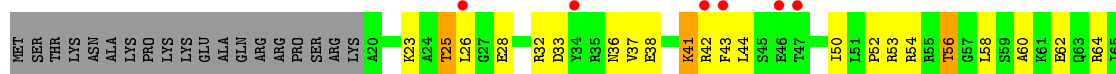
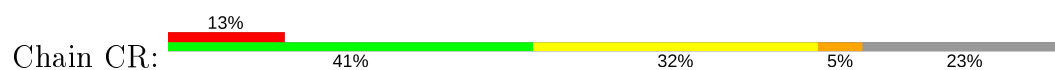




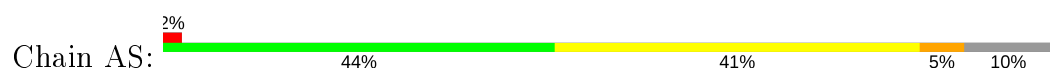
- Molecule 18: 30S ribosomal protein S18



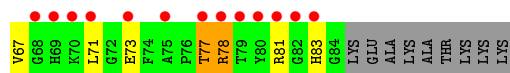
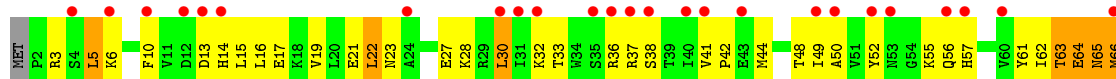
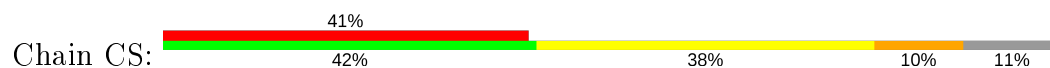
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

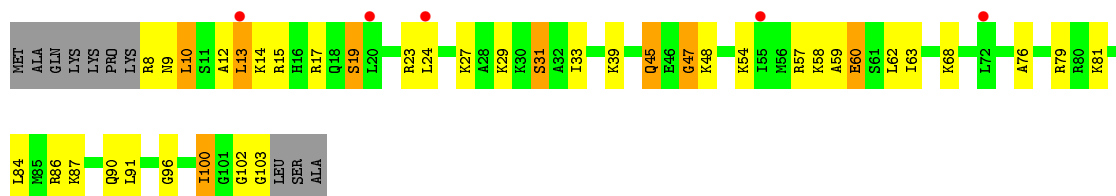


- Molecule 19: 30S ribosomal protein S19

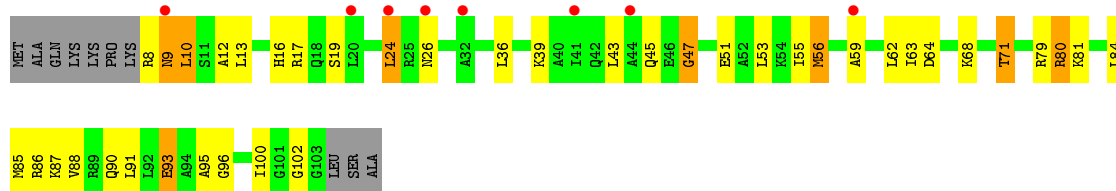


- Molecule 20: 30S ribosomal protein S20

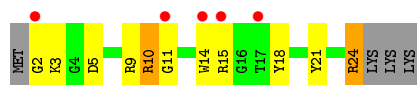




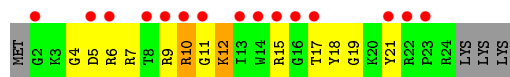
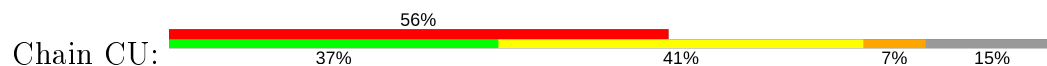
- Molecule 20: 30S ribosomal protein S20



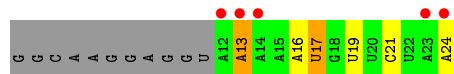
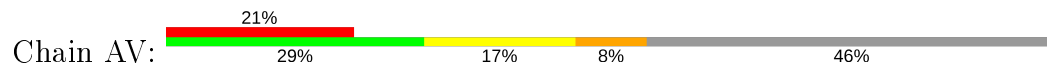
- Molecule 21: 30S ribosomal protein Thx



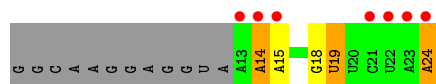
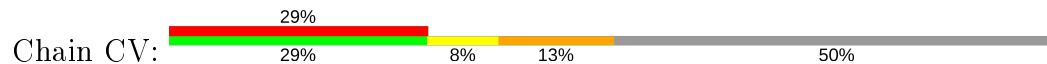
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA

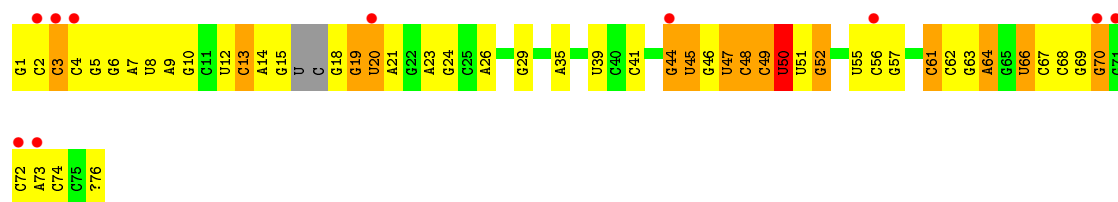


- Molecule 22: mRNA

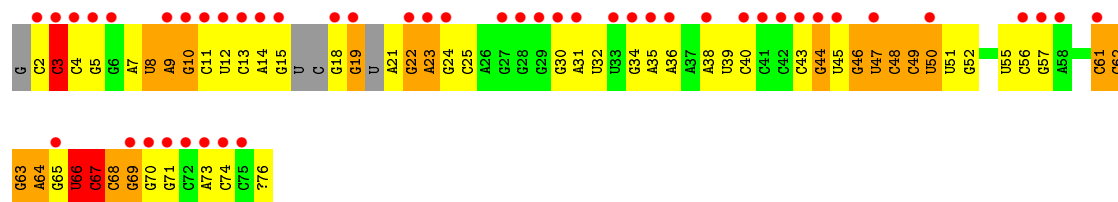
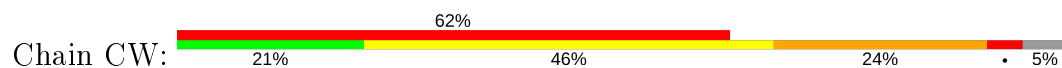


- Molecule 23: A-site tRNA

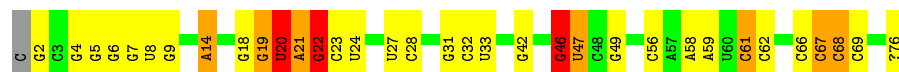




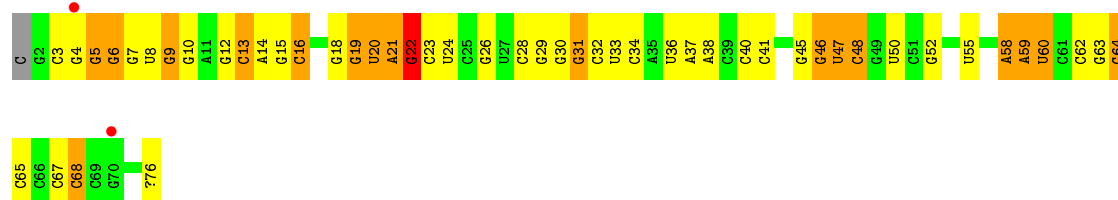
• Molecule 23: A-site tRNA



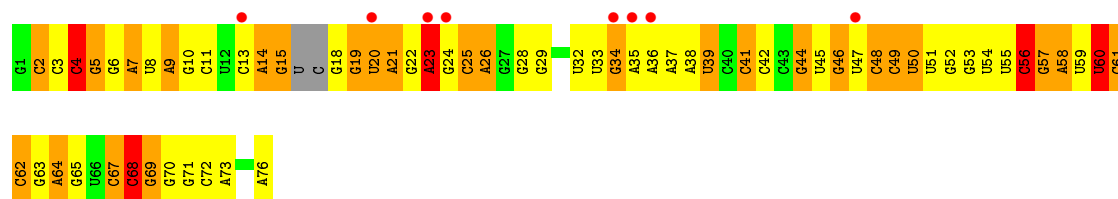
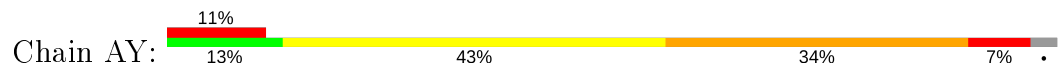
• Molecule 24: P-site tRNA



• Molecule 24: P-site tRNA

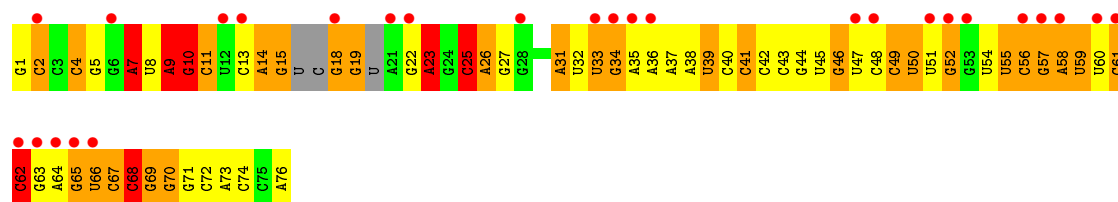


• Molecule 25: E-site tRNA

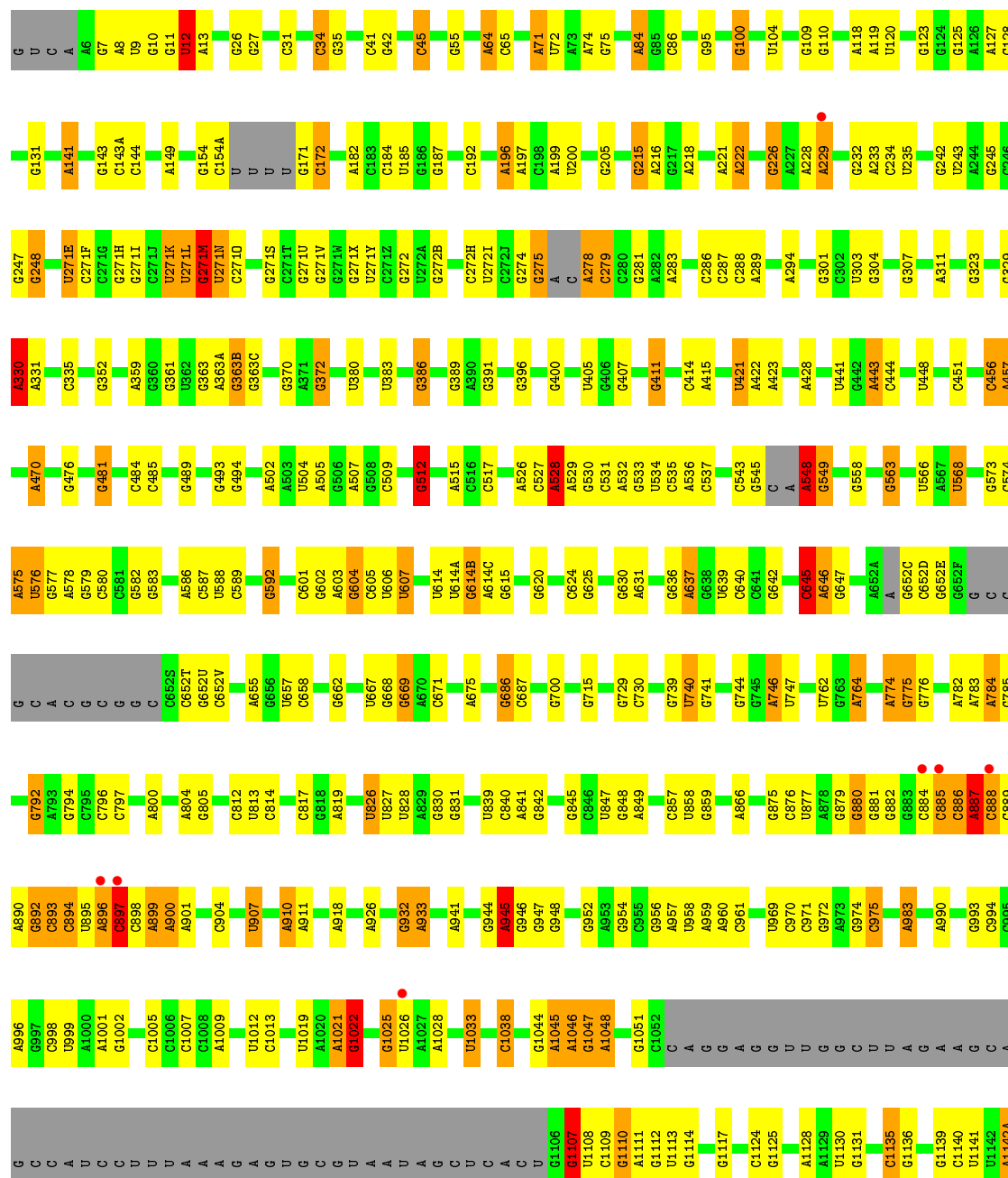


• Molecule 25: E-site tRNA

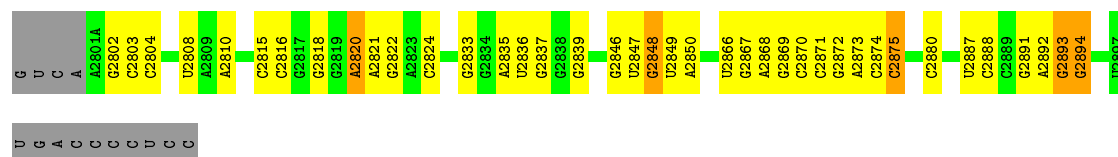




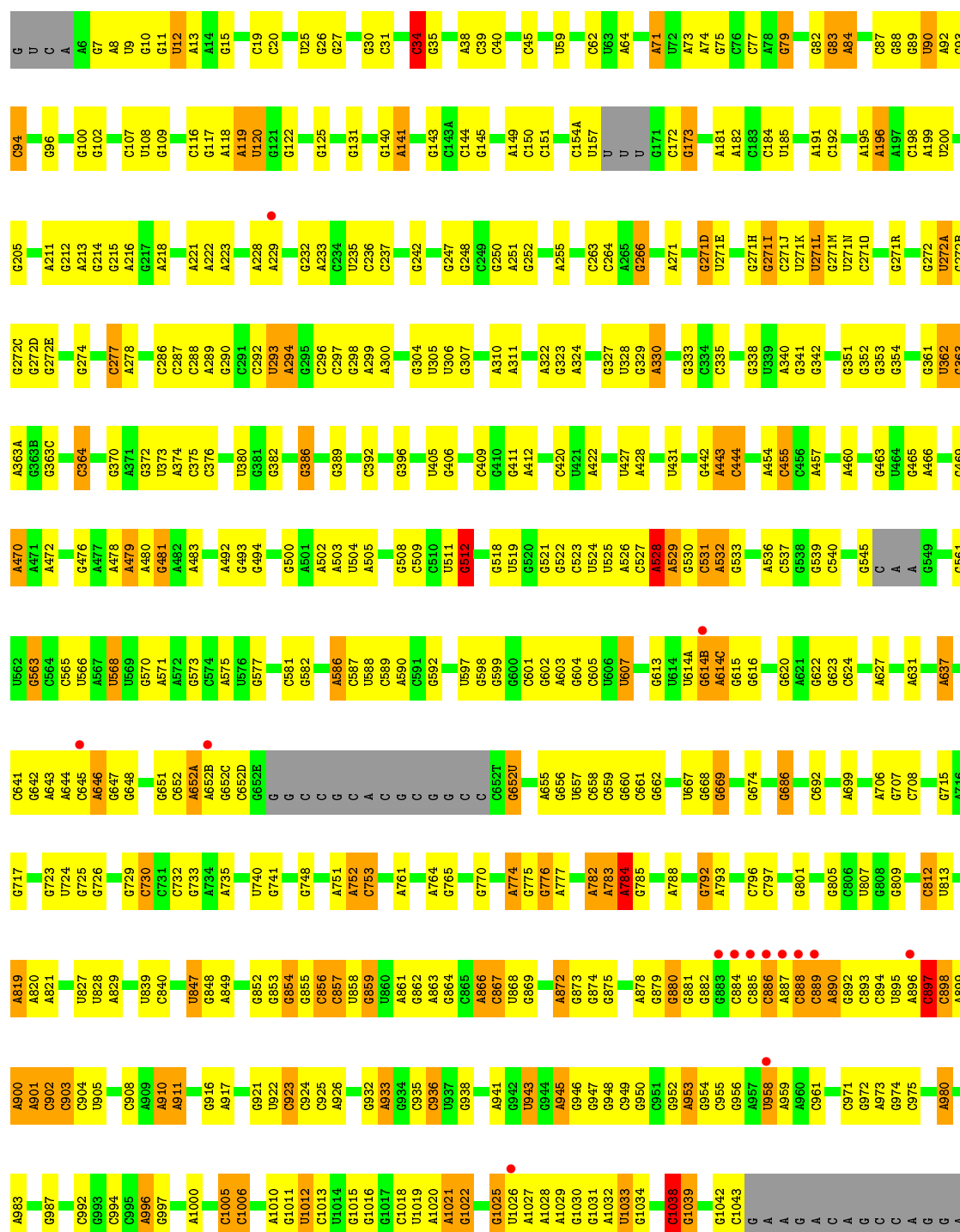
• Molecule 26: 23S Ribosomal RNA



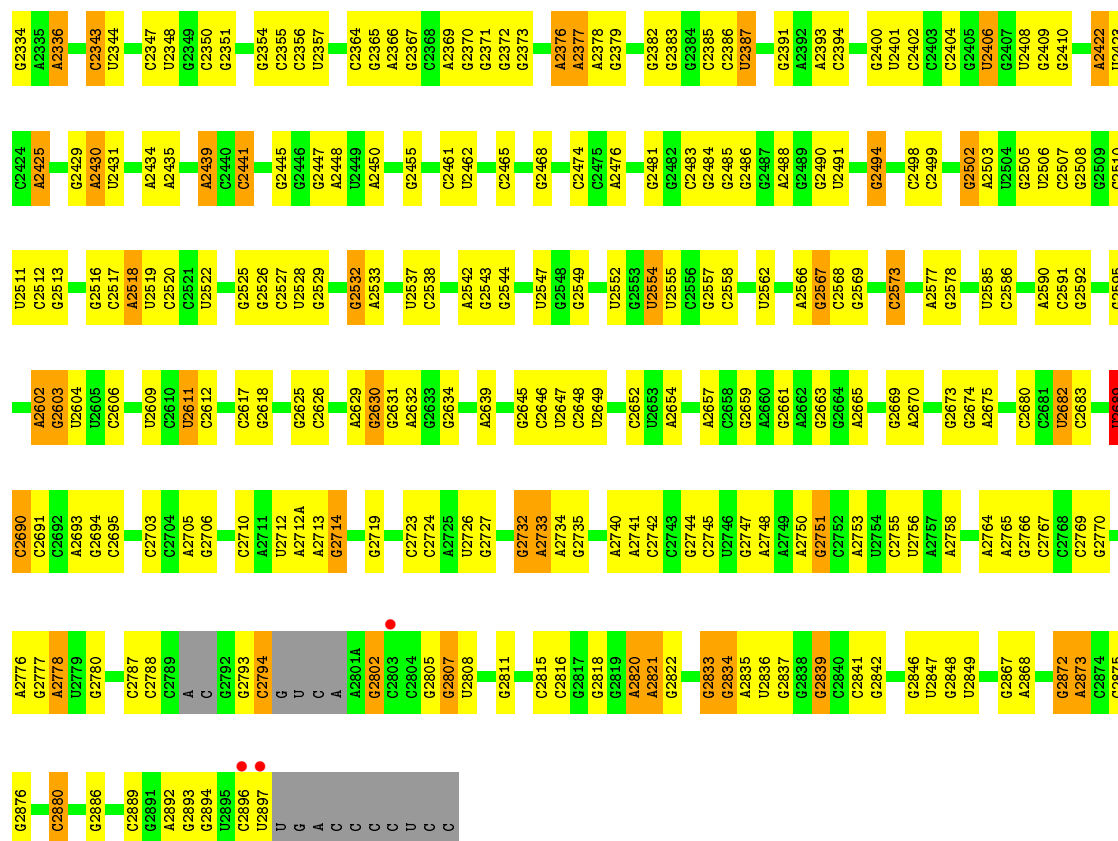
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| C2689 | A2534 | G2396 | U2296 | C2188 | A2126 | G2038 | C1914 | A1784 | A1669 | U | U1420 | A1274 | G1144 |
| C2691 | G2550 | C2297 | C2297 | U2189 | C2128 | U2041 | A1919 | A1785 | A1674 | A | G1421 | | C1153 |
| A2692 | U2554 | C2404 | A2298 | G2190 | C2129 | A2042 | A1919 | A1786 | | C | G1422 | A1278 | G1154 |
| C2694 | G2557 | U2406 | A2305 | G2192 | U2130 | C2043 | A1927 | A1791 | C1683 | G1537 | C1428 | U1292 | A1155 |
| U2698 | C2558 | | G2308 | G2193 | U2133 | G2049 | A1928 | U1794 | C1684 | G1538 | C1429 | C1293 | G1164 |
| C2699 | A2561 | G2414 | U2312 | A2198 | A2134 | C2055 | A1929 | C1795 | C1686 | G1539 | C1430 | C1297 | U1165 |
| C2703 | U2562 | G2418 | C2313 | C2200 | C2136 | G2056 | G1930 | U1796 | G1687 | U1540 | U1431 | | C1166 |
| G2706 | A2563 | U2448 | G2319 | G2206 | C2137 | A2059 | A1937 | U1798 | U1688 | C1543 | A1434 | U1300 | U1167 |
| G2709 | A2565 | U2449 | A2320 | G2207 | C2138 | A2060 | U1938 | G1799 | A1689 | A1564 | G1441 | A1301 | G1170 |
| G2710 | A2566 | A2422 | G2325 | A2208 | C2139 | A2062 | U1939 | G1800 | U1693 | C1557 | G1442 | A1302 | G1171 |
| A2711 | G2567 | G2425 | G2326 | U2218 | C2140 | A2062 | G1948 | A1803 | G1696 | A1558 | A1445 | G1310 | A1173 |
| U2712 | C2568 | A2426 | C2327 | A2225 | C2141 | G2067 | A1952 | G1814 | G1697 | A1566 | G1447 | U1313 | G1175 |
| A2712A | C2573 | G2429 | A2328 | A2233 | C2143 | U2068 | A1953 | G1815 | G1699 | | G1448 | C1314 | A1177 |
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| G2714 | | A2435 | G2330 | G2234 | C2145 | G2070 | U1955 | G1817 | A1701 | U1578 | G1450 | A1342 | C1180 |
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| A2764 | G2640 | C2499 | C2359 | A2274 | A2169 | U2109 | G2012 | A1876 | G1763 | A1636 | C1506 | U1405 | G1256 |
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| C2788 | A2657 | A2518 | G2367 | C2283 | C2175 | G2115 | U2022 | G1883 | G1769 | C1648 | G1515 | G1416 | C1270 |
| C2789 | G2658 | U2522 | A2377 | C2284 | C2177 | A2117 | G2023 | G1889 | A1773 | G1649 | C1516 | C1417 | G1271 |
| A2790 | G2659 | A2378 | A2378 | C2285 | C2178 | U2118 | U2028 | G1899 | U1776 | G1650 | G1517 | U1408 | A1272 |
| C2791 | G2659 | G2529 | G2383 | A2287 | U2180 | A2119 | G2030 | A1900 | G1777 | A1652 | G1519 | C1409 | |
| G2792 | C2683 | A2530 | G2384 | A2288 | G2181 | G2121 | A2031 | G1903 | U1778 | G1653 | C1520 | | |
| G2793 | G2683 | G2385 | G2385 | G2289 | U2182 | U2122 | G2032 | G1903 | A1780 | A1665 | C1530 | G1418 | |
| G2794 | U2687 | G2532 | | U2291 | C2183 | G2124 | A2033 | G1906 | | G1666 | C1532 | | |



• Molecule 26: 23S Ribosomal RNA







• Molecule 27: 5S Ribosomal RNA

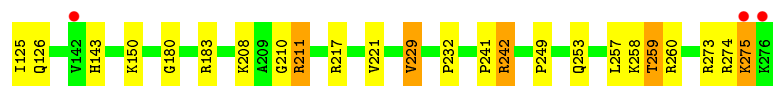
Chain BB: 71% 23% 5%

• Molecule 27: 5S Ribosomal RNA

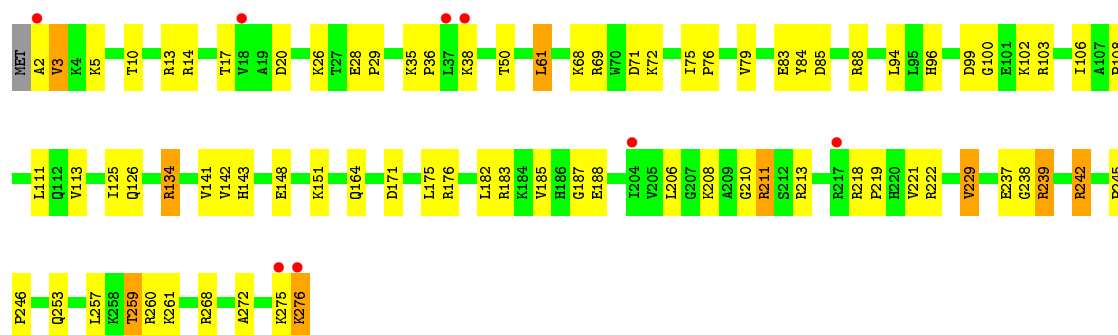
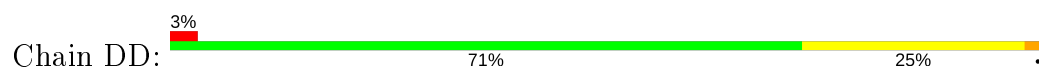
Chain DB: 29% 50% 19%

• Molecule 28: 50S ribosomal protein L2

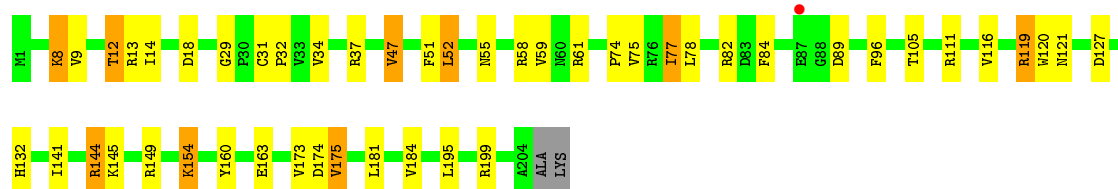
Chain BD: 79% 17%



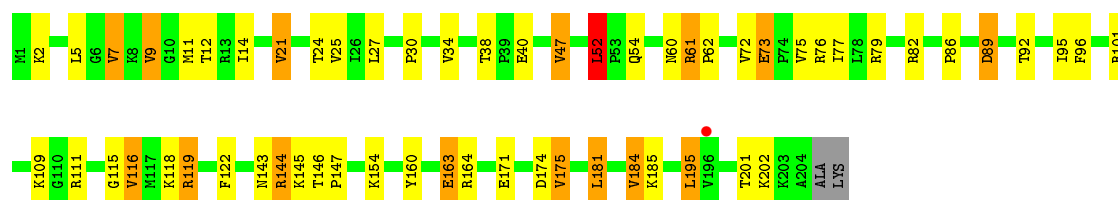
- Molecule 28: 50S ribosomal protein L2



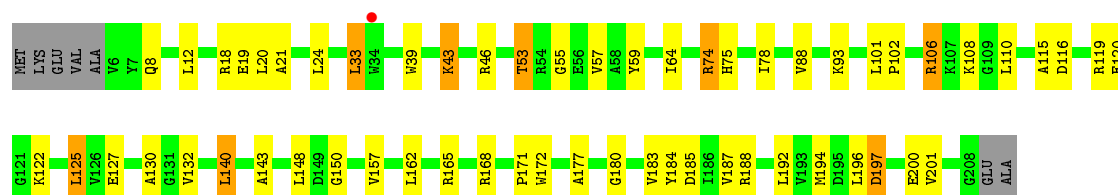
- Molecule 29: 50S ribosomal protein L3



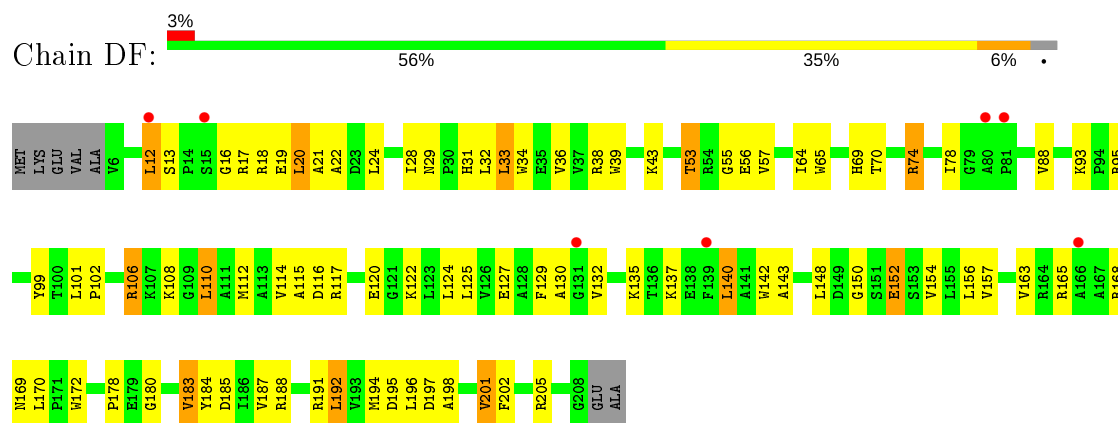
- Molecule 29: 50S ribosomal protein L3



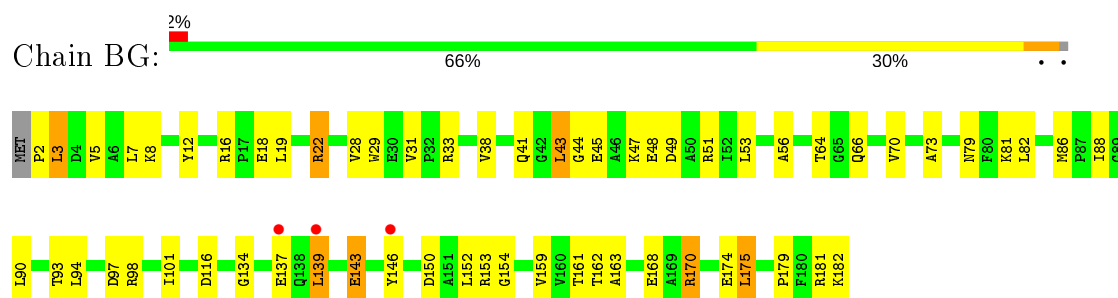
- Molecule 30: 50S ribosomal protein L4



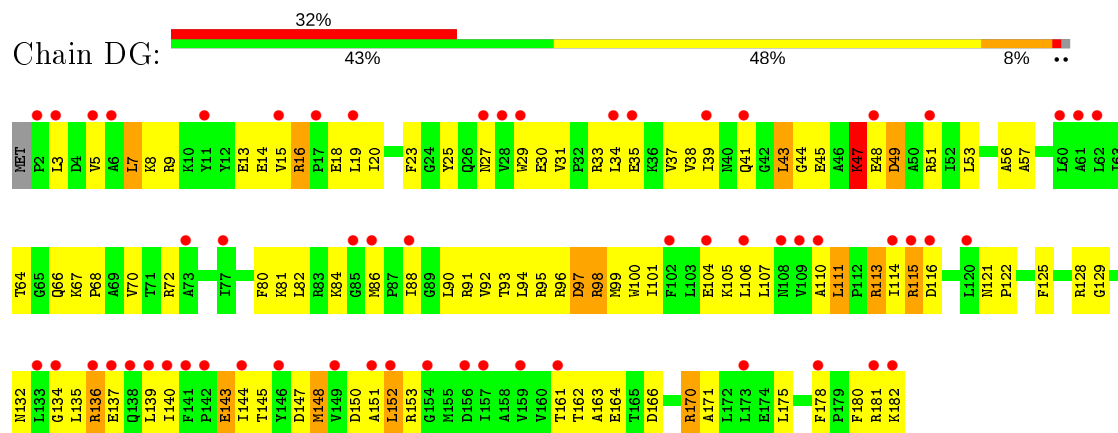
- Molecule 30: 50S ribosomal protein L4



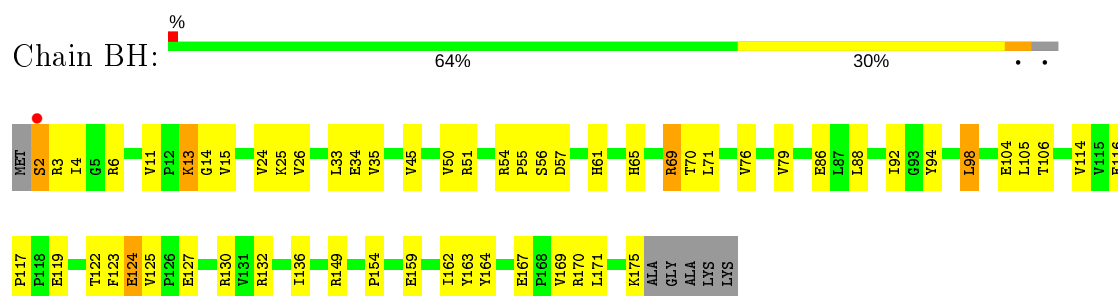
- Molecule 31: 50S ribosomal protein L5



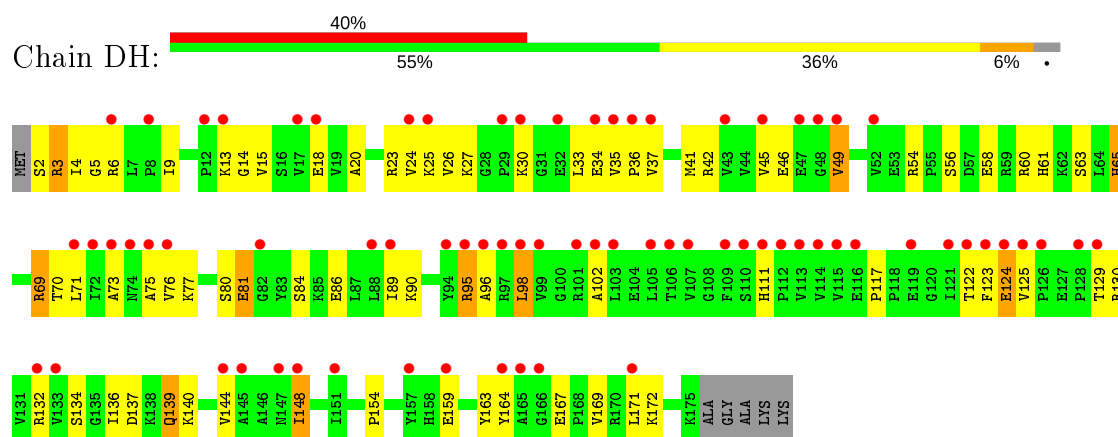
- Molecule 31: 50S ribosomal protein L5



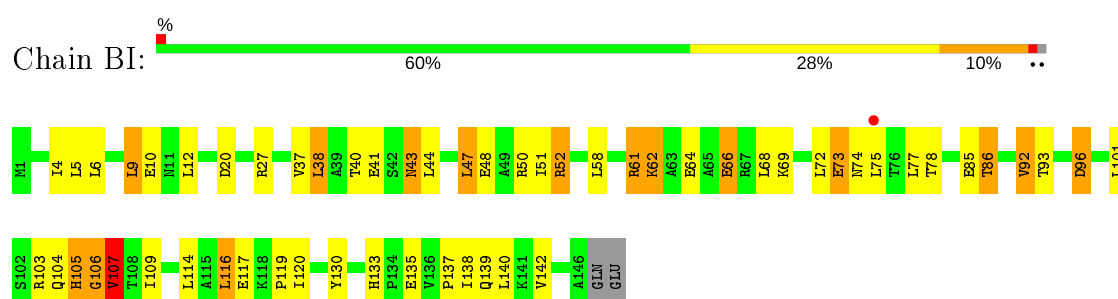
- Molecule 32: 50S ribosomal protein L6



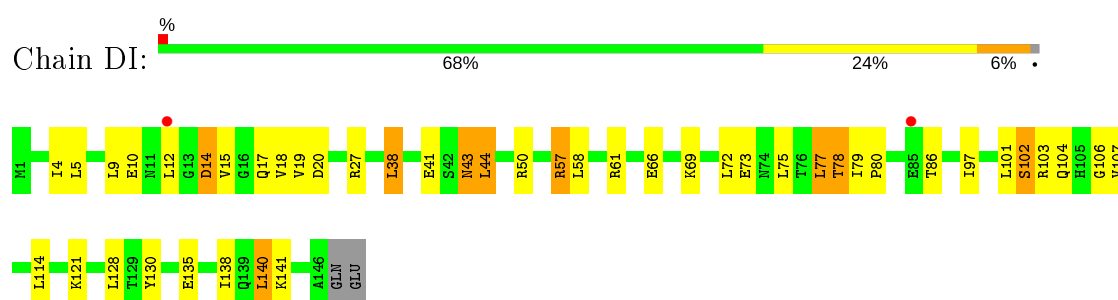
- Molecule 32: 50S ribosomal protein L6



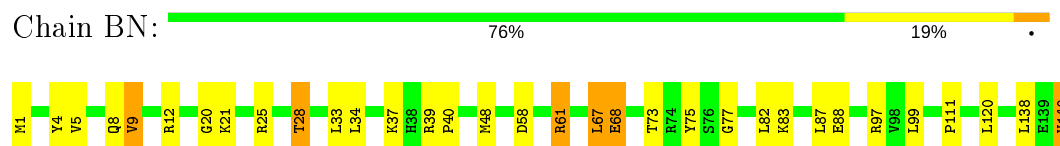
• Molecule 33: 50S ribosomal protein L9



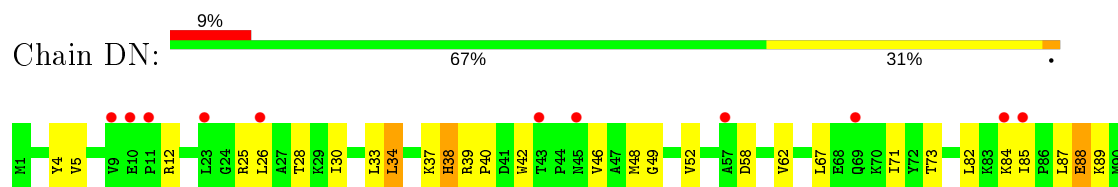
• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13

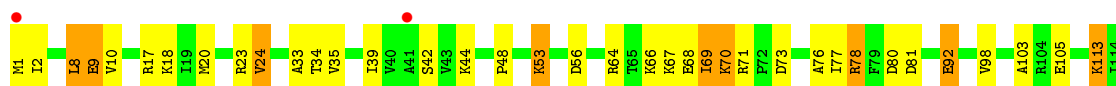




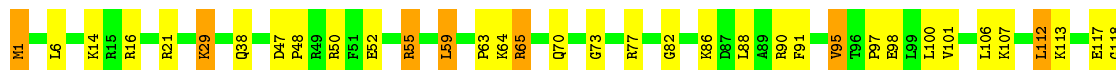
- Molecule 35: 50S ribosomal protein L14



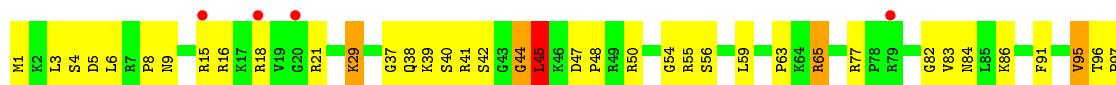
- Molecule 35: 50S ribosomal protein L14



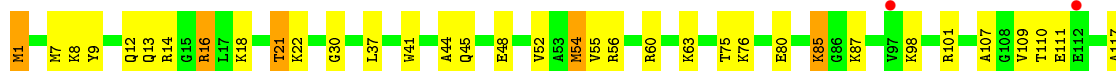
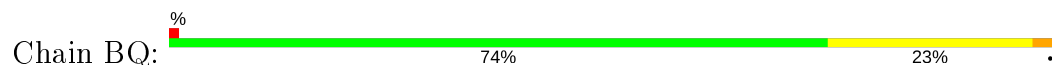
- Molecule 36: 50S ribosomal protein L15



- Molecule 36: 50S ribosomal protein L15

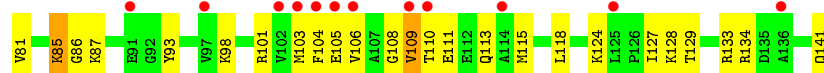
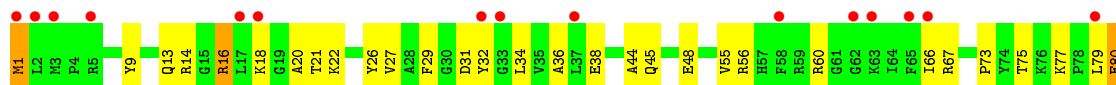


- Molecule 37: 50S ribosomal protein L16

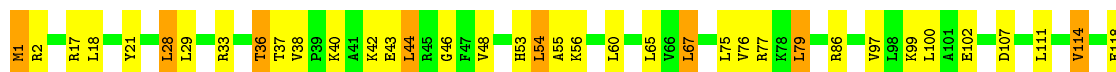




- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17



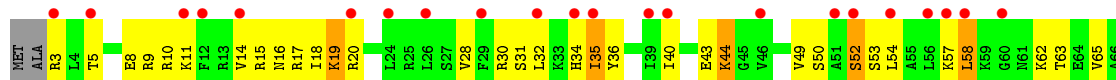
- Molecule 38: 50S ribosomal protein L17



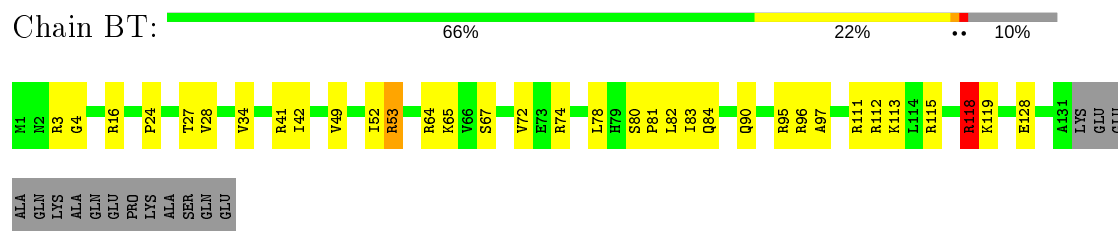
- Molecule 39: 50S ribosomal protein L18



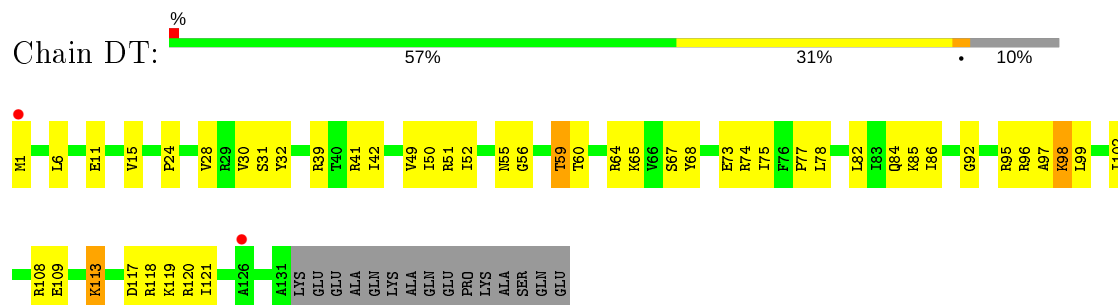
- Molecule 39: 50S ribosomal protein L18



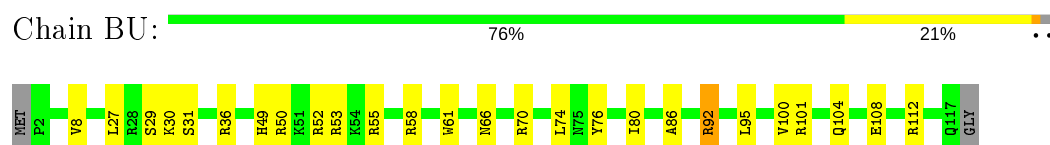
- Molecule 40: 50S ribosomal protein L19



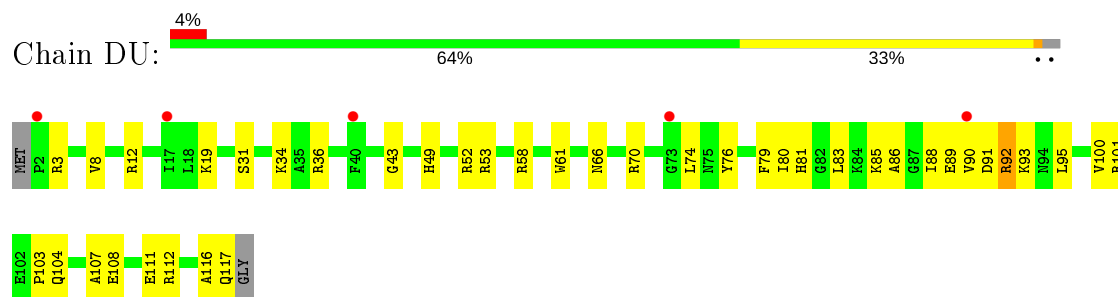
- Molecule 40: 50S ribosomal protein L19



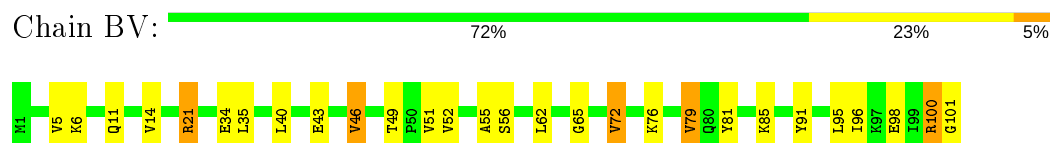
- Molecule 41: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L20

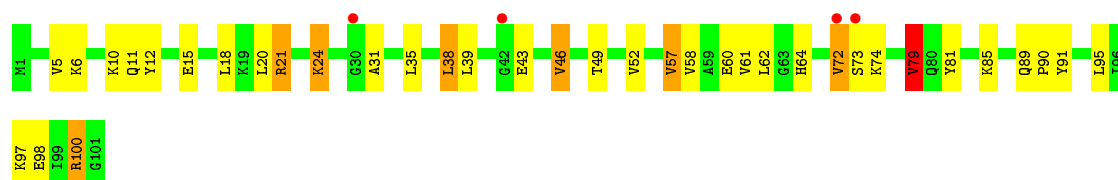


- Molecule 42: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L21





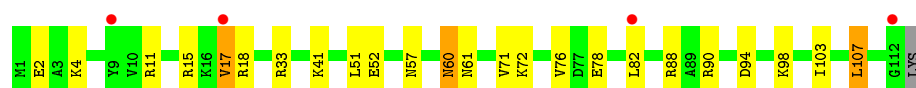
- Molecule 43: 50S ribosomal protein L22

Chain BW: 79% 18% . .



- Molecule 43: 50S ribosomal protein L22

Chain DW: 4% 78% 19% . .



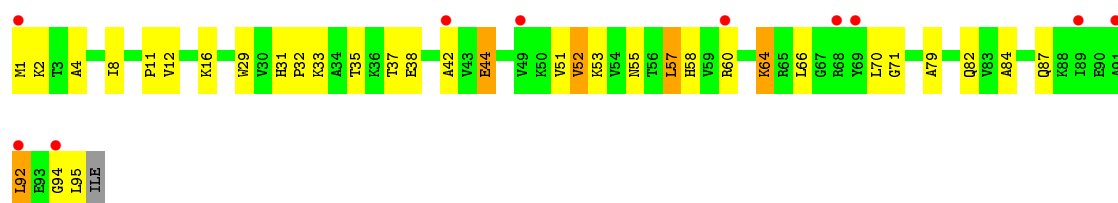
- Molecule 44: 50S ribosomal protein L23

Chain BX: 75% 20% . .



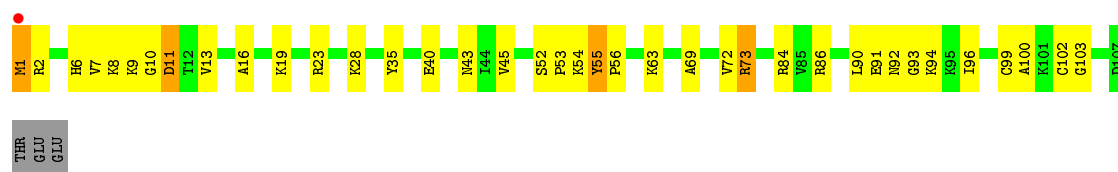
- Molecule 44: 50S ribosomal protein L23

Chain DX: 10% 64% 30% 5% .

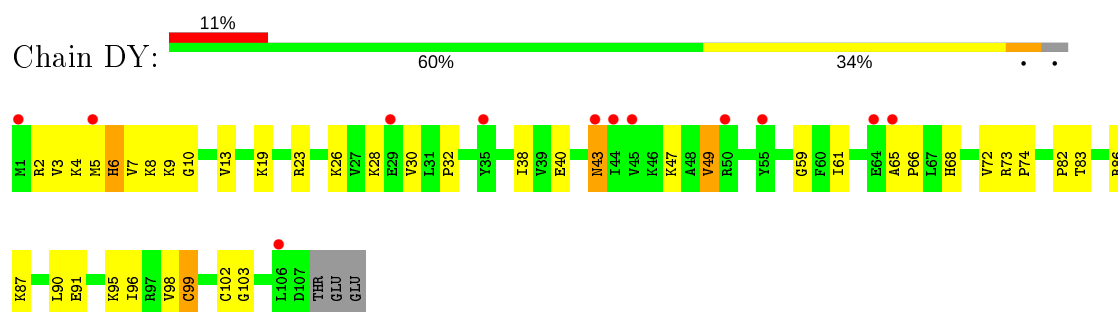


- Molecule 45: 50S ribosomal protein L24

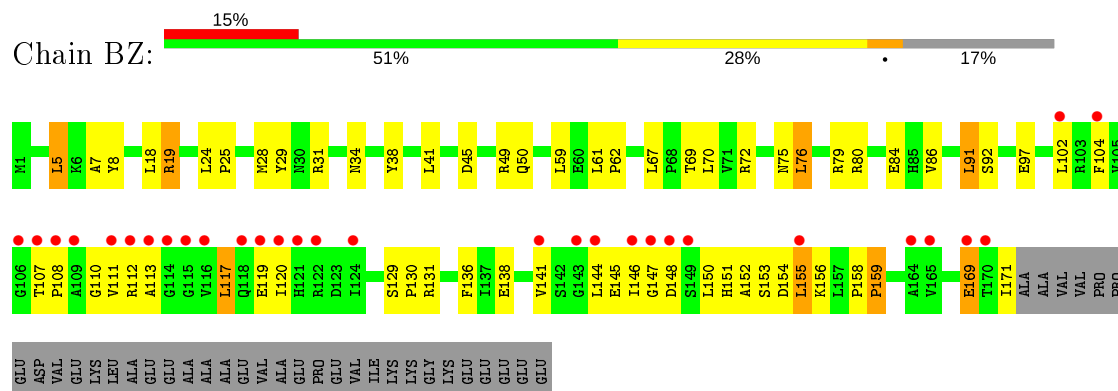
Chain BY: % 63% 31% . .



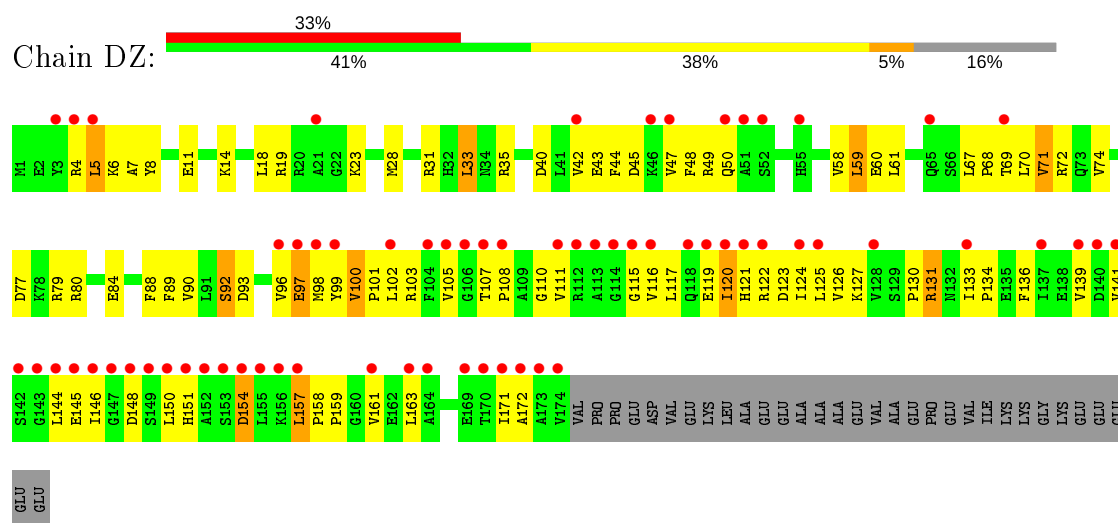
- Molecule 45: 50S ribosomal protein L24



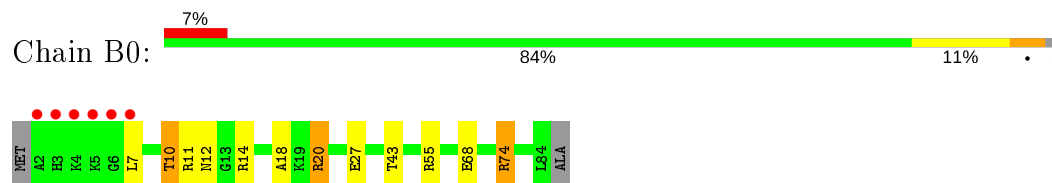
- Molecule 46: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L27

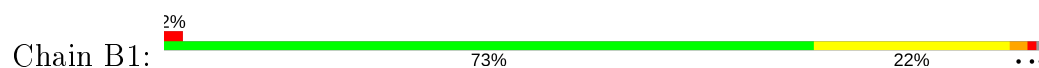


- Molecule 47: 50S ribosomal protein L27

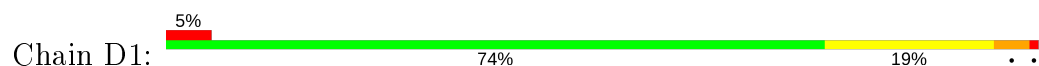




- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28



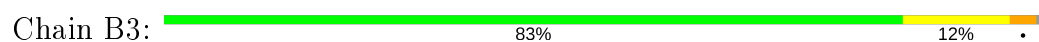
- Molecule 49: 50S ribosomal protein L29



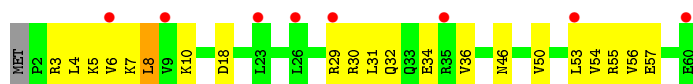
- Molecule 49: 50S ribosomal protein L29



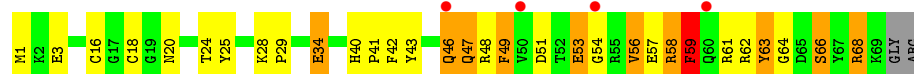
- Molecule 50: 50S ribosomal protein L30



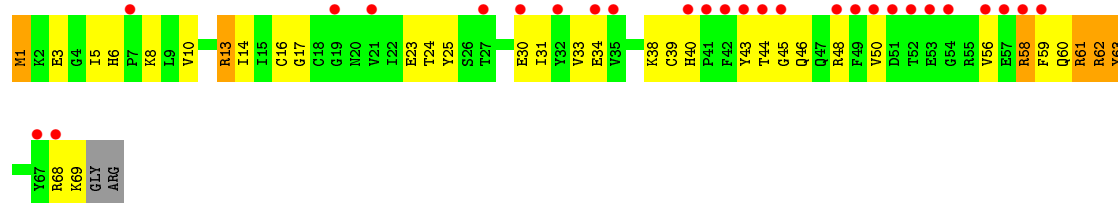
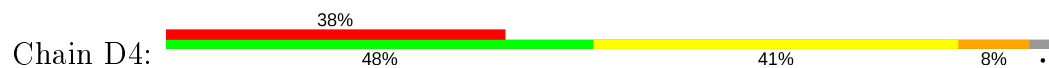
- Molecule 50: 50S ribosomal protein L30



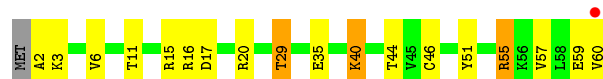
- Molecule 51: 50S ribosomal protein L31



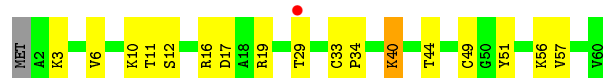
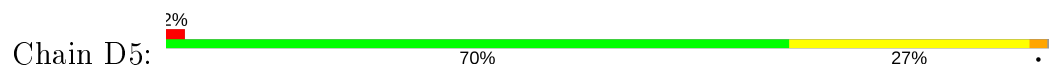
- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



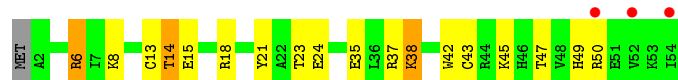
- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33

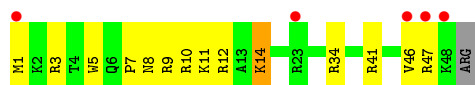


- Molecule 54: 50S ribosomal protein L34





- Molecule 54: 50S ribosomal protein L34



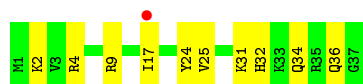
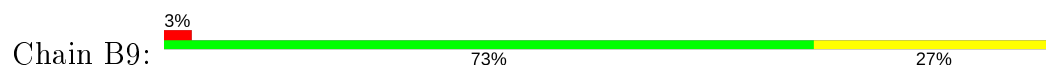
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 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 | 209.45Å 448.85Å 619.02Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 151.90 – 2.60 224.43 – 2.60 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (151.90-2.60) 99.9 (224.43-2.60) | Depositor EDS |
| R_{merge} | 0.23 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.22 (at 2.62Å) | Xtriage |
| Refinement program | PHENIX 1.8.2_1309 | Depositor |
| R, R_{free} | 0.223 , 0.264 0.224 , 0.265 | Depositor DCC |
| R_{free} test set | 88430 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 56.4 | Xtriage |
| Anisotropy | 0.077 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 60.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 297127 | wwPDB-VP |
| Average B, all atoms (Å ²) | 60.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: 5MU, ZN, MIA, SF4, MG, F3N, 31H, 5MC, 4SU, 7MG, K, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | AA | 0.38 | 0/36027 | 0.91 | 43/56227 (0.1%) |
| 1 | CA | 0.41 | 8/36170 (0.0%) | 1.01 | 101/56452 (0.2%) |
| 2 | AB | 0.30 | 0/1881 | 0.62 | 0/2542 |
| 2 | CB | 0.33 | 0/1860 | 0.67 | 2/2518 (0.1%) |
| 3 | AC | 0.27 | 0/1576 | 0.52 | 0/2130 |
| 3 | CC | 0.31 | 0/1568 | 0.61 | 1/2122 (0.0%) |
| 4 | AD | 0.29 | 0/1689 | 0.55 | 0/2267 |
| 4 | CD | 0.30 | 0/1708 | 0.55 | 0/2289 |
| 5 | AE | 0.30 | 0/1145 | 0.54 | 0/1543 |
| 5 | CE | 0.33 | 0/1149 | 0.61 | 0/1548 |
| 6 | AF | 0.30 | 0/825 | 0.52 | 0/1118 |
| 6 | CF | 0.32 | 0/833 | 0.55 | 0/1128 |
| 7 | AG | 0.28 | 0/1250 | 0.50 | 0/1679 |
| 7 | CG | 0.27 | 0/1254 | 0.53 | 0/1683 |
| 8 | AH | 0.28 | 0/1108 | 0.52 | 0/1494 |
| 8 | CH | 0.29 | 0/1108 | 0.54 | 0/1494 |
| 9 | AI | 0.29 | 0/1005 | 0.57 | 0/1350 |
| 9 | CI | 0.31 | 0/997 | 0.64 | 0/1343 |
| 10 | AJ | 0.27 | 0/722 | 0.54 | 0/982 |
| 10 | CJ | 0.33 | 0/727 | 0.62 | 0/988 |
| 11 | AK | 0.28 | 0/848 | 0.51 | 0/1149 |
| 11 | CK | 0.28 | 0/848 | 0.53 | 0/1149 |
| 12 | AL | 0.33 | 0/946 | 0.52 | 0/1274 |
| 12 | CL | 0.30 | 0/946 | 0.58 | 0/1274 |
| 13 | AM | 0.31 | 0/977 | 0.60 | 0/1310 |
| 13 | CM | 0.31 | 0/961 | 0.62 | 1/1291 (0.1%) |
| 14 | AN | 0.32 | 0/501 | 0.53 | 0/664 |
| 14 | CN | 0.33 | 0/501 | 0.57 | 0/664 |
| 15 | AO | 0.28 | 0/739 | 0.52 | 0/985 |
| 15 | CO | 0.29 | 0/739 | 0.54 | 0/985 |
| 16 | AP | 0.31 | 0/697 | 0.54 | 0/939 |
| 16 | CP | 0.29 | 0/693 | 0.51 | 0/935 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.29 | 0/836 | 0.53 | 0/1117 |
| 17 | CQ | 0.29 | 0/836 | 0.50 | 0/1117 |
| 18 | AR | 0.27 | 0/560 | 0.54 | 0/746 |
| 18 | CR | 0.29 | 0/560 | 0.56 | 0/746 |
| 19 | AS | 0.30 | 0/676 | 0.58 | 0/911 |
| 19 | CS | 0.33 | 0/661 | 0.71 | 0/893 |
| 20 | AT | 0.29 | 0/730 | 0.57 | 0/965 |
| 20 | CT | 0.28 | 0/733 | 0.55 | 0/969 |
| 21 | AU | 0.27 | 0/203 | 0.50 | 0/266 |
| 21 | CU | 0.33 | 0/203 | 0.53 | 0/266 |
| 22 | AV | 0.39 | 0/310 | 0.96 | 1/480 (0.2%) |
| 22 | CV | 0.42 | 0/282 | 0.99 | 2/437 (0.5%) |
| 23 | AW | 0.47 | 0/1577 | 1.20 | 7/2454 (0.3%) |
| 23 | CW | 0.53 | 0/1531 | 1.28 | 9/2379 (0.4%) |
| 24 | AX | 0.53 | 2/1700 (0.1%) | 1.20 | 22/2650 (0.8%) |
| 24 | CX | 0.46 | 0/1700 | 1.15 | 6/2650 (0.2%) |
| 25 | AY | 0.58 | 0/1602 | 1.35 | 20/2493 (0.8%) |
| 25 | CY | 0.59 | 0/1579 | 1.40 | 25/2455 (1.0%) |
| 26 | BA | 0.50 | 1/68013 (0.0%) | 0.93 | 91/106165 (0.1%) |
| 26 | DA | 0.41 | 1/67542 (0.0%) | 0.92 | 74/105428 (0.1%) |
| 27 | BB | 0.41 | 0/2878 | 0.86 | 1/4490 (0.0%) |
| 27 | DB | 0.44 | 0/2878 | 0.92 | 2/4490 (0.0%) |
| 28 | BD | 0.37 | 0/2186 | 0.59 | 0/2944 |
| 28 | DD | 0.33 | 0/2192 | 0.57 | 0/2951 |
| 29 | BE | 0.37 | 0/1592 | 0.57 | 0/2149 |
| 29 | DE | 0.33 | 0/1592 | 0.55 | 0/2149 |
| 30 | BF | 0.34 | 0/1619 | 0.55 | 0/2193 |
| 30 | DF | 0.32 | 0/1615 | 0.55 | 0/2188 |
| 31 | BG | 0.31 | 0/1450 | 0.54 | 1/1959 (0.1%) |
| 31 | DG | 0.33 | 0/1449 | 0.60 | 0/1958 |
| 32 | BH | 0.33 | 0/1356 | 0.54 | 0/1834 |
| 32 | DH | 0.29 | 0/1356 | 0.54 | 0/1834 |
| 33 | BI | 0.28 | 0/1100 | 0.56 | 0/1501 |
| 33 | DI | 0.29 | 0/1088 | 0.55 | 0/1484 |
| 34 | BN | 0.34 | 0/1144 | 0.53 | 0/1543 |
| 34 | DN | 0.31 | 0/1144 | 0.52 | 0/1543 |
| 35 | BO | 0.37 | 0/943 | 0.57 | 0/1269 |
| 35 | DO | 0.31 | 0/943 | 0.55 | 1/1269 (0.1%) |
| 36 | BP | 0.35 | 0/1156 | 0.57 | 0/1537 |
| 36 | DP | 0.32 | 0/1152 | 0.61 | 1/1533 (0.1%) |
| 37 | BQ | 0.35 | 0/1143 | 0.53 | 0/1527 |
| 37 | DQ | 0.32 | 0/1143 | 0.53 | 0/1527 |
| 38 | BR | 0.36 | 0/982 | 0.58 | 0/1312 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DR | 0.30 | 0/982 | 0.53 | 0/1312 |
| 39 | BS | 0.31 | 0/887 | 0.56 | 0/1180 |
| 39 | DS | 0.28 | 0/880 | 0.56 | 0/1172 |
| 40 | BT | 0.34 | 0/1105 | 0.56 | 1/1477 (0.1%) |
| 40 | DT | 0.31 | 0/1097 | 0.53 | 0/1468 |
| 41 | BU | 0.39 | 0/977 | 0.56 | 0/1301 |
| 41 | DU | 0.30 | 0/977 | 0.54 | 0/1301 |
| 42 | BV | 0.36 | 0/782 | 0.58 | 0/1049 |
| 42 | DV | 0.32 | 0/782 | 0.57 | 1/1049 (0.1%) |
| 43 | BW | 0.39 | 0/897 | 0.56 | 0/1205 |
| 43 | DW | 0.31 | 0/897 | 0.52 | 0/1205 |
| 44 | BX | 0.38 | 0/764 | 0.57 | 1/1025 (0.1%) |
| 44 | DX | 0.33 | 0/764 | 0.58 | 1/1025 (0.1%) |
| 45 | BY | 0.35 | 0/819 | 0.57 | 0/1095 |
| 45 | DY | 0.32 | 0/819 | 0.55 | 0/1095 |
| 46 | BZ | 0.32 | 0/1379 | 0.58 | 0/1873 |
| 46 | DZ | 0.30 | 0/1390 | 0.56 | 0/1890 |
| 47 | B0 | 0.35 | 0/662 | 0.55 | 0/881 |
| 47 | D0 | 0.32 | 0/662 | 0.53 | 0/881 |
| 48 | B1 | 0.35 | 0/762 | 0.54 | 0/1014 |
| 48 | D1 | 0.31 | 0/762 | 0.53 | 0/1014 |
| 49 | B2 | 0.31 | 0/590 | 0.53 | 0/781 |
| 49 | D2 | 0.28 | 0/590 | 0.46 | 0/781 |
| 50 | B3 | 0.34 | 0/474 | 0.57 | 0/635 |
| 50 | D3 | 0.27 | 0/469 | 0.55 | 0/630 |
| 51 | B4 | 0.31 | 0/571 | 0.70 | 0/768 |
| 51 | D4 | 0.32 | 0/545 | 0.67 | 0/737 |
| 52 | B5 | 0.35 | 0/469 | 0.65 | 0/635 |
| 52 | D5 | 0.31 | 0/469 | 0.50 | 0/635 |
| 53 | B6 | 0.37 | 0/460 | 0.52 | 0/613 |
| 53 | D6 | 0.29 | 0/456 | 0.49 | 0/608 |
| 54 | B7 | 0.40 | 0/426 | 0.57 | 0/561 |
| 54 | D7 | 0.33 | 0/426 | 0.54 | 0/561 |
| 55 | B8 | 0.37 | 0/525 | 0.59 | 0/691 |
| 55 | D8 | 0.32 | 0/525 | 0.51 | 0/691 |
| 56 | B9 | 0.37 | 0/310 | 0.50 | 0/407 |
| 56 | D9 | 0.33 | 0/310 | 0.52 | 0/407 |
| All | All | 0.41 | 12/316594 (0.0%) | 0.87 | 415/473940 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | AB | 0 | 2 |
| 2 | CB | 0 | 1 |
| 7 | AG | 0 | 2 |
| 20 | CT | 0 | 1 |
| 33 | BI | 0 | 1 |
| 35 | BO | 0 | 1 |
| 39 | BS | 0 | 1 |
| 51 | B4 | 0 | 1 |
| All | All | 0 | 10 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|--------|-------------|----------|
| 1 | CA | 1154 | G | N1-C2 | -10.90 | 1.29 | 1.37 |
| 1 | CA | 1119 | C | N3-C4 | -10.71 | 1.26 | 1.33 |
| 1 | CA | 1154 | G | C6-N1 | -10.47 | 1.32 | 1.39 |
| 26 | DA | 528 | A | N9-C4 | -6.80 | 1.33 | 1.37 |
| 1 | CA | 1154 | G | N7-C5 | -6.78 | 1.35 | 1.39 |
| 1 | CA | 1119 | C | C2-N3 | -6.04 | 1.30 | 1.35 |
| 26 | BA | 1142(A) | A | N9-C4 | -5.97 | 1.34 | 1.37 |
| 1 | CA | 1154 | G | C5-C4 | 5.82 | 1.42 | 1.38 |
| 24 | AX | 22 | G | N7-C5 | 5.60 | 1.42 | 1.39 |
| 24 | AX | 14 | A | N7-C5 | -5.36 | 1.36 | 1.39 |
| 1 | CA | 1154 | G | C8-N7 | -5.29 | 1.27 | 1.30 |
| 1 | CA | 1119 | C | N1-C2 | 5.25 | 1.45 | 1.40 |

All (415) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | CA | 1119 | C | N1-C2-O2 | 35.97 | 140.48 | 118.90 |
| 1 | CA | 1154 | G | C5-C6-O6 | 25.44 | 143.86 | 128.60 |
| 1 | CA | 1154 | G | N3-C2-N2 | 24.34 | 136.94 | 119.90 |
| 1 | CA | 1154 | G | N1-C2-N2 | -21.83 | 96.56 | 116.20 |
| 1 | CA | 1119 | C | N3-C2-O2 | -21.82 | 106.63 | 121.90 |
| 1 | CA | 1154 | G | C5-C6-N1 | -18.28 | 102.36 | 111.50 |
| 1 | CA | 1119 | C | C2-N3-C4 | 17.80 | 128.80 | 119.90 |
| 1 | CA | 1154 | G | C6-N1-C2 | 16.98 | 135.29 | 125.10 |
| 1 | CA | 1119 | C | C2-N1-C1' | 15.84 | 136.22 | 118.80 |
| 1 | CA | 1119 | C | N3-C4-N4 | -15.07 | 107.45 | 118.00 |
| 1 | CA | 1119 | C | C5-C4-N4 | 15.04 | 130.73 | 120.20 |
| 1 | CA | 1119 | C | C6-N1-C1' | -12.88 | 105.34 | 120.80 |
| 25 | CY | 66 | U | C5-C4-O4 | -11.57 | 118.96 | 125.90 |
| 1 | CA | 1154 | G | C2-N3-C4 | -11.37 | 106.22 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24 | AX | 46 | G | C6-N1-C2 | -11.23 | 118.36 | 125.10 |
| 1 | CA | 1154 | G | C4-N9-C1' | 10.50 | 140.15 | 126.50 |
| 26 | DA | 2139 | C | N1-C2-O2 | 10.43 | 125.16 | 118.90 |
| 1 | CA | 1154 | G | N1-C6-O6 | -10.31 | 113.72 | 119.90 |
| 24 | AX | 14 | A | C4-C5-C6 | 10.16 | 122.08 | 117.00 |
| 1 | CA | 1180 | A | C5-C6-N1 | -9.83 | 112.78 | 117.70 |
| 26 | DA | 2139 | C | C2-N1-C1' | 9.76 | 129.53 | 118.80 |
| 1 | CA | 1119 | C | N1-C2-N3 | -9.72 | 112.40 | 119.20 |
| 1 | CA | 1154 | G | C8-N9-C1' | -9.27 | 114.95 | 127.00 |
| 26 | DA | 34 | C | N1-C2-O2 | 9.06 | 124.33 | 118.90 |
| 24 | AX | 14 | A | C5-N7-C8 | 8.99 | 108.39 | 103.90 |
| 26 | DA | 2102 | U | N1-C2-O2 | 8.93 | 129.05 | 122.80 |
| 26 | DA | 528 | A | C2-N3-C4 | -8.89 | 106.15 | 110.60 |
| 25 | CY | 7 | A | C6-N1-C2 | -8.88 | 113.27 | 118.60 |
| 26 | DA | 2187 | G | C5-C6-O6 | -8.86 | 123.28 | 128.60 |
| 26 | DA | 2174 | C | C2-N1-C1' | 8.85 | 128.54 | 118.80 |
| 24 | AX | 22 | G | C5-N7-C8 | -8.78 | 99.91 | 104.30 |
| 25 | AY | 50 | U | C5-C4-O4 | 8.74 | 131.15 | 125.90 |
| 1 | CA | 1004 | A | O4'-C1'-N9 | 8.59 | 115.08 | 108.20 |
| 1 | CA | 1119 | C | C5-C6-N1 | 8.58 | 125.29 | 121.00 |
| 26 | BA | 512 | G | O4'-C1'-N9 | 8.51 | 115.01 | 108.20 |
| 24 | CX | 14 | A | C4-C5-C6 | 8.43 | 121.22 | 117.00 |
| 25 | AY | 68 | C | N1-C2-O2 | 8.36 | 123.92 | 118.90 |
| 26 | DA | 2682 | U | O5'-P-OP2 | -8.36 | 98.18 | 105.70 |
| 1 | CA | 1119 | C | C4-C5-C6 | -8.35 | 113.23 | 117.40 |
| 26 | DA | 2136 | C | N1-C2-O2 | 8.32 | 123.89 | 118.90 |
| 25 | AY | 50 | U | C2-N3-C4 | 8.32 | 131.99 | 127.00 |
| 1 | CA | 1180 | A | C2-N3-C4 | -8.29 | 106.46 | 110.60 |
| 26 | BA | 897 | C | C5-C6-N1 | 8.26 | 125.13 | 121.00 |
| 26 | DA | 2139 | C | C6-N1-C1' | -8.07 | 111.12 | 120.80 |
| 26 | DA | 2152 | G | N1-C6-O6 | 8.07 | 124.74 | 119.90 |
| 26 | DA | 2061 | G | O5'-P-OP2 | -8.04 | 98.47 | 105.70 |
| 25 | AY | 64 | A | C6-N1-C2 | 8.01 | 123.41 | 118.60 |
| 26 | BA | 2140 | C | C2-N1-C1' | 7.97 | 127.56 | 118.80 |
| 24 | AX | 22 | G | C4-C5-C6 | -7.92 | 114.05 | 118.80 |
| 1 | AA | 1027 | C | N1-C2-O2 | 7.92 | 123.65 | 118.90 |
| 24 | AX | 14 | A | C5-C6-N1 | -7.91 | 113.75 | 117.70 |
| 25 | CY | 68 | C | N1-C2-O2 | 7.88 | 123.62 | 118.90 |
| 26 | DA | 34 | C | C2-N1-C1' | 7.84 | 127.43 | 118.80 |
| 26 | DA | 2152 | G | C5-C6-O6 | -7.69 | 123.99 | 128.60 |
| 26 | DA | 897 | C | C2-N1-C1' | 7.61 | 127.17 | 118.80 |
| 25 | CY | 66 | U | N3-C4-O4 | 7.57 | 124.69 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | CA | 79 | G | C5-C6-O6 | 7.50 | 133.10 | 128.60 |
| 25 | AY | 64 | A | C5-C6-N6 | 7.47 | 129.67 | 123.70 |
| 26 | BA | 2140 | C | C6-N1-C2 | -7.46 | 117.32 | 120.30 |
| 24 | AX | 46 | G | N3-C2-N2 | -7.39 | 114.72 | 119.90 |
| 25 | CY | 7 | A | C5-C6-N1 | 7.38 | 121.39 | 117.70 |
| 1 | CA | 1154 | G | C4-C5-C6 | 7.34 | 123.20 | 118.80 |
| 26 | BA | 1963 | U | C2-N1-C1' | 7.32 | 126.48 | 117.70 |
| 26 | DA | 2136 | C | N3-C2-O2 | -7.30 | 116.79 | 121.90 |
| 26 | BA | 999 | U | O5'-P-OP2 | -7.28 | 99.14 | 105.70 |
| 23 | AW | 50 | U | C5-C6-N1 | 7.27 | 126.33 | 122.70 |
| 1 | AA | 1042 | G | O4'-C1'-N9 | 7.24 | 114.00 | 108.20 |
| 25 | AY | 56 | C | N1-C2-O2 | 7.24 | 123.25 | 118.90 |
| 26 | BA | 528 | A | C2-N3-C4 | -7.23 | 106.98 | 110.60 |
| 26 | BA | 12 | U | C2-N1-C1' | 7.20 | 126.34 | 117.70 |
| 1 | CA | 1137 | C | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 1 | AA | 997 | U | C5-C4-O4 | 7.14 | 130.18 | 125.90 |
| 1 | CA | 1004 | A | N1-C6-N6 | -7.13 | 114.32 | 118.60 |
| 26 | DA | 2153 | G | C5-C6-O6 | -7.12 | 124.33 | 128.60 |
| 25 | CY | 68 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 1 | AA | 1030(B) | C | C2-N1-C1' | 7.02 | 126.52 | 118.80 |
| 23 | AW | 70 | G | C4-N9-C1' | -7.01 | 117.39 | 126.50 |
| 26 | BA | 897 | C | C2-N1-C1' | 6.97 | 126.47 | 118.80 |
| 26 | BA | 2140 | C | N1-C2-O2 | 6.97 | 123.08 | 118.90 |
| 1 | CA | 1119 | C | C6-N1-C2 | -6.92 | 117.53 | 120.30 |
| 26 | DA | 2155 | G | C6-N1-C2 | 6.92 | 129.25 | 125.10 |
| 26 | DA | 2174 | C | C6-N1-C1' | -6.90 | 112.52 | 120.80 |
| 44 | DX | 57 | LEU | CA-CB-CG | 6.87 | 131.10 | 115.30 |
| 25 | CY | 66 | U | C2-N3-C4 | -6.86 | 122.88 | 127.00 |
| 26 | BA | 141 | A | N7-C8-N9 | 6.84 | 117.22 | 113.80 |
| 1 | AA | 1067 | A | P-O3'-C3' | 6.84 | 127.91 | 119.70 |
| 26 | BA | 2269 | A | O5'-P-OP1 | -6.84 | 99.55 | 105.70 |
| 26 | BA | 2141 | G | C5-C6-O6 | 6.83 | 132.70 | 128.60 |
| 1 | CA | 1225 | A | C5-C6-N6 | 6.82 | 129.16 | 123.70 |
| 25 | CY | 7 | A | N3-C4-N9 | 6.81 | 132.85 | 127.40 |
| 26 | BA | 1372 | U | C5-C4-O4 | -6.80 | 121.82 | 125.90 |
| 1 | AA | 1042 | G | C8-N9-C1' | 6.74 | 135.76 | 127.00 |
| 26 | BA | 330 | A | C2-N3-C4 | -6.73 | 107.23 | 110.60 |
| 23 | AW | 70 | G | C8-N9-C1' | 6.71 | 135.72 | 127.00 |
| 24 | AX | 46 | G | N1-C2-N3 | 6.71 | 127.92 | 123.90 |
| 26 | BA | 1021 | A | C2-N3-C4 | -6.70 | 107.25 | 110.60 |
| 1 | AA | 1002 | G | N3-C4-N9 | 6.69 | 130.01 | 126.00 |
| 1 | CA | 1150 | U | C5-C4-O4 | 6.68 | 129.91 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | AA | 1002 | G | C4-N9-C1' | 6.68 | 135.18 | 126.50 |
| 26 | BA | 2140 | C | N3-C2-O2 | -6.67 | 117.23 | 121.90 |
| 26 | DA | 2139 | C | N3-C2-O2 | -6.66 | 117.24 | 121.90 |
| 26 | BA | 1992 | G | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 26 | BA | 975 | C | N1-C2-O2 | -6.64 | 114.92 | 118.90 |
| 25 | AY | 4 | C | N3-C2-O2 | -6.61 | 117.27 | 121.90 |
| 1 | CA | 1042 | G | N3-C4-C5 | 6.58 | 131.89 | 128.60 |
| 1 | CA | 65 | U | P-O3'-C3' | 6.58 | 127.59 | 119.70 |
| 25 | CY | 18 | G | C4-N9-C1' | 6.57 | 135.04 | 126.50 |
| 1 | AA | 1150 | U | C5-C4-O4 | 6.57 | 129.84 | 125.90 |
| 26 | BA | 1142(A) | A | C2-N3-C4 | -6.56 | 107.32 | 110.60 |
| 25 | CY | 18 | G | C8-N9-C1' | -6.55 | 118.48 | 127.00 |
| 26 | BA | 945 | A | C2-N3-C4 | -6.55 | 107.33 | 110.60 |
| 24 | AX | 22 | G | C8-N9-C1' | 6.54 | 135.50 | 127.00 |
| 1 | AA | 346 | G | C4-N9-C1' | 6.52 | 134.98 | 126.50 |
| 24 | CX | 14 | A | C5-N7-C8 | 6.52 | 107.16 | 103.90 |
| 24 | CX | 46 | G | C6-N1-C2 | -6.52 | 121.19 | 125.10 |
| 26 | DA | 2139 | C | N3-C4-C5 | 6.52 | 124.51 | 121.90 |
| 26 | BA | 1372 | U | N3-C4-O4 | 6.52 | 123.96 | 119.40 |
| 26 | DA | 34 | C | N3-C2-O2 | -6.51 | 117.34 | 121.90 |
| 1 | AA | 1026 | G | C8-N9-C4 | -6.47 | 103.81 | 106.40 |
| 1 | CA | 848 | C | C5-C6-N1 | 6.46 | 124.23 | 121.00 |
| 26 | DA | 2153 | G | N1-C6-O6 | 6.45 | 123.77 | 119.90 |
| 1 | CA | 754 | C | C2-N1-C1' | 6.44 | 125.89 | 118.80 |
| 1 | AA | 841 | U | C5-C6-N1 | 6.44 | 125.92 | 122.70 |
| 25 | AY | 4 | C | C6-N1-C2 | -6.43 | 117.73 | 120.30 |
| 1 | CA | 1030 | C | C2-N1-C1' | 6.41 | 125.84 | 118.80 |
| 26 | DA | 1614 | A | O5'-P-OP1 | -6.40 | 99.94 | 105.70 |
| 1 | AA | 1002 | G | C8-N9-C1' | -6.36 | 118.73 | 127.00 |
| 26 | DA | 897 | C | C6-N1-C1' | -6.34 | 113.19 | 120.80 |
| 44 | BX | 57 | LEU | CA-CB-CG | 6.32 | 129.82 | 115.30 |
| 26 | BA | 1313 | U | N3-C2-O2 | -6.30 | 117.79 | 122.20 |
| 25 | CY | 23 | A | N1-C6-N6 | 6.30 | 122.38 | 118.60 |
| 25 | AY | 64 | A | C5-C6-N1 | -6.29 | 114.56 | 117.70 |
| 26 | BA | 1313 | U | C2-N1-C1' | 6.25 | 125.20 | 117.70 |
| 1 | CA | 1256 | A | O4'-C1'-N9 | -6.24 | 103.20 | 108.20 |
| 1 | AA | 839 | U | P-O3'-C3' | 6.23 | 127.18 | 119.70 |
| 23 | CW | 69 | G | O4'-C1'-N9 | -6.23 | 103.22 | 108.20 |
| 1 | CA | 1003 | G | N7-C8-N9 | 6.22 | 116.21 | 113.10 |
| 1 | AA | 1042 | G | C4-N9-C1' | -6.21 | 118.42 | 126.50 |
| 24 | AX | 22 | G | C5-C6-N1 | 6.21 | 114.60 | 111.50 |
| 26 | BA | 2100 | G | C5-C6-O6 | -6.21 | 124.88 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | AY | 23 | A | N1-C6-N6 | -6.20 | 114.88 | 118.60 |
| 1 | CA | 955 | U | C5-C4-O4 | 6.19 | 129.62 | 125.90 |
| 23 | AW | 70 | G | N3-C4-N9 | -6.18 | 122.29 | 126.00 |
| 26 | BA | 2848 | G | O4'-C1'-N9 | 6.16 | 113.12 | 108.20 |
| 1 | CA | 984 | C | C2-N3-C4 | 6.15 | 122.98 | 119.90 |
| 25 | CY | 68 | C | C2-N1-C1' | 6.13 | 125.55 | 118.80 |
| 1 | CA | 1003 | G | C4-N9-C1' | 6.13 | 134.47 | 126.50 |
| 13 | CM | 71 | ARG | NE-CZ-NH1 | 6.12 | 123.36 | 120.30 |
| 31 | BG | 3 | LEU | CA-CB-CG | 6.12 | 129.38 | 115.30 |
| 26 | BA | 645 | C | C2-N1-C1' | 6.12 | 125.53 | 118.80 |
| 26 | BA | 1639 | U | O5'-P-OP2 | -6.12 | 100.20 | 105.70 |
| 1 | AA | 1027 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 26 | BA | 2615 | U | O5'-P-OP1 | -6.10 | 100.21 | 105.70 |
| 1 | CA | 1225 | A | N1-C6-N6 | -6.09 | 114.94 | 118.60 |
| 26 | BA | 1614 | A | O5'-P-OP1 | -6.09 | 100.22 | 105.70 |
| 26 | DA | 512 | G | O4'-C1'-N9 | 6.09 | 113.07 | 108.20 |
| 1 | CA | 1126 | U | C2-N1-C1' | 6.08 | 125.00 | 117.70 |
| 26 | DA | 801 | G | O5'-P-OP2 | -6.08 | 100.23 | 105.70 |
| 25 | CY | 10 | G | N1-C6-O6 | 6.06 | 123.53 | 119.90 |
| 1 | CA | 1452 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 26 | DA | 1992 | G | C8-N9-C4 | -6.05 | 103.98 | 106.40 |
| 26 | BA | 933 | A | O4'-C1'-N9 | 6.02 | 113.02 | 108.20 |
| 24 | AX | 46 | G | C5-C6-N1 | 6.02 | 114.51 | 111.50 |
| 1 | CA | 1039 | C | C5-C6-N1 | 6.01 | 124.01 | 121.00 |
| 26 | DA | 2102 | U | C2-N3-C4 | 6.00 | 130.60 | 127.00 |
| 26 | BA | 2163 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 23 | CW | 10 | G | N3-C2-N2 | -5.99 | 115.71 | 119.90 |
| 26 | DA | 1531 | C | C2-N1-C1' | 5.99 | 125.38 | 118.80 |
| 26 | BA | 2248 | C | O5'-P-OP2 | -5.98 | 100.31 | 105.70 |
| 26 | DA | 2187 | G | N3-C4-N9 | 5.98 | 129.59 | 126.00 |
| 26 | DA | 2160 | G | C5-C6-O6 | 5.98 | 132.19 | 128.60 |
| 26 | DA | 2128 | C | C2-N3-C4 | 5.97 | 122.89 | 119.90 |
| 26 | DA | 2167 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 1 | AA | 991 | U | P-O3'-C3' | 5.95 | 126.83 | 119.70 |
| 26 | BA | 226 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 1 | CA | 998 | G | N9-C4-C5 | 5.94 | 107.78 | 105.40 |
| 26 | DA | 34 | C | C6-N1-C1' | -5.94 | 113.67 | 120.80 |
| 24 | AX | 22 | G | N3-C4-N9 | -5.94 | 122.44 | 126.00 |
| 26 | BA | 1300 | U | P-O3'-C3' | 5.94 | 126.82 | 119.70 |
| 26 | BA | 31 | C | O5'-P-OP1 | -5.93 | 100.36 | 105.70 |
| 42 | DV | 38 | LEU | CA-CB-CG | 5.93 | 128.94 | 115.30 |
| 26 | BA | 330 | A | N1-C2-N3 | 5.93 | 132.26 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | CA | 501 | C | O5'-P-OP1 | -5.93 | 100.36 | 105.70 |
| 26 | BA | 141 | A | C5-N7-C8 | -5.92 | 100.94 | 103.90 |
| 1 | AA | 1026 | G | N7-C8-N9 | 5.91 | 116.06 | 113.10 |
| 24 | AX | 22 | G | N1-C6-O6 | -5.91 | 116.35 | 119.90 |
| 26 | BA | 1493 | C | N1-C2-O2 | 5.91 | 122.44 | 118.90 |
| 1 | CA | 1003 | G | C8-N9-C4 | -5.91 | 104.04 | 106.40 |
| 1 | CA | 1220 | G | N3-C2-N2 | -5.91 | 115.77 | 119.90 |
| 26 | DA | 528 | A | N1-C2-N3 | 5.91 | 132.25 | 129.30 |
| 26 | BA | 1176 | G | OP1-P-O3' | 5.90 | 118.17 | 105.20 |
| 1 | CA | 955 | U | C2-N3-C4 | 5.90 | 130.54 | 127.00 |
| 26 | DA | 2190 | G | C5-C6-O6 | 5.90 | 132.14 | 128.60 |
| 26 | BA | 141 | A | O4'-C1'-N9 | 5.89 | 112.92 | 108.20 |
| 26 | BA | 1315 | C | O5'-P-OP2 | -5.88 | 100.41 | 105.70 |
| 1 | AA | 1123 | A | C6-N1-C2 | 5.87 | 122.12 | 118.60 |
| 26 | BA | 2061 | G | O5'-P-OP2 | -5.86 | 100.43 | 105.70 |
| 25 | AY | 15 | G | N3-C2-N2 | 5.85 | 124.00 | 119.90 |
| 26 | BA | 933 | A | N7-C8-N9 | 5.85 | 116.72 | 113.80 |
| 1 | CA | 1001(A) | G | C5-C6-O6 | -5.85 | 125.09 | 128.60 |
| 1 | AA | 1137 | C | O4'-C1'-N1 | -5.84 | 103.53 | 108.20 |
| 26 | DA | 1204 | A | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |
| 1 | CA | 1166 | G | N7-C8-N9 | 5.84 | 116.02 | 113.10 |
| 1 | CA | 1323 | G | N3-C4-N9 | 5.82 | 129.49 | 126.00 |
| 1 | CA | 1180 | A | C4-C5-C6 | 5.81 | 119.91 | 117.00 |
| 26 | DA | 2167 | U | N1-C2-O2 | 5.81 | 126.87 | 122.80 |
| 26 | BA | 2789 | C | C2-N1-C1' | -5.80 | 112.42 | 118.80 |
| 25 | CY | 4 | C | N1-C2-O2 | 5.79 | 122.38 | 118.90 |
| 25 | CY | 10 | G | C5-C6-O6 | -5.79 | 125.12 | 128.60 |
| 1 | CA | 1031 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 24 | CX | 14 | A | N1-C6-N6 | 5.78 | 122.07 | 118.60 |
| 26 | BA | 271(M) | G | P-O3'-C3' | 5.77 | 126.62 | 119.70 |
| 26 | BA | 528 | A | N3-C4-N9 | -5.74 | 122.81 | 127.40 |
| 23 | CW | 66 | U | P-O3'-C3' | 5.74 | 126.58 | 119.70 |
| 26 | BA | 887 | A | O4'-C1'-N9 | 5.73 | 112.79 | 108.20 |
| 27 | DB | 30 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 26 | BA | 2592 | G | O5'-P-OP1 | -5.71 | 100.56 | 105.70 |
| 24 | AX | 22 | G | C4-N9-C1' | -5.71 | 119.08 | 126.50 |
| 1 | AA | 1052 | U | N1-C2-O2 | 5.71 | 126.80 | 122.80 |
| 25 | AY | 60 | U | C2-N1-C1' | 5.70 | 124.54 | 117.70 |
| 1 | AA | 204 | U | C2-N1-C1' | 5.69 | 124.53 | 117.70 |
| 26 | BA | 975 | C | C2-N1-C1' | -5.69 | 112.54 | 118.80 |
| 26 | BA | 1776 | G | O5'-P-OP2 | -5.69 | 100.58 | 105.70 |
| 26 | DA | 897 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | BA | 548 | A | P-O3'-C3' | 5.69 | 126.52 | 119.70 |
| 25 | CY | 7 | A | N3-C4-C5 | -5.68 | 122.82 | 126.80 |
| 26 | BA | 1963 | U | N1-C2-O2 | 5.68 | 126.78 | 122.80 |
| 26 | DA | 2248 | C | O5'-P-OP2 | -5.68 | 100.59 | 105.70 |
| 1 | CA | 1154 | G | N3-C4-N9 | 5.67 | 129.41 | 126.00 |
| 26 | DA | 1300 | U | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 24 | AX | 20 | U | C2-N1-C1' | 5.67 | 124.51 | 117.70 |
| 26 | BA | 1784 | A | O5'-P-OP2 | -5.67 | 100.59 | 105.70 |
| 1 | AA | 1150 | U | C2-N3-C4 | 5.66 | 130.40 | 127.00 |
| 26 | DA | 2155 | G | N3-C2-N2 | 5.66 | 123.86 | 119.90 |
| 26 | DA | 2102 | U | N3-C2-O2 | -5.65 | 118.24 | 122.20 |
| 26 | BA | 271(M) | G | OP1-P-O3' | 5.64 | 117.62 | 105.20 |
| 26 | DA | 784 | A | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 1 | CA | 182 | U | N1-C2-O2 | -5.64 | 118.85 | 122.80 |
| 23 | CW | 36 | A | C6-N1-C2 | 5.63 | 121.98 | 118.60 |
| 1 | CA | 1126 | U | N1-C2-O2 | 5.63 | 126.74 | 122.80 |
| 25 | AY | 56 | C | N3-C2-O2 | -5.62 | 117.96 | 121.90 |
| 1 | CA | 1137 | C | C2-N1-C1' | -5.61 | 112.62 | 118.80 |
| 1 | CA | 204 | U | C2-N1-C1' | 5.61 | 124.43 | 117.70 |
| 24 | AX | 22 | G | N3-C4-C5 | 5.61 | 131.41 | 128.60 |
| 24 | AX | 46 | G | N9-C4-C5 | 5.61 | 107.64 | 105.40 |
| 1 | CA | 1023 | G | C4-N9-C1' | 5.61 | 133.79 | 126.50 |
| 1 | AA | 346 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 25 | AY | 68 | C | C5-C6-N1 | 5.60 | 123.80 | 121.00 |
| 26 | BA | 746 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 26 | DA | 1313 | U | C2-N1-C1' | 5.60 | 124.42 | 117.70 |
| 1 | AA | 1502 | A | N1-C2-N3 | 5.59 | 132.09 | 129.30 |
| 25 | CY | 31 | A | N1-C6-N6 | 5.58 | 121.95 | 118.60 |
| 1 | AA | 1206 | G | C5-C6-O6 | -5.58 | 125.25 | 128.60 |
| 1 | CA | 998 | G | C6-C5-N7 | 5.58 | 133.75 | 130.40 |
| 25 | AY | 68 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 26 | DA | 1992 | G | P-O3'-C3' | 5.57 | 126.38 | 119.70 |
| 1 | CA | 1039 | C | C2-N1-C1' | 5.56 | 124.92 | 118.80 |
| 1 | AA | 91 | C | C2-N1-C1' | 5.56 | 124.91 | 118.80 |
| 1 | CA | 1047 | G | N3-C4-N9 | 5.55 | 129.33 | 126.00 |
| 26 | DA | 2155 | G | N1-C2-N3 | -5.54 | 120.57 | 123.90 |
| 23 | CW | 67 | C | C2-N3-C4 | 5.54 | 122.67 | 119.90 |
| 1 | AA | 1165 | C | P-O3'-C3' | 5.54 | 126.34 | 119.70 |
| 26 | BA | 1021 | A | N1-C2-N3 | 5.53 | 132.06 | 129.30 |
| 26 | BA | 2593 | U | N3-C4-O4 | -5.53 | 115.53 | 119.40 |
| 1 | CA | 986 | A | C6-N1-C2 | -5.53 | 115.28 | 118.60 |
| 1 | CA | 1039 | C | C5-C4-N4 | -5.53 | 116.33 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 26 | DA | 2128 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 26 | BA | 1352 | U | O5'-P-OP1 | -5.52 | 100.73 | 105.70 |
| 24 | CX | 22 | G | C5-N7-C8 | -5.51 | 101.54 | 104.30 |
| 1 | CA | 1042 | G | N3-C4-N9 | -5.51 | 122.69 | 126.00 |
| 1 | CA | 992 | U | C5-C6-N1 | 5.50 | 125.45 | 122.70 |
| 25 | CY | 62 | C | C2-N3-C4 | 5.50 | 122.65 | 119.90 |
| 26 | BA | 1963 | U | C6-N1-C1' | -5.50 | 113.51 | 121.20 |
| 27 | BB | 85 | G | O4'-C1'-N9 | -5.49 | 103.81 | 108.20 |
| 1 | CA | 1180 | A | N1-C2-N3 | 5.48 | 132.04 | 129.30 |
| 1 | CA | 1154 | G | C5-N7-C8 | 5.48 | 107.04 | 104.30 |
| 26 | BA | 945 | A | C5-N7-C8 | -5.48 | 101.16 | 103.90 |
| 24 | AX | 14 | A | C4-N9-C1' | 5.47 | 136.16 | 126.30 |
| 1 | CA | 1030(B) | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 1 | CA | 998 | G | C4-C5-N7 | -5.47 | 108.61 | 110.80 |
| 26 | DA | 277 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 1 | AA | 1065 | U | P-O3'-C3' | 5.47 | 126.26 | 119.70 |
| 26 | DA | 2160 | G | C6-N1-C2 | 5.46 | 128.38 | 125.10 |
| 26 | DA | 2139 | C | C5-C6-N1 | 5.45 | 123.73 | 121.00 |
| 40 | BT | 118 | ARG | NE-CZ-NH1 | 5.45 | 123.02 | 120.30 |
| 26 | BA | 944 | G | C4-N9-C1' | 5.44 | 133.57 | 126.50 |
| 26 | BA | 1022 | G | N3-C2-N2 | -5.44 | 116.09 | 119.90 |
| 26 | BA | 1131 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 26 | DA | 2187 | G | C6-N1-C2 | -5.43 | 121.84 | 125.10 |
| 1 | AA | 1131 | G | C6-C5-N7 | -5.43 | 127.14 | 130.40 |
| 1 | CA | 997 | U | C5-C4-O4 | 5.42 | 129.15 | 125.90 |
| 26 | DA | 2187 | G | N1-C6-O6 | 5.42 | 123.15 | 119.90 |
| 1 | CA | 1183 | A | P-O3'-C3' | 5.41 | 126.20 | 119.70 |
| 22 | CV | 19 | U | C2-N3-C4 | 5.41 | 130.25 | 127.00 |
| 23 | CW | 3 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 1 | AA | 841 | U | C6-N1-C2 | -5.41 | 117.75 | 121.00 |
| 24 | AX | 14 | A | C8-N9-C1' | -5.40 | 117.99 | 127.70 |
| 1 | AA | 1030(B) | C | N1-C2-O2 | 5.39 | 122.14 | 118.90 |
| 23 | AW | 44 | G | C5-C6-O6 | 5.39 | 131.84 | 128.60 |
| 24 | AX | 46 | G | C4-C5-N7 | -5.39 | 108.64 | 110.80 |
| 26 | BA | 2167 | U | C2-N1-C1' | 5.39 | 124.16 | 117.70 |
| 26 | BA | 2134 | A | C3'-C2'-C1' | 5.38 | 105.81 | 101.50 |
| 1 | CA | 998 | G | N3-C4-N9 | -5.38 | 122.77 | 126.00 |
| 2 | CB | 154 | LEU | CA-CB-CG | 5.38 | 127.67 | 115.30 |
| 1 | CA | 942 | G | C5-C6-O6 | 5.38 | 131.83 | 128.60 |
| 1 | AA | 1285 | A | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 26 | BA | 141 | A | C8-N9-C4 | -5.34 | 103.66 | 105.80 |
| 23 | CW | 25 | C | C5-C4-N4 | 5.34 | 123.94 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | DA | 2153 | G | C8-N9-C1' | -5.33 | 120.07 | 127.00 |
| 1 | AA | 925 | G | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 1 | CA | 1123 | A | C5-C6-N6 | 5.33 | 127.96 | 123.70 |
| 1 | CA | 1216 | G | C4-N9-C1' | -5.33 | 119.58 | 126.50 |
| 26 | DA | 2153 | G | N3-C4-N9 | 5.32 | 129.19 | 126.00 |
| 24 | AX | 22 | G | N7-C8-N9 | 5.32 | 115.76 | 113.10 |
| 26 | BA | 1176 | G | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 1 | CA | 1054 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 3 | CC | 52 | LEU | CA-CB-CG | 5.31 | 127.50 | 115.30 |
| 26 | BA | 528 | A | N3-C4-C5 | 5.30 | 130.51 | 126.80 |
| 1 | CA | 1122 | U | C5-C4-O4 | 5.30 | 129.08 | 125.90 |
| 1 | CA | 1004 | A | C6-C5-N7 | 5.30 | 136.01 | 132.30 |
| 26 | DA | 528 | A | N3-C4-C5 | 5.30 | 130.51 | 126.80 |
| 26 | DA | 2153 | G | N9-C4-C5 | -5.30 | 103.28 | 105.40 |
| 26 | DA | 748 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 26 | BA | 2347 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 1 | CA | 992 | U | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 26 | DA | 2313 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 26 | BA | 2430 | A | C2-N3-C4 | 5.26 | 113.23 | 110.60 |
| 1 | CA | 1220 | G | N3-C4-N9 | -5.25 | 122.85 | 126.00 |
| 1 | CA | 1452 | C | C5-C6-N1 | 5.25 | 123.63 | 121.00 |
| 1 | AA | 1010 | G | N3-C4-N9 | 5.25 | 129.15 | 126.00 |
| 1 | CA | 79 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 25 | AY | 23 | A | C4-C5-C6 | -5.25 | 114.38 | 117.00 |
| 25 | CY | 50 | U | C5-C4-O4 | 5.24 | 129.05 | 125.90 |
| 26 | BA | 2191 | G | N7-C8-N9 | 5.24 | 115.72 | 113.10 |
| 26 | DA | 2889 | C | N1-C2-O2 | 5.24 | 122.05 | 118.90 |
| 24 | CX | 34 | C | C2-N1-C1' | 5.24 | 124.56 | 118.80 |
| 1 | CA | 998 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 26 | BA | 933 | A | C5-N7-C8 | -5.22 | 101.29 | 103.90 |
| 26 | DA | 2297 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | CA | 687 | A | P-O3'-C3' | 5.21 | 125.96 | 119.70 |
| 1 | AA | 266 | G | P-O3'-C3' | 5.21 | 125.96 | 119.70 |
| 1 | CA | 992 | U | C2-N1-C1' | 5.21 | 123.95 | 117.70 |
| 1 | CA | 182 | U | C2-N1-C1' | -5.21 | 111.45 | 117.70 |
| 26 | BA | 576 | U | O5'-P-OP1 | -5.20 | 101.02 | 105.70 |
| 22 | AV | 17 | U | C5-C4-O4 | 5.20 | 129.02 | 125.90 |
| 26 | BA | 1416 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 26 | BA | 2206 | G | C5-C6-O6 | -5.19 | 125.48 | 128.60 |
| 25 | AY | 50 | U | N3-C4-C5 | -5.19 | 111.49 | 114.60 |
| 26 | DA | 1937 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 2 | CB | 51 | LEU | CA-CB-CG | 5.17 | 127.20 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | BA | 575 | A | O5'-P-OP1 | -5.17 | 101.05 | 105.70 |
| 23 | CW | 44 | G | N3-C4-N9 | 5.17 | 129.10 | 126.00 |
| 26 | DA | 2689 | U | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 35 | DO | 8 | LEU | CA-CB-CG | 5.16 | 127.16 | 115.30 |
| 1 | CA | 754 | C | N1-C2-O2 | 5.16 | 121.99 | 118.90 |
| 25 | CY | 9 | A | C4-C5-C6 | -5.16 | 114.42 | 117.00 |
| 26 | BA | 2609 | U | C2-N1-C1' | -5.15 | 111.52 | 117.70 |
| 26 | BA | 1107 | G | N3-C4-C5 | -5.15 | 126.02 | 128.60 |
| 1 | CA | 1012 | U | N1-C2-N3 | 5.15 | 117.99 | 114.90 |
| 26 | BA | 2689 | U | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 26 | DA | 2153 | G | C6-C5-N7 | -5.14 | 127.32 | 130.40 |
| 26 | DA | 2174 | C | C5-C6-N1 | 5.14 | 123.57 | 121.00 |
| 36 | DP | 44 | GLY | C-N-CA | 5.14 | 134.54 | 121.70 |
| 1 | CA | 1030 | C | C6-N1-C1' | -5.13 | 114.64 | 120.80 |
| 26 | BA | 826 | U | OP1-P-O3' | 5.13 | 116.49 | 105.20 |
| 1 | CA | 999 | C | C2-N3-C4 | 5.13 | 122.47 | 119.90 |
| 26 | DA | 2178 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 1 | AA | 1042 | G | N3-C4-N9 | -5.13 | 122.92 | 126.00 |
| 24 | AX | 14 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 1 | CA | 1124 | G | N3-C4-N9 | 5.12 | 129.07 | 126.00 |
| 1 | AA | 1036 | G | C4-N9-C1' | 5.11 | 133.14 | 126.50 |
| 26 | BA | 2141 | G | C6-N1-C2 | 5.11 | 128.16 | 125.10 |
| 25 | CY | 25 | C | C2-N1-C1' | 5.11 | 124.42 | 118.80 |
| 26 | BA | 2174 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 1 | CA | 1221 | G | C6-N1-C2 | 5.09 | 128.16 | 125.10 |
| 22 | CV | 19 | U | C5-C4-O4 | 5.09 | 128.96 | 125.90 |
| 1 | CA | 953 | G | N3-C4-N9 | 5.09 | 129.06 | 126.00 |
| 26 | BA | 1021 | A | C8-N9-C4 | -5.09 | 103.77 | 105.80 |
| 27 | DB | 42 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 25 | AY | 9 | A | N1-C6-N6 | 5.08 | 121.65 | 118.60 |
| 1 | CA | 1166 | G | C8-N9-C4 | -5.08 | 104.37 | 106.40 |
| 1 | CA | 1064 | G | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 26 | DA | 1038 | C | C2-N1-C1' | 5.07 | 124.38 | 118.80 |
| 1 | CA | 1126 | U | C6-N1-C1' | -5.07 | 114.10 | 121.20 |
| 26 | DA | 2206 | G | C4-N9-C1' | -5.07 | 119.91 | 126.50 |
| 26 | DA | 2155 | G | N9-C4-C5 | -5.07 | 103.37 | 105.40 |
| 23 | AW | 70 | G | C6-C5-N7 | 5.06 | 133.44 | 130.40 |
| 26 | BA | 845 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 26 | DA | 2174 | C | N1-C2-O2 | 5.06 | 121.93 | 118.90 |
| 26 | BA | 2789 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 25 | CY | 68 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 26 | DA | 2153 | G | C4-N9-C1' | 5.05 | 133.07 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1067 | A | O4'-C1'-N9 | -5.05 | 104.16 | 108.20 |
| 26 | BA | 1022 | G | N3-C4-N9 | -5.05 | 122.97 | 126.00 |
| 26 | BA | 2319 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 23 | CW | 25 | C | C6-N1-C1' | 5.05 | 126.86 | 120.80 |
| 1 | CA | 65 | U | OP2-P-O3' | 5.04 | 116.30 | 105.20 |
| 26 | BA | 2183 | C | N1-C2-O2 | -5.04 | 115.88 | 118.90 |
| 25 | AY | 15 | G | N1-C2-N2 | -5.04 | 111.66 | 116.20 |
| 25 | CY | 50 | U | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 26 | BA | 2286 | A | N7-C8-N9 | 5.03 | 116.31 | 113.80 |
| 1 | AA | 1173 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 1 | AA | 1019 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 26 | DA | 1558 | A | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 1 | CA | 204 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | AA | 1026 | G | N3-C4-C5 | -5.02 | 126.09 | 128.60 |
| 1 | CA | 60 | A | P-O3'-C3' | 5.02 | 125.73 | 119.70 |
| 1 | CA | 998 | G | C8-N9-C1' | 5.02 | 133.53 | 127.00 |
| 25 | AY | 4 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 25 | CY | 7 | A | C6-C5-N7 | -5.02 | 128.79 | 132.30 |
| 26 | DA | 2139 | C | C4-C5-C6 | -5.02 | 114.89 | 117.40 |
| 1 | AA | 1502 | A | N7-C8-N9 | 5.01 | 116.30 | 113.80 |
| 25 | CY | 18 | G | N3-C4-N9 | 5.01 | 129.01 | 126.00 |
| 26 | BA | 383 | U | C2-N1-C1' | -5.00 | 111.70 | 117.70 |
| 23 | AW | 49 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | AB | 231 | GLU | Peptide |
| 2 | AB | 9 | GLU | Peptide |
| 7 | AG | 78 | ARG | Peptide |
| 7 | AG | 79 | ARG | Peptide |
| 51 | B4 | 59 | PHE | Peptide |
| 33 | BI | 9 | LEU | Peptide |
| 35 | BO | 80 | ASP | Peptide |
| 39 | BS | 58 | LEU | Peptide |
| 2 | CB | 9 | GLU | Peptide |
| 20 | CT | 9 | ASN | 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 | 32185 | 0 | 16245 | 536 | 0 |
| 1 | CA | 32312 | 0 | 16307 | 762 | 0 |
| 2 | AB | 1846 | 0 | 1867 | 81 | 0 |
| 2 | CB | 1825 | 0 | 1828 | 119 | 0 |
| 3 | AC | 1552 | 0 | 1546 | 60 | 0 |
| 3 | CC | 1544 | 0 | 1524 | 70 | 0 |
| 4 | AD | 1659 | 0 | 1676 | 56 | 0 |
| 4 | CD | 1678 | 0 | 1718 | 67 | 0 |
| 5 | AE | 1129 | 0 | 1185 | 27 | 0 |
| 5 | CE | 1133 | 0 | 1191 | 46 | 0 |
| 6 | AF | 812 | 0 | 804 | 18 | 0 |
| 6 | CF | 820 | 0 | 814 | 19 | 0 |
| 7 | AG | 1231 | 0 | 1238 | 21 | 0 |
| 7 | CG | 1235 | 0 | 1249 | 39 | 0 |
| 8 | AH | 1088 | 0 | 1126 | 35 | 0 |
| 8 | CH | 1088 | 0 | 1126 | 40 | 0 |
| 9 | AI | 986 | 0 | 995 | 43 | 0 |
| 9 | CI | 978 | 0 | 966 | 55 | 0 |
| 10 | AJ | 709 | 0 | 650 | 34 | 0 |
| 10 | CJ | 714 | 0 | 672 | 44 | 0 |
| 11 | AK | 833 | 0 | 836 | 19 | 0 |
| 11 | CK | 833 | 0 | 836 | 22 | 0 |
| 12 | AL | 930 | 0 | 980 | 27 | 0 |
| 12 | CL | 930 | 0 | 980 | 33 | 0 |
| 13 | AM | 966 | 0 | 1024 | 40 | 0 |
| 13 | CM | 950 | 0 | 988 | 74 | 0 |
| 14 | AN | 492 | 0 | 529 | 26 | 0 |
| 14 | CN | 492 | 0 | 529 | 34 | 0 |
| 15 | AO | 728 | 0 | 760 | 20 | 0 |
| 15 | CO | 728 | 0 | 760 | 22 | 0 |
| 16 | AP | 681 | 0 | 697 | 27 | 0 |
| 16 | CP | 677 | 0 | 686 | 22 | 0 |
| 17 | AQ | 823 | 0 | 891 | 26 | 0 |
| 17 | CQ | 823 | 0 | 891 | 19 | 0 |
| 18 | AR | 555 | 0 | 618 | 12 | 0 |
| 18 | CR | 555 | 0 | 618 | 24 | 0 |
| 19 | AS | 661 | 0 | 675 | 31 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | CS | 646 | 0 | 644 | 40 | 0 |
| 20 | AT | 728 | 0 | 798 | 26 | 0 |
| 20 | CT | 731 | 0 | 807 | 26 | 0 |
| 21 | AU | 199 | 0 | 208 | 8 | 0 |
| 21 | CU | 199 | 0 | 208 | 9 | 0 |
| 22 | AV | 277 | 0 | 140 | 3 | 0 |
| 22 | CV | 252 | 0 | 130 | 6 | 0 |
| 23 | AW | 1599 | 0 | 830 | 42 | 0 |
| 23 | CW | 1552 | 0 | 794 | 51 | 0 |
| 24 | AX | 1635 | 0 | 839 | 23 | 0 |
| 24 | CX | 1635 | 0 | 839 | 36 | 0 |
| 25 | AY | 1581 | 0 | 805 | 82 | 0 |
| 25 | CY | 1561 | 0 | 796 | 94 | 0 |
| 26 | BA | 60729 | 0 | 30622 | 666 | 0 |
| 26 | DA | 60311 | 0 | 30412 | 876 | 0 |
| 27 | BB | 2573 | 0 | 1306 | 20 | 0 |
| 27 | DB | 2573 | 0 | 1306 | 76 | 0 |
| 28 | BD | 2136 | 0 | 2218 | 42 | 0 |
| 28 | DD | 2142 | 0 | 2229 | 58 | 0 |
| 29 | BE | 1559 | 0 | 1618 | 25 | 0 |
| 29 | DE | 1559 | 0 | 1618 | 39 | 0 |
| 30 | BF | 1584 | 0 | 1625 | 39 | 0 |
| 30 | DF | 1580 | 0 | 1619 | 60 | 0 |
| 31 | BG | 1425 | 0 | 1443 | 38 | 0 |
| 31 | DG | 1424 | 0 | 1434 | 90 | 0 |
| 32 | BH | 1330 | 0 | 1407 | 34 | 0 |
| 32 | DH | 1330 | 0 | 1407 | 44 | 0 |
| 33 | BI | 1085 | 0 | 1114 | 37 | 0 |
| 33 | DI | 1073 | 0 | 1106 | 22 | 0 |
| 34 | BN | 1117 | 0 | 1184 | 23 | 0 |
| 34 | DN | 1117 | 0 | 1184 | 26 | 0 |
| 35 | BO | 933 | 0 | 996 | 25 | 0 |
| 35 | DO | 933 | 0 | 996 | 32 | 0 |
| 36 | BP | 1139 | 0 | 1223 | 41 | 0 |
| 36 | DP | 1135 | 0 | 1212 | 52 | 0 |
| 37 | BQ | 1122 | 0 | 1179 | 28 | 0 |
| 37 | DQ | 1122 | 0 | 1179 | 40 | 0 |
| 38 | BR | 968 | 0 | 1033 | 22 | 0 |
| 38 | DR | 968 | 0 | 1033 | 28 | 0 |
| 39 | BS | 877 | 0 | 938 | 20 | 0 |
| 39 | DS | 870 | 0 | 923 | 33 | 0 |
| 40 | BT | 1091 | 0 | 1151 | 26 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | DT | 1083 | 0 | 1136 | 37 | 0 |
| 41 | BU | 959 | 0 | 1019 | 18 | 0 |
| 41 | DU | 959 | 0 | 1018 | 30 | 0 |
| 42 | BV | 771 | 0 | 830 | 13 | 0 |
| 42 | DV | 771 | 0 | 830 | 24 | 0 |
| 43 | BW | 886 | 0 | 940 | 17 | 0 |
| 43 | DW | 886 | 0 | 940 | 13 | 0 |
| 44 | BX | 750 | 0 | 814 | 15 | 0 |
| 44 | DX | 750 | 0 | 814 | 27 | 0 |
| 45 | BY | 806 | 0 | 881 | 27 | 0 |
| 45 | DY | 806 | 0 | 881 | 30 | 0 |
| 46 | BZ | 1349 | 0 | 1355 | 44 | 0 |
| 46 | DZ | 1360 | 0 | 1363 | 70 | 0 |
| 47 | B0 | 653 | 0 | 674 | 13 | 0 |
| 47 | D0 | 653 | 0 | 674 | 22 | 0 |
| 48 | B1 | 755 | 0 | 826 | 16 | 0 |
| 48 | D1 | 755 | 0 | 826 | 18 | 0 |
| 49 | B2 | 588 | 0 | 643 | 11 | 0 |
| 49 | D2 | 588 | 0 | 643 | 14 | 0 |
| 50 | B3 | 469 | 0 | 518 | 6 | 0 |
| 50 | D3 | 464 | 0 | 514 | 13 | 0 |
| 51 | B4 | 558 | 0 | 544 | 37 | 0 |
| 51 | D4 | 532 | 0 | 503 | 25 | 0 |
| 52 | B5 | 455 | 0 | 465 | 14 | 0 |
| 52 | D5 | 455 | 0 | 465 | 13 | 0 |
| 53 | B6 | 453 | 0 | 473 | 13 | 0 |
| 53 | D6 | 449 | 0 | 469 | 12 | 0 |
| 54 | B7 | 418 | 0 | 467 | 10 | 0 |
| 54 | D7 | 418 | 0 | 467 | 13 | 0 |
| 55 | B8 | 517 | 0 | 582 | 17 | 0 |
| 55 | D8 | 517 | 0 | 582 | 15 | 0 |
| 56 | B9 | 307 | 0 | 335 | 7 | 0 |
| 56 | D9 | 307 | 0 | 335 | 11 | 0 |
| 57 | AA | 216 | 0 | 0 | 0 | 0 |
| 57 | AB | 1 | 0 | 0 | 0 | 0 |
| 57 | AE | 1 | 0 | 0 | 0 | 0 |
| 57 | AF | 1 | 0 | 0 | 0 | 0 |
| 57 | AK | 1 | 0 | 0 | 0 | 0 |
| 57 | AL | 2 | 0 | 0 | 0 | 0 |
| 57 | AM | 2 | 0 | 0 | 0 | 0 |
| 57 | AN | 2 | 0 | 0 | 0 | 0 |
| 57 | AT | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57 | AU | 1 | 0 | 0 | 0 | 0 |
| 57 | AW | 2 | 0 | 0 | 0 | 0 |
| 57 | AX | 15 | 0 | 0 | 0 | 0 |
| 57 | AY | 3 | 0 | 0 | 0 | 0 |
| 57 | B0 | 2 | 0 | 0 | 0 | 0 |
| 57 | B2 | 1 | 0 | 0 | 0 | 0 |
| 57 | B4 | 1 | 0 | 0 | 0 | 0 |
| 57 | B5 | 3 | 0 | 0 | 0 | 0 |
| 57 | B6 | 2 | 0 | 0 | 0 | 0 |
| 57 | B7 | 5 | 0 | 0 | 0 | 0 |
| 57 | B8 | 2 | 0 | 0 | 0 | 0 |
| 57 | B9 | 1 | 0 | 0 | 0 | 0 |
| 57 | BA | 814 | 0 | 0 | 0 | 0 |
| 57 | BB | 23 | 0 | 0 | 0 | 0 |
| 57 | BD | 10 | 0 | 0 | 0 | 0 |
| 57 | BE | 6 | 0 | 0 | 0 | 0 |
| 57 | BF | 11 | 0 | 0 | 0 | 0 |
| 57 | BG | 2 | 0 | 0 | 0 | 0 |
| 57 | BH | 1 | 0 | 0 | 0 | 0 |
| 57 | BN | 3 | 0 | 0 | 0 | 0 |
| 57 | BO | 1 | 0 | 0 | 0 | 0 |
| 57 | BP | 2 | 0 | 0 | 0 | 0 |
| 57 | BQ | 2 | 0 | 0 | 0 | 0 |
| 57 | BR | 2 | 0 | 0 | 0 | 0 |
| 57 | BU | 4 | 0 | 0 | 0 | 0 |
| 57 | BV | 5 | 0 | 0 | 0 | 0 |
| 57 | BW | 4 | 0 | 0 | 0 | 0 |
| 57 | BX | 1 | 0 | 0 | 0 | 0 |
| 57 | BY | 1 | 0 | 0 | 0 | 0 |
| 57 | BZ | 2 | 0 | 0 | 0 | 0 |
| 57 | CA | 169 | 0 | 0 | 0 | 0 |
| 57 | CD | 1 | 0 | 0 | 0 | 0 |
| 57 | CE | 2 | 0 | 0 | 0 | 0 |
| 57 | CF | 1 | 0 | 0 | 0 | 0 |
| 57 | CJ | 1 | 0 | 0 | 0 | 0 |
| 57 | CK | 1 | 0 | 0 | 0 | 0 |
| 57 | CT | 1 | 0 | 0 | 0 | 0 |
| 57 | CW | 1 | 0 | 0 | 0 | 0 |
| 57 | CX | 2 | 0 | 0 | 0 | 0 |
| 57 | D0 | 1 | 0 | 0 | 0 | 0 |
| 57 | D3 | 1 | 0 | 0 | 0 | 0 |
| 57 | D8 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57 | DA | 664 | 0 | 0 | 0 | 0 |
| 57 | DB | 13 | 0 | 0 | 0 | 0 |
| 57 | DD | 4 | 0 | 0 | 0 | 0 |
| 57 | DE | 7 | 0 | 0 | 0 | 0 |
| 57 | DF | 5 | 0 | 0 | 0 | 0 |
| 57 | DG | 1 | 0 | 0 | 0 | 0 |
| 57 | DN | 1 | 0 | 0 | 0 | 0 |
| 57 | DO | 2 | 0 | 0 | 0 | 0 |
| 57 | DP | 2 | 0 | 0 | 0 | 0 |
| 57 | DQ | 3 | 0 | 0 | 0 | 0 |
| 57 | DR | 1 | 0 | 0 | 0 | 0 |
| 57 | DU | 1 | 0 | 0 | 0 | 0 |
| 57 | DV | 1 | 0 | 0 | 0 | 0 |
| 57 | DW | 1 | 0 | 0 | 0 | 0 |
| 57 | DY | 1 | 0 | 0 | 0 | 0 |
| 58 | AD | 8 | 0 | 0 | 1 | 0 |
| 58 | CD | 8 | 0 | 0 | 1 | 0 |
| 59 | AN | 1 | 0 | 0 | 0 | 0 |
| 59 | B4 | 1 | 0 | 0 | 0 | 0 |
| 59 | B5 | 1 | 0 | 0 | 0 | 0 |
| 59 | B6 | 1 | 0 | 0 | 0 | 0 |
| 59 | B9 | 1 | 0 | 0 | 0 | 0 |
| 59 | BY | 1 | 0 | 0 | 0 | 0 |
| 59 | CN | 1 | 0 | 0 | 0 | 0 |
| 59 | D4 | 1 | 0 | 0 | 0 | 0 |
| 59 | D5 | 1 | 0 | 0 | 0 | 0 |
| 59 | D6 | 1 | 0 | 0 | 0 | 0 |
| 59 | D9 | 1 | 0 | 0 | 0 | 0 |
| 59 | DY | 1 | 0 | 0 | 0 | 0 |
| 60 | AX | 1 | 0 | 0 | 0 | 0 |
| 61 | AA | 210 | 0 | 0 | 13 | 0 |
| 61 | AD | 1 | 0 | 0 | 0 | 0 |
| 61 | AE | 2 | 0 | 0 | 0 | 0 |
| 61 | AJ | 1 | 0 | 0 | 0 | 0 |
| 61 | AL | 2 | 0 | 0 | 1 | 0 |
| 61 | AM | 2 | 0 | 0 | 0 | 0 |
| 61 | AV | 2 | 0 | 0 | 0 | 0 |
| 61 | AW | 4 | 0 | 0 | 0 | 0 |
| 61 | AX | 4 | 0 | 0 | 0 | 0 |
| 61 | AY | 1 | 0 | 0 | 0 | 0 |
| 61 | B0 | 6 | 0 | 0 | 0 | 0 |
| 61 | B1 | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61 | B3 | 2 | 0 | 0 | 0 | 0 |
| 61 | B5 | 4 | 0 | 0 | 0 | 0 |
| 61 | B6 | 2 | 0 | 0 | 0 | 0 |
| 61 | B7 | 3 | 0 | 0 | 2 | 0 |
| 61 | B8 | 13 | 0 | 0 | 0 | 0 |
| 61 | B9 | 1 | 0 | 0 | 0 | 0 |
| 61 | BA | 1406 | 0 | 0 | 56 | 0 |
| 61 | BB | 37 | 0 | 0 | 1 | 0 |
| 61 | BD | 15 | 0 | 0 | 2 | 0 |
| 61 | BE | 17 | 0 | 0 | 4 | 0 |
| 61 | BF | 11 | 0 | 0 | 0 | 0 |
| 61 | BG | 3 | 0 | 0 | 0 | 0 |
| 61 | BH | 1 | 0 | 0 | 0 | 0 |
| 61 | BI | 1 | 0 | 0 | 0 | 0 |
| 61 | BN | 1 | 0 | 0 | 0 | 0 |
| 61 | BO | 2 | 0 | 0 | 0 | 0 |
| 61 | BP | 13 | 0 | 0 | 0 | 0 |
| 61 | BQ | 4 | 0 | 0 | 0 | 0 |
| 61 | BR | 2 | 0 | 0 | 0 | 0 |
| 61 | BS | 2 | 0 | 0 | 0 | 0 |
| 61 | BT | 2 | 0 | 0 | 0 | 0 |
| 61 | BU | 4 | 0 | 0 | 0 | 0 |
| 61 | BV | 2 | 0 | 0 | 0 | 0 |
| 61 | BW | 3 | 0 | 0 | 1 | 0 |
| 61 | BX | 3 | 0 | 0 | 0 | 0 |
| 61 | BZ | 1 | 0 | 0 | 0 | 0 |
| 61 | CA | 156 | 0 | 0 | 11 | 0 |
| 61 | CE | 2 | 0 | 0 | 0 | 0 |
| 61 | CH | 1 | 0 | 0 | 0 | 0 |
| 61 | CJ | 1 | 0 | 0 | 0 | 0 |
| 61 | CK | 1 | 0 | 0 | 0 | 0 |
| 61 | CL | 1 | 0 | 0 | 1 | 0 |
| 61 | CT | 1 | 0 | 0 | 0 | 0 |
| 61 | CW | 2 | 0 | 0 | 2 | 0 |
| 61 | CX | 2 | 0 | 0 | 0 | 0 |
| 61 | CY | 1 | 0 | 0 | 0 | 0 |
| 61 | D0 | 4 | 0 | 0 | 0 | 0 |
| 61 | D1 | 1 | 0 | 0 | 0 | 0 |
| 61 | D3 | 2 | 0 | 0 | 0 | 0 |
| 61 | D5 | 1 | 0 | 0 | 0 | 0 |
| 61 | D6 | 1 | 0 | 0 | 0 | 0 |
| 61 | D8 | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61 | DA | 989 | 0 | 0 | 44 | 0 |
| 61 | DB | 9 | 0 | 0 | 0 | 0 |
| 61 | DD | 18 | 0 | 0 | 3 | 0 |
| 61 | DE | 5 | 0 | 0 | 0 | 0 |
| 61 | DF | 4 | 0 | 0 | 0 | 0 |
| 61 | DN | 2 | 0 | 0 | 0 | 0 |
| 61 | DP | 12 | 0 | 0 | 4 | 0 |
| 61 | DQ | 1 | 0 | 0 | 0 | 0 |
| 61 | DT | 4 | 0 | 0 | 0 | 0 |
| 61 | DU | 1 | 0 | 0 | 0 | 0 |
| 61 | DV | 1 | 0 | 0 | 0 | 0 |
| 61 | DW | 1 | 0 | 0 | 0 | 0 |
| 61 | DX | 2 | 0 | 0 | 0 | 0 |
| 61 | DY | 1 | 0 | 0 | 0 | 0 |
| All | All | 297127 | 0 | 196404 | 5502 | 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 12.

All (5502) 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) |
|------------------|------------------|--------------------------|-------------------|
| 26:DA:2139:C:N4 | 26:DA:2152:G:H1 | 1.46 | 1.14 |
| 1:CA:999:C:N4 | 1:CA:1042:G:H1 | 1.48 | 1.12 |
| 25:AY:49:C:N4 | 25:AY:65:G:H1 | 1.51 | 1.09 |
| 1:CA:985:C:N4 | 1:CA:1220:G:H1 | 1.50 | 1.09 |
| 1:CA:998:G:H1 | 1:CA:1043:C:N4 | 1.51 | 1.09 |
| 25:CY:7:A:N6 | 25:CY:66:U:H3 | 1.54 | 1.06 |
| 26:DA:2138:C:N4 | 26:DA:2153:G:H1 | 1.53 | 1.04 |
| 25:AY:53:G:H1 | 25:AY:61:C:N4 | 1.56 | 1.04 |
| 26:BA:2136:C:N4 | 26:BA:2155:G:H1 | 1.57 | 1.02 |
| 45:BY:92:ASN:HB2 | 45:BY:94:LYS:H | 1.21 | 1.02 |
| 26:BA:2102:U:H3 | 26:BA:2187:G:H1 | 1.06 | 1.00 |
| 1:CA:1245:A:H61 | 1:CA:1292:U:H3 | 1.09 | 1.00 |
| 1:CA:985:C:H42 | 1:CA:1220:G:H1 | 0.99 | 0.99 |
| 1:CA:1162:C:N4 | 1:CA:1174:G:H1 | 1.60 | 0.99 |
| 25:CY:10:G:H1 | 25:CY:25:C:H42 | 1.09 | 0.98 |
| 26:BA:2499:C:OP1 | 61:BA:5135:HOH:O | 1.83 | 0.97 |
| 4:CD:15:GLU:HG3 | 4:CD:63:LYS:HG3 | 1.47 | 0.96 |
| 26:BA:2138:C:H42 | 26:BA:2153:G:H1 | 1.09 | 0.96 |
| 1:CA:1000:U:H3 | 1:CA:1041:A:N6 | 1.63 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:CY:50:U:H3 | 25:CY:64:A:H61 | 1.02 | 0.95 |
| 26:DA:2127:G:C6 | 26:DA:2161:C:N4 | 2.34 | 0.95 |
| 23:AW:26:A:H61 | 23:AW:44:G:H1 | 1.06 | 0.94 |
| 47:B0:11:ARG:O | 47:B0:14:ARG:NH2 | 1.99 | 0.94 |
| 25:AY:29:G:H1 | 25:AY:41:C:N4 | 1.65 | 0.94 |
| 1:CA:76:C:N4 | 1:CA:93:G:H1 | 1.64 | 0.94 |
| 1:CA:1025:U:H3 | 1:CA:1036:G:H1 | 1.03 | 0.94 |
| 25:CY:22:G:N7 | 25:CY:46:7MG:N2 | 2.14 | 0.94 |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:HE1 | 1.31 | 0.94 |
| 1:CA:501:C:OP1 | 12:CL:124:LYS:NZ | 2.01 | 0.93 |
| 1:CA:1162:C:H42 | 1:CA:1174:G:H1 | 1.14 | 0.93 |
| 40:DT:55:ASN:H | 40:DT:59:THR:HG22 | 1.29 | 0.93 |
| 26:BA:1798:U:H5' | 28:BD:259:THR:HG22 | 1.50 | 0.93 |
| 2:CB:16:HIS:HB2 | 2:CB:204:ASN:HB3 | 1.47 | 0.93 |
| 23:AW:19:G:H1 | 23:AW:56:C:H42 | 1.17 | 0.93 |
| 1:CA:838:G:H1 | 1:CA:848:C:H42 | 1.10 | 0.93 |
| 35:BO:35:VAL:HG11 | 35:BO:103:ALA:HB3 | 1.51 | 0.92 |
| 26:BA:2121:G:H1 | 26:BA:2177:C:H42 | 1.13 | 0.92 |
| 46:DZ:5:LEU:HG | 46:DZ:47:VAL:HG21 | 1.50 | 0.92 |
| 25:CY:19:G:H1 | 25:CY:56:C:H42 | 1.12 | 0.92 |
| 25:CY:51:U:H3 | 25:CY:63:G:H1 | 1.17 | 0.91 |
| 23:AW:1:G:O6 | 23:AW:72:C:N3 | 2.04 | 0.91 |
| 26:DA:2121:G:H1 | 26:DA:2177:C:N4 | 1.68 | 0.91 |
| 26:DA:631:A:OP1 | 36:DP:65:ARG:NH1 | 2.04 | 0.91 |
| 1:CA:985:C:N3 | 1:CA:1220:G:N2 | 2.17 | 0.91 |
| 19:CS:42:PRO:HG3 | 51:D4:61:ARG:HG3 | 1.53 | 0.91 |
| 26:DA:2139:C:N4 | 26:DA:2152:G:N1 | 2.12 | 0.91 |
| 1:CA:1165:C:H42 | 1:CA:1171:G:H1 | 1.19 | 0.90 |
| 25:AY:53:G:H1 | 25:AY:61:C:H42 | 0.91 | 0.90 |
| 25:AY:29:G:H1 | 25:AY:41:C:H42 | 0.90 | 0.90 |
| 1:CA:656:C:O2' | 15:CO:28:GLN:NE2 | 2.06 | 0.89 |
| 26:DA:2121:G:H1 | 26:DA:2177:C:H42 | 0.95 | 0.89 |
| 2:AB:16:HIS:HB2 | 2:AB:204:ASN:HB3 | 1.55 | 0.89 |
| 1:CA:1244:C:H42 | 1:CA:1293:G:H1 | 1.12 | 0.89 |
| 25:AY:49:C:N3 | 25:AY:65:G:N2 | 2.21 | 0.89 |
| 1:CA:999:C:N3 | 1:CA:1042:G:N2 | 2.21 | 0.89 |
| 25:CY:19:G:N2 | 25:CY:56:C:N3 | 2.20 | 0.89 |
| 26:DA:1798:U:H5' | 28:DD:259:THR:HG22 | 1.55 | 0.89 |
| 25:CY:9:A:N6 | 25:CY:23:A:OP2 | 2.06 | 0.88 |
| 1:CA:998:G:N2 | 1:CA:1043:C:N3 | 2.20 | 0.88 |
| 1:AA:78:G:C6 | 1:AA:91:C:N4 | 2.40 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:AY:5:G:H1 | 25:AY:68:C:H42 | 1.16 | 0.88 |
| 46:DZ:110:GLY:HA3 | 46:DZ:145:GLU:HA | 1.55 | 0.88 |
| 1:AA:1316:G:H22 | 1:AA:1319:A:H5'' | 1.39 | 0.88 |
| 27:DB:41:U:H5 | 31:DG:70:VAL:H | 1.22 | 0.88 |
| 1:AA:78:G:C2 | 1:AA:91:C:N3 | 2.43 | 0.87 |
| 46:BZ:138:GLU:H | 46:BZ:156:LYS:HD3 | 1.36 | 0.87 |
| 1:AA:1166:G:N2 | 1:AA:1170:A:OP2 | 2.06 | 0.87 |
| 23:AW:1:G:N1 | 23:AW:72:C:O2 | 2.07 | 0.87 |
| 41:DU:76:TYR:OH | 41:DU:92:ARG:NH1 | 2.08 | 0.87 |
| 26:BA:1176:G:H1' | 26:BA:1177:A:H5' | 1.55 | 0.87 |
| 25:CY:15:G:H22 | 25:CY:48:C:H42 | 1.16 | 0.87 |
| 9:AI:17:VAL:HG21 | 9:AI:81:ILE:HG22 | 1.55 | 0.87 |
| 11:AK:48:ILE:HD12 | 11:AK:63:LEU:HB2 | 1.54 | 0.86 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:H1 | 1.21 | 0.86 |
| 1:CA:1226:C:O2' | 13:CM:111:LYS:NZ | 2.06 | 0.86 |
| 1:AA:1182:G:H4' | 1:AA:1183:A:H5' | 1.57 | 0.86 |
| 25:CY:50:U:H3 | 25:CY:64:A:N6 | 1.74 | 0.86 |
| 26:BA:2190:G:H2' | 26:BA:2191:G:H5'' | 1.56 | 0.86 |
| 26:DA:2139:C:N3 | 26:DA:2152:G:N2 | 2.23 | 0.86 |
| 1:AA:664:G:H22 | 1:AA:741:G:H1 | 1.23 | 0.86 |
| 19:AS:63:THR:H | 19:AS:66:MET:HE2 | 1.41 | 0.86 |
| 26:DA:2136:C:N3 | 26:DA:2155:G:N2 | 2.24 | 0.86 |
| 1:CA:76:C:H42 | 1:CA:93:G:H1 | 0.91 | 0.86 |
| 26:DA:2136:C:N4 | 26:DA:2155:G:N1 | 2.24 | 0.85 |
| 2:AB:195:ASP:O | 8:AH:68:ARG:NH2 | 2.10 | 0.85 |
| 26:DA:2807:G:N1 | 26:DA:2893:G:O6 | 2.08 | 0.85 |
| 26:BA:1310:G:OP2 | 54:B7:9:ARG:NH1 | 2.09 | 0.85 |
| 1:CA:1166:G:N2 | 1:CA:1170:A:OP2 | 2.09 | 0.85 |
| 46:BZ:72:ARG:NH2 | 46:BZ:97:GLU:O | 2.10 | 0.84 |
| 10:CJ:49:VAL:HG23 | 14:CN:41:ARG:HB2 | 1.58 | 0.84 |
| 16:CP:51:VAL:HG12 | 16:CP:53:VAL:H | 1.42 | 0.84 |
| 26:DA:2297:C:N3 | 26:DA:2321:G:N1 | 2.25 | 0.84 |
| 10:CJ:35:SER:HB3 | 10:CJ:73:ASP:HB2 | 1.59 | 0.84 |
| 26:BA:2134:A:H2' | 26:BA:2135:A:C8 | 2.13 | 0.84 |
| 13:CM:37:THR:O | 13:CM:55:ARG:NH1 | 2.10 | 0.84 |
| 26:BA:631:A:OP1 | 36:BP:65:ARG:NH1 | 2.10 | 0.84 |
| 1:CA:1075:C:OP1 | 2:CB:179:LYS:NZ | 2.10 | 0.84 |
| 26:DA:880:G:H22 | 26:DA:898:C:H1' | 1.40 | 0.84 |
| 32:DH:46:GLU:HB2 | 32:DH:49:VAL:HG12 | 1.58 | 0.84 |
| 37:DQ:109:VAL:HG13 | 37:DQ:113:GLN:HB3 | 1.60 | 0.84 |
| 19:AS:3:ARG:NH1 | 19:AS:8:GLY:O | 2.11 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:CA:958:A:N6 | 19:CS:77:THR:O | 2.11 | 0.84 |
| 1:AA:427:U:OP1 | 4:AD:13:ARG:NH2 | 2.11 | 0.83 |
| 26:DA:1039:G:O6 | 26:DA:1116:C:N4 | 2.11 | 0.83 |
| 1:CA:201:C:H42 | 1:CA:216:G:H1 | 1.21 | 0.83 |
| 1:CA:1286:A:H8 | 1:CA:1287:A:H4' | 1.43 | 0.83 |
| 5:CE:122:GLU:O | 5:CE:126:ARG:NH1 | 2.11 | 0.83 |
| 30:DF:53:THR:HG22 | 30:DF:56:GLU:HG3 | 1.59 | 0.83 |
| 42:DV:24:LYS:HG2 | 42:DV:64:HIS:HD2 | 1.43 | 0.83 |
| 26:DA:1204:A:H2 | 26:DA:1241:A:H62 | 1.22 | 0.83 |
| 19:CS:30:LEU:HD11 | 19:CS:32:LYS:HG3 | 1.60 | 0.83 |
| 23:CW:49:C:N4 | 23:CW:65:G:O6 | 2.12 | 0.83 |
| 25:CY:31:A:N1 | 25:CY:39:PSU:O2 | 2.12 | 0.83 |
| 1:CA:1162:C:N3 | 1:CA:1174:G:N2 | 2.26 | 0.83 |
| 5:CE:102:ALA:O | 5:CE:107:ARG:NH1 | 2.12 | 0.83 |
| 13:AM:122:LYS:HD3 | 13:AM:123:ALA:H | 1.43 | 0.83 |
| 26:DA:2165:G:H22 | 26:DA:2172:U:H5 | 1.24 | 0.82 |
| 26:DA:2136:C:N4 | 26:DA:2155:G:H1 | 1.77 | 0.82 |
| 26:DA:652(D):C:N4 | 26:DA:652(U):G:O6 | 2.09 | 0.82 |
| 1:CA:1106:G:H5'' | 3:CC:172:ARG:HG2 | 1.62 | 0.82 |
| 4:CD:122:ARG:NH1 | 4:CD:134:ASP:O | 2.12 | 0.82 |
| 26:BA:2136:C:N3 | 26:BA:2155:G:N2 | 2.27 | 0.82 |
| 40:BT:118:ARG:HH11 | 40:BT:118:ARG:HG3 | 1.45 | 0.82 |
| 1:CA:70:G:H1 | 1:CA:99:U:H3 | 1.28 | 0.82 |
| 1:CA:975:A:H4' | 1:CA:976:G:H5'' | 1.60 | 0.82 |
| 26:DA:1019:U:H3 | 26:DA:1142(A):A:H62 | 1.26 | 0.82 |
| 26:DA:2136:C:C4 | 26:DA:2155:G:N1 | 2.47 | 0.82 |
| 26:BA:1314:C:OP1 | 61:BA:4634:HOH:O | 1.98 | 0.82 |
| 1:CA:1065:U:OP2 | 1:CA:1190:G:N2 | 2.12 | 0.82 |
| 1:CA:983:A:N1 | 1:CA:1222:G:N2 | 2.28 | 0.81 |
| 27:DB:22:U:H3 | 27:DB:61:G:H1 | 1.24 | 0.81 |
| 36:DP:96:THR:H | 36:DP:99:LEU:HD21 | 1.43 | 0.81 |
| 1:CA:1133:G:H1 | 1:CA:1141:C:H42 | 1.24 | 0.81 |
| 2:AB:16:HIS:O | 2:AB:18:GLY:N | 2.13 | 0.81 |
| 9:CI:53:VAL:O | 9:CI:55:ALA:N | 2.12 | 0.81 |
| 26:DA:994:C:OP1 | 41:DU:53:ARG:NH2 | 2.12 | 0.81 |
| 1:AA:78:G:N1 | 1:AA:91:C:N4 | 2.29 | 0.81 |
| 25:AY:5:G:H1 | 25:AY:68:C:N4 | 1.78 | 0.81 |
| 3:AC:35:GLU:OE2 | 3:AC:59:ARG:NH2 | 2.14 | 0.81 |
| 1:CA:1030:C:H42 | 1:CA:1031:G:H1 | 1.24 | 0.81 |
| 1:CA:1318:A:H5'' | 19:CS:3:ARG:HH22 | 1.46 | 0.81 |
| 40:BT:16:ARG:NH2 | 40:BT:83:ILE:O | 2.14 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1000:U:H3 | 1:CA:1041:A:H61 | 0.87 | 0.81 |
| 2:CB:179:LYS:HA | 8:CH:72:PRO:HG3 | 1.62 | 0.81 |
| 28:DD:276:LYS:H | 28:DD:276:LYS:HD3 | 1.45 | 0.81 |
| 26:DA:2166:G:H3' | 26:DA:2167:U:H5'' | 1.62 | 0.81 |
| 23:AW:26:A:N6 | 23:AW:44:G:H1 | 1.78 | 0.80 |
| 26:BA:2867:G:OP2 | 40:BT:119:LYS:NZ | 2.14 | 0.80 |
| 25:CY:10:G:H1 | 25:CY:25:C:N4 | 1.78 | 0.80 |
| 1:AA:839:U:O2' | 1:AA:840:C:OP1 | 2.00 | 0.80 |
| 25:AY:8:4SU:H4' | 25:AY:48:C:H4' | 1.64 | 0.80 |
| 26:BA:1779:U:OP2 | 61:BA:5167:HOH:O | 1.99 | 0.80 |
| 25:CY:38:A:H3' | 25:CY:39:PSU:H5' | 1.62 | 0.80 |
| 46:DZ:45:ASP:OD2 | 46:DZ:49:ARG:NH1 | 2.14 | 0.80 |
| 1:AA:90:U:H2' | 1:AA:91:C:H5'' | 1.63 | 0.80 |
| 23:CW:4:C:N3 | 23:CW:69:G:N2 | 2.29 | 0.80 |
| 31:DG:145:THR:HG23 | 31:DG:147:ASP:H | 1.46 | 0.80 |
| 38:DR:97:VAL:HG22 | 38:DR:114:VAL:HG22 | 1.62 | 0.80 |
| 46:DZ:119:GLU:O | 46:DZ:122:ARG:NH1 | 2.15 | 0.80 |
| 4:CD:187:ARG:NH2 | 4:CD:193:ASP:OD2 | 2.15 | 0.80 |
| 27:DB:7:G:O6 | 27:DB:114:C:N4 | 2.14 | 0.80 |
| 25:AY:53:G:N2 | 25:AY:61:C:N3 | 2.29 | 0.80 |
| 25:AY:68:C:H2' | 25:AY:69:G:H5' | 1.63 | 0.80 |
| 26:BA:192:C:OP1 | 61:BA:4000:HOH:O | 1.99 | 0.80 |
| 1:CA:878:G:H5' | 8:CH:89:PRO:HG2 | 1.64 | 0.80 |
| 30:DF:53:THR:HG23 | 30:DF:55:GLY:H | 1.47 | 0.79 |
| 1:AA:347:G:O2' | 1:AA:348:G:OP1 | 2.00 | 0.79 |
| 1:AA:742:G:OP2 | 15:AO:35:ARG:NH2 | 2.16 | 0.79 |
| 1:CA:838:G:H1 | 1:CA:848:C:N4 | 1.79 | 0.79 |
| 26:BA:2683:C:O2 | 35:BO:70:LYS:NZ | 2.14 | 0.79 |
| 26:BA:956:G:OP2 | 37:BQ:14:ARG:NH2 | 2.15 | 0.79 |
| 1:CA:589:C:O2 | 1:CA:650:G:N2 | 2.13 | 0.79 |
| 26:BA:2102:U:O2 | 26:BA:2187:G:N2 | 2.13 | 0.79 |
| 28:DD:238:GLY:O | 61:DD:409:HOH:O | 2.00 | 0.79 |
| 25:AY:15:G:H22 | 25:AY:48:C:H42 | 1.30 | 0.79 |
| 23:CW:4:C:N4 | 23:CW:69:G:N1 | 2.29 | 0.79 |
| 1:AA:406:G:H5' | 4:AD:5:ILE:HD11 | 1.64 | 0.79 |
| 1:CA:1055:A:N7 | 1:CA:1200:C:N4 | 2.30 | 0.79 |
| 25:CY:4:C:H42 | 25:CY:69:G:H1 | 1.28 | 0.79 |
| 1:CA:1245:A:N6 | 1:CA:1292:U:H3 | 1.80 | 0.79 |
| 36:DP:100:LEU:HD12 | 36:DP:112:LEU:HD11 | 1.65 | 0.79 |
| 7:AG:38:LEU:HA | 7:AG:41:ARG:HD2 | 1.65 | 0.78 |
| 26:DA:2127:G:C2 | 26:DA:2161:C:N3 | 2.52 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1027:C:C2 | 1:AA:1034:G:N1 | 2.52 | 0.78 |
| 26:BA:1800:C:OP2 | 28:BD:183:ARG:NH2 | 2.17 | 0.78 |
| 33:BI:92:VAL:HG13 | 33:BI:120:ILE:HB | 1.65 | 0.78 |
| 6:CF:81:ILE:HD11 | 28:DD:125:ILE:HB | 1.64 | 0.78 |
| 44:BX:31:HIS:HD2 | 44:BX:33:LYS:H | 1.29 | 0.78 |
| 4:AD:155:LEU:HB3 | 4:AD:158:ILE:HD11 | 1.66 | 0.78 |
| 46:DZ:19:ARG:NH1 | 46:DZ:84:GLU:O | 2.17 | 0.78 |
| 1:AA:266:G:H5'' | 1:AA:268:C:H41 | 1.47 | 0.78 |
| 1:CA:1028:C:N3 | 1:CA:1033:G:C6 | 2.52 | 0.78 |
| 1:CA:838:G:N2 | 1:CA:848:C:N3 | 2.30 | 0.78 |
| 2:CB:187:LEU:HA | 2:CB:201:ILE:HB | 1.64 | 0.78 |
| 26:BA:2136:C:H42 | 26:BA:2155:G:H1 | 0.83 | 0.78 |
| 1:CA:664:G:H22 | 1:CA:741:G:H1 | 1.29 | 0.78 |
| 13:AM:84:ILE:HG13 | 13:AM:85:GLY:HA2 | 1.65 | 0.77 |
| 1:CA:1125:U:O2' | 1:CA:1126:U:H2' | 1.84 | 0.77 |
| 31:BG:12:TYR:HA | 31:BG:16:ARG:HG3 | 1.66 | 0.77 |
| 27:DB:20:C:N4 | 27:DB:63:G:O6 | 2.17 | 0.77 |
| 26:DA:2839:G:H5' | 38:DR:46:GLY:HA2 | 1.64 | 0.77 |
| 1:AA:78:G:N2 | 1:AA:91:C:N3 | 2.33 | 0.77 |
| 26:BA:2138:C:N4 | 26:BA:2153:G:H1 | 1.81 | 0.77 |
| 33:BI:104:GLN:O | 33:BI:106:GLY:N | 2.16 | 0.77 |
| 44:DX:60:ARG:HH12 | 54:D7:47:ARG:HH22 | 1.30 | 0.77 |
| 10:AJ:35:SER:HB3 | 10:AJ:73:ASP:HB2 | 1.67 | 0.77 |
| 23:AW:50:U:H5' | 23:AW:50:U:H6 | 1.48 | 0.77 |
| 25:AY:7:A:O2' | 25:AY:49:C:H5' | 1.85 | 0.77 |
| 1:AA:1027:C:N3 | 1:AA:1034:G:C6 | 2.53 | 0.77 |
| 1:AA:437:U:H5' | 4:AD:155:LEU:HD21 | 1.66 | 0.77 |
| 25:AY:5:G:N2 | 25:AY:68:C:N3 | 2.31 | 0.77 |
| 26:BA:517:C:OP1 | 52:B5:16:ARG:NH2 | 2.18 | 0.77 |
| 26:DA:2037:G:O6 | 61:DA:4191:HOH:O | 2.02 | 0.77 |
| 37:DQ:31:ASP:OD1 | 37:DQ:134:ARG:NH1 | 2.18 | 0.77 |
| 26:BA:1689:A:H62 | 26:BA:1698:A:H2 | 1.33 | 0.77 |
| 1:CA:1338:G:H21 | 24:CX:41:C:H1' | 1.49 | 0.77 |
| 1:AA:1025:U:O2' | 1:AA:1026:G:O4' | 2.02 | 0.77 |
| 25:CY:19:G:H1 | 25:CY:56:C:N4 | 1.82 | 0.77 |
| 32:DH:24:VAL:HG13 | 32:DH:37:VAL:HG21 | 1.66 | 0.77 |
| 26:BA:2130:U:H4' | 26:BA:2133:G:H4' | 1.67 | 0.76 |
| 1:CA:1134:G:H1 | 1:CA:1140:C:H42 | 1.29 | 0.76 |
| 51:D4:40:HIS:HB3 | 51:D4:43:TYR:HB2 | 1.67 | 0.76 |
| 26:DA:370:G:N7 | 61:DA:3786:HOH:O | 2.18 | 0.76 |
| 35:DO:35:VAL:HG11 | 35:DO:103:ALA:HB3 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:AS:27:GLU:HB3 | 19:AS:28:LYS:HA | 1.65 | 0.76 |
| 1:CA:1128:C:O2 | 1:CA:1147:C:N4 | 2.18 | 0.76 |
| 1:CA:504:C:OP1 | 61:CA:3202:HOH:O | 2.02 | 0.76 |
| 25:CY:51:U:O2 | 25:CY:63:G:N2 | 2.15 | 0.76 |
| 39:BS:39:ILE:HB | 39:BS:49:VAL:HG13 | 1.68 | 0.76 |
| 1:CA:1060:C:HO2' | 10:CJ:56:HIS:HD1 | 1.34 | 0.76 |
| 1:CA:406:G:H5' | 4:CD:5:ILE:HD11 | 1.65 | 0.76 |
| 26:BA:2162:G:H2' | 26:BA:2163:C:H5'' | 1.65 | 0.76 |
| 44:BX:88:LYS:NZ | 44:BX:90:GLU:OE1 | 2.18 | 0.76 |
| 24:CX:7:G:H5'' | 24:CX:8:4SU:H5 | 1.65 | 0.76 |
| 1:CA:1030:C:N4 | 1:CA:1031:G:H1 | 1.84 | 0.76 |
| 13:CM:84:ILE:O | 13:CM:86:CYS:N | 2.17 | 0.76 |
| 1:CA:1360:A:OP2 | 14:CN:35:ARG:NH2 | 2.18 | 0.76 |
| 25:CY:49:C:H42 | 25:CY:65:G:H1 | 1.33 | 0.76 |
| 39:BS:25:ARG:NH1 | 39:BS:42:ASP:OD1 | 2.18 | 0.76 |
| 1:AA:998:G:H1 | 1:AA:1043:C:H42 | 1.30 | 0.76 |
| 26:BA:1506:C:H2' | 26:BA:1507:A:H8 | 1.48 | 0.76 |
| 1:CA:1134:G:H1 | 1:CA:1140:C:N4 | 1.84 | 0.76 |
| 1:CA:76:C:N3 | 1:CA:93:G:N2 | 2.32 | 0.76 |
| 2:CB:54:THR:HG23 | 2:CB:199:TYR:HB3 | 1.67 | 0.76 |
| 1:CA:694:A:HO2' | 25:CY:38:A:HO2' | 1.32 | 0.76 |
| 26:DA:1169:G:H1 | 26:DA:1180:C:H42 | 1.31 | 0.76 |
| 26:DA:2134:A:N3 | 26:DA:2159:G:O2' | 2.17 | 0.76 |
| 31:DG:64:THR:HB | 31:DG:94:LEU:HD21 | 1.67 | 0.76 |
| 3:AC:3:ASN:OD1 | 3:AC:3:ASN:N | 2.18 | 0.75 |
| 26:BA:587:C:OP2 | 36:BP:21:ARG:NH2 | 2.20 | 0.75 |
| 55:D8:32:LEU:O | 55:D8:36:LYS:NZ | 2.18 | 0.75 |
| 26:BA:2121:G:H1 | 26:BA:2177:C:N4 | 1.84 | 0.75 |
| 4:CD:98:GLU:OE1 | 4:CD:103:ASN:ND2 | 2.19 | 0.75 |
| 9:CI:85:LEU:HB3 | 9:CI:92:TYR:HD2 | 1.51 | 0.75 |
| 46:DZ:126:VAL:HG11 | 46:DZ:161:VAL:HG23 | 1.67 | 0.75 |
| 36:BP:124:LYS:HG3 | 36:BP:144:GLU:HG2 | 1.69 | 0.75 |
| 26:DA:2113:U:H3 | 26:DA:2170:A:H61 | 1.33 | 0.75 |
| 25:CY:34:G:H2' | 25:CY:35:A:C8 | 2.21 | 0.75 |
| 1:CA:35:G:O2' | 12:CL:118:SER:O | 2.05 | 0.75 |
| 4:AD:166:LYS:NZ | 4:AD:179:GLU:OE2 | 2.20 | 0.75 |
| 1:CA:1030(A):G:N2 | 1:CA:1030(D):A:OP2 | 2.15 | 0.75 |
| 1:CA:1244:C:N4 | 1:CA:1293:G:H1 | 1.83 | 0.75 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:H1 | 1.32 | 0.75 |
| 48:D1:51:VAL:HG11 | 48:D1:74:VAL:HG21 | 1.68 | 0.75 |
| 3:AC:114:PRO:O | 3:AC:118:GLN:NE2 | 2.19 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:AY:67:C:H2' | 25:AY:68:C:C6 | 2.21 | 0.75 |
| 26:BA:2134:A:H2' | 26:BA:2135:A:H8 | 1.49 | 0.75 |
| 25:CY:68:C:H2' | 25:CY:69:G:H5' | 1.69 | 0.75 |
| 26:DA:2122:U:O4 | 26:DA:2176:A:N1 | 2.20 | 0.75 |
| 3:CC:100:ALA:O | 3:CC:102:ASN:ND2 | 2.20 | 0.75 |
| 1:CA:664:G:OP1 | 18:CR:64:ARG:NH2 | 2.19 | 0.75 |
| 1:CA:953:G:H5' | 1:CA:965:A:H61 | 1.51 | 0.74 |
| 3:CC:59:ARG:HG2 | 3:CC:64:VAL:HG13 | 1.68 | 0.74 |
| 1:CA:528:C:N4 | 12:CL:49:ASN:OD1 | 2.20 | 0.74 |
| 25:CY:38:A:C3' | 25:CY:39:PSU:H5' | 2.16 | 0.74 |
| 26:DA:1842:G:O2' | 28:DD:253:GLN:NE2 | 2.20 | 0.74 |
| 36:DP:42:SER:O | 61:DP:303:HOH:O | 2.05 | 0.74 |
| 46:DZ:77:ASP:OD1 | 46:DZ:80:ARG:NH1 | 2.18 | 0.74 |
| 26:BA:2116:G:N2 | 26:BA:2162:G:OP1 | 2.19 | 0.74 |
| 26:BA:885:C:H3' | 26:BA:886:C:H5'' | 1.70 | 0.74 |
| 2:CB:125:PRO:O | 2:CB:127:ILE:N | 2.20 | 0.74 |
| 38:DR:33:ARG:NH2 | 52:D5:57:VAL:O | 2.20 | 0.74 |
| 2:AB:178:ARG:HH21 | 8:AH:74:PRO:HB3 | 1.53 | 0.74 |
| 1:CA:1153:C:H42 | 1:CA:1154:G:H21 | 1.35 | 0.74 |
| 26:BA:1048:A:OP2 | 26:BA:1109:C:N4 | 2.21 | 0.74 |
| 26:BA:279:C:H42 | 26:BA:361:G:H1 | 1.33 | 0.74 |
| 1:AA:1007:C:N3 | 1:AA:1022:G:O6 | 2.19 | 0.74 |
| 26:BA:2287:A:H62 | 26:BA:2344:U:H3 | 1.31 | 0.74 |
| 26:BA:2353:G:N7 | 61:BA:4441:HOH:O | 2.20 | 0.74 |
| 37:BQ:111:GLU:OE1 | 37:BQ:133:ARG:NH2 | 2.19 | 0.74 |
| 1:CA:1011:G:H1 | 1:CA:1018:C:H42 | 1.33 | 0.74 |
| 26:DA:2357:U:OP1 | 47:D0:20:ARG:NH1 | 2.19 | 0.74 |
| 46:DZ:154:ASP:OD1 | 46:DZ:154:ASP:N | 2.20 | 0.74 |
| 1:AA:1086:U:H3 | 1:AA:1099:G:H22 | 1.35 | 0.74 |
| 26:BA:1842:G:O2' | 28:BD:253:GLN:NE2 | 2.20 | 0.74 |
| 1:CA:390:C:O3' | 16:CP:28:ARG:NH2 | 2.21 | 0.74 |
| 3:CC:58:GLU:HB3 | 10:CJ:92:THR:HG21 | 1.68 | 0.74 |
| 25:AY:49:C:H42 | 25:AY:65:G:H1 | 0.79 | 0.74 |
| 26:BA:2285:C:OP2 | 53:B6:6:ARG:NH1 | 2.20 | 0.74 |
| 1:CA:532:A:H61 | 3:CC:193:TYR:HB3 | 1.52 | 0.74 |
| 13:CM:5:ALA:HB1 | 13:CM:66:LEU:HD13 | 1.70 | 0.74 |
| 23:CW:30:G:H1 | 23:CW:40:C:H42 | 1.34 | 0.74 |
| 26:DA:11:G:N7 | 61:DA:4269:HOH:O | 2.21 | 0.74 |
| 26:DA:2138:C:H42 | 26:DA:2153:G:H1 | 0.77 | 0.74 |
| 31:DG:106:LEU:HA | 31:DG:110:ALA:HB3 | 1.70 | 0.74 |
| 1:CA:427:U:OP1 | 4:CD:13:ARG:NH2 | 2.20 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:DF:120:GLU:HB2 | 30:DF:122:LYS:HG2 | 1.68 | 0.73 |
| 1:CA:1005:A:OP2 | 1:CA:1024:G:N2 | 2.19 | 0.73 |
| 1:CA:1182:G:H4' | 1:CA:1183:A:H3' | 1.68 | 0.73 |
| 1:CA:992:U:H6 | 1:CA:992:U:H5'' | 1.53 | 0.73 |
| 2:CB:119:GLU:OE2 | 2:CB:153:ARG:NH1 | 2.22 | 0.73 |
| 24:CX:67:C:H2' | 24:CX:68:C:H5' | 1.69 | 0.73 |
| 1:AA:376:G:H5'' | 16:AP:5:ARG:HB3 | 1.70 | 0.73 |
| 32:BH:159:GLU:HG3 | 32:BH:169:VAL:HG11 | 1.68 | 0.73 |
| 1:CA:1054:C:C4 | 23:CW:34:G:H1' | 2.23 | 0.73 |
| 26:DA:2632:A:HO2' | 26:DA:2811:G:HO2' | 1.32 | 0.73 |
| 52:B5:40:LYS:NZ | 52:B5:44:THR:O | 2.18 | 0.73 |
| 1:CA:345:C:OP2 | 40:DT:39:ARG:NH2 | 2.21 | 0.73 |
| 26:BA:993:G:OP1 | 41:BU:50:ARG:NH2 | 2.22 | 0.73 |
| 26:BA:1602:U:O4 | 61:BA:4209:HOH:O | 2.06 | 0.73 |
| 26:BA:847:U:OP2 | 61:BA:4392:HOH:O | 2.06 | 0.73 |
| 45:BY:92:ASN:HB2 | 45:BY:94:LYS:N | 2.01 | 0.73 |
| 9:CI:8:GLY:HA3 | 9:CI:15:ALA:HB3 | 1.71 | 0.73 |
| 26:DA:952:G:OP1 | 37:DQ:16:ARG:NH2 | 2.21 | 0.73 |
| 23:AW:18:G:O2' | 23:AW:57:G:N2 | 2.14 | 0.73 |
| 1:CA:1321:C:H5'' | 1:CA:1322:C:H2' | 1.69 | 0.73 |
| 56:B9:17:ILE:HG22 | 56:B9:24:TYR:HB2 | 1.70 | 0.73 |
| 26:BA:243:U:OP1 | 55:B8:6:THR:OG1 | 2.07 | 0.73 |
| 1:AA:812:C:N3 | 61:AA:4038:HOH:O | 2.20 | 0.73 |
| 23:AW:19:G:N2 | 23:AW:56:C:N3 | 2.36 | 0.73 |
| 26:DA:2127:G:N1 | 26:DA:2161:C:C4 | 2.57 | 0.73 |
| 27:BB:33:G:H5' | 31:BG:2:PRO:HD3 | 1.70 | 0.73 |
| 1:CA:1323:G:N2 | 1:CA:1361:G:O2' | 2.22 | 0.73 |
| 1:AA:974:A:OP2 | 14:AN:41:ARG:NH1 | 2.21 | 0.72 |
| 25:AY:56:C:H2' | 25:AY:57:G:O4' | 1.88 | 0.72 |
| 1:AA:504:C:OP1 | 61:AA:4184:HOH:O | 2.07 | 0.72 |
| 3:CC:29:TYR:OH | 14:CN:54:PRO:O | 2.06 | 0.72 |
| 1:CA:26:A:O2' | 4:CD:209:ARG:NH2 | 2.22 | 0.72 |
| 26:DA:2138:C:N3 | 26:DA:2153:G:N2 | 2.34 | 0.72 |
| 1:AA:1183:A:O2' | 1:AA:1184:G:OP1 | 2.07 | 0.72 |
| 1:CA:117:G:OP2 | 61:CA:3236:HOH:O | 2.07 | 0.72 |
| 2:CB:95:GLN:HB2 | 2:CB:148:TYR:HD1 | 1.54 | 0.72 |
| 26:DA:191:A:N1 | 61:DA:4214:HOH:O | 2.22 | 0.72 |
| 1:AA:975:A:H4' | 1:AA:976:G:H5'' | 1.70 | 0.72 |
| 25:AY:33:U:H3' | 25:AY:34:G:H5'' | 1.71 | 0.72 |
| 23:CW:19:G:H1 | 23:CW:56:C:H42 | 1.37 | 0.72 |
| 26:DA:740:U:OP2 | 61:DA:4209:HOH:O | 2.07 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:DX:53:LYS:HB3 | 44:DX:82:GLN:HB3 | 1.69 | 0.72 |
| 51:B4:57:GLU:HB2 | 51:B4:58:ARG:HA | 1.72 | 0.72 |
| 13:CM:5:ALA:HB3 | 13:CM:22:ILE:HD12 | 1.69 | 0.72 |
| 42:DV:98:GLU:OE1 | 42:DV:100:ARG:NH1 | 2.23 | 0.72 |
| 26:BA:65:C:O2 | 26:BA:456:C:N4 | 2.20 | 0.72 |
| 23:CW:50:U:O4 | 23:CW:64:A:N1 | 2.22 | 0.72 |
| 25:CY:7:A:H61 | 25:CY:66:U:H3 | 0.79 | 0.72 |
| 43:BW:15:ARG:NH1 | 61:BW:4002:HOH:O | 2.21 | 0.72 |
| 26:BA:1385:G:O2' | 26:BA:1396:U:O2 | 2.07 | 0.72 |
| 2:CB:78:GLN:NE2 | 2:CB:95:GLN:OE1 | 2.23 | 0.72 |
| 5:CE:74:GLY:HA3 | 5:CE:116:THR:HG22 | 1.70 | 0.72 |
| 28:BD:17:THR:O | 28:BD:211:ARG:NH2 | 2.23 | 0.72 |
| 46:BZ:117:LEU:HD11 | 46:BZ:144:LEU:HD22 | 1.71 | 0.72 |
| 23:CW:61:C:O2' | 23:CW:62:C:O5' | 2.07 | 0.72 |
| 25:CY:15:G:H22 | 25:CY:48:C:N4 | 1.87 | 0.72 |
| 26:DA:1250:G:OP2 | 36:DP:21:ARG:NH1 | 2.23 | 0.72 |
| 1:AA:310:G:OP2 | 16:AP:27:LYS:NZ | 2.22 | 0.71 |
| 1:AA:934:C:OP1 | 61:AA:4086:HOH:O | 2.08 | 0.71 |
| 12:AL:24:VAL:HG12 | 12:AL:27:LEU:HB2 | 1.71 | 0.71 |
| 2:CB:212:GLN:NE2 | 2:CB:234:PRO:O | 2.23 | 0.71 |
| 2:AB:16:HIS:HB3 | 2:AB:210:SER:HB2 | 1.72 | 0.71 |
| 23:AW:7:A:H61 | 23:AW:66:U:H3 | 1.36 | 0.71 |
| 26:BA:2049:G:N7 | 61:BA:5132:HOH:O | 2.23 | 0.71 |
| 12:CL:117:ARG:HB3 | 12:CL:122:THR:HB | 1.73 | 0.71 |
| 49:D2:38:GLN:HB3 | 49:D2:44:LEU:HB2 | 1.72 | 0.71 |
| 26:DA:2206:G:H3' | 26:DA:2207:G:C8 | 2.25 | 0.71 |
| 48:B1:86:SER:OG | 48:B1:89:GLU:OE1 | 2.08 | 0.71 |
| 26:BA:604:G:OP2 | 36:BP:90:ARG:NH1 | 2.24 | 0.71 |
| 1:CA:1011:G:H1 | 1:CA:1018:C:N4 | 1.89 | 0.71 |
| 26:DA:143:G:H4' | 44:DX:35:THR:HG21 | 1.73 | 0.71 |
| 20:AT:57:ARG:HH12 | 20:AT:100:ILE:HD12 | 1.55 | 0.71 |
| 23:AW:19:G:H1 | 23:AW:56:C:N4 | 1.89 | 0.71 |
| 1:AA:1027:C:O2 | 1:AA:1034:G:C2 | 2.43 | 0.71 |
| 26:BA:1693:U:O2' | 28:BD:14:ARG:NH2 | 2.23 | 0.71 |
| 26:DA:1449:A:O2' | 26:DA:1529:G:N2 | 2.17 | 0.71 |
| 1:AA:538:G:H5'' | 12:AL:114:LYS:HB2 | 1.71 | 0.71 |
| 19:CS:77:THR:HG22 | 19:CS:78:ARG:HG2 | 1.71 | 0.71 |
| 26:DA:1800:C:OP2 | 28:DD:183:ARG:NH2 | 2.23 | 0.71 |
| 26:BA:1140:C:O3' | 34:BN:25:ARG:NH1 | 2.23 | 0.71 |
| 1:CA:1465:C:OP2 | 40:DT:108:ARG:NH2 | 2.22 | 0.71 |
| 2:CB:88:ALA:HB2 | 2:CB:219:VAL:HG13 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BA:899:A:O2' | 26:BA:900:A:O5' | 2.08 | 0.71 |
| 1:CA:986:A:O2' | 19:CS:55:LYS:O | 2.08 | 0.71 |
| 26:DA:2788:C:OP1 | 29:DE:61:ARG:NH2 | 2.23 | 0.71 |
| 28:DD:85:ASP:OD2 | 28:DD:88:ARG:NH1 | 2.21 | 0.71 |
| 4:CD:57:ARG:HH22 | 5:CE:107:ARG:HD3 | 1.55 | 0.71 |
| 5:CE:50:GLU:HB2 | 5:CE:53:LEU:HD13 | 1.73 | 0.71 |
| 27:DB:5:C:H42 | 27:DB:116:G:H1 | 1.39 | 0.71 |
| 6:AF:70:ASP:OD1 | 6:AF:70:ASP:N | 2.24 | 0.70 |
| 39:DS:15:ARG:O | 39:DS:19:LYS:HD3 | 1.90 | 0.70 |
| 26:BA:1380:G:OP2 | 61:BA:5119:HOH:O | 2.09 | 0.70 |
| 1:CA:1366:C:O2' | 10:CJ:60:ARG:NH2 | 2.24 | 0.70 |
| 31:DG:80:PHE:O | 31:DG:82:LEU:N | 2.22 | 0.70 |
| 33:DI:72:LEU:HD21 | 33:DI:107:VAL:HG11 | 1.74 | 0.70 |
| 54:B7:24:THR:HG22 | 54:B7:27:GLY:H | 1.56 | 0.70 |
| 26:BA:2239:G:OP2 | 61:BA:4313:HOH:O | 2.08 | 0.70 |
| 26:BA:2448:A:OP1 | 61:BA:5135:HOH:O | 2.09 | 0.70 |
| 1:CA:999:C:H42 | 1:CA:1042:G:H1 | 0.74 | 0.70 |
| 26:DA:1038:C:H42 | 26:DA:1117:G:H1 | 1.38 | 0.70 |
| 26:DA:2148:G:H2' | 26:DA:2149:G:C8 | 2.27 | 0.70 |
| 17:AQ:75:ARG:NH1 | 17:AQ:76:LEU:O | 2.25 | 0.70 |
| 1:CA:993:G:O6 | 1:CA:1045:C:N4 | 2.15 | 0.70 |
| 26:DA:1689:A:H62 | 26:DA:1698:A:H2 | 1.40 | 0.70 |
| 26:DA:900:A:H2' | 26:DA:901:A:H8 | 1.57 | 0.70 |
| 3:AC:19:GLU:HB3 | 3:AC:40:ARG:HH22 | 1.57 | 0.70 |
| 25:AY:51:U:H2' | 25:AY:52:G:H8 | 1.56 | 0.70 |
| 36:BP:126:VAL:HG12 | 36:BP:148:LEU:HD22 | 1.72 | 0.70 |
| 32:DH:159:GLU:HG3 | 32:DH:169:VAL:HG11 | 1.74 | 0.70 |
| 33:DI:78:THR:O | 33:DI:104:GLN:NE2 | 2.25 | 0.70 |
| 25:AY:15:G:N1 | 25:AY:48:C:N3 | 2.39 | 0.70 |
| 25:AY:22:G:N7 | 25:AY:46:7MG:O6 | 2.25 | 0.70 |
| 23:CW:4:C:N4 | 23:CW:69:G:C6 | 2.59 | 0.70 |
| 1:AA:1304:G:OP2 | 61:AA:4111:HOH:O | 2.10 | 0.70 |
| 5:AE:6:PHE:HB2 | 5:AE:34:VAL:HG22 | 1.73 | 0.70 |
| 12:AL:70:ILE:HG12 | 12:AL:100:ILE:HD12 | 1.72 | 0.70 |
| 1:CA:953:G:H5' | 1:CA:965:A:N6 | 2.07 | 0.70 |
| 27:DB:28:C:H2' | 27:DB:29:A:H8 | 1.57 | 0.70 |
| 1:CA:582:U:OP1 | 15:CO:68:ARG:NH1 | 2.24 | 0.70 |
| 46:DZ:44:PHE:O | 46:DZ:48:PHE:N | 2.21 | 0.70 |
| 1:AA:1159:U:OP1 | 2:AB:133:LYS:NZ | 2.25 | 0.69 |
| 12:AL:49:ASN:ND2 | 12:AL:92:ASP:OD2 | 2.20 | 0.69 |
| 26:BA:1238:G:OP2 | 61:BA:4983:HOH:O | 2.10 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:812:C:N3 | 61:CA:3212:HOH:O | 2.25 | 0.69 |
| 2:CB:161:ALA:HB1 | 2:CB:185:ILE:HD11 | 1.74 | 0.69 |
| 10:CJ:5:ARG:N | 10:CJ:73:ASP:HA | 2.07 | 0.69 |
| 26:DA:2404:C:O3' | 36:DP:77:ARG:NH2 | 2.25 | 0.69 |
| 28:BD:71:ASP:HB3 | 28:BD:103:ARG:HH22 | 1.57 | 0.69 |
| 12:CL:70:ILE:HD13 | 12:CL:77:LEU:HD12 | 1.72 | 0.69 |
| 26:DA:1033:U:OP1 | 56:D9:9:ARG:NH2 | 2.26 | 0.69 |
| 46:DZ:72:ARG:NH1 | 46:DZ:97:GLU:O | 2.25 | 0.69 |
| 26:BA:1434:A:H61 | 26:BA:1558:A:H62 | 1.39 | 0.69 |
| 1:CA:798:G:O6 | 61:CA:3223:HOH:O | 2.09 | 0.69 |
| 26:DA:300:A:OP1 | 45:DY:86:ARG:NH2 | 2.25 | 0.69 |
| 30:DF:197:ASP:OD1 | 30:DF:198:ALA:N | 2.25 | 0.69 |
| 36:DP:91:PHE:O | 36:DP:121:LYS:NZ | 2.21 | 0.69 |
| 9:AI:110:GLU:OE2 | 9:AI:113:LYS:NZ | 2.25 | 0.69 |
| 3:AC:58:GLU:HB3 | 10:AJ:92:THR:HG21 | 1.75 | 0.69 |
| 15:AO:55:GLY:HA2 | 15:AO:58:MET:HE2 | 1.73 | 0.69 |
| 26:BA:1297:C:OP1 | 61:BA:4340:HOH:O | 2.09 | 0.69 |
| 31:BG:41:GLN:NE2 | 31:BG:154:GLY:O | 2.25 | 0.69 |
| 1:CA:1128:C:H1' | 1:CA:1147:C:H42 | 1.56 | 0.69 |
| 1:CA:1359:C:O2 | 61:CA:3330:HOH:O | 2.09 | 0.69 |
| 1:CA:67:C:H2' | 1:CA:68:G:C8 | 2.28 | 0.69 |
| 8:CH:12:ARG:HH12 | 8:CH:27:PRO:HD2 | 1.58 | 0.69 |
| 25:CY:26:A:N1 | 25:CY:44:G:O6 | 2.26 | 0.69 |
| 26:DA:987:G:O2' | 26:DA:1000:A:N3 | 2.25 | 0.69 |
| 1:AA:1423:G:OP1 | 35:BO:49:ARG:NH2 | 2.24 | 0.69 |
| 4:AD:49:ARG:HE | 4:AD:49:ARG:H | 1.38 | 0.69 |
| 23:CW:56:C:H5 | 26:DA:897:C:H1' | 1.56 | 0.69 |
| 26:DA:2166:G:H3' | 26:DA:2167:U:C5' | 2.22 | 0.69 |
| 26:DA:2176:A:H2' | 26:DA:2177:C:C6 | 2.27 | 0.69 |
| 28:DD:275:LYS:HG3 | 28:DD:276:LYS:HA | 1.73 | 0.69 |
| 30:BF:185:ASP:HA | 30:BF:188:ARG:HD3 | 1.73 | 0.69 |
| 25:CY:69:G:H2' | 25:CY:70:G:O4' | 1.92 | 0.69 |
| 26:DA:2135:A:H2' | 26:DA:2136:C:C6 | 2.27 | 0.69 |
| 26:DA:2119:A:H2 | 26:DA:2171:A:H5' | 1.58 | 0.69 |
| 26:DA:878:A:N6 | 26:DA:899:A:O2' | 2.22 | 0.69 |
| 19:AS:27:GLU:HB2 | 19:AS:28:LYS:HD2 | 1.74 | 0.69 |
| 44:BX:35:THR:HG22 | 44:BX:38:GLU:H | 1.57 | 0.69 |
| 17:CQ:53:LEU:HD23 | 17:CQ:82:MET:HE1 | 1.75 | 0.69 |
| 19:CS:27:GLU:HB3 | 19:CS:28:LYS:HA | 1.75 | 0.69 |
| 1:AA:1033:G:H2' | 1:AA:1034:G:H8 | 1.58 | 0.69 |
| 10:AJ:47:PHE:HB2 | 10:AJ:63:PHE:HB2 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 26:BA:271(K):U:H1' | 33:BI:50:ARG:HD2 | 1.74 | 0.69 |
| 12:CL:124:LYS:HB2 | 12:CL:124:LYS:HZ2 | 1.57 | 0.69 |
| 29:BE:8:LYS:NZ | 61:BE:416:HOH:O | 2.18 | 0.69 |
| 1:CA:1060:C:O2' | 10:CJ:56:HIS:ND1 | 2.24 | 0.69 |
| 1:CA:1329:A:OP2 | 21:CU:7:ARG:NH2 | 2.22 | 0.69 |
| 1:CA:460:G:O6 | 1:CA:470:C:H5'' | 1.93 | 0.69 |
| 1:CA:1320:C:O4' | 19:CS:73:GLU:HG2 | 1.93 | 0.69 |
| 25:CY:5:G:H1 | 25:CY:68:C:H42 | 1.40 | 0.69 |
| 26:DA:89:G:H3' | 26:DA:90:U:H5'' | 1.75 | 0.69 |
| 26:DA:568:U:H5' | 26:DA:945:A:N1 | 2.08 | 0.69 |
| 7:AG:111:ARG:NH1 | 7:AG:113:GLU:OE2 | 2.23 | 0.69 |
| 25:AY:76:A:N6 | 26:BA:2422:A:O4' | 2.26 | 0.69 |
| 26:DA:1420:U:O2' | 26:DA:1421:G:OP1 | 2.10 | 0.69 |
| 2:AB:21:ARG:HB3 | 2:AB:39:ILE:HG12 | 1.75 | 0.69 |
| 5:AE:74:GLY:HA3 | 5:AE:116:THR:HG22 | 1.74 | 0.69 |
| 26:BA:952:G:OP1 | 37:BQ:16:ARG:NH2 | 2.26 | 0.69 |
| 46:DZ:93:ASP:HA | 46:DZ:131:ARG:HH22 | 1.57 | 0.69 |
| 23:AW:50:U:H3 | 23:AW:64:A:H61 | 1.39 | 0.68 |
| 26:BA:1840:G:N7 | 61:BA:4310:HOH:O | 2.26 | 0.68 |
| 47:B0:10:THR:HG22 | 47:B0:12:ASN:H | 1.57 | 0.68 |
| 20:CT:43:LEU:O | 20:CT:47:GLY:N | 2.17 | 0.68 |
| 1:AA:838:G:H1 | 1:AA:848:C:H42 | 1.40 | 0.68 |
| 1:CA:974:A:OP2 | 14:CN:41:ARG:NH1 | 2.27 | 0.68 |
| 31:DG:113:ARG:NH1 | 31:DG:139:LEU:O | 2.26 | 0.68 |
| 3:AC:6:HIS:HD2 | 3:AC:8:ILE:H | 1.40 | 0.68 |
| 14:AN:3:ARG:HH21 | 14:AN:3:ARG:HB3 | 1.57 | 0.68 |
| 26:BA:1714:G:H1 | 26:BA:1745(A):C:H42 | 1.41 | 0.68 |
| 33:BI:38:LEU:HD12 | 33:BI:38:LEU:H | 1.58 | 0.68 |
| 26:BA:1143:A:OP1 | 34:BN:25:ARG:NH2 | 2.26 | 0.68 |
| 25:CY:62:C:H2' | 25:CY:63:G:H8 | 1.58 | 0.68 |
| 51:D4:44:THR:O | 51:D4:46:GLN:N | 2.27 | 0.68 |
| 26:DA:1816:G:O6 | 28:DD:35:LYS:NZ | 2.20 | 0.68 |
| 26:DA:741:G:OP2 | 61:DA:4210:HOH:O | 2.12 | 0.68 |
| 1:AA:953:G:H5' | 1:AA:965:A:H61 | 1.56 | 0.68 |
| 37:BQ:18:LYS:O | 37:BQ:98:LYS:NZ | 2.22 | 0.68 |
| 8:CH:12:ARG:NH1 | 8:CH:27:PRO:HD2 | 2.09 | 0.68 |
| 47:D0:40:GLN:HE21 | 47:D0:57:PHE:HB3 | 1.58 | 0.68 |
| 26:DA:2128:C:H42 | 26:DA:2160:G:H1 | 1.42 | 0.68 |
| 26:DA:2502:G:N7 | 61:DA:4405:HOH:O | 2.26 | 0.68 |
| 26:DA:2689:U:H4' | 26:DA:2690:C:H5' | 1.75 | 0.68 |
| 30:DF:143:ALA:HB1 | 30:DF:148:LEU:HB2 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:AY:69:G:H2' | 25:AY:70:G:O4' | 1.94 | 0.68 |
| 26:BA:2123:G:H1 | 26:BA:2175:C:H42 | 1.40 | 0.68 |
| 1:CA:1002:G:H1 | 1:CA:1038:C:N4 | 1.91 | 0.68 |
| 1:CA:1166:G:H5'' | 1:CA:1166:G:H8 | 1.59 | 0.68 |
| 26:DA:1593:G:H2' | 26:DA:1594:G:C8 | 2.28 | 0.68 |
| 26:DA:2171:A:N3 | 26:DA:2172:U:N3 | 2.41 | 0.68 |
| 38:DR:33:ARG:NH1 | 38:DR:115:GLU:OE2 | 2.26 | 0.68 |
| 1:AA:339:C:OP2 | 35:BO:97:ARG:NH1 | 2.26 | 0.68 |
| 1:AA:559:A:OP1 | 5:AE:126:ARG:NH2 | 2.26 | 0.68 |
| 26:BA:1783:A:N7 | 61:BA:5029:HOH:O | 2.27 | 0.68 |
| 26:BA:543:C:N4 | 26:BA:549:G:O6 | 2.18 | 0.68 |
| 26:DA:1019:U:HO2' | 26:DA:1021:A:H2 | 1.42 | 0.68 |
| 26:DA:2183:C:H2' | 26:DA:2184:G:H8 | 1.59 | 0.68 |
| 30:DF:21:ALA:HB3 | 30:DF:22:ALA:HA | 1.75 | 0.68 |
| 1:AA:838:G:H1 | 1:AA:848:C:N4 | 1.91 | 0.68 |
| 10:AJ:49:VAL:HG23 | 14:AN:41:ARG:HB2 | 1.76 | 0.68 |
| 26:BA:548:A:O2' | 26:BA:549:G:OP1 | 2.10 | 0.68 |
| 27:BB:2:C:O2 | 27:BB:119:G:N2 | 2.20 | 0.68 |
| 1:CA:976:G:H5' | 1:CA:1358:U:O2' | 1.93 | 0.68 |
| 23:CW:43:C:H2' | 23:CW:44:G:C8 | 2.29 | 0.68 |
| 1:AA:123:C:OP1 | 1:AA:311:C:O2' | 2.11 | 0.68 |
| 26:BA:2447:G:OP2 | 61:BA:4544:HOH:O | 2.11 | 0.68 |
| 46:BZ:145:GLU:O | 46:BZ:148:ASP:N | 2.26 | 0.68 |
| 1:CA:750:G:N3 | 15:CO:23:GLY:HA3 | 2.08 | 0.68 |
| 26:DA:1189:A:OP2 | 61:DA:4174:HOH:O | 2.12 | 0.68 |
| 29:DE:111:ARG:HG3 | 29:DE:160:TYR:CD2 | 2.29 | 0.68 |
| 1:AA:1221:G:OP1 | 1:AA:1320:C:N4 | 2.26 | 0.68 |
| 1:CA:344:A:H5'' | 1:CA:345:C:H5 | 1.59 | 0.68 |
| 27:DB:55:U:O2' | 31:DG:27:ASN:ND2 | 2.26 | 0.68 |
| 39:DS:58:LEU:HD11 | 39:DS:65:VAL:HA | 1.75 | 0.68 |
| 2:AB:16:HIS:CG | 2:AB:17:PHE:H | 2.12 | 0.67 |
| 50:B3:8:LEU:HD13 | 50:B3:31:LEU:HD23 | 1.75 | 0.67 |
| 26:BA:602:G:O2' | 26:BA:655:A:N6 | 2.27 | 0.67 |
| 33:BI:106:GLY:HA2 | 33:BI:107:VAL:O | 1.93 | 0.67 |
| 35:BO:2:ILE:HD12 | 35:BO:6:THR:HG21 | 1.73 | 0.67 |
| 1:CA:1133:G:H2' | 1:CA:1134:G:H8 | 1.57 | 0.67 |
| 1:CA:1309:G:OP1 | 13:CM:88:ARG:NH1 | 2.26 | 0.67 |
| 4:CD:173:TRP:HB3 | 4:CD:187:ARG:HE | 1.59 | 0.67 |
| 1:AA:134:A:H61 | 16:AP:25:ARG:HH12 | 1.42 | 0.67 |
| 1:AA:572:A:OP1 | 61:AA:4084:HOH:O | 2.11 | 0.67 |
| 26:BA:2059:A:OP2 | 61:BA:4315:HOH:O | 2.11 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BA:2328:A:H2' | 26:BA:2329:G:C8 | 2.28 | 0.67 |
| 12:CL:124:LYS:HB2 | 12:CL:124:LYS:NZ | 2.08 | 0.67 |
| 24:CX:31:G:H3' | 24:CX:32:5MC:HM51 | 1.76 | 0.67 |
| 1:AA:1158:C:H5 | 1:AA:1181:G:H1 | 1.42 | 0.67 |
| 9:AI:53:VAL:O | 9:AI:55:ALA:N | 2.27 | 0.67 |
| 19:CS:27:GLU:HB2 | 19:CS:28:LYS:HD3 | 1.77 | 0.67 |
| 25:CY:15:G:N2 | 25:CY:48:C:H42 | 1.90 | 0.67 |
| 52:D5:16:ARG:NH1 | 52:D5:17:ASP:OD1 | 2.27 | 0.67 |
| 42:DV:43:GLU:OE2 | 42:DV:43:GLU:N | 2.27 | 0.67 |
| 1:AA:347:G:H2' | 1:AA:348:G:O4' | 1.94 | 0.67 |
| 16:AP:1:MET:N | 16:AP:1:MET:SD | 2.62 | 0.67 |
| 3:CC:91:LEU:HD23 | 3:CC:101:LEU:HD22 | 1.76 | 0.67 |
| 8:CH:4:ASP:OD2 | 8:CH:85:ARG:NH1 | 2.27 | 0.67 |
| 26:DA:2121:G:N2 | 26:DA:2177:C:N3 | 2.36 | 0.67 |
| 26:DA:526:A:OP1 | 61:DA:4183:HOH:O | 2.12 | 0.67 |
| 1:AA:1028:C:H2' | 1:AA:1029:C:H4' | 1.77 | 0.67 |
| 3:CC:129:ALA:HB3 | 3:CC:132:ARG:HB2 | 1.77 | 0.67 |
| 26:DA:2518:A:OP2 | 61:DA:3991:HOH:O | 2.12 | 0.67 |
| 3:AC:134:ILE:HG23 | 3:AC:151:VAL:HB | 1.76 | 0.67 |
| 26:BA:1452:A:OP2 | 61:BA:3995:HOH:O | 2.12 | 0.67 |
| 1:CA:1310:G:OP1 | 13:CM:77:ASN:ND2 | 2.27 | 0.67 |
| 5:CE:102:ALA:HB1 | 5:CE:106:PRO:HG2 | 1.77 | 0.67 |
| 18:CR:52:PRO:HB2 | 18:CR:54:ARG:HG2 | 1.77 | 0.67 |
| 26:DA:2224:G:OP1 | 28:DD:268:ARG:NE | 2.28 | 0.67 |
| 26:DA:2562:U:H1' | 35:DO:23:ARG:HH11 | 1.60 | 0.67 |
| 1:AA:160:A:N6 | 1:AA:345:C:OP2 | 2.27 | 0.67 |
| 1:CA:1022:G:H2' | 1:CA:1023:G:C8 | 2.29 | 0.67 |
| 13:CM:121:LYS:HZ2 | 13:CM:121:LYS:H | 1.43 | 0.67 |
| 1:AA:67:C:H2' | 1:AA:68:G:C8 | 2.30 | 0.67 |
| 2:AB:80:ILE:HD11 | 2:AB:212:GLN:HA | 1.76 | 0.67 |
| 1:AA:656:C:O2' | 15:AO:28:GLN:NE2 | 2.27 | 0.67 |
| 51:D4:38:LYS:O | 51:D4:40:HIS:N | 2.21 | 0.67 |
| 26:DA:1783:A:N7 | 61:DA:4510:HOH:O | 2.26 | 0.67 |
| 1:AA:1022:G:H2' | 1:AA:1023:G:H8 | 1.60 | 0.67 |
| 46:BZ:108:PRO:HB3 | 46:BZ:117:LEU:HD13 | 1.75 | 0.67 |
| 1:CA:560:U:O2' | 1:CA:561:U:OP2 | 2.13 | 0.67 |
| 9:CI:9:ARG:H | 9:CI:79:LEU:HD23 | 1.58 | 0.67 |
| 26:DA:131:G:OP1 | 61:DA:3791:HOH:O | 2.11 | 0.67 |
| 26:DA:2126:A:H61 | 26:DA:2172:U:H3' | 1.60 | 0.67 |
| 26:DA:2287:A:H62 | 26:DA:2344:U:H3 | 1.40 | 0.67 |
| 34:DN:115:ARG:HA | 34:DN:118:LYS:HE3 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:CY:9:A:OP2 | 25:CY:13:C:N4 | 2.26 | 0.67 |
| 26:DA:2127:G:N1 | 26:DA:2161:C:N4 | 2.42 | 0.67 |
| 26:DA:2148:G:H2' | 26:DA:2149:G:H8 | 1.58 | 0.67 |
| 26:DA:7:G:N2 | 26:DA:2896:C:O2 | 2.23 | 0.67 |
| 31:DG:13:GLU:O | 31:DG:15:VAL:N | 2.27 | 0.67 |
| 1:CA:673:G:H2' | 1:CA:674:G:C8 | 2.30 | 0.66 |
| 25:CY:62:C:H2' | 25:CY:63:G:C8 | 2.30 | 0.66 |
| 3:AC:70:VAL:HG22 | 3:AC:72:LYS:H | 1.59 | 0.66 |
| 26:BA:971:C:OP2 | 61:BA:5252:HOH:O | 2.11 | 0.66 |
| 1:CA:951:G:OP2 | 13:CM:102:ARG:NH1 | 2.29 | 0.66 |
| 2:CB:87:ARG:HH21 | 2:CB:233:SER:HB3 | 1.60 | 0.66 |
| 19:CS:49:ILE:HG13 | 19:CS:62:ILE:HD11 | 1.76 | 0.66 |
| 27:DB:50:G:OP1 | 39:DS:63:THR:N | 2.27 | 0.66 |
| 1:CA:1155:G:H2' | 1:CA:1156:G:C8 | 2.29 | 0.66 |
| 3:CC:22:TRP:CD2 | 3:CC:59:ARG:HD2 | 2.30 | 0.66 |
| 1:CA:1191:A:OP1 | 3:CC:3:ASN:ND2 | 2.28 | 0.66 |
| 7:CG:22:LEU:HG | 7:CG:62:PHE:HE2 | 1.60 | 0.66 |
| 37:BQ:54:MET:HG3 | 37:BQ:117:ALA:HB1 | 1.76 | 0.66 |
| 1:CA:1015:A:N3 | 1:CA:1218:C:O2' | 2.27 | 0.66 |
| 7:CG:59:LEU:HG | 7:CG:63:LYS:HE2 | 1.77 | 0.66 |
| 26:DA:2400:G:O3' | 53:D6:18:ARG:NH1 | 2.27 | 0.66 |
| 27:DB:76:G:N2 | 27:DB:101:G:O6 | 2.25 | 0.66 |
| 1:AA:1245:A:H61 | 1:AA:1292:U:H3 | 1.44 | 0.66 |
| 2:AB:93:VAL:HG21 | 2:AB:97:TRP:CD1 | 2.30 | 0.66 |
| 13:AM:34:LEU:HD13 | 13:AM:41:PRO:HA | 1.77 | 0.66 |
| 25:AY:6:G:O6 | 25:AY:7:A:N6 | 2.29 | 0.66 |
| 26:BA:2277:G:OP2 | 47:B0:10:THR:HG21 | 1.96 | 0.66 |
| 26:BA:123:G:OP2 | 61:BA:3977:HOH:O | 2.14 | 0.66 |
| 26:BA:2759:G:N7 | 61:BA:4108:HOH:O | 2.27 | 0.66 |
| 42:BV:34:GLU:HB3 | 42:BV:56:SER:HB2 | 1.75 | 0.66 |
| 2:AB:16:HIS:CD2 | 2:AB:17:PHE:H | 2.13 | 0.66 |
| 20:AT:15:ARG:O | 20:AT:19:SER:OG | 2.13 | 0.66 |
| 1:CA:1118:C:OP1 | 9:CI:104:ARG:NH1 | 2.28 | 0.66 |
| 1:CA:1316:G:H4' | 14:CN:18:VAL:HG13 | 1.77 | 0.66 |
| 26:DA:1278:A:OP1 | 38:DR:36:THR:HG23 | 1.96 | 0.66 |
| 1:CA:1348:U:H4' | 9:CI:120:ARG:HD3 | 1.78 | 0.66 |
| 3:CC:150:LYS:HB2 | 3:CC:173:VAL:HG21 | 1.77 | 0.66 |
| 26:BA:248:G:OP1 | 61:BA:4977:HOH:O | 2.13 | 0.66 |
| 8:AH:41:ARG:NH2 | 8:AH:123:GLU:OE2 | 2.29 | 0.66 |
| 26:BA:880:G:H2' | 26:BA:881:G:C8 | 2.30 | 0.66 |
| 1:CA:660:G:H1 | 1:CA:745:C:H42 | 1.43 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AE:20:GLN:NE2 | 5:AE:21:ALA:O | 2.29 | 0.66 |
| 26:BA:1405:U:H2' | 26:BA:1406:U:C6 | 2.31 | 0.66 |
| 26:BA:2080:G:O6 | 61:BA:4418:HOH:O | 2.12 | 0.66 |
| 26:BA:2140:C:C2 | 26:BA:2151:G:N2 | 2.64 | 0.66 |
| 26:BA:739:G:OP1 | 61:BA:5169:HOH:O | 2.13 | 0.66 |
| 26:BA:998:C:OP1 | 61:BA:4644:HOH:O | 2.14 | 0.66 |
| 26:BA:607:U:OP1 | 30:BF:102:PRO:HA | 1.96 | 0.66 |
| 35:BO:64:ARG:NH1 | 35:BO:81:ASP:OD1 | 2.29 | 0.66 |
| 1:AA:193:C:H2' | 1:AA:194:C:H6 | 1.59 | 0.65 |
| 1:CA:649:G:H2' | 1:CA:650:G:H5'' | 1.78 | 0.65 |
| 24:CX:9:G:O2' | 24:CX:10:G:N7 | 2.20 | 0.65 |
| 50:D3:7:LYS:NZ | 50:D3:32:GLN:O | 2.29 | 0.65 |
| 31:DG:16:ARG:O | 31:DG:20:ILE:HG13 | 1.95 | 0.65 |
| 2:AB:69:LEU:HB3 | 2:AB:162:ILE:HG22 | 1.78 | 0.65 |
| 7:AG:27:ILE:HD12 | 7:AG:40:ALA:HA | 1.77 | 0.65 |
| 23:AW:5:G:H2' | 23:AW:6:G:H8 | 1.60 | 0.65 |
| 26:BA:1174:A:H4' | 26:BA:1175:U:OP1 | 1.95 | 0.65 |
| 26:BA:1754:C:H5'' | 40:BT:113:LYS:HE3 | 1.77 | 0.65 |
| 26:BA:2722:G:OP2 | 61:BA:4098:HOH:O | 2.14 | 0.65 |
| 29:BE:105:THR:OG1 | 29:BE:199:ARG:NH2 | 2.30 | 0.65 |
| 1:CA:1026:G:O6 | 1:CA:1036:G:N2 | 2.28 | 0.65 |
| 1:CA:1286:A:C8 | 1:CA:1287:A:H4' | 2.30 | 0.65 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:N6 | 1.94 | 0.65 |
| 1:CA:977:A:O2' | 1:CA:981:U:N3 | 2.29 | 0.65 |
| 1:CA:1320:C:N3 | 19:CS:36:ARG:NH2 | 2.44 | 0.65 |
| 1:CA:1022:G:H2' | 1:CA:1023:G:H8 | 1.60 | 0.65 |
| 9:CI:46:ALA:HB2 | 9:CI:74:ILE:HG23 | 1.76 | 0.65 |
| 15:CO:54:ARG:NH1 | 15:CO:58:MET:SD | 2.70 | 0.65 |
| 25:CY:4:C:N4 | 25:CY:69:G:H1 | 1.94 | 0.65 |
| 30:DF:184:TYR:CE2 | 30:DF:188:ARG:HD2 | 2.32 | 0.65 |
| 36:DP:44:GLY:O | 61:DP:301:HOH:O | 2.14 | 0.65 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C6 | 2.32 | 0.65 |
| 1:AA:1442:G:O2' | 1:AA:1442(A):G:OP1 | 2.12 | 0.65 |
| 25:AY:29:G:N2 | 25:AY:41:C:N3 | 2.36 | 0.65 |
| 26:BA:880:G:H2' | 26:BA:881:G:H8 | 1.61 | 0.65 |
| 26:DA:323:G:HO2' | 26:DA:1205:U:H3 | 1.43 | 0.65 |
| 26:DA:857:C:OP2 | 47:D0:77:ARG:NH2 | 2.29 | 0.65 |
| 2:AB:93:VAL:HG21 | 2:AB:97:TRP:HD1 | 1.59 | 0.65 |
| 26:BA:278:A:H2' | 26:BA:279:C:C6 | 2.31 | 0.65 |
| 1:CA:954:G:H21 | 1:CA:1227:A:H62 | 1.44 | 0.65 |
| 26:BA:1342:A:OP2 | 61:BA:4209:HOH:O | 2.13 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1273:G:H3' | 1:CA:1274:G:H8 | 1.62 | 0.65 |
| 1:CA:1359:C:H1' | 1:CA:1362:C:H41 | 1.61 | 0.65 |
| 1:CA:501:C:H2' | 1:CA:502:G:C8 | 2.31 | 0.65 |
| 23:CW:3:C:N3 | 23:CW:70:G:O6 | 2.29 | 0.65 |
| 26:DA:500:G:N1 | 26:DA:503:A:OP2 | 2.30 | 0.65 |
| 9:AI:99:LEU:HB3 | 9:AI:101:PHE:CE1 | 2.32 | 0.65 |
| 27:BB:106:G:H5' | 46:BZ:31:ARG:HG2 | 1.79 | 0.65 |
| 26:DA:1693:U:O2' | 28:DD:14:ARG:NH2 | 2.29 | 0.65 |
| 31:DG:44:GLY:O | 31:DG:47:LYS:HB2 | 1.95 | 0.65 |
| 46:DZ:130:PRO:HA | 46:DZ:133:ILE:HD11 | 1.77 | 0.65 |
| 1:AA:1030(D):A:N6 | 1:AA:1031:G:H21 | 1.95 | 0.65 |
| 1:AA:1510:U:H2' | 1:AA:1511:G:C8 | 2.32 | 0.65 |
| 2:AB:102:LEU:HB3 | 2:AB:180:LEU:HD12 | 1.78 | 0.65 |
| 16:AP:53:VAL:HG13 | 16:AP:79:VAL:HG22 | 1.79 | 0.65 |
| 26:BA:1204:A:H2 | 26:BA:1241:A:H62 | 1.43 | 0.65 |
| 26:BA:131:G:OP1 | 61:BA:4045:HOH:O | 2.13 | 0.65 |
| 26:BA:2478:A:OP2 | 56:B9:2:LYS:NZ | 2.29 | 0.65 |
| 38:BR:67:LEU:HD13 | 38:BR:76:VAL:HG21 | 1.79 | 0.65 |
| 4:CD:157:LEU:O | 4:CD:161:ASN:ND2 | 2.29 | 0.65 |
| 8:CH:49:GLU:OE2 | 8:CH:62:TYR:OH | 2.14 | 0.65 |
| 3:AC:150:LYS:HG3 | 3:AC:169:ALA:HB2 | 1.79 | 0.64 |
| 26:DA:1803:A:O2' | 28:DD:259:THR:HG21 | 1.97 | 0.64 |
| 1:AA:1240:U:OP2 | 7:AG:116:ALA:N | 2.30 | 0.64 |
| 1:AA:942:G:H21 | 9:AI:124:GLN:NE2 | 1.95 | 0.64 |
| 25:AY:51:U:H2' | 25:AY:52:G:C8 | 2.32 | 0.64 |
| 51:B4:59:PHE:HA | 51:B4:61:ARG:H | 1.63 | 0.64 |
| 53:B6:6:ARG:NH1 | 53:B6:26:ASN:HB2 | 2.12 | 0.64 |
| 26:BA:1796:U:H2' | 26:BA:1797:C:C6 | 2.32 | 0.64 |
| 26:BA:882:G:N2 | 26:BA:895:U:O2 | 2.27 | 0.64 |
| 27:BB:23:G:O6 | 61:BB:3133:HOH:O | 2.10 | 0.64 |
| 47:D0:10:THR:HG22 | 47:D0:12:ASN:H | 1.61 | 0.64 |
| 26:DA:2794:C:N4 | 26:DA:2802:G:O6 | 2.30 | 0.64 |
| 40:BT:112:ARG:HG3 | 40:BT:115:ARG:HH21 | 1.62 | 0.64 |
| 51:D4:1:MET:HG2 | 51:D4:6:HIS:CD2 | 2.32 | 0.64 |
| 39:DS:28:VAL:HG13 | 39:DS:35:ILE:HD11 | 1.79 | 0.64 |
| 1:AA:1060:C:C5 | 3:AC:2:GLY:HA3 | 2.32 | 0.64 |
| 26:BA:1315:C:OP2 | 61:BA:4634:HOH:O | 2.14 | 0.64 |
| 26:BA:2162:G:C2' | 26:BA:2163:C:H5'' | 2.28 | 0.64 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:C8 | 2.33 | 0.64 |
| 1:CA:599:C:H2' | 1:CA:600:C:H5'' | 1.80 | 0.64 |
| 2:CB:218:ALA:O | 2:CB:222:ILE:HG23 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:DA:1648:C:OP1 | 61:DA:4201:HOH:O | 2.14 | 0.64 |
| 27:DB:24:G:N7 | 27:DB:56:G:H2' | 2.12 | 0.64 |
| 30:DF:116:ASP:OD2 | 36:DP:1:MET:N | 2.30 | 0.64 |
| 2:AB:13:ALA:HB2 | 2:AB:44:LEU:HG | 1.80 | 0.64 |
| 26:BA:2124:G:H1 | 26:BA:2174:C:H42 | 1.45 | 0.64 |
| 26:BA:744:G:OP1 | 61:BA:4683:HOH:O | 2.15 | 0.64 |
| 1:CA:664:G:P | 18:CR:64:ARG:HH22 | 2.19 | 0.64 |
| 11:CK:98:LEU:O | 11:CK:101:SER:OG | 2.14 | 0.64 |
| 26:DA:528:A:O2' | 26:DA:529:A:H5'' | 1.96 | 0.64 |
| 39:DS:10:ARG:NH2 | 39:DS:91:PRO:O | 2.27 | 0.64 |
| 26:BA:1993:U:OP2 | 61:BA:5277:HOH:O | 2.15 | 0.64 |
| 1:CA:1323:G:H4' | 1:CA:1363:C:C2 | 2.32 | 0.64 |
| 26:DA:236:C:H2' | 26:DA:237:C:H6 | 1.63 | 0.64 |
| 27:DB:66:A:H61 | 27:DB:109:C:H5'' | 1.63 | 0.64 |
| 33:DI:12:LEU:HD22 | 33:DI:19:VAL:HG21 | 1.78 | 0.64 |
| 18:AR:58:LEU:HB3 | 18:AR:62:GLU:HG3 | 1.77 | 0.64 |
| 48:B1:23:LYS:HB3 | 48:B1:29:GLY:HA3 | 1.78 | 0.64 |
| 1:CA:1002:G:C4 | 1:CA:1003:G:H8 | 2.15 | 0.64 |
| 26:DA:1792:G:O2' | 26:DA:1830:C:OP1 | 2.15 | 0.64 |
| 30:DF:101:LEU:HD12 | 30:DF:102:PRO:HD2 | 1.80 | 0.64 |
| 1:AA:195:A:OP1 | 20:AT:68:LYS:NZ | 2.30 | 0.64 |
| 23:AW:5:G:H2' | 23:AW:6:G:C8 | 2.33 | 0.64 |
| 45:BY:54:LYS:HA | 45:BY:56:PRO:HD3 | 1.80 | 0.64 |
| 5:CE:20:GLN:NE2 | 5:CE:21:ALA:O | 2.31 | 0.64 |
| 1:CA:1309:G:OP2 | 13:CM:99:ARG:NH2 | 2.28 | 0.64 |
| 26:DA:2323:G:O6 | 26:DA:2332:U:N3 | 2.18 | 0.64 |
| 33:DI:102:SER:O | 33:DI:106:GLY:N | 2.30 | 0.64 |
| 11:AK:98:LEU:O | 11:AK:101:SER:OG | 2.16 | 0.64 |
| 12:AL:33:ARG:HH11 | 12:AL:62:SER:HB3 | 1.62 | 0.64 |
| 26:BA:2849:U:OP2 | 40:BT:95:ARG:NH1 | 2.30 | 0.64 |
| 1:CA:1004:A:H2' | 1:CA:1038:C:H1' | 1.80 | 0.64 |
| 1:CA:1133:G:H1 | 1:CA:1141:C:N4 | 1.95 | 0.64 |
| 1:CA:1507:A:N6 | 1:CA:1528:U:O4 | 2.16 | 0.64 |
| 1:CA:444:C:H2' | 1:CA:445:G:H8 | 1.62 | 0.64 |
| 1:AA:56:U:H2' | 1:AA:57:G:C8 | 2.33 | 0.64 |
| 3:AC:37:GLN:NE2 | 14:AN:52:GLN:OE1 | 2.31 | 0.64 |
| 24:AX:19:G:H4' | 24:AX:20:U:OP2 | 1.97 | 0.64 |
| 32:BH:149:ARG:NH1 | 32:BH:167:GLU:OE2 | 2.30 | 0.64 |
| 32:BH:86:GLU:OE2 | 32:BH:132:ARG:NH2 | 2.30 | 0.64 |
| 43:BW:88:ARG:HG3 | 43:BW:92:ARG:HH21 | 1.61 | 0.64 |
| 1:AA:405:U:OP2 | 4:AD:3:ARG:NH2 | 2.32 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BA:441:U:O2 | 30:BF:46:ARG:NH2 | 2.26 | 0.63 |
| 1:AA:1464:G:OP2 | 40:BT:111:ARG:NH2 | 2.30 | 0.63 |
| 44:BX:31:HIS:CD2 | 44:BX:33:LYS:H | 2.14 | 0.63 |
| 1:CA:1129:C:H2' | 1:CA:1139:G:N7 | 2.11 | 0.63 |
| 1:CA:1165:C:N4 | 1:CA:1171:G:H1 | 1.93 | 0.63 |
| 2:CB:178:ARG:NH2 | 8:CH:68:ARG:HH22 | 1.95 | 0.63 |
| 29:DE:101:ARG:CZ | 29:DE:171:GLU:HB2 | 2.28 | 0.63 |
| 1:AA:1027:C:C2 | 1:AA:1034:G:C6 | 2.86 | 0.63 |
| 1:AA:894:G:N7 | 61:AA:4110:HOH:O | 2.30 | 0.63 |
| 25:AY:25:C:O2' | 25:AY:26:A:H8 | 1.82 | 0.63 |
| 26:BA:1165:U:H2' | 26:BA:1166:C:C6 | 2.33 | 0.63 |
| 26:BA:1418:G:OP2 | 61:BA:4561:HOH:O | 2.16 | 0.63 |
| 23:AW:55:PSU:O3' | 26:BA:897:C:H4' | 1.98 | 0.63 |
| 46:BZ:7:ALA:HB2 | 46:BZ:59:LEU:HD22 | 1.78 | 0.63 |
| 1:CA:1216:G:H5'' | 14:CN:5:ALA:HB2 | 1.79 | 0.63 |
| 1:CA:1305:G:O2' | 1:CA:1331:G:N2 | 2.31 | 0.63 |
| 1:CA:1318:A:OP1 | 19:CS:3:ARG:NH1 | 2.32 | 0.63 |
| 1:CA:1348:U:H2' | 1:CA:1349:A:H8 | 1.63 | 0.63 |
| 1:CA:1521:G:N3 | 61:CA:3217:HOH:O | 2.30 | 0.63 |
| 7:CG:72:ARG:HH22 | 7:CG:138:LYS:HZ1 | 1.45 | 0.63 |
| 11:CK:34:ASP:HB3 | 11:CK:40:ILE:HD11 | 1.79 | 0.63 |
| 1:CA:562:C:H1' | 12:CL:15:ARG:HB3 | 1.80 | 0.63 |
| 25:CY:31:A:N1 | 25:CY:39:PSU:C2 | 2.65 | 0.63 |
| 26:DA:971:C:OP2 | 61:DA:4615:HOH:O | 2.15 | 0.63 |
| 35:DO:115:VAL:HG13 | 35:DO:121:VAL:HG21 | 1.79 | 0.63 |
| 3:AC:181:ASN:ND2 | 3:AC:204:LEU:HD12 | 2.13 | 0.63 |
| 1:AA:1456:G:O3' | 20:AT:39:LYS:NZ | 2.31 | 0.63 |
| 26:BA:363(A):A:H2' | 26:BA:363(B):G:C8 | 2.34 | 0.63 |
| 1:CA:1013:G:N2 | 1:CA:1016:A:OP2 | 2.25 | 0.63 |
| 1:CA:533:A:O2' | 1:CA:535:A:OP2 | 2.17 | 0.63 |
| 26:DA:2127:G:C2 | 26:DA:2161:C:C4 | 2.87 | 0.63 |
| 26:DA:2805:G:H2' | 26:DA:2807:G:C8 | 2.34 | 0.63 |
| 27:DB:19:G:H2' | 27:DB:20:C:O4' | 1.99 | 0.63 |
| 26:DA:2880:C:O3' | 38:DR:90:ARG:NH1 | 2.30 | 0.63 |
| 6:AF:18:GLN:HA | 6:AF:21:LEU:HD12 | 1.79 | 0.63 |
| 25:AY:15:G:H22 | 25:AY:48:C:N4 | 1.96 | 0.63 |
| 26:BA:2312:U:H5' | 31:BG:88:ILE:HD11 | 1.81 | 0.63 |
| 7:CG:113:GLU:HB2 | 7:CG:119:ARG:HG2 | 1.81 | 0.63 |
| 16:CP:23:ASP:OD2 | 16:CP:25:ARG:NH1 | 2.32 | 0.63 |
| 13:AM:91:ARG:HB2 | 13:AM:98:VAL:HG13 | 1.81 | 0.63 |
| 20:AT:87:LYS:O | 20:AT:91:LEU:HG | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BA:2683:C:OP1 | 40:BT:53:ARG:NH2 | 2.31 | 0.63 |
| 26:DA:2206:G:H3' | 26:DA:2207:G:N7 | 2.13 | 0.63 |
| 28:DD:206:LEU:HD22 | 28:DD:211:ARG:HG2 | 1.80 | 0.63 |
| 32:DH:3:ARG:HH22 | 32:DH:5:GLY:H | 1.47 | 0.63 |
| 46:DZ:157:LEU:HD13 | 46:DZ:161:VAL:HG13 | 1.80 | 0.63 |
| 8:AH:34:GLU:OE2 | 8:AH:37:ARG:NH1 | 2.31 | 0.63 |
| 19:AS:64:GLU:O | 19:AS:67:VAL:HG23 | 1.98 | 0.63 |
| 25:AY:5:G:N1 | 25:AY:68:C:N4 | 2.31 | 0.63 |
| 33:BI:93:THR:OG1 | 33:BI:96:ASP:OD1 | 2.17 | 0.63 |
| 26:DA:1038:C:N4 | 26:DA:1117:G:H1 | 1.97 | 0.63 |
| 1:AA:1036:G:H3' | 1:AA:1037:C:H6 | 1.63 | 0.63 |
| 1:CA:539:A:H2' | 1:CA:540:G:C8 | 2.33 | 0.63 |
| 1:CA:957:U:O2' | 1:CA:959:A:N7 | 2.30 | 0.63 |
| 17:CQ:66:SER:O | 17:CQ:70:ARG:NH1 | 2.30 | 0.63 |
| 23:CW:76:F3N:OP2 | 61:CW:3102:HOH:O | 2.15 | 0.63 |
| 1:AA:1321:C:H5'' | 1:AA:1322:C:H2' | 1.78 | 0.63 |
| 1:CA:1002:G:H1 | 1:CA:1038:C:H42 | 1.44 | 0.63 |
| 1:CA:1402:C:N4 | 22:CV:18:G:OP2 | 2.31 | 0.63 |
| 26:DA:1021:A:H62 | 26:DA:1141:U:H3 | 1.44 | 0.63 |
| 26:DA:1637:A:OP2 | 61:DA:4544:HOH:O | 2.16 | 0.63 |
| 26:DA:1939:U:OP1 | 26:DA:2604:U:O2' | 2.17 | 0.63 |
| 26:DA:2173:A:H2' | 26:DA:2174:C:O4' | 1.99 | 0.63 |
| 1:CA:1150:U:O4 | 1:CA:1151:A:N6 | 2.32 | 0.63 |
| 4:CD:15:GLU:OE2 | 4:CD:66:ARG:NH1 | 2.31 | 0.63 |
| 8:CH:37:ARG:HH21 | 8:CH:38:ILE:HD11 | 1.63 | 0.63 |
| 10:CJ:17:ASP:OD1 | 10:CJ:70:ARG:NH1 | 2.31 | 0.63 |
| 26:DA:1602:U:O4 | 61:DA:3879:HOH:O | 2.11 | 0.63 |
| 31:DG:145:THR:HG22 | 31:DG:148:MET:SD | 2.38 | 0.63 |
| 1:AA:1025:U:O2 | 1:AA:1036:G:O6 | 2.16 | 0.62 |
| 23:AW:47:U:H5' | 23:AW:47:U:H6 | 1.64 | 0.62 |
| 26:BA:1566:A:OP1 | 28:BD:211:ARG:NH1 | 2.32 | 0.62 |
| 1:CA:1133:G:H2' | 1:CA:1134:G:C8 | 2.33 | 0.62 |
| 1:CA:1120:G:C6 | 1:CA:1154:G:N2 | 2.67 | 0.62 |
| 2:CB:216:SER:O | 2:CB:220:ASP:N | 2.21 | 0.62 |
| 29:DE:14:ILE:HG13 | 29:DE:21:VAL:HG13 | 1.80 | 0.62 |
| 1:AA:673:G:H2' | 1:AA:674:G:C8 | 2.34 | 0.62 |
| 12:AL:24:VAL:HG11 | 12:AL:27:LEU:HD22 | 1.82 | 0.62 |
| 26:BA:2532:G:O2' | 26:BA:2657:A:N1 | 2.31 | 0.62 |
| 26:BA:1155:A:OP1 | 41:BU:55:ARG:HD3 | 1.99 | 0.62 |
| 3:CC:125:GLU:OE2 | 3:CC:125:GLU:N | 2.26 | 0.62 |
| 11:CK:93:GLN:HA | 11:CK:93:GLN:HE21 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:CM:32:GLU:OE1 | 13:CM:59:TYR:OH | 2.16 | 0.62 |
| 20:CT:10:LEU:HB3 | 20:CT:12:ALA:H | 1.62 | 0.62 |
| 37:DQ:67:ARG:O | 37:DQ:101:ARG:NH2 | 2.30 | 0.62 |
| 47:B0:27:GLU:HG3 | 47:B0:68:GLU:HA | 1.81 | 0.62 |
| 1:CA:981:U:H5' | 14:CN:21:TYR:CZ | 2.35 | 0.62 |
| 3:CC:16:ARG:NH1 | 3:CC:181:ASN:OD1 | 2.31 | 0.62 |
| 5:CE:36:ASP:O | 5:CE:38:GLN:N | 2.27 | 0.62 |
| 26:DA:1300:U:H4' | 26:DA:1301:A:C5' | 2.29 | 0.62 |
| 25:CY:76:A:O2' | 26:DA:2394:C:N3 | 2.31 | 0.62 |
| 1:CA:1023:G:H3' | 1:CA:1024:G:H8 | 1.63 | 0.62 |
| 25:CY:31:A:C6 | 25:CY:39:PSU:O2 | 2.52 | 0.62 |
| 26:DA:902:C:H2' | 26:DA:903:C:C6 | 2.35 | 0.62 |
| 26:DA:322:A:OP2 | 30:DF:169:ASN:HB2 | 1.98 | 0.62 |
| 42:DV:72:VAL:HG13 | 42:DV:85:LYS:HB3 | 1.80 | 0.62 |
| 3:AC:56:ASP:HB2 | 3:AC:67:THR:HB | 1.81 | 0.62 |
| 1:AA:235:C:H5' | 17:AQ:70:ARG:HG2 | 1.80 | 0.62 |
| 36:BP:65:ARG:HG3 | 55:B8:25:MET:HG3 | 1.80 | 0.62 |
| 1:CA:946:A:H2' | 1:CA:947:G:C8 | 2.35 | 0.62 |
| 1:CA:951:G:N3 | 1:CA:970:C:O2' | 2.29 | 0.62 |
| 13:CM:20:THR:HA | 13:CM:25:ILE:HG22 | 1.81 | 0.62 |
| 1:CA:1218:C:OP2 | 14:CN:9:LYS:NZ | 2.33 | 0.62 |
| 37:DQ:85:LYS:HB2 | 47:D0:7:LEU:HD12 | 1.82 | 0.62 |
| 26:DA:1890:A:OP2 | 61:DA:4438:HOH:O | 2.16 | 0.62 |
| 24:AX:21:A:H61 | 24:AX:46:G:H2' | 1.64 | 0.62 |
| 1:CA:56:U:H2' | 1:CA:57:G:C8 | 2.35 | 0.62 |
| 1:CA:975:A:N1 | 10:CJ:48:THR:HB | 2.13 | 0.62 |
| 16:CP:28:ARG:NH1 | 16:CP:29:ASP:OD1 | 2.31 | 0.62 |
| 30:DF:122:LYS:NZ | 30:DF:152:GLU:OE2 | 2.30 | 0.62 |
| 43:DW:88:ARG:NH1 | 43:DW:94:ASP:OD2 | 2.32 | 0.62 |
| 45:DY:102:CYS:SG | 45:DY:103:GLY:N | 2.72 | 0.62 |
| 1:AA:1187:G:H4' | 9:AI:111:ARG:HH11 | 1.64 | 0.62 |
| 1:AA:1414:U:H3 | 1:AA:1486:G:H1 | 1.46 | 0.62 |
| 51:B4:63:TYR:N | 51:B4:64:GLY:HA2 | 2.15 | 0.62 |
| 1:CA:661:G:H1 | 1:CA:744:C:H42 | 1.46 | 0.62 |
| 1:CA:957:U:H2' | 1:CA:959:A:OP2 | 2.00 | 0.62 |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:CE1 | 2.23 | 0.62 |
| 31:DG:101:ILE:HD13 | 51:D4:25:TYR:HB2 | 1.82 | 0.62 |
| 26:DA:577:G:O2' | 26:DA:1254:A:OP1 | 2.18 | 0.62 |
| 26:DA:658:C:H2' | 26:DA:659:C:C6 | 2.34 | 0.62 |
| 1:AA:97:G:O2' | 1:AA:98:G:H5'' | 2.00 | 0.62 |
| 1:CA:54:C:N4 | 1:CA:353:A:OP2 | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:CM:23:TYR:HB3 | 13:CM:67:GLU:HA | 1.81 | 0.62 |
| 26:DA:2096:U:H3 | 26:DA:2193:G:H1 | 1.48 | 0.62 |
| 30:DF:28:ILE:HG23 | 30:DF:112:MET:HE3 | 1.81 | 0.62 |
| 1:AA:984:C:H42 | 1:AA:1221:G:H1 | 1.48 | 0.62 |
| 3:AC:82:GLU:HG2 | 3:AC:85:ARG:HH21 | 1.63 | 0.62 |
| 3:AC:39:ILE:HG23 | 3:AC:91:LEU:HD11 | 1.82 | 0.62 |
| 10:AJ:37:PRO:HA | 10:AJ:72:VAL:HG12 | 1.82 | 0.62 |
| 1:CA:1404:C:O2 | 1:CA:1519:A:O2' | 2.14 | 0.62 |
| 10:CJ:6:ILE:HG23 | 10:CJ:98:ILE:HG13 | 1.82 | 0.62 |
| 26:DA:2379:G:O2' | 39:DS:17:ARG:NH2 | 2.30 | 0.62 |
| 25:AY:25:C:O2' | 25:AY:26:A:O5' | 2.18 | 0.62 |
| 26:BA:271(L):U:OP1 | 33:BI:50:ARG:NH2 | 2.29 | 0.62 |
| 1:CA:742:G:OP2 | 15:CO:35:ARG:NH2 | 2.33 | 0.62 |
| 55:D8:33:ASN:HA | 55:D8:36:LYS:HD2 | 1.82 | 0.62 |
| 26:DA:1149:G:H2' | 26:DA:1150:C:C6 | 2.35 | 0.62 |
| 26:DA:2816:C:O3' | 38:DR:99:LYS:NZ | 2.32 | 0.62 |
| 33:DI:38:LEU:HD12 | 33:DI:38:LEU:H | 1.64 | 0.62 |
| 36:DP:39:LYS:HB2 | 36:DP:45:LEU:HG | 1.81 | 0.62 |
| 23:AW:76:F3N:N | 24:AX:76:31H:O2' | 2.33 | 0.61 |
| 26:BA:1859:A:N6 | 26:BA:1883:G:O2' | 2.32 | 0.61 |
| 30:DF:18:ARG:NH2 | 30:DF:127:GLU:OE1 | 2.31 | 0.61 |
| 31:DG:5:VAL:HG22 | 31:DG:8:LYS:H | 1.64 | 0.61 |
| 37:BQ:21:THR:HG21 | 37:BQ:101:ARG:HB2 | 1.82 | 0.61 |
| 12:CL:24:VAL:HG11 | 12:CL:27:LEU:HD22 | 1.81 | 0.61 |
| 26:DA:881:G:H1 | 26:DA:895:U:H3 | 1.48 | 0.61 |
| 1:AA:452:A:H4' | 16:AP:72:ARG:NH1 | 2.15 | 0.61 |
| 1:AA:62:U:OP1 | 1:AA:385:C:O2' | 2.17 | 0.61 |
| 51:B4:53:GLU:HB3 | 51:B4:54:GLY:HA2 | 1.82 | 0.61 |
| 26:BA:646:A:H2' | 26:BA:647:G:O4' | 2.01 | 0.61 |
| 30:BF:184:TYR:O | 30:BF:188:ARG:HG3 | 2.00 | 0.61 |
| 1:CA:662:G:H2' | 1:CA:663:A:C8 | 2.34 | 0.61 |
| 2:CB:101:MET:HA | 2:CB:108:ILE:HG13 | 1.82 | 0.61 |
| 1:CA:1376:U:H3' | 7:CG:94:ARG:HH21 | 1.65 | 0.61 |
| 10:CJ:49:VAL:HG12 | 10:CJ:61:GLU:O | 2.00 | 0.61 |
| 26:BA:1447:G:N7 | 61:BA:4947:HOH:O | 2.31 | 0.61 |
| 29:BE:29:GLY:HA3 | 61:BE:408:HOH:O | 1.99 | 0.61 |
| 31:BG:43:LEU:HD11 | 31:BG:153:ARG:HG2 | 1.83 | 0.61 |
| 45:BY:102:CYS:SG | 45:BY:103:GLY:N | 2.73 | 0.61 |
| 1:CA:1397:C:OP2 | 5:CE:24:ARG:NH2 | 2.33 | 0.61 |
| 26:DA:1031:G:H5'' | 56:D9:8:LYS:HE3 | 1.80 | 0.61 |
| 26:DA:1028:A:N6 | 26:DA:1125:G:H2' | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DA:796:C:H2' | 26:DA:797:C:C6 | 2.34 | 0.61 |
| 27:DB:45:A:O4' | 31:DG:95:ARG:NH1 | 2.33 | 0.61 |
| 41:DU:83:LEU:HD12 | 41:DU:88:ILE:HD12 | 1.81 | 0.61 |
| 1:AA:1036:G:H3' | 1:AA:1037:C:C6 | 2.34 | 0.61 |
| 1:AA:139:G:N2 | 1:AA:224:C:O2 | 2.28 | 0.61 |
| 11:AK:91:ARG:HG3 | 11:AK:92:GLU:N | 2.15 | 0.61 |
| 42:BV:40:LEU:HB2 | 42:BV:46:VAL:HG13 | 1.81 | 0.61 |
| 46:BZ:24:LEU:HB2 | 46:BZ:41:LEU:HD23 | 1.81 | 0.61 |
| 1:CA:1297:C:OP1 | 13:CM:44:ARG:NH2 | 2.27 | 0.61 |
| 1:CA:769:G:H4' | 1:CA:1513:A:H4' | 1.82 | 0.61 |
| 26:DA:1371:G:O6 | 61:DA:3964:HOH:O | 2.12 | 0.61 |
| 23:AW:26:A:N1 | 23:AW:44:G:N2 | 2.44 | 0.61 |
| 26:BA:2430:A:N3 | 26:BA:2430:A:H2' | 2.15 | 0.61 |
| 30:BF:101:LEU:O | 30:BF:106:ARG:NH1 | 2.32 | 0.61 |
| 2:CB:16:HIS:CD2 | 2:CB:17:PHE:H | 2.18 | 0.61 |
| 1:CA:1193:G:O2' | 5:CE:25:ARG:NH2 | 2.34 | 0.61 |
| 6:CF:61:LEU:HB3 | 6:CF:63:TYR:HE1 | 1.65 | 0.61 |
| 7:CG:22:LEU:HG | 7:CG:62:PHE:CE2 | 2.36 | 0.61 |
| 12:CL:113:ARG:NH2 | 61:CL:201:HOH:O | 2.33 | 0.61 |
| 13:CM:91:ARG:HB2 | 13:CM:98:VAL:HG13 | 1.82 | 0.61 |
| 27:DB:106:G:H5' | 46:DZ:31:ARG:HG2 | 1.83 | 0.61 |
| 26:DA:958:U:OP2 | 37:DQ:14:ARG:NH1 | 2.33 | 0.61 |
| 26:BA:1113:U:H2' | 26:BA:1114:G:C8 | 2.36 | 0.61 |
| 26:BA:1843:C:H5' | 28:BD:253:GLN:NE2 | 2.15 | 0.61 |
| 27:BB:105:A:OP1 | 46:BZ:72:ARG:NH1 | 2.34 | 0.61 |
| 8:CH:45:ILE:HG22 | 8:CH:63:LEU:HA | 1.83 | 0.61 |
| 44:DX:60:ARG:HH12 | 54:D7:47:ARG:NH2 | 1.98 | 0.61 |
| 36:BP:59:LEU:HD21 | 55:B8:10:ALA:HA | 1.82 | 0.61 |
| 26:BA:2305:A:H5'' | 31:BG:134:GLY:HA3 | 1.83 | 0.61 |
| 4:CD:154:ASN:HA | 4:CD:159:ARG:HH21 | 1.65 | 0.61 |
| 10:CJ:29:ARG:HB2 | 10:CJ:84:GLN:HE22 | 1.65 | 0.61 |
| 56:D9:25:VAL:HB | 56:D9:34:GLN:HB2 | 1.81 | 0.61 |
| 26:DA:2114:A:N6 | 26:DA:2119:A:N7 | 2.48 | 0.61 |
| 35:DO:71:ARG:NE | 35:DO:105:GLU:OE2 | 2.32 | 0.61 |
| 25:AY:15:G:N2 | 25:AY:48:C:H42 | 1.99 | 0.61 |
| 30:BF:8:GLN:HE21 | 30:BF:8:GLN:HA | 1.65 | 0.61 |
| 1:CA:1240:U:OP2 | 7:CG:116:ALA:N | 2.34 | 0.61 |
| 1:CA:735:C:H2' | 1:CA:736:C:H6 | 1.64 | 0.61 |
| 2:CB:113:HIS:O | 2:CB:117:GLU:N | 2.32 | 0.61 |
| 26:DA:2169:A:H2' | 26:DA:2170:A:C8 | 2.35 | 0.61 |
| 1:AA:69:G:H2' | 1:AA:70:G:C8 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:AK:51:LYS:HD3 | 11:AK:55:LYS:HE2 | 1.83 | 0.61 |
| 1:CA:1128:C:O2' | 1:CA:1147:C:N3 | 2.23 | 0.61 |
| 2:CB:13:ALA:N | 2:CB:14:GLY:HA3 | 2.16 | 0.61 |
| 2:CB:16:HIS:CG | 2:CB:17:PHE:H | 2.19 | 0.61 |
| 9:CI:3:GLN:OE1 | 9:CI:20:ARG:NH2 | 2.34 | 0.61 |
| 26:DA:1557:C:OP2 | 26:DA:1558:A:O2' | 2.17 | 0.61 |
| 26:DA:2022:U:O2' | 26:DA:2617:C:H5' | 2.01 | 0.61 |
| 26:DA:1140:C:O3' | 34:DN:25:ARG:NH1 | 2.34 | 0.61 |
| 1:AA:1075:C:OP1 | 2:AB:179:LYS:NZ | 2.20 | 0.60 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:N1 | 1.95 | 0.60 |
| 11:AK:79:SER:HA | 11:AK:104:GLN:HB2 | 1.82 | 0.60 |
| 13:AM:23:TYR:HB3 | 13:AM:67:GLU:HA | 1.83 | 0.60 |
| 18:AR:26:LEU:HD21 | 18:AR:39:VAL:HG13 | 1.82 | 0.60 |
| 54:B7:34:ARG:NH1 | 54:B7:41:ARG:O | 2.34 | 0.60 |
| 26:BA:1913:A:H4' | 26:BA:1914:C:H5'' | 1.83 | 0.60 |
| 27:BB:41:U:H5 | 31:BG:70:VAL:H | 1.49 | 0.60 |
| 1:CA:728:A:H2' | 1:CA:729:A:C8 | 2.36 | 0.60 |
| 1:CA:947:G:O3' | 13:CM:109:THR:OG1 | 2.19 | 0.60 |
| 4:CD:175:SER:HB3 | 4:CD:186:LEU:HD11 | 1.82 | 0.60 |
| 26:DA:1550:C:OP1 | 26:DA:1720:U:O2' | 2.17 | 0.60 |
| 26:DA:821:A:N1 | 61:DA:4084:HOH:O | 2.31 | 0.60 |
| 26:DA:93:G:H2' | 26:DA:94:C:C6 | 2.36 | 0.60 |
| 12:AL:32:PHE:HB3 | 12:AL:84:LEU:HD11 | 1.82 | 0.60 |
| 14:AN:21:TYR:OH | 14:AN:23:ARG:NH2 | 2.33 | 0.60 |
| 1:CA:1329:A:H5' | 13:CM:29:ARG:HD2 | 1.82 | 0.60 |
| 26:DA:1231:G:H2' | 26:DA:1232:G:C8 | 2.36 | 0.60 |
| 26:DA:2312:U:H5' | 31:DG:88:ILE:HD11 | 1.83 | 0.60 |
| 26:DA:1250:G:N7 | 36:DP:18:ARG:NH2 | 2.49 | 0.60 |
| 26:BA:1179:C:H2' | 26:BA:1180:C:H6 | 1.66 | 0.60 |
| 26:BA:2096:U:H3 | 26:BA:2193:G:H1 | 1.49 | 0.60 |
| 26:BA:2822:G:N7 | 61:BA:5279:HOH:O | 2.32 | 0.60 |
| 1:CA:222:U:H2' | 1:CA:223:U:C6 | 2.35 | 0.60 |
| 1:CA:289:G:OP2 | 61:CA:3236:HOH:O | 2.16 | 0.60 |
| 4:CD:100:ARG:NH1 | 4:CD:137:SER:OG | 2.34 | 0.60 |
| 1:CA:1297:C:O3' | 7:CG:114:ARG:NH2 | 2.34 | 0.60 |
| 19:AS:31:ILE:HB | 19:AS:49:ILE:HG23 | 1.83 | 0.60 |
| 25:AY:62:C:H2' | 25:AY:63:G:H8 | 1.66 | 0.60 |
| 26:BA:288:C:H2' | 26:BA:289:A:H8 | 1.66 | 0.60 |
| 26:BA:568:U:H5' | 26:BA:945:A:N1 | 2.16 | 0.60 |
| 30:BF:116:ASP:OD1 | 30:BF:119:ARG:NH2 | 2.34 | 0.60 |
| 54:D7:34:ARG:NH1 | 54:D7:41:ARG:O | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:243:A:H4' | 1:AA:244:U:H5'' | 1.82 | 0.60 |
| 1:AA:26:A:O2' | 4:AD:209:ARG:NH2 | 2.34 | 0.60 |
| 26:BA:1278:A:OP1 | 38:BR:36:THR:HG23 | 2.02 | 0.60 |
| 1:CA:1135:U:H2' | 1:CA:1137:C:C2 | 2.36 | 0.60 |
| 17:CQ:81:ARG:HB3 | 17:CQ:84:LEU:HD12 | 1.83 | 0.60 |
| 26:DA:2130:U:H4' | 26:DA:2133:G:H4' | 1.82 | 0.60 |
| 1:AA:1183:A:H3' | 1:AA:1184:G:H5'' | 1.84 | 0.60 |
| 1:AA:1106:G:H5'' | 3:AC:172:ARG:HG2 | 1.82 | 0.60 |
| 1:CA:501:C:H2' | 1:CA:502:G:H8 | 1.67 | 0.60 |
| 8:CH:20:TYR:HA | 8:CH:65:TYR:CZ | 2.37 | 0.60 |
| 9:CI:14:VAL:HG23 | 9:CI:66:ARG:HB3 | 1.83 | 0.60 |
| 25:CY:15:G:N1 | 25:CY:48:C:N3 | 2.46 | 0.60 |
| 46:DZ:111:VAL:HG21 | 46:DZ:117:LEU:HB2 | 1.84 | 0.60 |
| 26:BA:1025:G:C4 | 26:BA:1135:C:H1' | 2.37 | 0.60 |
| 1:AA:1064:G:H4' | 1:AA:1065:U:OP1 | 2.00 | 0.60 |
| 1:AA:1241:G:OP1 | 7:AG:35:LYS:NZ | 2.35 | 0.60 |
| 1:AA:1351:U:O4 | 9:AI:118:LYS:NZ | 2.35 | 0.60 |
| 13:CM:14:ARG:HB2 | 13:CM:17:VAL:HG23 | 1.83 | 0.60 |
| 49:D2:29:LYS:HG2 | 49:D2:57:ILE:HD13 | 1.84 | 0.60 |
| 26:DA:2185:C:H2' | 26:DA:2186:G:O4' | 2.01 | 0.60 |
| 35:DO:53:LYS:NZ | 35:DO:56:ASP:OD1 | 2.34 | 0.60 |
| 26:DA:483:A:O2' | 45:DY:49:VAL:O | 2.10 | 0.60 |
| 46:DZ:93:ASP:HA | 46:DZ:131:ARG:NH2 | 2.17 | 0.60 |
| 5:AE:12:LEU:HB3 | 5:AE:31:LEU:HB2 | 1.83 | 0.60 |
| 26:BA:636:G:OP1 | 36:BP:132:LYS:HE2 | 2.02 | 0.60 |
| 33:BI:104:GLN:HB3 | 33:BI:105:HIS:HD2 | 1.67 | 0.60 |
| 1:CA:148:G:H2' | 1:CA:149:A:H8 | 1.66 | 0.60 |
| 18:AR:70:ILE:HG23 | 18:AR:79:LEU:HD12 | 1.84 | 0.60 |
| 23:AW:7:A:N6 | 23:AW:66:U:H3 | 2.00 | 0.60 |
| 26:BA:1507:A:O2' | 26:BA:1508:A:O4' | 2.20 | 0.60 |
| 26:BA:71:A:OP2 | 26:BA:71:A:H3' | 2.02 | 0.60 |
| 28:BD:108:PRO:HB3 | 28:BD:143:HIS:CE1 | 2.37 | 0.60 |
| 38:BR:97:VAL:HG22 | 38:BR:114:VAL:HG13 | 1.84 | 0.60 |
| 46:BZ:117:LEU:HD21 | 46:BZ:144:LEU:HD13 | 1.84 | 0.60 |
| 46:BZ:138:GLU:N | 46:BZ:156:LYS:HD3 | 2.13 | 0.60 |
| 1:CA:19:C:H5'' | 5:CE:86:ALA:HB3 | 1.83 | 0.60 |
| 15:CO:5:LYS:H | 15:CO:5:LYS:HD3 | 1.67 | 0.60 |
| 1:CA:1456:G:N1 | 20:CT:51:GLU:OE2 | 2.30 | 0.60 |
| 51:D4:16:CYS:HA | 51:D4:33:VAL:HB | 1.83 | 0.60 |
| 26:DA:2836:U:H2' | 26:DA:2837:G:C8 | 2.37 | 0.60 |
| 1:AA:450:G:OP1 | 16:AP:43:LYS:NZ | 2.34 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1366:C:H2' | 1:CA:1367:C:C6 | 2.37 | 0.59 |
| 1:CA:662:G:H2' | 1:CA:663:A:H8 | 1.67 | 0.59 |
| 3:CC:70:VAL:HG22 | 3:CC:72:LYS:H | 1.66 | 0.59 |
| 26:DA:307:G:N1 | 26:DA:310:A:OP2 | 2.33 | 0.59 |
| 31:DG:41:GLN:HB3 | 31:DG:43:LEU:HD22 | 1.83 | 0.59 |
| 33:DI:4:ILE:HG12 | 33:DI:18:VAL:HG22 | 1.84 | 0.59 |
| 46:DZ:59:LEU:HD11 | 46:DZ:69:THR:HG21 | 1.81 | 0.59 |
| 1:AA:148:G:H2' | 1:AA:149:A:H8 | 1.66 | 0.59 |
| 9:AI:128:ARG:NH2 | 24:AX:33:U:OP2 | 2.34 | 0.59 |
| 7:AG:37:ASN:ND2 | 9:AI:39:GLY:O | 2.33 | 0.59 |
| 9:AI:49:PRO:HG3 | 9:AI:101:PHE:HD2 | 1.65 | 0.59 |
| 1:AA:1125:U:H4' | 10:AJ:5:ARG:HH22 | 1.67 | 0.59 |
| 2:CB:92:TYR:N | 2:CB:151:GLY:O | 2.32 | 0.59 |
| 9:CI:96:LEU:HD22 | 9:CI:101:PHE:HB2 | 1.84 | 0.59 |
| 26:DA:144:C:H2' | 26:DA:145:G:H8 | 1.67 | 0.59 |
| 26:DA:2815:C:H5' | 52:D5:29:THR:HG21 | 1.83 | 0.59 |
| 1:AA:1292:U:P | 7:AG:41:ARG:HH22 | 2.25 | 0.59 |
| 23:AW:9:A:OP2 | 23:AW:13:C:N4 | 2.30 | 0.59 |
| 26:BA:1359:A:H61 | 26:BA:1372:U:H3 | 1.49 | 0.59 |
| 1:CA:1062:U:H2' | 1:CA:1063:C:C6 | 2.37 | 0.59 |
| 5:CE:100:VAL:O | 5:CE:107:ARG:NH2 | 2.36 | 0.59 |
| 25:CY:50:U:O2 | 25:CY:64:A:N1 | 2.35 | 0.59 |
| 26:DA:1310:G:OP2 | 54:D7:9:ARG:NH1 | 2.35 | 0.59 |
| 26:DA:2127:G:N2 | 26:DA:2161:C:N3 | 2.50 | 0.59 |
| 40:DT:30:VAL:HG22 | 40:DT:86:ILE:HG12 | 1.83 | 0.59 |
| 46:DZ:5:LEU:HD22 | 46:DZ:6:LYS:H | 1.68 | 0.59 |
| 1:AA:262:A:H2' | 1:AA:263:A:C8 | 2.38 | 0.59 |
| 9:AI:117:HIS:HB2 | 9:AI:121:ARG:HG3 | 1.84 | 0.59 |
| 11:CK:54:ARG:NH1 | 25:CY:39:PSU:O2' | 2.35 | 0.59 |
| 12:CL:117:ARG:CZ | 12:CL:117:ARG:HB2 | 2.32 | 0.59 |
| 26:DA:2336:A:H61 | 47:D0:43:THR:HG22 | 1.67 | 0.59 |
| 3:AC:50:ALA:HB1 | 3:AC:70:VAL:HG21 | 1.84 | 0.59 |
| 4:AD:173:TRP:CZ3 | 4:AD:174:LEU:HG | 2.38 | 0.59 |
| 26:BA:1359:A:N6 | 26:BA:1372:U:H3 | 2.00 | 0.59 |
| 28:BD:68:LYS:HD2 | 28:BD:70:TRP:CZ2 | 2.38 | 0.59 |
| 1:CA:646:U:H2' | 1:CA:647:C:C6 | 2.37 | 0.59 |
| 26:DA:668:G:H5' | 26:DA:669:G:OP2 | 2.01 | 0.59 |
| 26:BA:2136:C:N4 | 26:BA:2155:G:N1 | 2.30 | 0.59 |
| 36:BP:91:PHE:O | 36:BP:121:LYS:NZ | 2.35 | 0.59 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:H6 | 1.67 | 0.59 |
| 1:CA:986:A:N3 | 19:CS:52:TYR:OH | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:CB:133:LYS:O | 2:CB:137:ARG:N | 2.32 | 0.59 |
| 2:CB:15:VAL:HG12 | 2:CB:209:ARG:HB3 | 1.85 | 0.59 |
| 39:DS:43:GLU:HB3 | 39:DS:44:LYS:HE2 | 1.82 | 0.59 |
| 39:DS:5:THR:OG1 | 39:DS:8:GLU:OE2 | 2.13 | 0.59 |
| 10:AJ:62:HIS:HB3 | 14:AN:59:ALA:HB3 | 1.84 | 0.59 |
| 36:BP:52:GLU:OE1 | 36:BP:55:ARG:NH1 | 2.31 | 0.59 |
| 46:BZ:111:VAL:HG12 | 46:BZ:112:ARG:H | 1.68 | 0.59 |
| 1:CA:1302:U:OP2 | 13:CM:21:TYR:OH | 2.17 | 0.59 |
| 2:CB:91:PRO:HB3 | 2:CB:154:LEU:HB3 | 1.83 | 0.59 |
| 26:DA:2140:C:H2' | 26:DA:2141:G:H5' | 1.85 | 0.59 |
| 26:DA:2745:C:O2' | 32:DH:139:GLN:O | 2.20 | 0.59 |
| 1:AA:1025:U:O2' | 1:AA:1026:G:H8 | 1.86 | 0.59 |
| 1:AA:1202:G:O4' | 14:AN:29:ARG:NH1 | 2.35 | 0.59 |
| 9:AI:17:VAL:HG23 | 9:AI:63:ILE:HG12 | 1.83 | 0.59 |
| 50:B3:3:ARG:NH1 | 50:B3:60:GLU:OE2 | 2.35 | 0.59 |
| 1:CA:1298:C:P | 7:CG:114:ARG:HH22 | 2.26 | 0.59 |
| 10:CJ:46:ARG:HG2 | 10:CJ:64:GLU:HB3 | 1.83 | 0.59 |
| 16:CP:52:ASP:O | 16:CP:54:GLU:N | 2.36 | 0.59 |
| 26:DA:2315:G:H2' | 26:DA:2316:C:C6 | 2.37 | 0.59 |
| 26:DA:2646:C:OP2 | 26:DA:2732:G:O2' | 2.20 | 0.59 |
| 30:DF:185:ASP:HA | 30:DF:188:ARG:HD3 | 1.84 | 0.59 |
| 37:DQ:34:LEU:HB2 | 37:DQ:118:LEU:HD22 | 1.84 | 0.59 |
| 40:DT:56:GLY:O | 40:DT:59:THR:HG23 | 2.02 | 0.59 |
| 26:DA:481:G:O5' | 45:DY:47:LYS:NZ | 2.35 | 0.59 |
| 3:AC:40:ARG:NH2 | 3:AC:55:VAL:O | 2.36 | 0.59 |
| 17:AQ:9:VAL:HG21 | 17:AQ:84:LEU:HD13 | 1.84 | 0.59 |
| 26:BA:2141:G:H22 | 26:BA:2149:G:H22 | 1.51 | 0.59 |
| 26:BA:307:G:H21 | 26:BA:330:A:H62 | 1.49 | 0.59 |
| 35:BO:63:VAL:HG12 | 35:BO:106:LEU:HD11 | 1.84 | 0.59 |
| 7:CG:72:ARG:N | 7:CG:142:GLU:OE2 | 2.30 | 0.59 |
| 8:CH:4:ASP:OD1 | 8:CH:7:ALA:N | 2.25 | 0.59 |
| 1:CA:375:U:OP1 | 16:CP:69:THR:HG21 | 2.02 | 0.59 |
| 26:DA:2273:A:H2' | 26:DA:2274:A:C8 | 2.38 | 0.59 |
| 34:DN:38:HIS:CE1 | 34:DN:39:ARG:HG3 | 2.37 | 0.59 |
| 1:AA:1320:C:H5'' | 19:AS:70:LYS:HG3 | 1.84 | 0.59 |
| 26:BA:1019:U:H3 | 26:BA:1142(A):A:H62 | 1.51 | 0.59 |
| 26:BA:1478:G:O2' | 26:BA:1558:A:N1 | 2.35 | 0.59 |
| 1:CA:573:A:N3 | 1:CA:883:C:O2' | 2.29 | 0.59 |
| 1:CA:1104:G:O5' | 2:CB:111:ARG:HD2 | 2.02 | 0.59 |
| 2:CB:121:LEU:H | 2:CB:125:PRO:HG2 | 1.68 | 0.59 |
| 26:DA:1025:G:C4 | 26:DA:1135:C:H1' | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:DP:86:LYS:HB3 | 36:DP:118:GLY:HA3 | 1.83 | 0.59 |
| 1:AA:46:G:O2' | 1:AA:365:U:O2 | 2.21 | 0.58 |
| 26:BA:1170:G:C2 | 26:BA:1171:G:H1' | 2.38 | 0.58 |
| 39:BS:15:ARG:O | 39:BS:19:LYS:HG2 | 2.02 | 0.58 |
| 1:CA:1049:U:C5 | 1:CA:1201:A:H5' | 2.37 | 0.58 |
| 1:CA:1120:G:C6 | 1:CA:1121:U:C4 | 2.91 | 0.58 |
| 1:CA:129(A):G:C6 | 1:CA:189(E):U:H4' | 2.38 | 0.58 |
| 2:CB:57:PHE:HE2 | 2:CB:185:ILE:HD12 | 1.67 | 0.58 |
| 2:CB:73:THR:HA | 2:CB:94:ASN:O | 2.02 | 0.58 |
| 19:CS:38:SER:HB2 | 19:CS:71:LEU:HD22 | 1.84 | 0.58 |
| 1:CA:1305:G:H5' | 21:CU:4:GLY:HA3 | 1.84 | 0.58 |
| 49:D2:22:GLU:OE2 | 49:D2:68:ARG:NH2 | 2.35 | 0.58 |
| 13:AM:3:ARG:HG3 | 13:AM:4:ILE:N | 2.18 | 0.58 |
| 2:CB:55:PHE:O | 2:CB:59:GLU:N | 2.25 | 0.58 |
| 3:CC:6:HIS:HD2 | 3:CC:8:ILE:H | 1.51 | 0.58 |
| 27:DB:11:C:OP2 | 27:DB:12:C:N4 | 2.30 | 0.58 |
| 2:AB:19:HIS:HE1 | 2:AB:189:ASP:HB3 | 1.69 | 0.58 |
| 1:CA:922:G:H4' | 5:CE:20:GLN:HA | 1.86 | 0.58 |
| 50:D3:5:LYS:NZ | 50:D3:34:GLU:OE2 | 2.19 | 0.58 |
| 26:DA:888:C:H2' | 26:DA:889:C:C4 | 2.38 | 0.58 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:H6 | 1.68 | 0.58 |
| 26:BA:1045:A:H1' | 26:BA:1047:G:N3 | 2.18 | 0.58 |
| 26:BA:2173:A:H3' | 26:BA:2174:C:H6 | 1.69 | 0.58 |
| 26:BA:2206:G:H5' | 26:BA:2207:G:N7 | 2.18 | 0.58 |
| 28:BD:79:VAL:HG21 | 28:BD:111:LEU:HD11 | 1.85 | 0.58 |
| 40:BT:65:LYS:HE2 | 40:BT:67:SER:HB2 | 1.85 | 0.58 |
| 46:BZ:110:GLY:N | 46:BZ:144:LEU:O | 2.32 | 0.58 |
| 1:CA:1004:A:N7 | 1:CA:1037:C:H2' | 2.18 | 0.58 |
| 1:CA:396:G:O2' | 1:CA:398:C:OP1 | 2.11 | 0.58 |
| 2:CB:87:ARG:NH2 | 2:CB:233:SER:HB3 | 2.18 | 0.58 |
| 13:CM:121:LYS:H | 13:CM:121:LYS:NZ | 2.01 | 0.58 |
| 18:CR:60:ALA:O | 18:CR:64:ARG:HG3 | 2.02 | 0.58 |
| 25:CY:8:4SU:H1' | 25:CY:48:C:O2 | 2.04 | 0.58 |
| 47:D0:11:ARG:O | 47:D0:14:ARG:NH2 | 2.36 | 0.58 |
| 26:DA:1639:U:H2' | 26:DA:1640:C:H5'' | 1.85 | 0.58 |
| 1:AA:1309:G:OP2 | 13:AM:99:ARG:NH2 | 2.33 | 0.58 |
| 1:AA:1305:G:N2 | 1:AA:1331:G:H1' | 2.18 | 0.58 |
| 21:AU:5:ASP:O | 21:AU:11:GLY:HA3 | 2.03 | 0.58 |
| 25:AY:60:U:H5'' | 25:AY:61:C:H5 | 1.69 | 0.58 |
| 45:BY:90:LEU:HD21 | 45:BY:96:ILE:HG12 | 1.85 | 0.58 |
| 10:CJ:38:ILE:HD11 | 10:CJ:71:LEU:HD23 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DA:1371:G:H2' | 26:DA:1372:U:H5 | 1.69 | 0.58 |
| 26:DA:2680:C:OP2 | 29:DE:111:ARG:NH2 | 2.36 | 0.58 |
| 35:DO:24:VAL:HA | 35:DO:39:ILE:HG22 | 1.86 | 0.58 |
| 1:AA:473:G:H2' | 1:AA:474:G:H8 | 1.68 | 0.58 |
| 1:AA:731:G:H5' | 1:AA:766:A:H4' | 1.85 | 0.58 |
| 13:AM:11:ARG:HB2 | 13:AM:46:LYS:HB3 | 1.86 | 0.58 |
| 26:BA:1021:A:H62 | 26:BA:1141:U:H3 | 1.49 | 0.58 |
| 26:BA:880:G:N2 | 26:BA:898:C:N3 | 2.44 | 0.58 |
| 42:BV:72:VAL:HG13 | 42:BV:85:LYS:HB3 | 1.85 | 0.58 |
| 1:CA:1028:C:C2 | 1:CA:1033:G:N1 | 2.72 | 0.58 |
| 1:CA:1122:U:C4 | 1:CA:1123:A:N7 | 2.72 | 0.58 |
| 1:CA:1298:C:H4' | 1:CA:1299:A:H5' | 1.85 | 0.58 |
| 13:CM:92:HIS:CD2 | 13:CM:98:VAL:HG21 | 2.39 | 0.58 |
| 26:DA:362:U:O2' | 26:DA:363:G:H5'' | 2.03 | 0.58 |
| 1:AA:1026:G:C2 | 1:AA:1027:C:H4' | 2.38 | 0.58 |
| 5:AE:53:LEU:HD12 | 5:AE:53:LEU:H | 1.68 | 0.58 |
| 26:BA:301:G:OP2 | 45:BY:84:ARG:NH2 | 2.37 | 0.58 |
| 1:CA:1063:C:OP2 | 1:CA:1064:G:O2' | 2.20 | 0.58 |
| 36:DP:63:PRO:HG2 | 55:D8:25:MET:HB2 | 1.86 | 0.58 |
| 32:DH:58:GLU:OE2 | 32:DH:60:ARG:NH1 | 2.37 | 0.58 |
| 1:AA:279:A:C5 | 17:AQ:98:LEU:HD23 | 2.38 | 0.58 |
| 1:AA:78:G:N2 | 1:AA:92:C:N3 | 2.51 | 0.58 |
| 1:AA:998:G:H1 | 1:AA:1043:C:N4 | 1.98 | 0.58 |
| 9:AI:3:GLN:OE1 | 9:AI:20:ARG:NH2 | 2.36 | 0.58 |
| 26:BA:882:G:H1 | 26:BA:894:C:H42 | 1.50 | 0.58 |
| 1:CA:148:G:H2' | 1:CA:149:A:C8 | 2.39 | 0.58 |
| 1:CA:328:C:H4' | 1:CA:329:A:H5' | 1.86 | 0.58 |
| 3:CC:54:ARG:HB3 | 3:CC:54:ARG:HH11 | 1.68 | 0.58 |
| 10:CJ:89:ASP:O | 10:CJ:91:PRO:HD3 | 2.04 | 0.58 |
| 26:DA:1412:A:H2' | 26:DA:1413:G:H8 | 1.68 | 0.58 |
| 26:DA:2127:G:C5 | 26:DA:2161:C:N4 | 2.71 | 0.58 |
| 31:DG:15:VAL:HG22 | 31:DG:175:LEU:HB3 | 1.85 | 0.58 |
| 46:DZ:150:LEU:H | 46:DZ:172:ALA:HB3 | 1.68 | 0.58 |
| 1:AA:1104:G:H4' | 2:AB:111:ARG:NH1 | 2.18 | 0.58 |
| 26:BA:1815:A:OP2 | 28:BD:54:ARG:NH2 | 2.35 | 0.58 |
| 26:BA:2404:C:O3' | 36:BP:77:ARG:NH2 | 2.37 | 0.58 |
| 1:CA:407:G:OP1 | 4:CD:115:ARG:NH2 | 2.35 | 0.58 |
| 26:DA:1166:C:H2' | 26:DA:1167:U:C6 | 2.39 | 0.58 |
| 26:DA:858:U:H1' | 26:DA:2268:A:H2' | 1.84 | 0.58 |
| 26:DA:903:C:H2' | 26:DA:904:C:C6 | 2.38 | 0.58 |
| 1:AA:72:C:H2' | 1:AA:73:G:O4' | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:158:LEU:HD21 | 2:AB:180:LEU:HD13 | 1.86 | 0.58 |
| 28:BD:180:GLY:HA3 | 28:BD:275:LYS:HB2 | 1.86 | 0.58 |
| 30:BF:116:ASP:OD2 | 36:BP:1:MET:N | 2.29 | 0.58 |
| 45:BY:92:ASN:N | 45:BY:93:GLY:HA2 | 2.18 | 0.58 |
| 1:CA:978:A:O2' | 1:CA:1321:C:N4 | 2.36 | 0.58 |
| 1:CA:964:A:N3 | 1:CA:969:A:O2' | 2.33 | 0.58 |
| 3:CC:65:ALA:HA | 3:CC:100:ALA:HB3 | 1.86 | 0.58 |
| 9:CI:21:PRO:HA | 9:CI:59:PHE:HA | 1.85 | 0.58 |
| 24:CX:16:C:H5' | 24:CX:59:A:N1 | 2.19 | 0.58 |
| 25:CX:56:C:O4' | 26:DA:2169:A:H1' | 2.04 | 0.58 |
| 28:DD:28:GLU:OE2 | 61:DD:416:HOH:O | 2.17 | 0.58 |
| 31:DG:43:LEU:HD12 | 31:DG:45:GLU:HG3 | 1.86 | 0.58 |
| 43:DW:57:ASN:HA | 43:DW:61:ASN:HD22 | 1.69 | 0.58 |
| 1:AA:1456:G:O6 | 20:AT:54:LYS:NZ | 2.30 | 0.57 |
| 1:AA:21:G:OP1 | 61:AA:4104:HOH:O | 2.17 | 0.57 |
| 6:AF:99:ALA:HB1 | 18:AR:23:LYS:HE2 | 1.86 | 0.57 |
| 56:B9:25:VAL:HB | 56:B9:34:GLN:HB2 | 1.86 | 0.57 |
| 26:BA:2113:U:N3 | 26:BA:2114:A:N7 | 2.52 | 0.57 |
| 1:CA:998:G:H1 | 1:CA:1043:C:H42 | 0.74 | 0.57 |
| 2:CB:52:GLU:O | 2:CB:56:ARG:HG2 | 2.04 | 0.57 |
| 9:CI:77:ILE:O | 9:CI:81:ILE:HG22 | 2.04 | 0.57 |
| 42:DV:6:LYS:HG2 | 42:DV:11:GLN:HG2 | 1.85 | 0.57 |
| 2:AB:95:GLN:HG3 | 2:AB:147:LYS:HD3 | 1.85 | 0.57 |
| 10:AJ:38:ILE:HD11 | 10:AJ:71:LEU:HB3 | 1.86 | 0.57 |
| 35:BO:80:ASP:OD1 | 40:BT:64:ARG:NH2 | 2.36 | 0.57 |
| 1:CA:114:U:H2' | 1:CA:115:G:C8 | 2.39 | 0.57 |
| 2:CB:25:ASN:OD1 | 2:CB:27:LYS:HG2 | 2.04 | 0.57 |
| 23:CW:21:A:N6 | 23:CW:46:7MG:C4 | 2.72 | 0.57 |
| 25:CX:49:C:N3 | 25:CX:65:G:N2 | 2.46 | 0.57 |
| 26:DA:1857:G:O2' | 26:DA:1885:A:N6 | 2.32 | 0.57 |
| 26:DA:2144:U:N3 | 26:DA:2146:C:N3 | 2.52 | 0.57 |
| 26:DA:848:G:H2' | 26:DA:849:A:C8 | 2.39 | 0.57 |
| 1:AA:1392:G:H21 | 1:AA:1502:A:H8 | 1.53 | 0.57 |
| 2:AB:71:VAL:HG11 | 2:AB:170:GLU:HG2 | 1.86 | 0.57 |
| 54:B7:34:ARG:NH2 | 61:B7:202:HOH:O | 2.36 | 0.57 |
| 26:BA:630:G:OP2 | 55:B8:15:LYS:NZ | 2.30 | 0.57 |
| 26:BA:831:G:O2' | 36:BP:38:GLN:NE2 | 2.38 | 0.57 |
| 35:BO:64:ARG:NH2 | 35:BO:99:PHE:O | 2.37 | 0.57 |
| 43:BW:68:ARG:HH11 | 43:BW:111:HIS:HA | 1.67 | 0.57 |
| 1:CA:1119:C:N3 | 1:CA:1154:G:O6 | 2.36 | 0.57 |
| 1:CA:45:U:H2' | 1:CA:46:G:C8 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CC:47:LEU:O | 3:CC:51:GLY:N | 2.34 | 0.57 |
| 5:CE:33:VAL:HG13 | 5:CE:112:LEU:HD12 | 1.86 | 0.57 |
| 7:CG:27:ILE:HD13 | 7:CG:40:ALA:HA | 1.86 | 0.57 |
| 23:CW:4:C:N3 | 23:CW:69:G:C2 | 2.72 | 0.57 |
| 26:DA:1022:G:H22 | 26:DA:1142(A):A:H2 | 1.50 | 0.57 |
| 26:BA:1267:U:OP1 | 61:BA:5075:HOH:O | 2.17 | 0.57 |
| 26:BA:668:G:H5' | 26:BA:669:G:OP2 | 2.05 | 0.57 |
| 23:AW:52:G:H4' | 37:BQ:56:ARG:NH2 | 2.20 | 0.57 |
| 1:CA:1097:C:H1' | 1:CA:1170:A:H1' | 1.86 | 0.57 |
| 4:CD:25:ARG:NH1 | 4:CD:30:LYS:O | 2.36 | 0.57 |
| 7:CG:111:ARG:NH1 | 7:CG:113:GLU:OE1 | 2.37 | 0.57 |
| 23:CW:30:G:H1 | 23:CW:40:C:N4 | 2.03 | 0.57 |
| 26:DA:2070:G:OP2 | 61:DA:4461:HOH:O | 2.17 | 0.57 |
| 26:DA:643:A:N1 | 26:DA:2369:A:O2' | 2.36 | 0.57 |
| 28:DD:108:PRO:HG2 | 28:DD:111:LEU:HB2 | 1.87 | 0.57 |
| 35:DO:92:GLU:OE2 | 35:DO:113:LYS:HD3 | 2.05 | 0.57 |
| 42:DV:60:GLU:HB2 | 42:DV:97:LYS:HE2 | 1.85 | 0.57 |
| 1:AA:406:G:N3 | 4:AD:119:GLN:NE2 | 2.43 | 0.57 |
| 2:AB:137:ARG:NH1 | 2:AB:137:ARG:HB3 | 2.19 | 0.57 |
| 12:AL:34:ARG:NH2 | 61:AL:301:HOH:O | 2.36 | 0.57 |
| 26:BA:2123:G:H1 | 26:BA:2175:C:N4 | 2.02 | 0.57 |
| 1:CA:1051:C:H2' | 1:CA:1052:U:C6 | 2.40 | 0.57 |
| 1:CA:1157:A:H4' | 1:CA:1158:C:O5' | 2.04 | 0.57 |
| 1:CA:1168:A:H2' | 1:CA:1169:A:C8 | 2.39 | 0.57 |
| 1:CA:1305:G:N2 | 1:CA:1331:G:H1' | 2.20 | 0.57 |
| 1:CA:998:G:H2' | 1:CA:999:C:O4' | 2.04 | 0.57 |
| 4:CD:61:LYS:NZ | 4:CD:72:GLU:OE1 | 2.35 | 0.57 |
| 13:CM:93:ARG:NH1 | 26:DA:888:C:O5' | 2.37 | 0.57 |
| 23:CW:3:C:O2 | 23:CW:70:G:N1 | 2.29 | 0.57 |
| 24:CX:55:PSU:N3 | 24:CX:58:A:OP2 | 2.26 | 0.57 |
| 29:DE:30:PRO:HB3 | 29:DE:92:THR:HG22 | 1.86 | 0.57 |
| 37:DQ:111:GLU:O | 37:DQ:115:MET:HG2 | 2.05 | 0.57 |
| 1:AA:1000:U:O2 | 1:AA:1042:G:N2 | 2.37 | 0.57 |
| 26:BA:2187:G:O2' | 26:BA:2188:C:OP1 | 2.20 | 0.57 |
| 38:BR:28:LEU:HD12 | 38:BR:48:VAL:HG21 | 1.86 | 0.57 |
| 1:CA:1209:C:O2' | 1:CA:1214:C:N4 | 2.38 | 0.57 |
| 1:CA:444:C:H2' | 1:CA:445:G:C8 | 2.39 | 0.57 |
| 16:CP:57:ARG:NH2 | 16:CP:79:VAL:O | 2.38 | 0.57 |
| 30:DF:195:ASP:OD1 | 30:DF:196:LEU:N | 2.38 | 0.57 |
| 1:AA:184:G:H2' | 1:AA:185:A:H8 | 1.70 | 0.57 |
| 6:AF:81:ILE:HD11 | 28:BD:125:ILE:HB | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:AY:33:U:H2' | 25:AY:34:G:H3' | 1.86 | 0.57 |
| 54:B7:33:ARG:NH2 | 61:B7:201:HOH:O | 2.38 | 0.57 |
| 45:BY:86:ARG:HD2 | 45:BY:100:ALA:HA | 1.87 | 0.57 |
| 1:CA:1154:G:N7 | 1:CA:1155:G:C4 | 2.72 | 0.57 |
| 2:CB:16:HIS:O | 2:CB:18:GLY:N | 2.37 | 0.57 |
| 26:DA:686:G:N2 | 26:DA:788:A:H61 | 2.02 | 0.57 |
| 28:DD:3:VAL:HG13 | 28:DD:17:THR:HB | 1.86 | 0.57 |
| 30:DF:13:SER:OG | 30:DF:16:GLY:O | 2.21 | 0.57 |
| 26:DA:674:G:H1' | 30:DF:74:ARG:HD3 | 1.85 | 0.57 |
| 26:DA:1188:U:H4' | 42:DV:79:VAL:HG22 | 1.86 | 0.57 |
| 1:AA:1057:G:OP2 | 61:AA:4024:HOH:O | 2.16 | 0.57 |
| 1:AA:1157:A:H4' | 1:AA:1158:C:O5' | 2.05 | 0.57 |
| 1:AA:159:G:H2' | 1:AA:161:A:OP2 | 2.05 | 0.57 |
| 26:BA:892:G:H3' | 26:BA:893:C:C6 | 2.39 | 0.57 |
| 31:BG:5:VAL:HG22 | 31:BG:8:LYS:H | 1.69 | 0.57 |
| 1:CA:1001:A:H2' | 1:CA:1001(A):G:C8 | 2.39 | 0.57 |
| 1:CA:1012:U:O2 | 1:CA:1017:G:O6 | 2.23 | 0.57 |
| 3:CC:18:TRP:H | 3:CC:18:TRP:HE3 | 1.52 | 0.57 |
| 1:CA:619:U:N3 | 4:CD:134:ASP:OD1 | 2.32 | 0.57 |
| 26:DA:479:A:N3 | 26:DA:481:G:H5'' | 2.19 | 0.57 |
| 27:DB:3:C:H2' | 27:DB:4:C:C6 | 2.39 | 0.57 |
| 13:AM:40:ASN:O | 13:AM:43:THR:OG1 | 2.23 | 0.57 |
| 25:AY:15:G:O6 | 25:AY:48:C:O2 | 2.23 | 0.57 |
| 1:CA:1442:G:O2' | 1:CA:1442(A):G:OP1 | 2.15 | 0.57 |
| 1:CA:297:G:N2 | 1:CA:300:A:OP2 | 2.38 | 0.57 |
| 15:CO:55:GLY:HA2 | 15:CO:58:MET:HE2 | 1.86 | 0.57 |
| 31:DG:151:ALA:HB3 | 31:DG:153:ARG:HH11 | 1.70 | 0.57 |
| 46:DZ:159:PRO:HA | 46:DZ:161:VAL:N | 2.20 | 0.57 |
| 5:AE:100:VAL:O | 5:AE:107:ARG:NH2 | 2.34 | 0.57 |
| 1:AA:375:U:OP1 | 16:AP:69:THR:HG21 | 2.05 | 0.57 |
| 26:BA:1173:G:O2' | 26:BA:1174:A:O4' | 2.17 | 0.57 |
| 26:BA:2357:U:OP1 | 47:B0:20:ARG:NH1 | 2.38 | 0.57 |
| 1:CA:1204:A:OP1 | 14:CN:3:ARG:NH1 | 2.37 | 0.57 |
| 1:CA:588:G:O6 | 1:CA:651:C:N4 | 2.33 | 0.57 |
| 3:CC:3:ASN:HD22 | 3:CC:4:LYS:HG3 | 1.69 | 0.57 |
| 24:CX:21:A:N6 | 24:CX:46:G:H2' | 2.19 | 0.57 |
| 26:DA:1169:G:H1 | 26:DA:1180:C:N4 | 2.01 | 0.57 |
| 26:DA:614(C):A:C4 | 30:DF:180:GLY:HA2 | 2.40 | 0.57 |
| 45:DY:28:LYS:HD2 | 45:DY:40:GLU:HG3 | 1.87 | 0.57 |
| 46:DZ:92:SER:O | 46:DZ:130:PRO:HG2 | 2.05 | 0.57 |
| 1:AA:1118:C:H2' | 1:AA:1119:C:H6 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:AO:18:PHE:HB2 | 15:AO:19:PRO:HD2 | 1.86 | 0.56 |
| 15:AO:74:ASP:CG | 15:AO:77:ARG:HG3 | 2.26 | 0.56 |
| 49:B2:65:ASN:OD1 | 49:B2:69:ARG:NH1 | 2.38 | 0.56 |
| 26:DA:2137:C:H2' | 26:DA:2138:C:C6 | 2.40 | 0.56 |
| 26:DA:247:G:H4' | 26:DA:386:G:C5 | 2.40 | 0.56 |
| 35:DO:1:MET:HG3 | 35:DO:67:LYS:HG2 | 1.86 | 0.56 |
| 36:DP:96:THR:H | 36:DP:99:LEU:CD2 | 2.17 | 0.56 |
| 45:DY:6:HIS:CD2 | 45:DY:7:VAL:HG23 | 2.40 | 0.56 |
| 26:BA:222:A:H5'' | 26:BA:421:U:OP1 | 2.05 | 0.56 |
| 1:CA:1183:A:H5' | 1:CA:1183:A:H8 | 1.69 | 0.56 |
| 8:CH:41:ARG:NH2 | 8:CH:123:GLU:OE2 | 2.38 | 0.56 |
| 13:CM:16:ASP:HB3 | 13:CM:34:LEU:HD11 | 1.87 | 0.56 |
| 47:D0:27:GLU:HG3 | 47:D0:68:GLU:HA | 1.86 | 0.56 |
| 26:DA:2062:A:OP1 | 61:DA:3826:HOH:O | 2.17 | 0.56 |
| 26:DA:2522:U:O2' | 26:DA:2647:U:OP1 | 2.18 | 0.56 |
| 26:DA:2532:G:O2' | 26:DA:2657:A:N1 | 2.36 | 0.56 |
| 26:DA:422:A:OP2 | 61:DA:3787:HOH:O | 2.17 | 0.56 |
| 26:DA:740:U:H2' | 26:DA:741:G:C8 | 2.39 | 0.56 |
| 31:DG:101:ILE:HG22 | 31:DG:105:LYS:HE2 | 1.86 | 0.56 |
| 36:DP:99:LEU:O | 36:DP:103:ALA:N | 2.37 | 0.56 |
| 44:DX:35:THR:HG22 | 44:DX:38:GLU:H | 1.70 | 0.56 |
| 1:AA:1392:G:N2 | 1:AA:1502:A:H8 | 2.03 | 0.56 |
| 1:AA:1189:C:P | 10:AJ:51:ARG:HH22 | 2.27 | 0.56 |
| 10:AJ:11:PHE:HE1 | 10:AJ:67:THR:HG22 | 1.70 | 0.56 |
| 20:AT:10:LEU:HB3 | 20:AT:12:ALA:H | 1.70 | 0.56 |
| 26:BA:1300:U:H4' | 26:BA:1301:A:C5' | 2.36 | 0.56 |
| 26:BA:2138:C:N3 | 26:BA:2153:G:N2 | 2.52 | 0.56 |
| 26:BA:800:A:H8 | 26:BA:800:A:OP1 | 1.88 | 0.56 |
| 26:BA:9:U:H3 | 26:BA:2629:A:H2 | 1.54 | 0.56 |
| 42:BV:76:LYS:HB2 | 42:BV:81:TYR:HB3 | 1.87 | 0.56 |
| 12:CL:24:VAL:HG12 | 12:CL:27:LEU:HB2 | 1.86 | 0.56 |
| 26:DA:2184:G:H2' | 26:DA:2185:C:C6 | 2.39 | 0.56 |
| 26:DA:614(A):U:H4' | 26:DA:614(B):G:H5' | 1.86 | 0.56 |
| 46:DZ:150:LEU:N | 46:DZ:172:ALA:HB3 | 2.20 | 0.56 |
| 1:AA:93:G:H2' | 1:AA:96:U:O4' | 2.06 | 0.56 |
| 9:AI:23:ASN:ND2 | 9:AI:60:ASP:OD2 | 2.38 | 0.56 |
| 13:AM:88:ARG:HG3 | 13:AM:98:VAL:HG12 | 1.87 | 0.56 |
| 26:BA:2127:G:H21 | 26:BA:2173:A:H1' | 1.71 | 0.56 |
| 1:CA:1247:U:H1' | 1:CA:1291:G:N2 | 2.20 | 0.56 |
| 2:CB:134:GLU:HA | 2:CB:137:ARG:HB2 | 1.87 | 0.56 |
| 10:CJ:55:LYS:HE3 | 10:CJ:56:HIS:NE2 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:CM:29:ARG:HG3 | 13:CM:64:TRP:CZ3 | 2.39 | 0.56 |
| 13:CM:71:ARG:CG | 13:CM:71:ARG:HH11 | 2.18 | 0.56 |
| 17:CQ:78:GLU:OE2 | 17:CQ:81:ARG:NH1 | 2.37 | 0.56 |
| 18:CR:43:PHE:HD1 | 18:CR:56:THR:HG22 | 1.69 | 0.56 |
| 26:DA:1412:A:H2' | 26:DA:1413:G:C8 | 2.41 | 0.56 |
| 26:DA:236:C:H2' | 26:DA:237:C:C6 | 2.41 | 0.56 |
| 27:DB:28:C:H2' | 27:DB:29:A:C8 | 2.39 | 0.56 |
| 1:AA:1068:G:OP2 | 1:AA:1068:G:H8 | 1.88 | 0.56 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:C6 | 2.41 | 0.56 |
| 1:AA:1328:C:OP1 | 21:AU:21:TYR:OH | 2.23 | 0.56 |
| 1:AA:198:G:O6 | 1:AA:219:C:N4 | 2.39 | 0.56 |
| 1:AA:972:C:O2' | 10:AJ:55:LYS:O | 2.22 | 0.56 |
| 2:AB:54:THR:HG23 | 2:AB:199:TYR:HB3 | 1.87 | 0.56 |
| 26:BA:2279:G:N7 | 47:B0:14:ARG:NH1 | 2.53 | 0.56 |
| 26:BA:1796:U:H2' | 26:BA:1797:C:H6 | 1.68 | 0.56 |
| 26:BA:2646:C:OP2 | 26:BA:2732:G:O2' | 2.20 | 0.56 |
| 26:BA:2839:G:H5' | 38:BR:46:GLY:HA2 | 1.87 | 0.56 |
| 26:BA:363(A):A:H2' | 26:BA:363(B):G:H8 | 1.71 | 0.56 |
| 31:BG:28:VAL:O | 31:BG:31:VAL:HG12 | 2.05 | 0.56 |
| 43:BW:14:PRO:HG2 | 43:BW:78:GLU:HG2 | 1.86 | 0.56 |
| 7:CG:15:ASP:HB3 | 7:CG:24:THR:HG23 | 1.86 | 0.56 |
| 26:DA:2112:G:C5 | 26:DA:2113:U:H1' | 2.40 | 0.56 |
| 26:DA:518:G:H2' | 26:DA:519:U:C6 | 2.41 | 0.56 |
| 1:AA:562:C:H1' | 12:AL:15:ARG:HB3 | 1.87 | 0.56 |
| 26:BA:1173:G:O2' | 26:BA:1174:A:O5' | 2.23 | 0.56 |
| 26:BA:2243:U:H2' | 26:BA:2244:U:C6 | 2.40 | 0.56 |
| 26:BA:2719:G:OP2 | 61:BA:4851:HOH:O | 2.18 | 0.56 |
| 40:BT:24:PRO:HD3 | 40:BT:52:ILE:HD12 | 1.88 | 0.56 |
| 26:BA:1187:G:H5'' | 42:BV:81:TYR:CE1 | 2.39 | 0.56 |
| 1:CA:532:A:H61 | 3:CC:193:TYR:CB | 2.16 | 0.56 |
| 23:CW:18:G:O2' | 23:CW:57:G:N2 | 2.26 | 0.56 |
| 26:DA:1231:G:H2' | 26:DA:1232:G:H8 | 1.69 | 0.56 |
| 26:DA:84:A:H5' | 45:DY:8:LYS:HG2 | 1.86 | 0.56 |
| 27:DB:42:C:O2' | 31:DG:67:LYS:O | 2.16 | 0.56 |
| 26:DA:2867:G:OP2 | 40:DT:119:LYS:NZ | 2.39 | 0.56 |
| 1:AA:45:U:H2' | 1:AA:46:G:C8 | 2.40 | 0.56 |
| 3:AC:15:THR:HG21 | 3:AC:181:ASN:HA | 1.88 | 0.56 |
| 10:AJ:35:SER:N | 10:AJ:73:ASP:O | 2.33 | 0.56 |
| 25:AY:33:U:C3' | 25:AY:34:G:H5'' | 2.35 | 0.56 |
| 26:BA:1045:A:OP1 | 26:BA:1046:A:H3' | 2.05 | 0.56 |
| 29:BE:55:ASN:HB3 | 29:BE:58:ARG:HG3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DA:2061:G:H5'' | 26:DA:2503:A:C2 | 2.40 | 0.56 |
| 26:DA:2142:C:N3 | 26:DA:2149:G:O6 | 2.39 | 0.56 |
| 26:DA:330:A:H2 | 26:DA:1210:A:HO2' | 1.54 | 0.56 |
| 1:AA:1278:U:H5' | 1:AA:1279:A:O4' | 2.06 | 0.56 |
| 1:AA:976:G:H5' | 1:AA:1358:U:O2' | 2.06 | 0.56 |
| 2:AB:109:SER:O | 2:AB:112:VAL:HG22 | 2.06 | 0.56 |
| 13:AM:122:LYS:HD3 | 13:AM:123:ALA:N | 2.18 | 0.56 |
| 17:AQ:66:SER:O | 17:AQ:70:ARG:NH1 | 2.38 | 0.56 |
| 26:BA:2130:U:O2 | 26:BA:2131:G:N2 | 2.38 | 0.56 |
| 44:BX:53:LYS:HB3 | 44:BX:82:GLN:HB3 | 1.88 | 0.56 |
| 1:CA:587:G:N2 | 1:CA:754:C:OP2 | 2.37 | 0.56 |
| 4:CD:191:ARG:NH1 | 4:CD:191:ARG:O | 2.38 | 0.56 |
| 15:CO:17:ARG:HG3 | 15:CO:17:ARG:HH11 | 1.69 | 0.56 |
| 26:DA:1579:A:H2' | 26:DA:1580:A:C8 | 2.41 | 0.56 |
| 1:AA:1003:G:C2 | 1:AA:1004:A:N3 | 2.73 | 0.56 |
| 3:AC:29:TYR:OH | 14:AN:54:PRO:O | 2.20 | 0.56 |
| 15:AO:56:LEU:O | 15:AO:60:VAL:HG23 | 2.05 | 0.56 |
| 25:AY:38:A:C2' | 25:AY:39:PSU:H5'' | 2.35 | 0.56 |
| 26:BA:1171:G:H3' | 26:BA:1173:G:H5' | 1.88 | 0.56 |
| 1:CA:1154:G:N7 | 1:CA:1155:G:N9 | 2.54 | 0.56 |
| 5:CE:140:ARG:O | 5:CE:143:ARG:NH2 | 2.39 | 0.56 |
| 9:CI:8:GLY:O | 9:CI:15:ALA:N | 2.35 | 0.56 |
| 6:CF:50:TYR:CE2 | 18:CR:77:GLY:HA2 | 2.41 | 0.56 |
| 1:AA:78:G:C2 | 1:AA:91:C:C4 | 2.94 | 0.56 |
| 5:AE:110:LEU:HD13 | 5:AE:118:ILE:HG21 | 1.86 | 0.56 |
| 9:AI:29:ASN:OD1 | 9:AI:65:VAL:N | 2.37 | 0.56 |
| 13:AM:87:TYR:O | 13:AM:91:ARG:HG2 | 2.06 | 0.56 |
| 39:BS:14:VAL:O | 39:BS:18:ILE:HG12 | 2.06 | 0.56 |
| 2:CB:8:LYS:HD2 | 2:CB:9:GLU:H | 1.71 | 0.56 |
| 5:CE:84:PHE:N | 5:CE:87:SER:O | 2.33 | 0.56 |
| 13:CM:71:ARG:HH11 | 13:CM:71:ARG:HG3 | 1.69 | 0.56 |
| 37:DQ:77:LYS:NZ | 37:DQ:86:GLY:O | 2.39 | 0.56 |
| 1:AA:193:C:H2' | 1:AA:194:C:C6 | 2.41 | 0.56 |
| 2:AB:16:HIS:CG | 2:AB:17:PHE:N | 2.73 | 0.56 |
| 24:AX:21:A:H5' | 24:AX:22:G:OP1 | 2.05 | 0.56 |
| 49:B2:23:LYS:O | 49:B2:27:GLU:HG3 | 2.06 | 0.56 |
| 26:BA:1588:C:H2' | 26:BA:1589:C:C6 | 2.40 | 0.56 |
| 26:BA:456:C:H4' | 61:BA:3937:HOH:O | 2.04 | 0.56 |
| 35:BO:1:MET:HG3 | 35:BO:67:LYS:HG2 | 1.87 | 0.56 |
| 26:BA:64:A:O3' | 44:BX:71:GLY:HA3 | 2.05 | 0.56 |
| 1:CA:1057:G:H2' | 1:CA:1058:G:O4' | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1084:G:H5' | 1:CA:1102:A:OP2 | 2.06 | 0.56 |
| 1:CA:1095:U:H5'' | 1:CA:1109:C:O2 | 2.05 | 0.56 |
| 25:CY:19:G:N1 | 25:CY:56:C:N4 | 2.41 | 0.56 |
| 26:DA:1316:U:H2' | 26:DA:1317:A:H8 | 1.71 | 0.56 |
| 26:DA:2327:A:H2' | 26:DA:2328:A:C8 | 2.41 | 0.56 |
| 46:DZ:100:VAL:HG21 | 46:DZ:134:PRO:HG2 | 1.88 | 0.56 |
| 1:AA:946:A:H2' | 1:AA:947:G:C8 | 2.40 | 0.55 |
| 10:AJ:61:GLU:OE2 | 14:AN:45:ARG:NE | 2.32 | 0.55 |
| 10:AJ:8:LEU:HB2 | 10:AJ:70:ARG:HB2 | 1.88 | 0.55 |
| 26:BA:1033:U:OP1 | 56:B9:9:ARG:NH2 | 2.39 | 0.55 |
| 26:BA:2023:G:H5' | 26:BA:2617:C:H4' | 1.87 | 0.55 |
| 26:BA:278:A:O2' | 26:BA:279:C:OP1 | 2.16 | 0.55 |
| 26:BA:911:A:H2' | 37:BQ:9:TYR:OH | 2.05 | 0.55 |
| 1:CA:757:U:H2' | 1:CA:758:G:O4' | 2.06 | 0.55 |
| 4:CD:43:HIS:ND1 | 4:CD:46:LYS:HE2 | 2.20 | 0.55 |
| 23:CW:51:U:H3 | 23:CW:63:G:H1 | 1.54 | 0.55 |
| 44:DX:60:ARG:NH1 | 54:D7:47:ARG:HH22 | 2.01 | 0.55 |
| 26:DA:299:A:N1 | 26:DA:322:A:O2' | 2.30 | 0.55 |
| 26:DA:478:A:N1 | 26:DA:500:G:H4' | 2.21 | 0.55 |
| 26:DA:2723:C:H5'' | 38:DR:1:MET:HE2 | 1.88 | 0.55 |
| 41:DU:76:TYR:CZ | 41:DU:80:ILE:HG13 | 2.42 | 0.55 |
| 1:AA:68:G:C2 | 1:AA:69:G:H1' | 2.42 | 0.55 |
| 26:BA:389:G:N1 | 36:BP:70:GLN:HG3 | 2.22 | 0.55 |
| 1:CA:1028:C:C4 | 1:CA:1033:G:O6 | 2.59 | 0.55 |
| 20:CT:10:LEU:HD23 | 20:CT:12:ALA:HB2 | 1.88 | 0.55 |
| 23:CW:44:G:H2' | 23:CW:45:U:H5' | 1.88 | 0.55 |
| 26:DA:2776:A:H4' | 26:DA:2777:G:H5'' | 1.87 | 0.55 |
| 26:DA:586:A:N1 | 26:DA:809:G:O2' | 2.31 | 0.55 |
| 1:AA:167:G:H2' | 1:AA:168:G:H8 | 1.72 | 0.55 |
| 1:AA:181:G:O2' | 1:AA:183:G:O6 | 2.18 | 0.55 |
| 1:AA:652:U:O4 | 1:AA:752:G:O2' | 2.13 | 0.55 |
| 1:AA:674:G:H2' | 1:AA:675:A:H8 | 1.69 | 0.55 |
| 3:AC:36:ASP:O | 3:AC:40:ARG:HG3 | 2.06 | 0.55 |
| 5:AE:122:GLU:O | 5:AE:126:ARG:NH1 | 2.39 | 0.55 |
| 36:BP:63:PRO:HG2 | 55:B8:25:MET:HB2 | 1.87 | 0.55 |
| 26:BA:2848:G:C8 | 40:BT:97:ALA:HB2 | 2.41 | 0.55 |
| 26:BA:588:U:H2' | 26:BA:589:C:C6 | 2.40 | 0.55 |
| 3:CC:56:ASP:HB2 | 3:CC:67:THR:HB | 1.88 | 0.55 |
| 27:DB:55:U:H1' | 31:DG:29:TRP:CD1 | 2.42 | 0.55 |
| 29:DE:116:VAL:HG13 | 29:DE:122:PHE:HB2 | 1.88 | 0.55 |
| 29:DE:163:GLU:HG2 | 29:DE:164:ARG:N | 2.20 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:222:U:H2' | 1:AA:223:U:C6 | 2.42 | 0.55 |
| 10:AJ:30:SER:O | 10:AJ:81:THR:HG21 | 2.07 | 0.55 |
| 33:BI:114:LEU:HD12 | 33:BI:130:TYR:HA | 1.87 | 0.55 |
| 26:BA:535:C:O3' | 41:BU:53:ARG:NH1 | 2.39 | 0.55 |
| 1:CA:1023:G:H3' | 1:CA:1024:G:C8 | 2.41 | 0.55 |
| 1:CA:420:U:O2' | 1:CA:423:G:O6 | 2.13 | 0.55 |
| 1:CA:527:G:O2' | 1:CA:535:A:N1 | 2.34 | 0.55 |
| 1:CA:521:G:H4' | 12:CL:73:GLU:HG2 | 1.87 | 0.55 |
| 18:CR:43:PHE:CD1 | 18:CR:56:THR:HG22 | 2.41 | 0.55 |
| 26:DA:1446:C:H42 | 26:DA:1465:G:H1 | 1.52 | 0.55 |
| 26:DA:2674:G:H2' | 26:DA:2675:A:C8 | 2.41 | 0.55 |
| 26:DA:2753:A:N3 | 56:D9:15:LYS:NZ | 2.43 | 0.55 |
| 26:DA:888:C:H5'' | 26:DA:889:C:OP2 | 2.07 | 0.55 |
| 28:DD:71:ASP:HB3 | 28:DD:103:ARG:HH22 | 1.71 | 0.55 |
| 1:AA:922:G:H4' | 5:AE:20:GLN:HA | 1.89 | 0.55 |
| 26:BA:1540:U:H2' | 26:BA:1541:G:O4' | 2.07 | 0.55 |
| 26:BA:2207:G:O2' | 26:BA:2208:A:OP1 | 2.24 | 0.55 |
| 26:BA:2567:G:H2' | 26:BA:2568:C:C6 | 2.41 | 0.55 |
| 1:CA:1223:C:H5'' | 1:CA:1224:G:H5'' | 1.88 | 0.55 |
| 1:CA:984:C:O5' | 1:CA:984:C:H6 | 1.88 | 0.55 |
| 2:CB:162:ILE:O | 2:CB:185:ILE:HG12 | 2.06 | 0.55 |
| 5:CE:137:GLU:HG2 | 5:CE:140:ARG:HH11 | 1.71 | 0.55 |
| 6:CF:97:PHE:HE1 | 18:CR:62:GLU:HG2 | 1.71 | 0.55 |
| 48:D1:59:THR:O | 48:D1:91:LYS:NZ | 2.26 | 0.55 |
| 26:DA:2787:C:H1' | 29:DE:62:PRO:HG3 | 1.88 | 0.55 |
| 26:DA:39:C:H2' | 26:DA:40:C:C6 | 2.42 | 0.55 |
| 26:DA:848:G:C4 | 26:DA:933:A:H8 | 2.24 | 0.55 |
| 38:DR:55:ALA:HB2 | 38:DR:79:LEU:HD13 | 1.88 | 0.55 |
| 40:DT:50:ILE:HA | 40:DT:99:LEU:HD12 | 1.89 | 0.55 |
| 2:AB:167:PRO:HG3 | 2:AB:186:ALA:HB1 | 1.88 | 0.55 |
| 26:BA:1021:A:H8 | 26:BA:1022:G:H5'' | 1.71 | 0.55 |
| 26:BA:2108:C:H2' | 26:BA:2109:U:H6 | 1.71 | 0.55 |
| 26:BA:330:A:H2 | 26:BA:1210:A:H2' | 1.71 | 0.55 |
| 33:BI:93:THR:HG22 | 33:BI:119:PRO:HB3 | 1.88 | 0.55 |
| 1:CA:1028:C:N3 | 1:CA:1033:G:O6 | 2.40 | 0.55 |
| 1:CA:1316:G:H22 | 1:CA:1319:A:H5'' | 1.72 | 0.55 |
| 23:CW:19:G:H1 | 23:CW:56:C:N4 | 2.03 | 0.55 |
| 26:DA:1434:A:H61 | 26:DA:1558:A:H62 | 1.54 | 0.55 |
| 9:AI:24:GLY:HA2 | 9:AI:59:PHE:O | 2.07 | 0.55 |
| 1:AA:750:G:O2' | 15:AO:22:THR:O | 2.14 | 0.55 |
| 23:AW:50:U:H3 | 23:AW:64:A:N6 | 2.05 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1299:A:H2' | 1:CA:1299:A:N3 | 2.21 | 0.55 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:C6 | 2.41 | 0.55 |
| 1:CA:1104:G:H4' | 2:CB:111:ARG:NH1 | 2.21 | 0.55 |
| 2:CB:122:PHE:CE2 | 2:CB:139:LYS:HG2 | 2.42 | 0.55 |
| 2:CB:87:ARG:NH1 | 2:CB:220:ASP:OD1 | 2.39 | 0.55 |
| 5:CE:6:PHE:HB2 | 5:CE:34:VAL:HG22 | 1.89 | 0.55 |
| 48:D1:76:ARG:HH11 | 48:D1:97:LEU:HD22 | 1.71 | 0.55 |
| 26:DA:2126:A:N6 | 26:DA:2162:G:O2' | 2.39 | 0.55 |
| 26:DA:2630:G:H2' | 26:DA:2631:G:C8 | 2.42 | 0.55 |
| 26:DA:84:A:H5'' | 45:DY:8:LYS:HE3 | 1.89 | 0.55 |
| 3:AC:58:GLU:HB2 | 3:AC:65:ALA:HB3 | 1.88 | 0.55 |
| 27:BB:66:A:H61 | 27:BB:108:U:H2' | 1.72 | 0.55 |
| 4:CD:22:LYS:HB2 | 4:CD:26:CYS:SG | 2.47 | 0.55 |
| 26:DA:1528:A:OP2 | 61:DA:3982:HOH:O | 2.18 | 0.55 |
| 26:DA:2098:U:H3 | 26:DA:2191:G:H1 | 1.53 | 0.55 |
| 26:DA:528:A:C2 | 26:DA:2042:A:H2' | 2.42 | 0.55 |
| 26:DA:566:U:H5'' | 36:DP:29:LYS:HE3 | 1.87 | 0.55 |
| 26:DA:2303:G:O2' | 31:DG:132:ASN:HB2 | 2.07 | 0.55 |
| 1:AA:814:A:H2' | 1:AA:816:A:H5'' | 1.89 | 0.55 |
| 18:CR:25:THR:O | 18:CR:25:THR:OG1 | 2.19 | 0.55 |
| 21:CU:5:ASP:O | 21:CU:11:GLY:HA3 | 2.06 | 0.55 |
| 48:D1:83:GLU:OE1 | 48:D1:83:GLU:N | 2.39 | 0.55 |
| 50:D3:7:LYS:HB2 | 50:D3:34:GLU:HG3 | 1.89 | 0.55 |
| 55:D8:6:THR:HG22 | 55:D8:63:PRO:HD2 | 1.88 | 0.55 |
| 26:DA:1889:A:H2' | 26:DA:1890:A:C8 | 2.42 | 0.55 |
| 26:DA:900:A:H2' | 26:DA:901:A:C8 | 2.41 | 0.55 |
| 38:DR:36:THR:HG22 | 38:DR:37:THR:H | 1.72 | 0.55 |
| 44:DX:4:ALA:HB1 | 44:DX:42:ALA:HA | 1.89 | 0.55 |
| 1:AA:1005:A:H1' | 1:AA:1036:G:N2 | 2.21 | 0.55 |
| 1:AA:954:G:H21 | 1:AA:1227:A:H62 | 1.55 | 0.55 |
| 1:AA:79:G:C2 | 1:AA:90:U:O2 | 2.60 | 0.55 |
| 4:AD:98:GLU:OE1 | 4:AD:103:ASN:ND2 | 2.38 | 0.55 |
| 26:BA:1420:U:O2' | 26:BA:1421:G:OP1 | 2.22 | 0.55 |
| 26:BA:2190:G:C2' | 26:BA:2191:G:H5'' | 2.34 | 0.55 |
| 37:BQ:14:ARG:HG2 | 37:BQ:41:TRP:HH2 | 1.71 | 0.55 |
| 1:CA:1352:C:H2' | 1:CA:1353:G:C8 | 2.42 | 0.55 |
| 1:CA:692:U:O2' | 1:CA:694:A:N7 | 2.34 | 0.55 |
| 23:CW:11:C:H42 | 23:CW:24:G:H1 | 1.54 | 0.55 |
| 47:D0:32:ARG:H | 47:D0:35:ASN:ND2 | 2.05 | 0.55 |
| 26:DA:1292:U:H2' | 26:DA:1293:C:C6 | 2.42 | 0.55 |
| 26:DA:2298:A:H1' | 26:DA:2321:G:H21 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DA:2848:G:C8 | 40:DT:97:ALA:HB2 | 2.42 | 0.55 |
| 28:DD:10:THR:OG1 | 28:DD:13:ARG:HG2 | 2.07 | 0.55 |
| 36:DP:48:PRO:O | 55:D8:57:ARG:NH2 | 2.37 | 0.55 |
| 37:DQ:36:ALA:HA | 37:DQ:129:THR:HG22 | 1.89 | 0.55 |
| 14:AN:33:VAL:HA | 14:AN:40:CYS:HA | 1.89 | 0.54 |
| 51:B4:53:GLU:HB3 | 51:B4:54:GLY:CA | 2.37 | 0.54 |
| 26:BA:330:A:HO2' | 26:BA:331:A:H8 | 1.56 | 0.54 |
| 32:BH:154:PRO:HB3 | 32:BH:163:TYR:CZ | 2.42 | 0.54 |
| 33:BI:116:LEU:HD21 | 33:BI:119:PRO:HA | 1.89 | 0.54 |
| 1:CA:1004:A:H62 | 1:CA:1037:C:H2' | 1.71 | 0.54 |
| 1:CA:1262:C:H42 | 1:CA:1273:G:H1 | 1.53 | 0.54 |
| 1:CA:1359:C:H3' | 14:CN:35:ARG:HH21 | 1.72 | 0.54 |
| 26:DA:1011:G:OP2 | 41:DU:66:ASN:ND2 | 2.39 | 0.54 |
| 26:DA:2592:G:OP1 | 61:DA:4233:HOH:O | 2.18 | 0.54 |
| 26:DA:2595:G:N7 | 61:DA:4305:HOH:O | 2.34 | 0.54 |
| 26:DA:297:C:H2' | 26:DA:298:G:O4' | 2.07 | 0.54 |
| 1:AA:757:U:H2' | 1:AA:758:G:O4' | 2.08 | 0.54 |
| 2:AB:16:HIS:CD2 | 2:AB:17:PHE:N | 2.75 | 0.54 |
| 19:AS:67:VAL:HG21 | 51:B4:59:PHE:CD1 | 2.42 | 0.54 |
| 26:BA:2687:U:H2' | 26:BA:2688:U:O4' | 2.07 | 0.54 |
| 36:BP:50:ARG:HD3 | 55:B8:7:HIS:CD2 | 2.42 | 0.54 |
| 1:CA:1055:A:N3 | 3:CC:156:ARG:NH1 | 2.51 | 0.54 |
| 1:CA:1118:C:C2 | 1:CA:1119:C:H5 | 2.26 | 0.54 |
| 1:CA:1376:U:O5' | 7:CG:94:ARG:NH2 | 2.40 | 0.54 |
| 2:CB:63:MET:HG2 | 2:CB:225:ALA:HB1 | 1.89 | 0.54 |
| 19:CS:19:VAL:O | 19:CS:23:ASN:ND2 | 2.40 | 0.54 |
| 24:CX:19:G:H4' | 24:CX:20:U:OP2 | 2.07 | 0.54 |
| 26:DA:1796:U:H2' | 26:DA:1797:C:C6 | 2.42 | 0.54 |
| 28:DD:36:PRO:HA | 28:DD:61:LEU:HD12 | 1.88 | 0.54 |
| 30:DF:34:TRP:CE2 | 36:DP:8:PRO:HG3 | 2.43 | 0.54 |
| 37:DQ:18:LYS:O | 37:DQ:98:LYS:NZ | 2.33 | 0.54 |
| 5:AE:68:GLU:HG2 | 5:AE:70:PRO:HD3 | 1.87 | 0.54 |
| 1:CA:1118:C:H1' | 1:CA:1179:A:C5 | 2.42 | 0.54 |
| 1:CA:1165:C:N3 | 1:CA:1171:G:N2 | 2.56 | 0.54 |
| 1:CA:920:U:H2' | 1:CA:921:U:C6 | 2.41 | 0.54 |
| 4:CD:60:GLU:HG2 | 4:CD:202:LEU:HB2 | 1.89 | 0.54 |
| 26:DA:2113:U:H3 | 26:DA:2170:A:N6 | 2.03 | 0.54 |
| 31:DG:41:GLN:HE22 | 31:DG:153:ARG:HB3 | 1.71 | 0.54 |
| 31:DG:18:GLU:HG2 | 31:DG:175:LEU:HD21 | 1.89 | 0.54 |
| 33:DI:61:ARG:HA | 33:DI:61:ARG:NE | 2.22 | 0.54 |
| 36:DP:44:GLY:CA | 36:DP:45:LEU:HB2 | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:DR:95:THR:HG22 | 38:DR:116:LEU:HD23 | 1.90 | 0.54 |
| 1:AA:1026:G:C6 | 1:AA:1027:C:H1' | 2.42 | 0.54 |
| 1:AA:456:C:C2' | 1:AA:457:C:H5' | 2.37 | 0.54 |
| 12:AL:97:ARG:HB2 | 12:AL:98:TYR:CE1 | 2.42 | 0.54 |
| 26:BA:1786:A:H1' | 26:BA:1938:A:N6 | 2.22 | 0.54 |
| 26:BA:2327:A:H2' | 26:BA:2328:A:C8 | 2.42 | 0.54 |
| 26:BA:2336:A:H61 | 47:B0:43:THR:CG2 | 2.21 | 0.54 |
| 26:BA:620:G:N3 | 26:BA:620:G:H5' | 2.23 | 0.54 |
| 26:BA:671:C:N4 | 61:BA:4880:HOH:O | 2.39 | 0.54 |
| 46:BZ:75:ASN:O | 46:BZ:84:GLU:HG2 | 2.08 | 0.54 |
| 1:CA:674:G:H2' | 1:CA:675:A:H8 | 1.72 | 0.54 |
| 4:CD:70:ILE:HG12 | 4:CD:74:GLN:HB3 | 1.88 | 0.54 |
| 26:DA:1005:C:H2' | 26:DA:1006:C:C6 | 2.43 | 0.54 |
| 26:DA:1805:U:O2 | 28:DD:50:THR:HB | 2.08 | 0.54 |
| 26:DA:2533:A:OP1 | 26:DA:2665:A:O2' | 2.20 | 0.54 |
| 26:BA:323:G:C8 | 30:BF:171:PRO:HG3 | 2.43 | 0.54 |
| 26:BA:614(C):A:C4 | 30:BF:180:GLY:HA2 | 2.42 | 0.54 |
| 26:BA:729:G:C6 | 28:BD:208:LYS:HB2 | 2.42 | 0.54 |
| 26:BA:886:C:H4' | 26:BA:886:C:OP1 | 2.08 | 0.54 |
| 30:BF:18:ARG:NH2 | 30:BF:127:GLU:OE1 | 2.37 | 0.54 |
| 36:BP:97:PRO:HD3 | 36:BP:126:VAL:O | 2.08 | 0.54 |
| 42:BV:98:GLU:OE2 | 42:BV:100:ARG:NH1 | 2.41 | 0.54 |
| 1:CA:1132:C:H42 | 1:CA:1142:G:H1 | 1.55 | 0.54 |
| 1:CA:991:U:C4 | 1:CA:1212:U:H1' | 2.42 | 0.54 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:H6 | 1.73 | 0.54 |
| 1:CA:430:A:P | 4:CD:22:LYS:HZ1 | 2.31 | 0.54 |
| 2:CB:16:HIS:HB2 | 2:CB:204:ASN:CB | 2.30 | 0.54 |
| 4:CD:150:GLU:OE2 | 4:CD:151:LYS:N | 2.41 | 0.54 |
| 50:D3:3:ARG:HH21 | 50:D3:36:VAL:HG11 | 1.73 | 0.54 |
| 51:D4:59:PHE:HA | 51:D4:61:ARG:N | 2.23 | 0.54 |
| 52:D5:49:CYS:O | 52:D5:56:LYS:NZ | 2.40 | 0.54 |
| 26:DA:590:A:OP1 | 30:DF:95:ARG:NH1 | 2.41 | 0.54 |
| 30:DF:165:ARG:HG2 | 30:DF:168:ARG:HH21 | 1.73 | 0.54 |
| 37:DQ:1:MET:HB2 | 37:DQ:44:ALA:HB1 | 1.89 | 0.54 |
| 2:AB:178:ARG:HH22 | 8:AH:68:ARG:HH12 | 1.55 | 0.54 |
| 4:AD:178:VAL:HG12 | 4:AD:179:GLU:H | 1.72 | 0.54 |
| 7:AG:152:ALA:O | 7:AG:155:ARG:HB3 | 2.07 | 0.54 |
| 10:AJ:5:ARG:NH2 | 10:AJ:73:ASP:OD2 | 2.24 | 0.54 |
| 26:BA:100:G:O2' | 49:B2:7:ARG:NH2 | 2.40 | 0.54 |
| 1:CA:1348:U:OP2 | 1:CA:1373:G:N2 | 2.32 | 0.54 |
| 1:CA:266:G:H5'' | 1:CA:268:C:H41 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:185:ILE:HG22 | 2:CB:199:TYR:HB2 | 1.88 | 0.54 |
| 23:CW:7:A:H5' | 23:CW:8:4SU:H5 | 1.88 | 0.54 |
| 24:CX:23:C:H2' | 24:CX:24:U:C6 | 2.43 | 0.54 |
| 26:DA:1639:U:OP1 | 61:DA:4007:HOH:O | 2.19 | 0.54 |
| 31:DG:44:GLY:N | 31:DG:88:ILE:O | 2.40 | 0.54 |
| 26:DA:954:G:H5'' | 37:DQ:13:GLN:HB3 | 1.89 | 0.54 |
| 37:DQ:32:TYR:HB2 | 37:DQ:106:VAL:HG23 | 1.88 | 0.54 |
| 1:AA:1399:C:C2 | 1:AA:1502:A:N6 | 2.76 | 0.54 |
| 5:AE:78:HIS:HD1 | 8:AH:104:ARG:HD2 | 1.72 | 0.54 |
| 6:AF:69:GLU:O | 6:AF:72:VAL:HG12 | 2.08 | 0.54 |
| 25:AY:63:G:H2' | 25:AY:64:A:O4' | 2.08 | 0.54 |
| 26:BA:1779:U:H2' | 61:BA:5029:HOH:O | 2.07 | 0.54 |
| 26:BA:2815:C:H5' | 52:B5:29:THR:HG21 | 1.88 | 0.54 |
| 26:BA:2445:G:OP1 | 30:BF:74:ARG:NH2 | 2.41 | 0.54 |
| 34:BN:75:TYR:CE2 | 34:BN:77:GLY:HA2 | 2.43 | 0.54 |
| 1:CA:1153:C:H42 | 1:CA:1154:G:N2 | 2.04 | 0.54 |
| 2:CB:12:GLU:O | 2:CB:15:VAL:N | 2.34 | 0.54 |
| 11:CK:48:ILE:HD11 | 11:CK:64:ALA:HA | 1.89 | 0.54 |
| 26:DA:2139:C:C4 | 26:DA:2153:G:C2 | 2.96 | 0.54 |
| 26:DA:2285:C:OP2 | 53:D6:6:ARG:NH1 | 2.38 | 0.54 |
| 26:DA:370:G:OP2 | 61:DA:3787:HOH:O | 2.18 | 0.54 |
| 33:DI:27:ARG:HD2 | 48:D1:71:TYR:CE2 | 2.43 | 0.54 |
| 38:DR:21:TYR:OH | 38:DR:43:GLU:HG2 | 2.08 | 0.54 |
| 1:AA:1298:C:H4' | 1:AA:1299:A:H5'' | 1.89 | 0.54 |
| 1:AA:79:G:N1 | 1:AA:90:U:N3 | 2.56 | 0.54 |
| 19:AS:65:ASN:HD22 | 19:AS:65:ASN:N | 2.05 | 0.54 |
| 37:BQ:85:LYS:HB2 | 47:B0:7:LEU:HD12 | 1.90 | 0.54 |
| 26:BA:1044:G:HO2' | 26:BA:1111:A:H61 | 1.56 | 0.54 |
| 26:BA:1799:G:H4' | 26:BA:1800:C:H5'' | 1.89 | 0.54 |
| 1:CA:1003:G:H2' | 1:CA:1004:A:H1' | 1.89 | 0.54 |
| 1:CA:1245:A:H2' | 1:CA:1246:C:O4' | 2.07 | 0.54 |
| 26:DA:1859:A:N6 | 26:DA:1883:G:O2' | 2.41 | 0.54 |
| 26:DA:2552:U:OP2 | 61:DA:4518:HOH:O | 2.18 | 0.54 |
| 26:DA:305:U:H2' | 26:DA:306:U:C6 | 2.42 | 0.54 |
| 35:DO:80:ASP:OD1 | 40:DT:64:ARG:NH2 | 2.41 | 0.54 |
| 1:AA:1258:G:O2' | 1:AA:1259:C:H5' | 2.08 | 0.54 |
| 1:AA:560:U:O2' | 1:AA:561:U:OP2 | 2.21 | 0.54 |
| 13:AM:57:ARG:O | 13:AM:61:GLU:HG2 | 2.08 | 0.54 |
| 2:CB:105:PHE:CE1 | 2:CB:155:LEU:HD12 | 2.42 | 0.54 |
| 3:CC:130:VAL:O | 3:CC:134:ILE:HG12 | 2.07 | 0.54 |
| 4:CD:108:LEU:HD13 | 4:CD:174:LEU:HD13 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:CM:107:ALA:HB3 | 13:CM:111:LYS:HD2 | 1.89 | 0.54 |
| 26:DA:1010:A:OP2 | 61:DA:4178:HOH:O | 2.18 | 0.54 |
| 26:DA:1514:U:H2' | 26:DA:1515:G:H8 | 1.73 | 0.54 |
| 26:DA:2153:G:C6 | 26:DA:2154:G:C6 | 2.96 | 0.54 |
| 26:DA:289:A:H2' | 26:DA:290:G:O4' | 2.08 | 0.54 |
| 30:DF:101:LEU:O | 30:DF:106:ARG:NH1 | 2.34 | 0.54 |
| 30:DF:192:LEU:HD13 | 30:DF:194:MET:HE2 | 1.89 | 0.54 |
| 32:DH:3:ARG:NH2 | 32:DH:5:GLY:H | 2.05 | 0.54 |
| 46:DZ:69:THR:HG22 | 46:DZ:90:VAL:HA | 1.90 | 0.54 |
| 1:AA:1316:G:N2 | 1:AA:1319:A:H5'' | 2.17 | 0.54 |
| 1:AA:950:U:H2' | 1:AA:951:G:H8 | 1.73 | 0.54 |
| 2:AB:69:LEU:HD12 | 2:AB:91:PRO:HB2 | 1.90 | 0.54 |
| 12:AL:53:ARG:HG3 | 12:AL:93:LEU:HD21 | 1.90 | 0.54 |
| 25:AY:58:A:HO2' | 25:AY:60:U:H5 | 1.55 | 0.54 |
| 26:BA:2101:G:H2' | 26:BA:2102:U:C6 | 2.43 | 0.54 |
| 26:BA:2141:G:N7 | 26:BA:2151:G:N2 | 2.56 | 0.54 |
| 26:BA:2690:C:OP1 | 38:BR:17:ARG:NH1 | 2.38 | 0.54 |
| 26:BA:910:A:H62 | 37:BQ:12:GLN:HA | 1.73 | 0.54 |
| 34:BN:21:LYS:HE3 | 34:BN:140:VAL:OXT | 2.08 | 0.54 |
| 1:CA:1120:G:O6 | 1:CA:1154:G:N2 | 2.41 | 0.54 |
| 1:CA:1510:U:H2' | 1:CA:1511:G:C8 | 2.42 | 0.54 |
| 2:CB:115:LEU:HD11 | 2:CB:153:ARG:HD2 | 1.90 | 0.54 |
| 9:CI:23:ASN:HD22 | 9:CI:23:ASN:N | 2.06 | 0.54 |
| 19:CS:48:THR:HG22 | 19:CS:61:TYR:HA | 1.88 | 0.54 |
| 25:CY:5:G:H1 | 25:CY:68:C:N4 | 2.06 | 0.54 |
| 31:DG:39:ILE:HB | 31:DG:92:VAL:HG13 | 1.90 | 0.54 |
| 1:AA:78:G:N1 | 1:AA:91:C:C4 | 2.76 | 0.53 |
| 4:AD:173:TRP:NE1 | 4:AD:193:ASP:OD2 | 2.38 | 0.53 |
| 5:AE:80:ILE:HG22 | 5:AE:91:LEU:HB2 | 1.89 | 0.53 |
| 25:AY:19:G:H4' | 25:AY:20:U:OP2 | 2.06 | 0.53 |
| 51:B4:57:GLU:CB | 51:B4:58:ARG:HA | 2.38 | 0.53 |
| 26:BA:1230:C:H2' | 26:BA:1231:G:C8 | 2.43 | 0.53 |
| 26:BA:226:G:H21 | 26:BA:228:A:H62 | 1.56 | 0.53 |
| 31:BG:170:ARG:NH2 | 31:BG:182:LYS:O | 2.41 | 0.53 |
| 1:CA:1033:G:C2' | 1:CA:1034:G:H5' | 2.38 | 0.53 |
| 10:CJ:81:THR:HA | 10:CJ:84:GLN:HB2 | 1.89 | 0.53 |
| 16:CP:51:VAL:HG12 | 16:CP:53:VAL:N | 2.19 | 0.53 |
| 26:DA:2144:U:H1' | 26:DA:2148:G:N2 | 2.23 | 0.53 |
| 1:AA:202:U:O2' | 1:AA:203:U:O5' | 2.13 | 0.53 |
| 19:AS:65:ASN:HA | 51:B4:58:ARG:HG3 | 1.89 | 0.53 |
| 26:BA:1378:A:OP1 | 54:B7:10:ARG:NH2 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BA:1019:U:HO2' | 26:BA:1021:A:H2 | 1.55 | 0.53 |
| 26:BA:2142:C:O2' | 26:BA:2143:C:H5' | 2.08 | 0.53 |
| 26:BA:2151:G:H2' | 26:BA:2152:G:C8 | 2.42 | 0.53 |
| 26:BA:614(B):G:OP1 | 61:BA:5228:HOH:O | 2.19 | 0.53 |
| 44:BX:94:GLY:N | 44:BX:95:LEU:HA | 2.23 | 0.53 |
| 1:CA:1301:U:O2' | 1:CA:1302:U:H5' | 2.08 | 0.53 |
| 1:CA:890:G:O2' | 1:CA:906:G:O6 | 2.21 | 0.53 |
| 1:CA:951:G:HO2' | 1:CA:972:C:H5 | 1.56 | 0.53 |
| 1:CA:952:U:H2' | 1:CA:953:G:C8 | 2.43 | 0.53 |
| 2:CB:186:ALA:O | 2:CB:201:ILE:N | 2.40 | 0.53 |
| 6:CF:69:GLU:H | 6:CF:69:GLU:CD | 2.09 | 0.53 |
| 7:CG:72:ARG:NH1 | 7:CG:142:GLU:OE2 | 2.41 | 0.53 |
| 8:CH:51:VAL:HG11 | 8:CH:60:ARG:HH11 | 1.73 | 0.53 |
| 9:CI:6:GLY:HA3 | 9:CI:80:GLY:O | 2.09 | 0.53 |
| 23:CW:50:U:H3 | 23:CW:64:A:H2 | 1.54 | 0.53 |
| 61:CW:3102:HOH:O | 47:D0:2:ALA:N | 2.41 | 0.53 |
| 26:DA:144:C:H2' | 26:DA:145:G:C8 | 2.44 | 0.53 |
| 26:DA:973:A:H8 | 26:DA:973:A:OP1 | 1.92 | 0.53 |
| 27:DB:28:C:OP1 | 39:DS:36:TYR:OH | 2.16 | 0.53 |
| 26:BA:141:A:H8 | 26:BA:1408:C:HO2' | 1.55 | 0.53 |
| 5:CE:6:PHE:HD1 | 5:CE:36:ASP:HB3 | 1.72 | 0.53 |
| 26:DA:2261:C:O2' | 26:DA:2262:U:H5' | 2.08 | 0.53 |
| 39:DS:67:ARG:O | 39:DS:71:ARG:HG3 | 2.08 | 0.53 |
| 1:AA:1030(D):A:H2' | 1:AA:1031:G:O4' | 2.08 | 0.53 |
| 1:AA:646:U:H2' | 1:AA:647:C:C6 | 2.43 | 0.53 |
| 11:AK:99:GLN:HG2 | 11:AK:105:VAL:HG21 | 1.89 | 0.53 |
| 26:BA:197:A:N6 | 26:BA:2430:A:O2' | 2.40 | 0.53 |
| 26:BA:642:G:H21 | 26:BA:646:A:H2 | 1.56 | 0.53 |
| 26:BA:667:U:O2 | 55:B8:2:PRO:HD2 | 2.08 | 0.53 |
| 31:BG:161:THR:HG22 | 31:BG:163:ALA:H | 1.73 | 0.53 |
| 26:BA:2659:G:O2' | 32:BH:175:LYS:NZ | 2.41 | 0.53 |
| 1:CA:1250:A:N3 | 1:CA:1370:G:O2' | 2.35 | 0.53 |
| 20:CT:36:LEU:HD12 | 20:CT:55:ILE:HG23 | 1.90 | 0.53 |
| 1:CA:1457:G:OP1 | 20:CT:39:LYS:NZ | 2.41 | 0.53 |
| 26:DA:2590:A:OP2 | 28:DD:238:GLY:HA2 | 2.08 | 0.53 |
| 1:AA:1028:C:H2' | 1:AA:1029:C:C4' | 2.37 | 0.53 |
| 1:AA:1118:C:H2' | 1:AA:1119:C:C6 | 2.43 | 0.53 |
| 1:AA:1270:C:OP2 | 21:AU:24:ARG:NH2 | 2.42 | 0.53 |
| 8:AH:86:ILE:HG13 | 8:AH:133:LEU:HD22 | 1.89 | 0.53 |
| 20:AT:27:LYS:O | 20:AT:31:SER:OG | 2.27 | 0.53 |
| 26:BA:71:A:N7 | 44:BX:31:HIS:HE1 | 2.05 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BI:27:ARG:HD2 | 48:B1:71:TYR:CE1 | 2.44 | 0.53 |
| 46:BZ:28:MET:HE1 | 46:BZ:67:LEU:HD12 | 1.91 | 0.53 |
| 1:CA:1057:G:O3' | 3:CC:197:GLY:HA3 | 2.09 | 0.53 |
| 1:CA:1152:A:H2' | 1:CA:1153:C:H6 | 1.73 | 0.53 |
| 1:CA:243:A:H4' | 1:CA:244:U:H5'' | 1.90 | 0.53 |
| 3:CC:52:LEU:HD13 | 3:CC:118:GLN:HE22 | 1.73 | 0.53 |
| 9:CI:17:VAL:HG23 | 9:CI:63:ILE:HG12 | 1.89 | 0.53 |
| 25:CY:70:G:H2' | 25:CY:71:G:H5' | 1.91 | 0.53 |
| 26:DA:2128:C:H5' | 26:DA:2173:A:N3 | 2.23 | 0.53 |
| 26:DA:2364:C:OP1 | 47:D0:55:ARG:NH1 | 2.41 | 0.53 |
| 39:DS:77:ALA:HB1 | 39:DS:82:ILE:HB | 1.89 | 0.53 |
| 35:DO:120:GLU:HB2 | 40:DT:68:TYR:HE2 | 1.74 | 0.53 |
| 46:DZ:50:GLN:OE1 | 46:DZ:50:GLN:N | 2.34 | 0.53 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:H62 | 1.57 | 0.53 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.44 | 0.53 |
| 26:BA:1107:G:H2' | 26:BA:1107:G:N3 | 2.23 | 0.53 |
| 26:BA:1047:G:H2' | 26:BA:1110:G:H22 | 1.74 | 0.53 |
| 30:BF:20:LEU:HD22 | 30:BF:21:ALA:H | 1.73 | 0.53 |
| 1:CA:1166:G:H5' | 1:CA:1168:A:OP2 | 2.08 | 0.53 |
| 1:CA:316:G:OP2 | 1:CA:351:G:O2' | 2.24 | 0.53 |
| 1:CA:97:G:O2' | 1:CA:98:G:H5'' | 2.08 | 0.53 |
| 25:CY:68:C:C2' | 25:CY:69:G:H5' | 2.38 | 0.53 |
| 53:D6:35:GLU:OE2 | 53:D6:50:ARG:NH1 | 2.42 | 0.53 |
| 26:DA:1593:G:H2' | 26:DA:1594:G:H8 | 1.73 | 0.53 |
| 26:DA:2302:G:H2' | 26:DA:2303:G:H5' | 1.91 | 0.53 |
| 23:CW:76:F3N:O2' | 26:DA:2585:U:O4 | 2.15 | 0.53 |
| 31:DG:97:ASP:HA | 31:DG:100:TRP:HD1 | 1.73 | 0.53 |
| 40:DT:28:VAL:HG13 | 40:DT:86:ILE:HG23 | 1.89 | 0.53 |
| 41:DU:92:ARG:HA | 41:DU:95:LEU:HB2 | 1.91 | 0.53 |
| 3:AC:152:ILE:HB | 3:AC:199:LYS:HB2 | 1.91 | 0.53 |
| 20:AT:86:ARG:O | 20:AT:90:GLN:NE2 | 2.37 | 0.53 |
| 25:AY:60:U:H5'' | 25:AY:61:C:C5 | 2.43 | 0.53 |
| 26:BA:1688:U:O2 | 26:BA:1700:A:H5' | 2.09 | 0.53 |
| 26:BA:2887:U:H2' | 26:BA:2888:C:C6 | 2.44 | 0.53 |
| 26:BA:624:C:O2' | 26:BA:657:U:OP1 | 2.24 | 0.53 |
| 30:BF:197:ASP:OD1 | 30:BF:197:ASP:N | 2.41 | 0.53 |
| 31:BG:179:PRO:HB2 | 51:B4:42:PHE:HE1 | 1.73 | 0.53 |
| 41:BU:66:ASN:O | 41:BU:70:ARG:HG3 | 2.09 | 0.53 |
| 1:CA:1173:G:H2' | 1:CA:1174:G:H8 | 1.73 | 0.53 |
| 1:CA:1376:U:H2' | 1:CA:1377:A:C8 | 2.43 | 0.53 |
| 1:CA:142:G:H2' | 1:CA:143:A:C8 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:876:G:O5' | 8:CH:14:ARG:NH1 | 2.41 | 0.53 |
| 12:CL:32:PHE:HB3 | 12:CL:84:LEU:HD11 | 1.89 | 0.53 |
| 18:CR:53:ARG:HA | 18:CR:56:THR:OG1 | 2.08 | 0.53 |
| 26:DA:1309:G:H3' | 54:D7:9:ARG:HH12 | 1.73 | 0.53 |
| 26:DA:1645:G:H5'' | 26:DA:1646:C:H5' | 1.89 | 0.53 |
| 26:DA:2430:A:H2' | 26:DA:2430:A:N3 | 2.23 | 0.53 |
| 27:DB:110:G:H2' | 27:DB:111:G:H5' | 1.90 | 0.53 |
| 32:DH:154:PRO:HB3 | 32:DH:163:TYR:CE2 | 2.43 | 0.53 |
| 34:DN:67:LEU:O | 34:DN:88:GLU:HG2 | 2.08 | 0.53 |
| 35:DO:77:ILE:HB | 40:DT:74:ARG:HD3 | 1.91 | 0.53 |
| 40:DT:60:THR:HG22 | 40:DT:77:PRO:HA | 1.90 | 0.53 |
| 1:AA:1238:A:OP2 | 61:AA:4136:HOH:O | 2.18 | 0.53 |
| 15:AO:39:LEU:HD13 | 15:AO:56:LEU:HB2 | 1.91 | 0.53 |
| 17:AQ:53:LEU:HD23 | 17:AQ:82:MET:HE1 | 1.91 | 0.53 |
| 23:AW:47:U:H5' | 23:AW:47:U:C6 | 2.44 | 0.53 |
| 26:BA:242:G:C8 | 55:B8:5:LYS:HG2 | 2.44 | 0.53 |
| 26:BA:969:U:H2' | 26:BA:970:C:C6 | 2.44 | 0.53 |
| 1:CA:1119:C:C4 | 1:CA:1154:G:O6 | 2.62 | 0.53 |
| 2:CB:70:PHE:HE1 | 2:CB:163:PHE:HD2 | 1.56 | 0.53 |
| 4:CD:159:ARG:O | 4:CD:163:GLU:N | 2.40 | 0.53 |
| 4:CD:78:LEU:HD22 | 4:CD:96:LEU:HB3 | 1.90 | 0.53 |
| 1:CA:522:C:H41 | 12:CL:53:ARG:NH2 | 2.07 | 0.53 |
| 26:DA:1405:U:H2' | 26:DA:1406:U:C6 | 2.43 | 0.53 |
| 26:DA:1839:G:C8 | 26:DA:1927:A:H1' | 2.44 | 0.53 |
| 26:DA:2127:G:N2 | 26:DA:2161:C:C2 | 2.77 | 0.53 |
| 26:DA:2206:G:H5' | 26:DA:2207:G:N7 | 2.24 | 0.53 |
| 26:DA:852:G:H2' | 26:DA:853:G:C8 | 2.44 | 0.53 |
| 26:DA:8:A:H2' | 26:DA:9:U:H6 | 1.74 | 0.53 |
| 27:DB:66:A:N6 | 27:DB:109:C:H5'' | 2.24 | 0.53 |
| 31:DG:7:LEU:HD13 | 31:DG:104:GLU:HA | 1.91 | 0.53 |
| 46:DZ:145:GLU:H | 46:DZ:148:ASP:HB2 | 1.73 | 0.53 |
| 1:AA:877:C:H5'' | 8:AH:88:LYS:HD3 | 1.90 | 0.53 |
| 26:BA:1176:G:H1' | 26:BA:1177:A:C5' | 2.33 | 0.53 |
| 26:BA:2334:G:O6 | 47:B0:74:ARG:NH2 | 2.42 | 0.53 |
| 33:BI:104:GLN:HB3 | 33:BI:105:HIS:CD2 | 2.43 | 0.53 |
| 39:BS:46:VAL:HG12 | 39:BS:48:LEU:HD12 | 1.91 | 0.53 |
| 1:CA:1023:G:C4 | 1:CA:1024:G:C8 | 2.97 | 0.53 |
| 1:CA:1133:G:C4 | 1:CA:1134:G:C8 | 2.97 | 0.53 |
| 1:CA:429:U:H3' | 4:CD:9:CYS:SG | 2.49 | 0.53 |
| 26:DA:1688:U:O2 | 26:DA:1700:A:H5' | 2.09 | 0.53 |
| 26:DA:2023:G:H5' | 26:DA:2617:C:H4' | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DA:601:C:OP1 | 30:DF:108:LYS:NZ | 2.23 | 0.53 |
| 26:DA:90:U:H1' | 26:DA:92:A:C8 | 2.44 | 0.53 |
| 1:AA:1241:G:C2' | 1:AA:1242:C:H5' | 2.38 | 0.53 |
| 1:AA:79:G:C6 | 1:AA:90:U:N3 | 2.77 | 0.53 |
| 1:AA:841:U:P | 1:AA:841:U:H6 | 2.32 | 0.53 |
| 4:AD:173:TRP:CE3 | 4:AD:174:LEU:HG | 2.44 | 0.53 |
| 27:BB:2:C:H2' | 27:BB:3:C:C6 | 2.43 | 0.53 |
| 32:BH:88:LEU:HD13 | 32:BH:130:ARG:HG2 | 1.91 | 0.53 |
| 42:BV:14:VAL:HB | 42:BV:96:ILE:HG13 | 1.90 | 0.53 |
| 1:CA:1330:U:H4' | 13:CM:23:TYR:CE1 | 2.43 | 0.53 |
| 1:CA:309:G:O2' | 1:CA:607:A:N1 | 2.42 | 0.53 |
| 2:CB:33:TYR:HB2 | 2:CB:43:ASP:HA | 1.91 | 0.53 |
| 8:CH:103:VAL:HG11 | 8:CH:136:GLU:HB2 | 1.91 | 0.53 |
| 9:CI:29:ASN:OD1 | 9:CI:64:THR:HA | 2.09 | 0.53 |
| 51:D4:58:ARG:HB3 | 51:D4:59:PHE:HD1 | 1.74 | 0.53 |
| 32:DH:26:VAL:HG21 | 32:DH:75:ALA:HB1 | 1.90 | 0.53 |
| 34:DN:4:TYR:HB2 | 41:DU:101:ARG:HH12 | 1.74 | 0.53 |
| 41:DU:79:PHE:CZ | 41:DU:83:LEU:HD21 | 2.43 | 0.53 |
| 1:AA:539:A:H2' | 1:AA:540:G:C8 | 2.42 | 0.52 |
| 8:AH:51:VAL:HG12 | 8:AH:52:ASP:H | 1.74 | 0.52 |
| 26:BA:1223:G:N2 | 26:BA:1226:A:OP2 | 2.35 | 0.52 |
| 26:BA:2611:U:C4 | 52:B5:3:LYS:HG2 | 2.44 | 0.52 |
| 1:CA:263:A:OP1 | 20:CT:79:ARG:NH1 | 2.41 | 0.52 |
| 1:CA:714:G:H2' | 1:CA:715:A:C8 | 2.44 | 0.52 |
| 1:CA:952:U:H2' | 1:CA:953:G:H8 | 1.73 | 0.52 |
| 7:CG:78:ARG:NH1 | 7:CG:154:TYR:O | 2.41 | 0.52 |
| 20:CT:13:LEU:O | 20:CT:17:ARG:HG3 | 2.09 | 0.52 |
| 27:DB:56:G:OP1 | 31:DG:27:ASN:ND2 | 2.42 | 0.52 |
| 46:DZ:111:VAL:HA | 46:DZ:115:GLY:HA3 | 1.91 | 0.52 |
| 1:AA:1035:A:H8 | 1:AA:1035:A:O5' | 1.92 | 0.52 |
| 1:AA:714:G:H2' | 1:AA:715:A:C8 | 2.44 | 0.52 |
| 23:AW:47:U:O2' | 23:AW:48:C:OP1 | 2.23 | 0.52 |
| 53:B6:35:GLU:OE2 | 53:B6:50:ARG:NH1 | 2.43 | 0.52 |
| 26:BA:2168:G:C6 | 26:BA:2171:A:H8 | 2.27 | 0.52 |
| 26:BA:271(E):U:H2' | 26:BA:271(F):C:C6 | 2.44 | 0.52 |
| 46:BZ:144:LEU:HD21 | 46:BZ:148:ASP:O | 2.08 | 0.52 |
| 1:CA:1066:C:H2' | 1:CA:1067:A:C8 | 2.45 | 0.52 |
| 1:CA:1198:G:H2' | 1:CA:1199:U:C6 | 2.45 | 0.52 |
| 1:CA:952:U:O2' | 1:CA:965:A:N6 | 2.41 | 0.52 |
| 1:CA:975:A:H4' | 1:CA:976:G:C5' | 2.35 | 0.52 |
| 3:CC:43:LEU:HD11 | 3:CC:91:LEU:HD11 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CD:208:SER:OG | 5:CE:101:ILE:HD12 | 2.09 | 0.52 |
| 25:CY:27:G:O6 | 25:CY:43:C:N3 | 2.42 | 0.52 |
| 55:D8:26:LYS:HB2 | 55:D8:44:LYS:O | 2.10 | 0.52 |
| 26:DA:589:C:H2' | 26:DA:590:A:C8 | 2.44 | 0.52 |
| 45:DY:49:VAL:HG21 | 45:DY:61:ILE:HG23 | 1.91 | 0.52 |
| 46:DZ:33:LEU:HD21 | 46:DZ:90:VAL:HG21 | 1.90 | 0.52 |
| 1:AA:662:G:H2' | 1:AA:663:A:C8 | 2.44 | 0.52 |
| 4:AD:49:ARG:NE | 4:AD:49:ARG:H | 2.07 | 0.52 |
| 5:AE:79:GLU:HG3 | 5:AE:93:PRO:HD2 | 1.92 | 0.52 |
| 19:AS:48:THR:HG22 | 19:AS:61:TYR:HA | 1.91 | 0.52 |
| 26:BA:2126:A:N3 | 26:BA:2127:G:H1' | 2.24 | 0.52 |
| 26:BA:2870:C:H2' | 26:BA:2871:C:O4' | 2.09 | 0.52 |
| 1:CA:1069:C:O2' | 1:CA:1192:C:H1' | 2.09 | 0.52 |
| 1:CA:1095:U:C4 | 1:CA:1096:C:C4 | 2.98 | 0.52 |
| 1:CA:1264:C:O2 | 1:CA:1272:G:N2 | 2.41 | 0.52 |
| 26:DA:646:A:H2' | 26:DA:647:G:O4' | 2.09 | 0.52 |
| 26:DA:885:C:H1' | 26:DA:892:G:H22 | 1.75 | 0.52 |
| 46:DZ:6:LYS:HD2 | 46:DZ:8:TYR:OH | 2.10 | 0.52 |
| 3:AC:40:ARG:O | 3:AC:44:GLU:HB2 | 2.10 | 0.52 |
| 26:BA:2110:G:C2 | 26:BA:2120:G:H1' | 2.44 | 0.52 |
| 35:BO:104:ARG:CZ | 40:BT:34:VAL:HG21 | 2.39 | 0.52 |
| 1:CA:1039:C:H2' | 1:CA:1040:U:O4' | 2.09 | 0.52 |
| 1:CA:1318:A:H5'' | 19:CS:3:ARG:NH2 | 2.20 | 0.52 |
| 1:CA:302:G:N3 | 1:CA:556:C:H4' | 2.24 | 0.52 |
| 1:CA:56:U:H2' | 1:CA:57:G:H8 | 1.74 | 0.52 |
| 26:DA:83:G:OP1 | 45:DY:95:LYS:NZ | 2.32 | 0.52 |
| 27:DB:66:A:N6 | 27:DB:108:U:H3' | 2.25 | 0.52 |
| 29:DE:111:ARG:HA | 38:DR:1:MET:SD | 2.50 | 0.52 |
| 39:DS:14:VAL:O | 39:DS:18:ILE:HG12 | 2.10 | 0.52 |
| 46:DZ:105:VAL:N | 46:DZ:139:VAL:O | 2.39 | 0.52 |
| 1:AA:1118:C:OP1 | 9:AI:104:ARG:NH1 | 2.41 | 0.52 |
| 1:AA:626:U:H2' | 1:AA:627:G:C8 | 2.45 | 0.52 |
| 16:AP:58:TYR:O | 16:AP:62:VAL:HG23 | 2.09 | 0.52 |
| 31:BG:48:GLU:HA | 31:BG:51:ARG:HG2 | 1.91 | 0.52 |
| 1:CA:1004:A:N6 | 1:CA:1037:C:C2 | 2.77 | 0.52 |
| 1:CA:1286:A:N1 | 21:CU:18:TYR:OH | 2.42 | 0.52 |
| 3:CC:119:ARG:HG2 | 3:CC:123:GLN:HE21 | 1.75 | 0.52 |
| 13:CM:29:ARG:HG3 | 13:CM:64:TRP:CH2 | 2.45 | 0.52 |
| 25:CY:9:A:H5' | 25:CY:46:7MG:H1' | 1.91 | 0.52 |
| 26:DA:2815:C:C5' | 52:D5:29:THR:HG21 | 2.39 | 0.52 |
| 26:DA:2117:A:O2' | 26:DA:2118:U:H5'' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DA:2126:A:N6 | 26:DA:2172:U:H3' | 2.24 | 0.52 |
| 26:DA:2128:C:H2' | 26:DA:2129:C:O4' | 2.10 | 0.52 |
| 26:DA:2350:C:H2' | 26:DA:2351:G:O4' | 2.10 | 0.52 |
| 26:DA:729:G:H5' | 26:DA:730:C:H5'' | 1.91 | 0.52 |
| 27:DB:110:G:C2' | 27:DB:111:G:H5' | 2.39 | 0.52 |
| 28:DD:175:LEU:HD12 | 28:DD:185:VAL:HG21 | 1.92 | 0.52 |
| 35:DO:73:ASP:HB2 | 40:DT:82:LEU:HD13 | 1.92 | 0.52 |
| 1:AA:1279:A:H4' | 1:AA:1281:U:H5 | 1.75 | 0.52 |
| 1:AA:946:A:O2' | 1:AA:1333:A:N3 | 2.35 | 0.52 |
| 20:AT:9:ASN:O | 20:AT:10:LEU:HB2 | 2.10 | 0.52 |
| 53:B6:6:ARG:NE | 53:B6:24:GLU:OE1 | 2.32 | 0.52 |
| 53:B6:13:CYS:SG | 53:B6:47:THR:HG21 | 2.49 | 0.52 |
| 26:BA:1028:A:H61 | 26:BA:1125:G:H2' | 1.75 | 0.52 |
| 26:BA:2173:A:H3' | 26:BA:2174:C:C6 | 2.45 | 0.52 |
| 26:BA:848:G:C4 | 26:BA:933:A:H8 | 2.26 | 0.52 |
| 31:BG:143:GLU:O | 51:B4:28:LYS:NZ | 2.32 | 0.52 |
| 37:BQ:30:GLY:HA2 | 37:BQ:107:ALA:HB2 | 1.92 | 0.52 |
| 26:BA:1153:C:OP1 | 41:BU:92:ARG:NH1 | 2.43 | 0.52 |
| 45:BY:35:TYR:CE2 | 45:BY:69:ALA:HB3 | 2.44 | 0.52 |
| 2:CB:100:GLY:O | 2:CB:108:ILE:HD11 | 2.10 | 0.52 |
| 2:CB:158:LEU:HD23 | 2:CB:182:ILE:HD11 | 1.91 | 0.52 |
| 3:CC:125:GLU:HG3 | 3:CC:190:ARG:O | 2.10 | 0.52 |
| 9:CI:9:ARG:O | 9:CI:104:ARG:HG3 | 2.09 | 0.52 |
| 25:CY:33:U:C3' | 25:CY:34:G:H5'' | 2.40 | 0.52 |
| 26:DA:200:U:O4 | 26:DA:250:G:N2 | 2.43 | 0.52 |
| 34:DN:38:HIS:ND1 | 34:DN:39:ARG:HG3 | 2.25 | 0.52 |
| 1:AA:1144:G:N2 | 1:AA:1146:A:H62 | 2.08 | 0.52 |
| 1:AA:353:A:H5' | 1:AA:353:A:H8 | 1.74 | 0.52 |
| 1:AA:950:U:H2' | 1:AA:951:G:C8 | 2.45 | 0.52 |
| 8:AH:121:ASP:OD2 | 8:AH:121:ASP:N | 2.43 | 0.52 |
| 30:BF:53:THR:CG2 | 30:BF:55:GLY:H | 2.22 | 0.52 |
| 35:BO:73:ASP:HB2 | 40:BT:82:LEU:HD13 | 1.91 | 0.52 |
| 1:CA:1353:G:OP1 | 21:CU:10:ARG:NH1 | 2.43 | 0.52 |
| 1:CA:171:A:H2' | 1:CA:172:A:C8 | 2.45 | 0.52 |
| 1:CA:448:A:P | 1:CA:485:G:H22 | 2.33 | 0.52 |
| 18:CR:70:ILE:HG23 | 18:CR:79:LEU:HD12 | 1.92 | 0.52 |
| 26:DA:79:G:H1 | 26:DA:107:C:H42 | 1.58 | 0.52 |
| 26:DA:2155:G:H2' | 26:DA:2156:G:O4' | 2.10 | 0.52 |
| 26:DA:77:C:H42 | 26:DA:109:G:H1 | 1.57 | 0.52 |
| 27:DB:17:C:O2 | 27:DB:67:G:N2 | 2.35 | 0.52 |
| 30:DF:184:TYR:O | 30:DF:188:ARG:HG3 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1125:U:H4' | 10:AJ:5:ARG:NH2 | 2.24 | 0.52 |
| 1:AA:677:U:H3 | 1:AA:713:G:H22 | 1.58 | 0.52 |
| 6:AF:10:LEU:HB2 | 6:AF:59:TYR:HB3 | 1.92 | 0.52 |
| 23:AW:52:G:H4' | 37:BQ:56:ARG:CZ | 2.39 | 0.52 |
| 24:AX:21:A:N6 | 24:AX:46:G:H2' | 2.24 | 0.52 |
| 26:BA:892:G:H3' | 26:BA:893:C:H6 | 1.74 | 0.52 |
| 29:BE:111:ARG:HG3 | 29:BE:160:TYR:CD2 | 2.44 | 0.52 |
| 26:BA:1653:G:H3' | 38:BR:2:ARG:HD3 | 1.90 | 0.52 |
| 1:CA:142:G:H2' | 1:CA:143:A:H8 | 1.74 | 0.52 |
| 1:CA:457:C:H2' | 1:CA:458:C:H6 | 1.75 | 0.52 |
| 26:DA:1341:U:OP1 | 26:DA:1397:U:N3 | 2.35 | 0.52 |
| 26:DA:1608:A:H1' | 26:DA:1610:A:OP2 | 2.10 | 0.52 |
| 26:DA:1827:C:OP2 | 28:DD:222:ARG:NH1 | 2.43 | 0.52 |
| 26:DA:263:C:H2' | 26:DA:264:C:O4' | 2.10 | 0.52 |
| 26:DA:528:A:OP2 | 34:DN:114:ARG:NH1 | 2.43 | 0.52 |
| 39:DS:34:HIS:ND1 | 39:DS:53:SER:OG | 2.35 | 0.52 |
| 1:AA:1024:G:H2' | 1:AA:1025:U:H5'' | 1.92 | 0.52 |
| 1:AA:69:G:H2' | 1:AA:70:G:H8 | 1.74 | 0.52 |
| 4:AD:128:VAL:HG12 | 4:AD:129:ASN:ND2 | 2.25 | 0.52 |
| 1:AA:619:U:N3 | 4:AD:134:ASP:OD2 | 2.38 | 0.52 |
| 9:AI:9:ARG:H | 9:AI:79:LEU:HD23 | 1.75 | 0.52 |
| 26:BA:1406:U:H2' | 26:BA:1407:C:C6 | 2.45 | 0.52 |
| 26:BA:639:U:H2' | 26:BA:640:C:C6 | 2.45 | 0.52 |
| 1:CA:1030(A):G:N2 | 1:CA:1030(C):G:H3' | 2.25 | 0.52 |
| 1:CA:1513:A:H2' | 1:CA:1514:C:C6 | 2.45 | 0.52 |
| 1:CA:346:G:OP1 | 40:DT:41:ARG:NH2 | 2.42 | 0.52 |
| 3:CC:22:TRP:CB | 3:CC:59:ARG:HB2 | 2.40 | 0.52 |
| 12:CL:34:ARG:HG3 | 12:CL:105:TYR:CE2 | 2.44 | 0.52 |
| 19:CS:17:GLU:O | 19:CS:21:GLU:N | 2.36 | 0.52 |
| 25:CY:18:G:N2 | 25:CY:55:PSU:C4 | 2.77 | 0.52 |
| 56:D9:17:ILE:HG22 | 56:D9:24:TYR:HB2 | 1.92 | 0.52 |
| 26:DA:2114:A:N6 | 26:DA:2115:G:H21 | 2.08 | 0.52 |
| 26:DA:637:A:H8 | 36:DP:117:GLU:HG3 | 1.75 | 0.52 |
| 1:AA:347:G:HO2' | 1:AA:348:G:P | 2.33 | 0.52 |
| 1:AA:582:U:OP1 | 15:AO:64:ARG:NH1 | 2.43 | 0.52 |
| 12:AL:77:LEU:HD21 | 12:AL:107:ALA:HA | 1.92 | 0.52 |
| 13:AM:15:VAL:HB | 13:AM:34:LEU:HD11 | 1.92 | 0.52 |
| 52:B5:55:ARG:NH1 | 52:B5:57:VAL:HG22 | 2.25 | 0.52 |
| 28:BD:101:GLU:OE1 | 28:BD:103:ARG:NH1 | 2.42 | 0.52 |
| 29:BE:77:ILE:HD13 | 29:BE:195:LEU:HD12 | 1.92 | 0.52 |
| 1:CA:545:C:O2' | 1:CA:549:C:OP1 | 2.22 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:CF:3:ARG:HD3 | 6:CF:64:GLN:NE2 | 2.25 | 0.52 |
| 12:CL:69:TYR:HE2 | 12:CL:71:PRO:HA | 1.73 | 0.52 |
| 20:CT:56:MET:HE3 | 20:CT:85:MET:HA | 1.90 | 0.52 |
| 22:CV:14:A:C2 | 22:CV:15:A:C4 | 2.98 | 0.52 |
| 26:DA:93:G:H2' | 26:DA:94:C:H6 | 1.74 | 0.52 |
| 30:DF:32:LEU:O | 30:DF:36:VAL:HG23 | 2.09 | 0.52 |
| 38:DR:74:LYS:HG2 | 38:DR:77:ARG:HH21 | 1.74 | 0.52 |
| 40:DT:51:ARG:HG3 | 40:DT:98:LYS:HZ3 | 1.75 | 0.52 |
| 42:DV:21:ARG:HG2 | 42:DV:91:TYR:CD2 | 2.45 | 0.52 |
| 43:DW:60:ASN:HD22 | 43:DW:60:ASN:N | 2.07 | 0.52 |
| 1:AA:1022:G:H2' | 1:AA:1023:G:C8 | 2.44 | 0.51 |
| 8:AH:112:LEU:HA | 8:AH:134:ILE:HG12 | 1.92 | 0.51 |
| 25:AY:13:C:H2' | 25:AY:14:A:C8 | 2.45 | 0.51 |
| 26:BA:1028:A:N6 | 26:BA:1125:G:H2' | 2.25 | 0.51 |
| 26:BA:1345:C:OP2 | 61:BA:4016:HOH:O | 2.18 | 0.51 |
| 26:BA:2875:C:OP1 | 40:BT:3:ARG:NH1 | 2.42 | 0.51 |
| 46:BZ:29:TYR:HB3 | 46:BZ:34:ASN:HD22 | 1.75 | 0.51 |
| 46:BZ:92:SER:O | 46:BZ:130:PRO:HG2 | 2.10 | 0.51 |
| 2:CB:135:GLN:O | 2:CB:139:LYS:HB2 | 2.10 | 0.51 |
| 1:CA:1250:A:H4' | 9:CI:68:GLY:N | 2.25 | 0.51 |
| 23:CW:76:F3N:N | 24:CX:76:31H:O2' | 2.43 | 0.51 |
| 24:CX:67:C:C2' | 24:CX:68:C:H5' | 2.40 | 0.51 |
| 26:DA:1032:A:H2 | 26:DA:1122:G:H22 | 1.59 | 0.51 |
| 26:DA:2124:G:H1 | 26:DA:2174:C:H42 | 1.58 | 0.51 |
| 26:DA:2400:G:H2' | 26:DA:2401:U:H6 | 1.74 | 0.51 |
| 26:DA:323:G:O2' | 26:DA:1205:U:N3 | 2.35 | 0.51 |
| 31:DG:106:LEU:O | 31:DG:111:LEU:HD22 | 2.10 | 0.51 |
| 31:DG:48:GLU:HA | 31:DG:51:ARG:HG2 | 1.90 | 0.51 |
| 26:DA:956:G:H5' | 37:DQ:77:LYS:HD2 | 1.92 | 0.51 |
| 1:AA:524:G:H2' | 1:AA:525:C:C6 | 2.46 | 0.51 |
| 1:AA:606:G:N2 | 1:AA:631:G:N7 | 2.58 | 0.51 |
| 24:AX:61:C:H2' | 24:AX:62:C:H6 | 1.76 | 0.51 |
| 24:AX:66:C:H2' | 24:AX:67:C:O4' | 2.10 | 0.51 |
| 53:B6:14:THR:HG21 | 53:B6:48:VAL:HG22 | 1.92 | 0.51 |
| 26:BA:86:C:H4' | 26:BA:104:U:H1' | 1.92 | 0.51 |
| 26:BA:2191:G:H5' | 26:BA:2191:G:H8 | 1.74 | 0.51 |
| 23:AW:19:G:C5 | 26:BA:882:G:H4' | 2.45 | 0.51 |
| 39:BS:11:LYS:O | 39:BS:15:ARG:HG3 | 2.10 | 0.51 |
| 43:BW:2:GLU:OE2 | 43:BW:72:LYS:HE2 | 2.10 | 0.51 |
| 1:CA:1028:C:H2' | 1:CA:1029:C:C6 | 2.45 | 0.51 |
| 1:CA:1343:G:H2' | 1:CA:1344:C:C6 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1359:C:H3' | 14:CN:35:ARG:NH2 | 2.25 | 0.51 |
| 2:CB:219:VAL:O | 2:CB:222:ILE:HG12 | 2.11 | 0.51 |
| 4:CD:18:LYS:NZ | 4:CD:31:CYS:SG | 2.84 | 0.51 |
| 8:CH:15:ASN:O | 8:CH:19:VAL:HG23 | 2.10 | 0.51 |
| 19:CS:33:THR:HG21 | 19:CS:71:LEU:HD21 | 1.91 | 0.51 |
| 26:DA:1721:G:N1 | 26:DA:1739:U:OP2 | 2.43 | 0.51 |
| 26:DA:2537:U:H2' | 26:DA:2538:C:C6 | 2.45 | 0.51 |
| 26:DA:2645:G:N2 | 26:DA:2767:C:OP2 | 2.43 | 0.51 |
| 27:DB:48:A:P | 39:DS:30:ARG:HH12 | 2.33 | 0.51 |
| 29:DE:115:GLY:O | 29:DE:119:ARG:HB2 | 2.11 | 0.51 |
| 44:DX:11:PRO:HB3 | 44:DX:92:LEU:HD11 | 1.91 | 0.51 |
| 3:AC:18:TRP:HE3 | 3:AC:18:TRP:H | 1.58 | 0.51 |
| 11:AK:16:SER:O | 11:AK:35:PRO:HD3 | 2.11 | 0.51 |
| 13:AM:14:ARG:HB2 | 13:AM:17:VAL:HG23 | 1.91 | 0.51 |
| 26:BA:2110:G:OP1 | 26:BA:2118:U:N3 | 2.27 | 0.51 |
| 26:BA:2751:G:C2 | 32:BH:2:SER:HB3 | 2.45 | 0.51 |
| 26:BA:41:C:H2' | 26:BA:42:G:O4' | 2.10 | 0.51 |
| 1:CA:1218:C:H2' | 1:CA:1219:U:C6 | 2.45 | 0.51 |
| 24:CX:48:C:C2 | 24:CX:59:A:H1' | 2.45 | 0.51 |
| 26:DA:1366:A:OP1 | 48:D1:3:LYS:NZ | 2.30 | 0.51 |
| 27:DB:7:G:N1 | 27:DB:114:C:N3 | 2.48 | 0.51 |
| 27:DB:94:C:H2' | 27:DB:95:C:H6 | 1.75 | 0.51 |
| 1:AA:265:G:H2' | 1:AA:267:C:H5 | 1.74 | 0.51 |
| 1:AA:619:U:C2 | 4:AD:135:LEU:HD22 | 2.46 | 0.51 |
| 24:AX:8:4SU:H6 | 24:AX:8:4SU:O5' | 2.11 | 0.51 |
| 48:B1:51:VAL:HG11 | 48:B1:74:VAL:HG21 | 1.92 | 0.51 |
| 26:BA:330:A:H2 | 26:BA:1210:A:HO2' | 1.58 | 0.51 |
| 26:BA:687:C:H5'' | 54:B7:2:LYS:HE2 | 1.91 | 0.51 |
| 46:BZ:59:LEU:HD12 | 46:BZ:69:THR:HG21 | 1.92 | 0.51 |
| 1:CA:1134:G:N2 | 1:CA:1140:C:N3 | 2.54 | 0.51 |
| 14:CN:6:LEU:HB3 | 14:CN:23:ARG:HH22 | 1.75 | 0.51 |
| 25:CY:31:A:C2 | 25:CY:39:PSU:N3 | 2.79 | 0.51 |
| 26:DA:1325:G:OP1 | 26:DA:1647:G:O2' | 2.15 | 0.51 |
| 26:DA:708:C:H42 | 26:DA:723:G:H1 | 1.57 | 0.51 |
| 46:DZ:108:PRO:HG3 | 46:DZ:141:VAL:HB | 1.91 | 0.51 |
| 20:AT:47:GLY:HA2 | 20:AT:48:LYS:C | 2.30 | 0.51 |
| 25:AY:7:A:HO2' | 25:AY:49:C:H5' | 1.72 | 0.51 |
| 26:BA:271(M):G:H4' | 26:BA:271(N):U:OP1 | 2.10 | 0.51 |
| 26:BA:601:C:OP1 | 30:BF:108:LYS:HE3 | 2.11 | 0.51 |
| 1:CA:1011:G:N2 | 1:CA:1018:C:N3 | 2.53 | 0.51 |
| 1:CA:1028:C:O2 | 1:CA:1033:G:N1 | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1333:A:H2' | 1:CA:1334:G:O4' | 2.10 | 0.51 |
| 51:D4:59:PHE:HA | 51:D4:60:GLN:C | 2.29 | 0.51 |
| 26:DA:2394:C:OP2 | 55:D8:30:ARG:NH1 | 2.43 | 0.51 |
| 26:DA:1187:G:H5' | 42:DV:81:TYR:CE1 | 2.45 | 0.51 |
| 26:DA:392:C:H5'' | 26:DA:409:C:H5'' | 1.93 | 0.51 |
| 26:DA:528:A:C2' | 26:DA:529:A:H5'' | 2.40 | 0.51 |
| 31:DG:105:LYS:NZ | 31:DG:143:GLU:OE1 | 2.43 | 0.51 |
| 34:DN:58:ASP:OD1 | 34:DN:58:ASP:N | 2.41 | 0.51 |
| 46:DZ:59:LEU:HD21 | 46:DZ:69:THR:OG1 | 2.10 | 0.51 |
| 1:AA:309:G:O2' | 1:AA:607:A:N1 | 2.44 | 0.51 |
| 4:AD:119:GLN:HG2 | 4:AD:123:HIS:CD2 | 2.46 | 0.51 |
| 19:AS:3:ARG:NH1 | 19:AS:10:PHE:HB2 | 2.26 | 0.51 |
| 25:AY:38:A:H2' | 25:AY:39:PSU:H5'' | 1.91 | 0.51 |
| 43:BW:25:ARG:NH2 | 43:BW:74:ALA:O | 2.40 | 0.51 |
| 1:CA:1120:G:C6 | 1:CA:1154:G:C2 | 2.99 | 0.51 |
| 9:CI:125:TYR:HD1 | 9:CI:126:SER:N | 2.09 | 0.51 |
| 9:CI:85:LEU:HB3 | 9:CI:92:TYR:CD2 | 2.40 | 0.51 |
| 13:CM:71:ARG:NH1 | 13:CM:71:ARG:HG3 | 2.25 | 0.51 |
| 26:DA:667:U:O2 | 55:D8:2:PRO:HD2 | 2.10 | 0.51 |
| 26:DA:184:C:H2' | 26:DA:185:U:C6 | 2.45 | 0.51 |
| 27:DB:95:C:H2' | 27:DB:96:U:C6 | 2.46 | 0.51 |
| 28:DD:20:ASP:OD1 | 28:DD:20:ASP:N | 2.44 | 0.51 |
| 42:DV:35:LEU:HB2 | 42:DV:57:VAL:HG23 | 1.93 | 0.51 |
| 1:AA:625:G:H4' | 16:AP:16:HIS:CD2 | 2.45 | 0.51 |
| 26:BA:2183:C:H2' | 26:BA:2184:G:H8 | 1.76 | 0.51 |
| 26:BA:457:A:H5'' | 61:BA:3937:HOH:O | 2.10 | 0.51 |
| 36:BP:59:LEU:HD11 | 55:B8:10:ALA:HB2 | 1.91 | 0.51 |
| 45:BY:86:ARG:HH11 | 45:BY:100:ALA:HB1 | 1.76 | 0.51 |
| 1:CA:1347:G:HO2' | 1:CA:1373:G:H1 | 1.59 | 0.51 |
| 9:CI:28:VAL:HG22 | 9:CI:63:ILE:HB | 1.92 | 0.51 |
| 24:CX:23:C:H2' | 24:CX:24:U:H6 | 1.75 | 0.51 |
| 25:CY:33:U:H3' | 25:CY:34:G:H5'' | 1.92 | 0.51 |
| 26:DA:1246:A:OP1 | 30:DF:38:ARG:NH1 | 2.43 | 0.51 |
| 26:DA:1378:A:OP1 | 54:D7:10:ARG:NH2 | 2.44 | 0.51 |
| 26:DA:2126:A:N3 | 26:DA:2127:G:H1' | 2.26 | 0.51 |
| 26:DA:872:A:H2' | 26:DA:873:G:C8 | 2.45 | 0.51 |
| 27:DB:80:U:H2' | 27:DB:81:G:C8 | 2.44 | 0.51 |
| 32:DH:30:LYS:HG3 | 32:DH:80:SER:O | 2.10 | 0.51 |
| 41:DU:49:HIS:HA | 41:DU:52:ARG:HB3 | 1.91 | 0.51 |
| 43:DW:18:ARG:NH1 | 43:DW:76:VAL:O | 2.44 | 0.51 |
| 1:AA:1183:A:HO2' | 1:AA:1184:G:P | 2.32 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:328:C:H4' | 1:AA:329:A:H5' | 1.93 | 0.51 |
| 1:AA:841:U:C4 | 1:AA:848:C:H1' | 2.45 | 0.51 |
| 1:AA:78:G:N2 | 1:AA:91:C:C2 | 2.79 | 0.51 |
| 2:AB:137:ARG:CZ | 2:AB:137:ARG:HB3 | 2.41 | 0.51 |
| 8:AH:39:LEU:HB3 | 8:AH:45:ILE:HG12 | 1.92 | 0.51 |
| 9:AI:99:LEU:HB3 | 9:AI:101:PHE:CD1 | 2.44 | 0.51 |
| 13:AM:19:LEU:HD21 | 13:AM:56:LEU:HD11 | 1.92 | 0.51 |
| 25:AY:68:C:C2' | 25:AY:69:G:H5' | 2.40 | 0.51 |
| 33:BI:140:LEU:HD22 | 33:BI:142:VAL:HG22 | 1.92 | 0.51 |
| 1:CA:1517:G:H1' | 26:DA:1919:A:O3' | 2.11 | 0.51 |
| 3:CC:63:ASN:HB2 | 3:CC:98:ASN:HB2 | 1.93 | 0.51 |
| 6:CF:87:ARG:HH11 | 6:CF:87:ARG:HB2 | 1.75 | 0.51 |
| 11:CK:101:SER:HB2 | 11:CK:103:LEU:HD23 | 1.92 | 0.51 |
| 13:CM:25:ILE:HG23 | 13:CM:29:ARG:HB3 | 1.92 | 0.51 |
| 15:CO:39:LEU:HD13 | 15:CO:56:LEU:HB2 | 1.92 | 0.51 |
| 26:DA:71:A:N7 | 44:DX:31:HIS:HE1 | 2.08 | 0.51 |
| 1:AA:1001:A:H2' | 1:AA:1001(A):G:C8 | 2.46 | 0.51 |
| 1:AA:1022:G:H4' | 1:AA:1022:G:OP1 | 2.11 | 0.51 |
| 1:AA:1068:G:N2 | 1:AA:1191:A:N3 | 2.47 | 0.51 |
| 1:AA:1226:C:O2' | 13:AM:111:LYS:NZ | 2.41 | 0.51 |
| 13:AM:123:ALA:HB2 | 23:AW:39:PSU:H1' | 1.93 | 0.51 |
| 20:AT:76:ALA:HA | 20:AT:79:ARG:NH1 | 2.26 | 0.51 |
| 51:B4:63:TYR:CD1 | 51:B4:63:TYR:N | 2.77 | 0.51 |
| 29:BE:47:VAL:HG22 | 29:BE:84:PHE:O | 2.11 | 0.51 |
| 1:CA:1038:C:H2' | 1:CA:1039:C:H5'' | 1.91 | 0.51 |
| 1:CA:1264:C:H42 | 1:CA:1271:G:H1 | 1.58 | 0.51 |
| 8:CH:69:ARG:HG3 | 8:CH:76:PRO:HA | 1.93 | 0.51 |
| 26:DA:1410:G:H2' | 26:DA:1411:C:C6 | 2.46 | 0.51 |
| 26:DA:218:A:C2 | 26:DA:235:U:H4' | 2.46 | 0.51 |
| 27:DB:3:C:H2' | 27:DB:4:C:H6 | 1.76 | 0.51 |
| 27:DB:42:C:O2' | 31:DG:66:GLN:HG2 | 2.11 | 0.51 |
| 34:DN:30:ILE:HG22 | 34:DN:34:LEU:HD22 | 1.93 | 0.51 |
| 46:DZ:145:GLU:HG2 | 46:DZ:146:ILE:HD12 | 1.93 | 0.51 |
| 1:AA:1189:C:OP1 | 10:AJ:51:ARG:NH2 | 2.27 | 0.51 |
| 9:AI:48:GLU:HB3 | 9:AI:101:PHE:HE2 | 1.76 | 0.51 |
| 18:AR:56:THR:HB | 18:AR:58:LEU:HD22 | 1.93 | 0.51 |
| 19:AS:50:ALA:HB1 | 19:AS:57:HIS:HB3 | 1.92 | 0.51 |
| 24:AX:19:G:H3' | 24:AX:20:U:H6 | 1.76 | 0.51 |
| 26:BA:1048:A:P | 26:BA:1109:C:H42 | 2.32 | 0.51 |
| 26:BA:2319:G:N2 | 39:BS:3:ARG:HA | 2.26 | 0.51 |
| 26:BA:880:G:N2 | 26:BA:898:C:C2 | 2.79 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BA:893:C:O2' | 26:BA:894:C:H5' | 2.10 | 0.51 |
| 33:BI:96:ASP:OD1 | 33:BI:96:ASP:N | 2.44 | 0.51 |
| 26:BA:907:U:HO2' | 37:BQ:101:ARG:HH22 | 1.58 | 0.51 |
| 1:CA:160:A:H61 | 1:CA:347:G:H1' | 1.76 | 0.51 |
| 1:CA:839:U:O2' | 1:CA:840:C:OP1 | 2.27 | 0.51 |
| 1:CA:982:U:O2 | 1:CA:1222:G:N1 | 2.43 | 0.51 |
| 2:CB:19:HIS:CE1 | 2:CB:206:ASP:HB2 | 2.44 | 0.51 |
| 3:CC:125:GLU:O | 3:CC:127:ARG:NH1 | 2.41 | 0.51 |
| 8:CH:73:ASP:OD1 | 8:CH:75:ARG:HD3 | 2.10 | 0.51 |
| 26:DA:2376:A:H3' | 26:DA:2377:A:H8 | 1.76 | 0.51 |
| 26:DA:2769:C:H2' | 26:DA:2770:G:O4' | 2.11 | 0.51 |
| 26:DA:997:G:OP1 | 41:DU:92:ARG:HG2 | 2.10 | 0.51 |
| 28:DD:79:VAL:HG21 | 28:DD:111:LEU:HD11 | 1.93 | 0.51 |
| 30:DF:24:LEU:HD23 | 30:DF:115:ALA:HA | 1.93 | 0.51 |
| 30:DF:150:GLY:HA2 | 30:DF:172:TRP:CE3 | 2.46 | 0.51 |
| 32:DH:154:PRO:HB3 | 32:DH:163:TYR:CZ | 2.46 | 0.51 |
| 32:DH:20:ALA:HB3 | 32:DH:23:ARG:HG3 | 1.93 | 0.51 |
| 40:DT:24:PRO:HD3 | 40:DT:52:ILE:HD12 | 1.93 | 0.51 |
| 1:AA:46:G:O6 | 61:AA:4164:HOH:O | 2.16 | 0.50 |
| 1:AA:735:C:H2' | 1:AA:736:C:H6 | 1.76 | 0.50 |
| 1:AA:96:U:O2' | 1:AA:97:G:H5' | 2.11 | 0.50 |
| 1:AA:976:G:OP2 | 1:AA:1358:U:O2' | 2.21 | 0.50 |
| 25:AY:28:G:H2' | 25:AY:29:G:C8 | 2.46 | 0.50 |
| 52:B5:16:ARG:NH1 | 52:B5:17:ASP:OD1 | 2.44 | 0.50 |
| 40:BT:118:ARG:HG3 | 40:BT:118:ARG:NH1 | 2.14 | 0.50 |
| 1:CA:344:A:H4' | 1:CA:345:C:OP2 | 2.11 | 0.50 |
| 1:CA:707:C:H2' | 1:CA:708:C:C6 | 2.46 | 0.50 |
| 1:CA:735:C:H2' | 1:CA:736:C:C6 | 2.45 | 0.50 |
| 4:CD:12:CYS:SG | 4:CD:19:LEU:HB2 | 2.51 | 0.50 |
| 5:CE:18:ARG:HG2 | 5:CE:19:MET:N | 2.27 | 0.50 |
| 8:CH:20:TYR:CE2 | 8:CH:76:PRO:HG2 | 2.46 | 0.50 |
| 18:CR:38:GLU:O | 18:CR:41:LYS:NZ | 2.45 | 0.50 |
| 20:CT:9:ASN:O | 20:CT:10:LEU:HB2 | 2.11 | 0.50 |
| 21:CU:7:ARG:NH1 | 21:CU:21:TYR:OH | 2.43 | 0.50 |
| 23:CW:21:A:H1' | 23:CW:48:C:N4 | 2.26 | 0.50 |
| 26:DA:1299:G:OP1 | 61:DA:4540:HOH:O | 2.19 | 0.50 |
| 26:DA:2103:C:C2' | 26:DA:2104:G:H5' | 2.40 | 0.50 |
| 26:DA:656:G:H2' | 26:DA:657:U:O4' | 2.10 | 0.50 |
| 26:DA:662:G:H5'' | 36:DP:16:ARG:HG2 | 1.92 | 0.50 |
| 1:AA:523:A:H61 | 12:AL:92:ASP:HB2 | 1.76 | 0.50 |
| 26:BA:1803:A:O2' | 28:BD:259:THR:HG21 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 26:BA:184:C:H2' | 26:BA:185:U:C6 | 2.47 | 0.50 |
| 26:BA:1996:C:H4' | 26:BA:1997:G:OP1 | 2.11 | 0.50 |
| 26:BA:2176:A:H2' | 26:BA:2177:C:C6 | 2.46 | 0.50 |
| 26:BA:2748:A:H5' | 32:BH:4:ILE:HD12 | 1.93 | 0.50 |
| 26:BA:848:G:H2' | 26:BA:849:A:C8 | 2.46 | 0.50 |
| 38:BR:38:VAL:HG12 | 38:BR:42:LYS:HE3 | 1.92 | 0.50 |
| 1:CA:1164:G:C2' | 1:CA:1165:C:H5' | 2.40 | 0.50 |
| 1:CA:580:U:H5'' | 15:CO:58:MET:HG2 | 1.92 | 0.50 |
| 2:CB:120:ALA:O | 2:CB:121:LEU:HB3 | 2.11 | 0.50 |
| 20:CT:86:ARG:NH1 | 20:CT:90:GLN:HE22 | 2.10 | 0.50 |
| 26:DA:2611:U:C4 | 52:D5:3:LYS:HG2 | 2.46 | 0.50 |
| 26:DA:2139:C:N4 | 26:DA:2152:G:C6 | 2.79 | 0.50 |
| 28:DD:148:GLU:HB2 | 28:DD:151:LYS:HD2 | 1.91 | 0.50 |
| 31:DG:5:VAL:HG22 | 31:DG:8:LYS:HB2 | 1.93 | 0.50 |
| 44:DX:31:HIS:CD2 | 44:DX:33:LYS:H | 2.29 | 0.50 |
| 26:BA:2133:G:O2' | 26:BA:2156:G:N2 | 2.43 | 0.50 |
| 26:BA:2816:C:O3' | 38:BR:99:LYS:NZ | 2.40 | 0.50 |
| 26:BA:2869:G:H2' | 26:BA:2870:C:O4' | 2.11 | 0.50 |
| 26:BA:657:U:H2' | 26:BA:658:C:C6 | 2.45 | 0.50 |
| 35:BO:34:THR:OG1 | 35:BO:35:VAL:N | 2.43 | 0.50 |
| 1:CA:1007:C:H2' | 1:CA:1008:C:H6 | 1.75 | 0.50 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:C6 | 2.46 | 0.50 |
| 26:DA:2046:G:H5' | 52:D5:19:ARG:HA | 1.92 | 0.50 |
| 26:DA:272(A):U:H5 | 26:DA:272(C):G:OP1 | 1.95 | 0.50 |
| 26:DA:571:A:H5' | 26:DA:2030:A:N7 | 2.27 | 0.50 |
| 27:DB:27:C:H5'' | 39:DS:54:LEU:HD21 | 1.94 | 0.50 |
| 1:AA:1034:G:H3' | 1:AA:1035:A:C8 | 2.46 | 0.50 |
| 1:AA:551:U:H2' | 1:AA:552:U:C6 | 2.47 | 0.50 |
| 1:AA:642:A:N3 | 8:AH:113:SER:OG | 2.38 | 0.50 |
| 1:AA:752:G:H4' | 15:AO:69:TYR:OH | 2.12 | 0.50 |
| 51:B4:46:GLN:O | 51:B4:48:ARG:N | 2.44 | 0.50 |
| 53:B6:9:LEU:HD13 | 53:B6:51:GLU:HG3 | 1.92 | 0.50 |
| 26:BA:2893:G:H4' | 26:BA:2894:G:O5' | 2.11 | 0.50 |
| 26:BA:652(C):G:H1 | 26:BA:652(V):C:H42 | 1.59 | 0.50 |
| 1:CA:1119:C:H2' | 1:CA:1120:G:C8 | 2.46 | 0.50 |
| 1:CA:1154:G:N7 | 1:CA:1155:G:C8 | 2.80 | 0.50 |
| 1:CA:473:G:H2' | 1:CA:474:G:H8 | 1.76 | 0.50 |
| 4:CD:155:LEU:O | 4:CD:159:ARG:HG3 | 2.11 | 0.50 |
| 25:CY:59:U:H3' | 25:CY:60:U:O2 | 2.12 | 0.50 |
| 26:DA:271(R):G:H5'' | 48:D1:97:LEU:HD21 | 1.93 | 0.50 |
| 50:D3:18:ASP:N | 50:D3:18:ASP:OD1 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DA:361:G:O2' | 26:DA:362:U:H5' | 2.12 | 0.50 |
| 26:DA:866:A:H2 | 26:DA:867:C:C4 | 2.29 | 0.50 |
| 26:DA:873:G:N2 | 26:DA:905:U:C2 | 2.80 | 0.50 |
| 41:DU:61:TRP:CH2 | 41:DU:93:LYS:HB2 | 2.47 | 0.50 |
| 1:AA:1346:A:N1 | 1:AA:1374:A:H5'' | 2.26 | 0.50 |
| 1:AA:186:C:H2' | 1:AA:187:C:C6 | 2.47 | 0.50 |
| 4:AD:65:ARG:HG2 | 4:AD:75:PHE:CD1 | 2.47 | 0.50 |
| 20:AT:45:GLN:HA | 20:AT:91:LEU:HB3 | 1.94 | 0.50 |
| 26:BA:1113:U:H2' | 26:BA:1114:G:H8 | 1.75 | 0.50 |
| 26:BA:1177:A:O2' | 26:BA:1178:C:O4' | 2.24 | 0.50 |
| 26:BA:2238:G:N3 | 26:BA:2238:G:H2' | 2.25 | 0.50 |
| 26:BA:566:U:H5'' | 36:BP:29:LYS:HE3 | 1.93 | 0.50 |
| 45:BY:16:ALA:HB2 | 45:BY:73:ARG:HD3 | 1.94 | 0.50 |
| 1:CA:1033:G:H2' | 1:CA:1034:G:H5' | 1.93 | 0.50 |
| 1:CA:1119:C:OP2 | 9:CI:9:ARG:NH1 | 2.35 | 0.50 |
| 1:CA:1492:A:H2' | 1:CA:1493:A:C8 | 2.46 | 0.50 |
| 1:CA:344:A:H5'' | 1:CA:345:C:C5 | 2.43 | 0.50 |
| 3:CC:22:TRP:HB3 | 3:CC:59:ARG:HB2 | 1.93 | 0.50 |
| 1:CA:376:G:H5'' | 16:CP:5:ARG:HB2 | 1.93 | 0.50 |
| 25:CY:1:G:H1 | 25:CY:72:C:H42 | 1.60 | 0.50 |
| 25:CY:26:A:N1 | 25:CY:44:G:C6 | 2.80 | 0.50 |
| 26:DA:1166:C:H1' | 26:DA:1184:G:N2 | 2.27 | 0.50 |
| 26:DA:2252:G:H2' | 26:DA:2253:G:C8 | 2.47 | 0.50 |
| 26:DA:2364:C:H2' | 26:DA:2365:G:O4' | 2.12 | 0.50 |
| 26:DA:2528:U:O2' | 26:DA:2529:G:H3' | 2.12 | 0.50 |
| 26:DA:289:A:H62 | 26:DA:351:G:H21 | 1.59 | 0.50 |
| 29:DE:174:ASP:OD1 | 29:DE:175:VAL:N | 2.44 | 0.50 |
| 32:DH:73:ALA:O | 32:DH:76:VAL:HG12 | 2.11 | 0.50 |
| 35:DO:78:ARG:HG2 | 40:DT:73:GLU:HB2 | 1.93 | 0.50 |
| 7:AG:78:ARG:NH2 | 7:AG:154:TYR:O | 2.43 | 0.50 |
| 25:AY:25:C:C2 | 25:AY:26:A:C8 | 3.00 | 0.50 |
| 25:AY:44:G:H8 | 25:AY:44:G:OP2 | 1.95 | 0.50 |
| 26:BA:2150:U:C2' | 26:BA:2151:G:H5' | 2.41 | 0.50 |
| 26:BA:2564:A:C2 | 26:BA:2647:U:H4' | 2.46 | 0.50 |
| 1:CA:1342:C:H2' | 1:CA:1343:G:C8 | 2.46 | 0.50 |
| 6:CF:15:ASP:OD1 | 6:CF:18:GLN:N | 2.24 | 0.50 |
| 8:CH:121:ASP:OD1 | 8:CH:121:ASP:N | 2.39 | 0.50 |
| 13:CM:57:ARG:NH1 | 51:D4:34:GLU:HA | 2.27 | 0.50 |
| 13:CM:121:LYS:HZ3 | 23:CW:40:C:H4' | 1.77 | 0.50 |
| 23:CW:61:C:O2' | 23:CW:62:C:H6 | 1.95 | 0.50 |
| 26:DA:1379:A:H4' | 26:DA:1380:G:OP2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DA:601:C:O2 | 26:DA:605:C:H4' | 2.11 | 0.50 |
| 27:DB:66:A:H61 | 27:DB:108:U:H3' | 1.76 | 0.50 |
| 26:BA:222:A:H3' | 26:BA:421:U:H5' | 1.94 | 0.50 |
| 26:BA:857:C:N4 | 26:BA:858:U:O4 | 2.45 | 0.50 |
| 34:BN:73:THR:OG1 | 34:BN:82:LEU:HD11 | 2.11 | 0.50 |
| 26:BA:662:G:H5'' | 36:BP:16:ARG:HG2 | 1.94 | 0.50 |
| 38:BR:21:TYR:OH | 38:BR:43:GLU:HG2 | 2.11 | 0.50 |
| 1:CA:109:A:C6 | 1:CA:326:G:C6 | 3.00 | 0.50 |
| 1:CA:811:C:O2' | 1:CA:901:A:N1 | 2.40 | 0.50 |
| 2:CB:134:GLU:O | 2:CB:138:LEU:HG | 2.11 | 0.50 |
| 4:CD:38:TYR:CZ | 4:CD:45:GLN:HG3 | 2.47 | 0.50 |
| 5:CE:31:LEU:HD22 | 5:CE:43:LEU:HD11 | 1.94 | 0.50 |
| 10:CJ:27:ALA:HA | 10:CJ:81:THR:CG2 | 2.41 | 0.50 |
| 12:CL:71:PRO:O | 12:CL:102:ARG:HD2 | 2.12 | 0.50 |
| 26:DA:1038:C:N3 | 26:DA:1117:G:N2 | 2.50 | 0.50 |
| 26:DA:2001:A:H2' | 26:DA:2002:G:C8 | 2.46 | 0.50 |
| 26:DA:304:G:O6 | 61:DA:4181:HOH:O | 2.18 | 0.50 |
| 26:DA:570:G:H5'' | 61:DA:3844:HOH:O | 2.11 | 0.50 |
| 26:DA:2748:A:O2' | 32:DH:63:SER:O | 2.18 | 0.50 |
| 33:DI:14:ASP:N | 33:DI:17:GLN:OE1 | 2.44 | 0.50 |
| 37:DQ:38:GLU:HG3 | 37:DQ:127:ILE:HB | 1.94 | 0.50 |
| 1:AA:1064:G:N2 | 1:AA:1191:A:OP2 | 2.41 | 0.50 |
| 1:AA:977:A:H1' | 1:AA:982:U:O4 | 2.12 | 0.50 |
| 2:AB:185:ILE:HG23 | 2:AB:199:TYR:HB2 | 1.93 | 0.50 |
| 26:BA:2689:U:H4' | 26:BA:2690:C:H5' | 1.93 | 0.50 |
| 26:BA:84:A:H5'' | 45:BY:8:LYS:HG3 | 1.93 | 0.50 |
| 33:BI:72:LEU:C | 33:BI:74:ASN:H | 2.14 | 0.50 |
| 1:CA:1035:A:H2' | 1:CA:1036:G:C8 | 2.46 | 0.50 |
| 1:CA:1049:U:C6 | 1:CA:1201:A:H5' | 2.47 | 0.50 |
| 1:CA:1137:C:H5'' | 1:CA:1138:G:OP1 | 2.12 | 0.50 |
| 1:CA:457:C:H2' | 1:CA:458:C:C6 | 2.46 | 0.50 |
| 24:CX:8:4SU:O2' | 24:CX:21:A:N1 | 2.28 | 0.50 |
| 25:CY:34:G:C6 | 25:CY:35:A:C6 | 3.00 | 0.50 |
| 26:DA:2240:C:OP2 | 61:DA:3953:HOH:O | 2.19 | 0.50 |
| 29:DE:89:ASP:N | 29:DE:89:ASP:OD1 | 2.43 | 0.50 |
| 30:DF:137:LYS:HA | 30:DF:140:LEU:HD23 | 1.93 | 0.50 |
| 31:DG:125:PHE:CZ | 31:DG:170:ARG:HA | 2.47 | 0.50 |
| 39:DS:50:SER:O | 39:DS:76:LYS:NZ | 2.45 | 0.50 |
| 1:AA:1002:G:C4 | 1:AA:1003:G:H1' | 2.47 | 0.50 |
| 1:AA:250:A:H4' | 1:AA:251:G:O5' | 2.10 | 0.50 |
| 2:AB:30:ARG:HH21 | 2:AB:194:PRO:HB2 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 26:BA:2612:C:OP2 | 52:B5:2:ALA:N | 2.45 | 0.50 |
| 26:BA:2846:G:H2' | 26:BA:2847:U:O4' | 2.11 | 0.50 |
| 27:BB:87:G:N2 | 27:BB:90:A:OP2 | 2.30 | 0.50 |
| 41:BU:58:ARG:HA | 41:BU:61:TRP:CE3 | 2.46 | 0.50 |
| 1:CA:1256:A:N6 | 1:CA:1278:U:H1' | 2.26 | 0.50 |
| 2:CB:141:GLU:O | 2:CB:145:LEU:HG | 2.12 | 0.50 |
| 5:CE:137:GLU:HA | 5:CE:140:ARG:HB3 | 1.94 | 0.50 |
| 1:CA:1342:C:O2' | 9:CI:124:GLN:HG2 | 2.12 | 0.50 |
| 9:CI:26:VAL:HG13 | 9:CI:61:ALA:HB3 | 1.92 | 0.50 |
| 16:CP:22:THR:HA | 16:CP:33:ILE:HG13 | 1.94 | 0.50 |
| 23:CW:66:U:H2' | 23:CW:67:C:O4' | 2.12 | 0.50 |
| 26:DA:1184:G:H5' | 50:D3:29:ARG:HH11 | 1.77 | 0.50 |
| 26:DA:2750:A:H8 | 26:DA:2750:A:OP1 | 1.95 | 0.50 |
| 26:DA:686:G:H21 | 26:DA:788:A:H61 | 1.58 | 0.50 |
| 28:DD:17:THR:O | 28:DD:211:ARG:NH2 | 2.43 | 0.50 |
| 30:DF:110:LEU:HD12 | 30:DF:202:PHE:CE1 | 2.47 | 0.50 |
| 26:DA:2305:A:H5'' | 31:DG:134:GLY:HA3 | 1.94 | 0.50 |
| 31:DG:37:VAL:O | 31:DG:94:LEU:N | 2.41 | 0.50 |
| 35:DO:24:VAL:HB | 35:DO:33:ALA:HB2 | 1.92 | 0.50 |
| 1:AA:1027:C:C4 | 1:AA:1034:G:O6 | 2.64 | 0.49 |
| 1:AA:79:G:N1 | 1:AA:90:U:C2 | 2.80 | 0.49 |
| 1:AA:92:C:H2' | 1:AA:93:G:C8 | 2.47 | 0.49 |
| 3:AC:47:LEU:HD13 | 3:AC:68:VAL:HG11 | 1.94 | 0.49 |
| 15:AO:17:ARG:HH11 | 15:AO:17:ARG:HG3 | 1.75 | 0.49 |
| 17:AQ:28:PRO:HA | 17:AQ:35:VAL:HA | 1.94 | 0.49 |
| 51:B4:59:PHE:CA | 51:B4:61:ARG:H | 2.24 | 0.49 |
| 26:BA:1274:A:N3 | 26:BA:1297:C:H1' | 2.27 | 0.49 |
| 26:BA:1507:A:O2' | 26:BA:1508:A:O5' | 2.26 | 0.49 |
| 26:BA:2646:C:H2' | 26:BA:2647:U:O4' | 2.12 | 0.49 |
| 26:BA:271(V):G:O6 | 61:BA:4929:HOH:O | 2.19 | 0.49 |
| 26:BA:2691:C:O3' | 26:BA:2871:C:H4' | 2.12 | 0.49 |
| 26:BA:614(A):U:H5'' | 61:BA:5227:HOH:O | 2.12 | 0.49 |
| 36:BP:82:GLY:HA2 | 36:BP:113:LYS:O | 2.11 | 0.49 |
| 46:BZ:111:VAL:C | 46:BZ:113:ALA:H | 2.15 | 0.49 |
| 1:CA:1016:A:C5 | 1:CA:1017:G:H1' | 2.47 | 0.49 |
| 1:CA:1128:C:H4' | 1:CA:1148:U:O2 | 2.12 | 0.49 |
| 1:CA:1316:G:O2' | 1:CA:1318:A:N7 | 2.37 | 0.49 |
| 1:CA:404:U:H5' | 4:CD:122:ARG:HD3 | 1.94 | 0.49 |
| 1:CA:54:C:H2' | 1:CA:352:C:H41 | 1.77 | 0.49 |
| 25:CY:4:C:H2' | 25:CY:5:G:H5' | 1.92 | 0.49 |
| 26:DA:1357:U:H2' | 26:DA:1358:G:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DA:2025:C:N4 | 61:DA:4191:HOH:O | 2.45 | 0.49 |
| 26:DA:526:A:O2' | 26:DA:2043:C:O2 | 2.24 | 0.49 |
| 27:DB:44:G:OP1 | 31:DG:98:ARG:NH2 | 2.45 | 0.49 |
| 27:DB:98:G:H2' | 27:DB:99:G:O4' | 2.12 | 0.49 |
| 34:DN:4:TYR:CD2 | 41:DU:100:VAL:HG11 | 2.47 | 0.49 |
| 1:AA:1007:C:O2 | 1:AA:1022:G:N1 | 2.31 | 0.49 |
| 1:AA:1366:C:O2' | 10:AJ:60:ARG:NH2 | 2.44 | 0.49 |
| 4:AD:53:ASP:O | 4:AD:57:ARG:HG3 | 2.12 | 0.49 |
| 5:AE:18:ARG:HE | 5:AE:27:ARG:HH21 | 1.60 | 0.49 |
| 50:B3:18:ASP:OD1 | 50:B3:18:ASP:N | 2.40 | 0.49 |
| 26:BA:1866:C:H2' | 26:BA:1876:A:O4' | 2.12 | 0.49 |
| 26:BA:247:G:H4' | 26:BA:386:G:C5 | 2.47 | 0.49 |
| 1:CA:1028:C:C2 | 1:CA:1033:G:C6 | 3.00 | 0.49 |
| 1:CA:1152:A:H2' | 1:CA:1153:C:C6 | 2.46 | 0.49 |
| 1:CA:1279:A:O2' | 1:CA:1281:U:OP2 | 2.26 | 0.49 |
| 1:CA:1452:C:H6 | 1:CA:1452:C:O5' | 1.95 | 0.49 |
| 1:CA:441:A:H3' | 1:CA:442:C:C6 | 2.48 | 0.49 |
| 1:CA:65:U:H5' | 1:CA:65:U:C6 | 2.47 | 0.49 |
| 1:CA:716:A:N3 | 11:CK:118:GLY:HA2 | 2.27 | 0.49 |
| 1:CA:954:G:H21 | 1:CA:1227:A:N6 | 2.10 | 0.49 |
| 1:CA:986:A:H1' | 19:CS:55:LYS:HA | 1.94 | 0.49 |
| 1:CA:992:U:C6 | 1:CA:992:U:H5'' | 2.41 | 0.49 |
| 1:CA:1291:G:H4' | 9:CI:39:GLY:HA3 | 1.93 | 0.49 |
| 13:CM:3:ARG:HB2 | 51:D4:34:GLU:HG2 | 1.94 | 0.49 |
| 1:CA:195:A:OP1 | 20:CT:68:LYS:NZ | 2.44 | 0.49 |
| 26:DA:141:A:C8 | 26:DA:1408:C:O2' | 2.64 | 0.49 |
| 26:DA:2153:G:H3' | 26:DA:2154:G:H8 | 1.77 | 0.49 |
| 26:DA:443:A:H5'' | 26:DA:444:C:OP1 | 2.13 | 0.49 |
| 26:DA:900:A:O2' | 26:DA:901:A:OP1 | 2.29 | 0.49 |
| 30:DF:178:PRO:HB2 | 30:DF:201:VAL:HG21 | 1.94 | 0.49 |
| 32:DH:69:ARG:HG3 | 32:DH:70:THR:N | 2.27 | 0.49 |
| 34:DN:30:ILE:HG23 | 34:DN:52:VAL:HG11 | 1.94 | 0.49 |
| 2:AB:112:VAL:O | 2:AB:116:GLU:HG3 | 2.11 | 0.49 |
| 13:AM:79:LYS:HA | 13:AM:82:MET:HE2 | 1.95 | 0.49 |
| 1:AA:279:A:C4 | 17:AQ:98:LEU:HD23 | 2.47 | 0.49 |
| 51:B4:53:GLU:HG2 | 51:B4:56:VAL:HG22 | 1.94 | 0.49 |
| 26:BA:645:C:H5' | 26:BA:646:A:OP2 | 2.12 | 0.49 |
| 29:BE:52:LEU:HD12 | 29:BE:77:ILE:HD11 | 1.94 | 0.49 |
| 31:BG:139:LEU:HD12 | 31:BG:139:LEU:H | 1.75 | 0.49 |
| 33:BI:6:LEU:HD11 | 33:BI:37:VAL:HG23 | 1.93 | 0.49 |
| 1:CA:1251:A:H2' | 1:CA:1252:A:C8 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:CA:1324:A:H4' | 1:CA:1362:C:O3' | 2.12 | 0.49 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C6 | 2.47 | 0.49 |
| 1:CA:1249:C:O2' | 9:CI:73:GLN:NE2 | 2.44 | 0.49 |
| 13:CM:19:LEU:HD21 | 13:CM:56:LEU:HD11 | 1.94 | 0.49 |
| 3:CC:6:HIS:ND1 | 14:CN:49:HIS:HB3 | 2.27 | 0.49 |
| 25:CY:61:C:H2' | 25:CY:62:C:C6 | 2.48 | 0.49 |
| 26:DA:1991:U:H2' | 26:DA:1992:G:H5'' | 1.93 | 0.49 |
| 26:DA:2557:G:H2' | 26:DA:2558:C:C6 | 2.47 | 0.49 |
| 28:DD:108:PRO:HB3 | 28:DD:143:HIS:CE1 | 2.47 | 0.49 |
| 35:DO:64:ARG:NH1 | 35:DO:81:ASP:OD1 | 2.45 | 0.49 |
| 1:AA:131:C:O2' | 1:AA:262:A:N3 | 2.41 | 0.49 |
| 26:BA:272:G:N7 | 26:BA:421:U:H2' | 2.27 | 0.49 |
| 46:BZ:45:ASP:OD2 | 46:BZ:49:ARG:NH1 | 2.45 | 0.49 |
| 1:CA:1003:G:H2' | 1:CA:1004:A:C1' | 2.42 | 0.49 |
| 1:CA:814:A:H2' | 1:CA:816:A:H5'' | 1.94 | 0.49 |
| 13:CM:60:VAL:HA | 13:CM:63:THR:OG1 | 2.11 | 0.49 |
| 23:CW:70:G:H2' | 23:CW:71:G:H8 | 1.76 | 0.49 |
| 55:D8:15:LYS:HG2 | 55:D8:16:ILE:N | 2.26 | 0.49 |
| 26:DA:1509(B):A:H2' | 26:DA:1510:G:H8 | 1.76 | 0.49 |
| 26:DA:1264:G:H2' | 26:DA:2014:A:N6 | 2.28 | 0.49 |
| 26:DA:2135:A:H2' | 26:DA:2136:C:C5 | 2.47 | 0.49 |
| 26:DA:2314:C:H2' | 26:DA:2315:G:C8 | 2.47 | 0.49 |
| 26:DA:624:C:OP1 | 61:DA:3854:HOH:O | 2.20 | 0.49 |
| 28:DD:182:LEU:HB2 | 28:DD:272:ALA:HB3 | 1.95 | 0.49 |
| 29:DE:73:GLU:OE2 | 29:DE:73:GLU:N | 2.41 | 0.49 |
| 30:DF:29:ASN:O | 30:DF:112:MET:HE1 | 2.12 | 0.49 |
| 39:DS:58:LEU:HD21 | 39:DS:65:VAL:HG13 | 1.94 | 0.49 |
| 44:DX:31:HIS:HD2 | 44:DX:33:LYS:H | 1.59 | 0.49 |
| 46:DZ:108:PRO:HB2 | 46:DZ:111:VAL:HG23 | 1.94 | 0.49 |
| 1:AA:335:C:O2' | 1:AA:1433:A:N3 | 2.41 | 0.49 |
| 10:AJ:61:GLU:OE1 | 14:AN:58:LYS:NZ | 2.43 | 0.49 |
| 26:BA:1044:G:H5' | 26:BA:1045:A:OP2 | 2.12 | 0.49 |
| 26:BA:1713:U:H2' | 26:BA:1714:G:H8 | 1.77 | 0.49 |
| 26:BA:2533:A:H2' | 26:BA:2534:A:O4' | 2.13 | 0.49 |
| 26:BA:443:A:H1' | 26:BA:1201:C:O4' | 2.12 | 0.49 |
| 26:BA:625:G:O6 | 36:BP:107:LYS:NZ | 2.46 | 0.49 |
| 33:BI:66:GLU:HA | 33:BI:69:LYS:HB3 | 1.93 | 0.49 |
| 34:BN:4:TYR:HB2 | 41:BU:101:ARG:NH1 | 2.28 | 0.49 |
| 36:BP:121:LYS:HB3 | 36:BP:123:LEU:HG | 1.95 | 0.49 |
| 36:BP:138:LEU:HD23 | 36:BP:145:PRO:HB3 | 1.94 | 0.49 |
| 46:BZ:152:ALA:HA | 46:BZ:155:LEU:HD22 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CC:110:ASN:O | 3:CC:141:VAL:HG22 | 2.12 | 0.49 |
| 3:CC:157:ILE:HD12 | 3:CC:164:ARG:HB3 | 1.94 | 0.49 |
| 7:CG:26:PHE:CE1 | 7:CG:30:ILE:HD11 | 2.48 | 0.49 |
| 10:CJ:51:ARG:O | 14:CN:45:ARG:NH1 | 2.45 | 0.49 |
| 13:CM:34:LEU:HD13 | 13:CM:41:PRO:HB3 | 1.94 | 0.49 |
| 15:CO:8:LYS:O | 15:CO:12:ILE:HG13 | 2.12 | 0.49 |
| 23:CW:68:C:H2' | 23:CW:69:G:H8 | 1.76 | 0.49 |
| 25:CY:74:C:H4' | 48:D1:23:LYS:HE3 | 1.93 | 0.49 |
| 26:DA:2343:C:O2' | 26:DA:2373:G:O2' | 2.22 | 0.49 |
| 26:DA:2602:A:H4' | 26:DA:2603:G:O5' | 2.12 | 0.49 |
| 26:DA:335:C:H4' | 45:DY:73:ARG:NE | 2.27 | 0.49 |
| 27:DB:45:A:H2' | 27:DB:46:A:C8 | 2.47 | 0.49 |
| 30:DF:64:ILE:HG21 | 30:DF:78:ILE:HG23 | 1.95 | 0.49 |
| 1:AA:1343:G:H2' | 1:AA:1344:C:C6 | 2.47 | 0.49 |
| 8:AH:64:LYS:HG2 | 8:AH:79:VAL:HG21 | 1.94 | 0.49 |
| 1:AA:110:C:O2' | 16:AP:25:ARG:O | 2.26 | 0.49 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CD2 | 2.48 | 0.49 |
| 23:AW:69:G:H2' | 23:AW:69:G:N3 | 2.28 | 0.49 |
| 24:AX:7:G:O2' | 24:AX:49:G:H5' | 2.13 | 0.49 |
| 26:BA:2522:U:O2' | 26:BA:2647:U:OP1 | 2.20 | 0.49 |
| 26:BA:657:U:H2' | 26:BA:658:C:H6 | 1.77 | 0.49 |
| 41:BU:29:SER:OG | 41:BU:30:LYS:NZ | 2.40 | 0.49 |
| 1:CA:1347:G:N2 | 1:CA:1373:G:H2' | 2.27 | 0.49 |
| 2:CB:105:PHE:HE1 | 2:CB:155:LEU:HD12 | 1.78 | 0.49 |
| 2:CB:127:ILE:O | 2:CB:128:GLU:HB2 | 2.12 | 0.49 |
| 5:CE:80:ILE:HD11 | 8:CH:104:ARG:HH21 | 1.77 | 0.49 |
| 1:CA:585:G:OP1 | 17:CQ:37:LYS:NZ | 2.45 | 0.49 |
| 25:CY:19:G:C2 | 25:CY:57:G:C6 | 3.01 | 0.49 |
| 26:DA:1514:U:H2' | 26:DA:1515:G:C8 | 2.48 | 0.49 |
| 26:DA:2164:C:H5 | 26:DA:2165:G:N3 | 2.11 | 0.49 |
| 26:DA:692:C:O2' | 28:DD:38:LYS:NZ | 2.44 | 0.49 |
| 44:DX:52:VAL:HG12 | 44:DX:82:GLN:O | 2.13 | 0.49 |
| 1:AA:1014:A:H4' | 19:AS:14:HIS:CE1 | 2.46 | 0.49 |
| 1:AA:1316:G:N1 | 1:AA:1319:A:OP2 | 2.43 | 0.49 |
| 1:AA:256:U:H2' | 1:AA:257:G:H8 | 1.77 | 0.49 |
| 1:AA:266:G:O3' | 17:AQ:67:LYS:HB2 | 2.13 | 0.49 |
| 2:AB:42:ILE:HD12 | 2:AB:203:GLY:HA2 | 1.93 | 0.49 |
| 3:AC:181:ASN:HD21 | 3:AC:204:LEU:HD12 | 1.77 | 0.49 |
| 16:AP:22:THR:HA | 16:AP:33:ILE:HG12 | 1.93 | 0.49 |
| 19:AS:63:THR:OG1 | 19:AS:65:ASN:ND2 | 2.45 | 0.49 |
| 25:AY:50:U:H2' | 25:AY:51:U:C6 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BA:1045:A:OP1 | 26:BA:1045:A:H4' | 2.12 | 0.49 |
| 26:BA:2439:A:C8 | 26:BA:2439:A:H5' | 2.48 | 0.49 |
| 26:BA:400:G:N7 | 61:BA:4974:HOH:O | 2.34 | 0.49 |
| 26:BA:579:G:H2' | 26:BA:580:C:C6 | 2.48 | 0.49 |
| 45:BY:28:LYS:HD2 | 45:BY:40:GLU:HG3 | 1.94 | 0.49 |
| 1:CA:1324:A:O4' | 1:CA:1362:C:H4' | 2.13 | 0.49 |
| 1:CA:343:U:H2' | 1:CA:345:C:C5 | 2.47 | 0.49 |
| 2:CB:140:HIS:O | 2:CB:143:GLU:HB2 | 2.12 | 0.49 |
| 19:CS:64:GLU:O | 19:CS:67:VAL:HG23 | 2.11 | 0.49 |
| 26:DA:2528:U:H5'' | 56:D9:31:LYS:HE2 | 1.94 | 0.49 |
| 26:DA:1508:A:H4' | 26:DA:1509(A):A:C5 | 2.47 | 0.49 |
| 26:DA:1952:A:OP1 | 35:DO:42:SER:OG | 2.29 | 0.49 |
| 26:DA:2602:A:H4' | 26:DA:2603:G:C5' | 2.42 | 0.49 |
| 26:DA:854:G:H2' | 26:DA:855:G:H8 | 1.77 | 0.49 |
| 33:DI:130:TYR:HB3 | 33:DI:138:ILE:HB | 1.94 | 0.49 |
| 37:DQ:85:LYS:HG2 | 47:D0:7:LEU:HB3 | 1.94 | 0.49 |
| 39:DS:31:SER:OG | 39:DS:32:LEU:N | 2.46 | 0.49 |
| 40:DT:24:PRO:HA | 40:DT:49:VAL:HG23 | 1.95 | 0.49 |
| 1:AA:346:G:C4 | 1:AA:347:G:H1' | 2.48 | 0.49 |
| 2:AB:115:LEU:HD13 | 2:AB:145:LEU:HB3 | 1.93 | 0.49 |
| 4:AD:155:LEU:HD22 | 4:AD:157:LEU:H | 1.77 | 0.49 |
| 8:AH:6:ILE:HD11 | 8:AH:31:PHE:HD2 | 1.78 | 0.49 |
| 31:BG:66:GLN:HG3 | 51:B4:1:MET:HE1 | 1.94 | 0.49 |
| 53:B6:6:ARG:HH12 | 53:B6:26:ASN:HB2 | 1.78 | 0.49 |
| 33:BI:109:ILE:HG23 | 33:BI:130:TYR:CZ | 2.48 | 0.49 |
| 44:BX:5:TYR:CZ | 49:B2:30:ARG:HB2 | 2.48 | 0.49 |
| 1:CA:1003:G:N2 | 1:CA:1025:U:O4 | 2.46 | 0.49 |
| 1:CA:542:G:OP1 | 4:CD:10:ARG:NH2 | 2.30 | 0.49 |
| 1:CA:834:C:H2' | 1:CA:835:U:C6 | 2.47 | 0.49 |
| 1:CA:1151:A:H5' | 10:CJ:41:PRO:HA | 1.95 | 0.49 |
| 26:DA:242:G:N2 | 26:DA:255:A:OP2 | 2.38 | 0.49 |
| 30:DF:183:VAL:O | 30:DF:187:VAL:HG23 | 2.13 | 0.49 |
| 1:AA:1137:C:H5'' | 1:AA:1138:G:OP1 | 2.13 | 0.49 |
| 1:AA:628:G:H2' | 1:AA:629:G:C8 | 2.48 | 0.49 |
| 13:AM:65:LYS:NZ | 51:B4:53:GLU:OE1 | 2.45 | 0.49 |
| 19:AS:27:GLU:CB | 19:AS:28:LYS:HA | 2.38 | 0.49 |
| 26:BA:887:A:O2' | 26:BA:888:C:OP2 | 2.28 | 0.49 |
| 31:BG:170:ARG:HD3 | 31:BG:174:GLU:HG3 | 1.94 | 0.49 |
| 32:BH:154:PRO:HD3 | 32:BH:162:ILE:O | 2.12 | 0.49 |
| 32:BH:154:PRO:HB3 | 32:BH:163:TYR:CE2 | 2.48 | 0.49 |
| 1:CA:1010:G:N2 | 1:CA:1020:U:O2 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:976:G:C8 | 1:CA:1362:C:N4 | 2.80 | 0.49 |
| 1:CA:250:A:H4' | 1:CA:251:G:O5' | 2.12 | 0.49 |
| 1:CA:392:G:H2' | 1:CA:393:A:C8 | 2.48 | 0.49 |
| 1:CA:429:U:H1' | 1:CA:430:A:H5'' | 1.95 | 0.49 |
| 1:CA:589:C:N3 | 1:CA:650:G:N1 | 2.41 | 0.49 |
| 25:CY:35:A:N6 | 25:CY:36:A:N1 | 2.61 | 0.49 |
| 26:DA:1300:U:H4' | 26:DA:1301:A:H5' | 1.94 | 0.49 |
| 26:DA:1313:U:H4' | 26:DA:1332:G:H4' | 1.95 | 0.49 |
| 26:DA:1652:A:OP1 | 38:DR:8:ARG:NH1 | 2.46 | 0.49 |
| 26:DA:1657:C:H2' | 26:DA:1658:C:C6 | 2.48 | 0.49 |
| 26:DA:465:G:OP1 | 54:D7:12:ARG:NH2 | 2.41 | 0.49 |
| 42:DV:24:LYS:HG2 | 42:DV:64:HIS:CD2 | 2.35 | 0.49 |
| 1:AA:1020:U:H2' | 1:AA:1021:G:C8 | 2.48 | 0.49 |
| 1:AA:1356:G:H2' | 1:AA:1357:A:C8 | 2.48 | 0.49 |
| 1:AA:262:A:C6 | 1:AA:263:A:C6 | 3.00 | 0.49 |
| 1:AA:736:C:H2' | 1:AA:737:A:C8 | 2.48 | 0.49 |
| 1:AA:1249:C:O2' | 9:AI:73:GLN:NE2 | 2.46 | 0.49 |
| 9:AI:93:ARG:HB2 | 9:AI:93:ARG:HH11 | 1.78 | 0.49 |
| 1:AA:111:G:H5'' | 16:AP:27:LYS:HG2 | 1.93 | 0.49 |
| 19:AS:38:SER:HB2 | 19:AS:71:LEU:HD13 | 1.95 | 0.49 |
| 24:AX:7:G:H1 | 24:AX:66:C:H42 | 1.61 | 0.49 |
| 51:B4:24:THR:OG1 | 51:B4:25:TYR:N | 2.45 | 0.49 |
| 26:BA:2124:G:H1 | 26:BA:2174:C:N4 | 2.11 | 0.49 |
| 26:BA:2022:U:O2' | 26:BA:2617:C:H5' | 2.13 | 0.49 |
| 26:BA:576:U:H2' | 26:BA:577:G:C8 | 2.47 | 0.49 |
| 32:BH:11:VAL:HG21 | 32:BH:50:VAL:HG23 | 1.94 | 0.49 |
| 39:BS:65:VAL:O | 39:BS:69:VAL:HG13 | 2.13 | 0.49 |
| 1:CA:434:U:H2' | 1:CA:435:C:C6 | 2.48 | 0.49 |
| 3:CC:78:GLY:HA3 | 3:CC:83:ARG:H | 1.77 | 0.49 |
| 5:CE:12:LEU:O | 5:CE:30:ALA:HA | 2.13 | 0.49 |
| 23:CW:21:A:N6 | 23:CW:46:7MG:N3 | 2.61 | 0.49 |
| 26:DA:1339:G:N2 | 26:DA:1603:A:H1' | 2.27 | 0.49 |
| 26:DA:648:G:O2' | 26:DA:2351:G:OP1 | 2.23 | 0.49 |
| 26:DA:724:U:H2' | 26:DA:725:G:O4' | 2.13 | 0.49 |
| 27:DB:118:G:H2' | 27:DB:119:G:H5' | 1.95 | 0.49 |
| 27:DB:20:C:H2' | 27:DB:21:G:H5' | 1.93 | 0.49 |
| 30:DF:154:VAL:HG22 | 30:DF:191:ARG:HB2 | 1.94 | 0.49 |
| 36:DP:84:ASN:OD1 | 36:DP:117:GLU:HB2 | 2.13 | 0.49 |
| 1:AA:1027:C:C2 | 1:AA:1034:G:C2 | 3.01 | 0.48 |
| 1:AA:1131:G:O5' | 1:AA:1131:G:H8 | 1.96 | 0.48 |
| 3:AC:81:GLY:O | 3:AC:85:ARG:HG3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AF:69:GLU:CD | 6:AF:69:GLU:H | 2.12 | 0.48 |
| 13:AM:80:ARG:NH2 | 19:AS:69:HIS:HE1 | 2.11 | 0.48 |
| 23:AW:1:G:C6 | 23:AW:72:C:N3 | 2.79 | 0.48 |
| 49:B2:31:GLU:HB3 | 49:B2:53:LEU:HD11 | 1.94 | 0.48 |
| 26:BA:1021:A:C8 | 26:BA:1021:A:H3' | 2.47 | 0.48 |
| 26:BA:1588:C:H2' | 26:BA:1589:C:H6 | 1.78 | 0.48 |
| 26:BA:2763:G:OP2 | 61:BA:4693:HOH:O | 2.20 | 0.48 |
| 26:BA:578:A:OP2 | 61:BA:4085:HOH:O | 2.20 | 0.48 |
| 32:BH:86:GLU:OE2 | 32:BH:130:ARG:NH1 | 2.46 | 0.48 |
| 34:BN:67:LEU:O | 34:BN:88:GLU:HG3 | 2.13 | 0.48 |
| 36:BP:121:LYS:O | 36:BP:123:LEU:N | 2.42 | 0.48 |
| 42:BV:21:ARG:HG2 | 42:BV:91:TYR:CD1 | 2.48 | 0.48 |
| 1:CA:976:G:C8 | 1:CA:1358:U:C2 | 3.01 | 0.48 |
| 15:CO:26:GLU:N | 15:CO:26:GLU:OE2 | 2.43 | 0.48 |
| 15:CO:25:THR:HG21 | 15:CO:70:LEU:HB2 | 1.94 | 0.48 |
| 26:DA:196:A:H2' | 26:DA:196:A:N3 | 2.28 | 0.48 |
| 26:DA:2693:A:H2' | 26:DA:2694:G:H8 | 1.78 | 0.48 |
| 26:DA:539:G:H2' | 26:DA:540:C:H6 | 1.78 | 0.48 |
| 29:DE:9:VAL:HG13 | 29:DE:25:VAL:O | 2.13 | 0.48 |
| 1:AA:1122:U:H2' | 1:AA:1123:A:O4' | 2.13 | 0.48 |
| 4:AD:165:MET:C | 4:AD:168:ARG:HH12 | 2.17 | 0.48 |
| 7:AG:26:PHE:O | 7:AG:30:ILE:HG13 | 2.13 | 0.48 |
| 9:AI:77:ILE:O | 9:AI:81:ILE:HG23 | 2.13 | 0.48 |
| 26:BA:1164:G:H2' | 26:BA:1165:U:C6 | 2.49 | 0.48 |
| 26:BA:1587:A:H2' | 26:BA:1588:C:C6 | 2.49 | 0.48 |
| 26:BA:2141:G:C2 | 26:BA:2142:C:C2 | 3.02 | 0.48 |
| 26:BA:2286:A:H4' | 26:BA:2287:A:O4' | 2.13 | 0.48 |
| 30:BF:64:ILE:HD11 | 30:BF:75:HIS:HB2 | 1.94 | 0.48 |
| 1:CA:834:C:H2' | 1:CA:835:U:H6 | 1.78 | 0.48 |
| 1:CA:936:C:H2' | 1:CA:937:A:O4' | 2.13 | 0.48 |
| 1:CA:938:A:C6 | 1:CA:939:G:C5 | 3.01 | 0.48 |
| 2:CB:210:SER:OG | 2:CB:211:ILE:N | 2.46 | 0.48 |
| 4:CD:175:SER:OG | 4:CD:184:LYS:HB2 | 2.12 | 0.48 |
| 14:CN:29:ARG:HD3 | 14:CN:40:CYS:HB2 | 1.94 | 0.48 |
| 23:CW:8:4SU:H1' | 23:CW:48:C:H1' | 1.95 | 0.48 |
| 26:DA:1434:A:H61 | 26:DA:1558:A:N6 | 2.11 | 0.48 |
| 26:DA:191:A:H2' | 26:DA:192:C:C6 | 2.48 | 0.48 |
| 26:DA:2552:U:H2' | 26:DA:2554:U:H5'' | 1.96 | 0.48 |
| 26:DA:607:U:OP1 | 30:DF:102:PRO:HA | 2.13 | 0.48 |
| 36:DP:39:LYS:CB | 36:DP:45:LEU:HG | 2.43 | 0.48 |
| 1:AA:1182:G:C4' | 1:AA:1183:A:H5' | 2.35 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:AQ:58:GLU:O | 17:AQ:74:LEU:N | 2.41 | 0.48 |
| 54:B7:46:VAL:HG13 | 54:B7:48:LYS:HE3 | 1.95 | 0.48 |
| 56:B9:2:LYS:HE2 | 56:B9:31:LYS:O | 2.12 | 0.48 |
| 26:BA:1019:U:O2' | 26:BA:1021:A:H2 | 1.96 | 0.48 |
| 26:BA:1379:A:H4' | 26:BA:1380:G:OP2 | 2.13 | 0.48 |
| 26:BA:762:U:H5'' | 61:BA:4793:HOH:O | 2.13 | 0.48 |
| 35:BO:24:VAL:HB | 35:BO:33:ALA:HB2 | 1.95 | 0.48 |
| 45:BY:6:HIS:CD2 | 45:BY:6:HIS:H | 2.30 | 0.48 |
| 1:CA:1053:G:O5' | 1:CA:1054:C:H5' | 2.13 | 0.48 |
| 1:CA:1169:A:H2' | 1:CA:1170:A:C8 | 2.48 | 0.48 |
| 1:CA:1181:G:O2' | 1:CA:1182:G:N7 | 2.38 | 0.48 |
| 1:CA:979:C:H2' | 1:CA:980:C:H5' | 1.95 | 0.48 |
| 2:CB:16:HIS:CG | 2:CB:17:PHE:N | 2.81 | 0.48 |
| 2:CB:27:LYS:HG3 | 2:CB:194:PRO:HD2 | 1.95 | 0.48 |
| 1:CA:1060:C:C5 | 3:CC:2:GLY:HA3 | 2.49 | 0.48 |
| 7:CG:76:ARG:HB3 | 7:CG:156:TRP:HH2 | 1.78 | 0.48 |
| 7:CG:20:ASP:OD2 | 7:CG:23:VAL:HG23 | 2.14 | 0.48 |
| 8:CH:134:ILE:HG22 | 8:CH:135:CYS:SG | 2.54 | 0.48 |
| 54:D7:9:ARG:HE | 54:D7:47:ARG:HB2 | 1.78 | 0.48 |
| 26:DA:1218:C:H42 | 26:DA:1231:G:H1 | 1.61 | 0.48 |
| 26:DA:1998:G:O2' | 26:DA:2724:C:O2' | 2.25 | 0.48 |
| 26:DA:2183:C:H2' | 26:DA:2184:G:C8 | 2.46 | 0.48 |
| 26:DA:223:A:O2' | 26:DA:420:C:O2 | 2.31 | 0.48 |
| 26:DA:531:C:H4' | 26:DA:532:A:H5'' | 1.95 | 0.48 |
| 26:DA:858:U:OP1 | 47:D0:44:ARG:NH2 | 2.44 | 0.48 |
| 35:DO:98:VAL:HG22 | 35:DO:118:ALA:HA | 1.95 | 0.48 |
| 1:AA:1243:C:H2' | 1:AA:1244:C:C6 | 2.48 | 0.48 |
| 1:AA:963:G:H5' | 61:AA:4173:HOH:O | 2.12 | 0.48 |
| 3:AC:181:ASN:HD22 | 3:AC:204:LEU:HB2 | 1.78 | 0.48 |
| 1:AA:1525:G:OP1 | 11:AK:120:ARG:NH2 | 2.46 | 0.48 |
| 19:AS:19:VAL:O | 19:AS:23:ASN:ND2 | 2.47 | 0.48 |
| 48:B1:85:LEU:HB3 | 48:B1:89:GLU:CG | 2.43 | 0.48 |
| 26:BA:1714:G:H1 | 26:BA:1745(A):C:N4 | 2.11 | 0.48 |
| 26:BA:234:C:H2' | 26:BA:235:U:H6 | 1.79 | 0.48 |
| 26:BA:2693:A:H2' | 26:BA:2694:G:H8 | 1.77 | 0.48 |
| 27:BB:22:U:H2' | 27:BB:23:G:C8 | 2.49 | 0.48 |
| 1:CA:988:G:H1 | 1:CA:1217:C:H42 | 1.60 | 0.48 |
| 1:CA:1376:U:OP1 | 7:CG:98:SER:OG | 2.29 | 0.48 |
| 1:CA:1399:C:C2 | 1:CA:1502:A:N6 | 2.81 | 0.48 |
| 1:CA:17:U:H2' | 1:CA:18:C:C6 | 2.49 | 0.48 |
| 1:CA:736:C:H2' | 1:CA:737:A:C8 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:73:G:C6 | 1:CA:97:G:C6 | 3.01 | 0.48 |
| 5:CE:24:ARG:NH1 | 22:CV:24:A:OP2 | 2.46 | 0.48 |
| 1:CA:1126:U:O4 | 10:CJ:71:LEU:HD13 | 2.14 | 0.48 |
| 17:CQ:40:LYS:HD2 | 17:CQ:42:TYR:CZ | 2.49 | 0.48 |
| 23:CW:22:G:H2' | 23:CW:23:A:C8 | 2.48 | 0.48 |
| 26:DA:2348:U:O4 | 26:DA:2382:G:N1 | 2.47 | 0.48 |
| 26:DA:250:G:C6 | 26:DA:251:A:C6 | 3.01 | 0.48 |
| 26:DA:894:C:H2' | 26:DA:895:U:C6 | 2.48 | 0.48 |
| 27:DB:43:C:OP1 | 51:D4:6:HIS:NE2 | 2.42 | 0.48 |
| 46:DZ:103:ARG:O | 46:DZ:139:VAL:N | 2.45 | 0.48 |
| 10:AJ:5:ARG:HD3 | 10:AJ:71:LEU:HD11 | 1.95 | 0.48 |
| 3:AC:13:GLY:HA3 | 14:AN:57:ARG:NH2 | 2.27 | 0.48 |
| 17:AQ:26:GLN:HG2 | 17:AQ:37:LYS:HG2 | 1.95 | 0.48 |
| 24:AX:67:C:H2' | 24:AX:68:C:H5' | 1.94 | 0.48 |
| 26:BA:2127:G:C6 | 26:BA:2128:C:C4 | 3.01 | 0.48 |
| 26:BA:900:A:H2' | 26:BA:901:A:C8 | 2.49 | 0.48 |
| 1:CA:1030:C:N3 | 1:CA:1031:G:N2 | 2.54 | 0.48 |
| 1:CA:203:U:OP2 | 1:CA:203:U:H2' | 2.13 | 0.48 |
| 10:CJ:55:LYS:O | 10:CJ:57:LYS:N | 2.46 | 0.48 |
| 12:CL:67:THR:OG1 | 12:CL:95:GLY:O | 2.31 | 0.48 |
| 26:DA:2839:G:H5' | 38:DR:46:GLY:CA | 2.37 | 0.48 |
| 26:DA:455:C:N3 | 26:DA:472:A:H2' | 2.28 | 0.48 |
| 26:DA:539:G:H2' | 26:DA:540:C:C6 | 2.48 | 0.48 |
| 36:DP:50:ARG:HD3 | 55:D8:7:HIS:CD2 | 2.49 | 0.48 |
| 39:DS:11:LYS:O | 39:DS:15:ARG:HG3 | 2.13 | 0.48 |
| 40:DT:109:GLU:O | 40:DT:113:LYS:HB2 | 2.13 | 0.48 |
| 44:DX:12:VAL:HG22 | 44:DX:29:TRP:CE2 | 2.48 | 0.48 |
| 1:AA:36:C:OP1 | 12:AL:123:LYS:NZ | 2.24 | 0.48 |
| 2:AB:33:TYR:HB2 | 2:AB:43:ASP:HB2 | 1.96 | 0.48 |
| 4:AD:107:ARG:HH22 | 4:AD:194:LEU:HD11 | 1.78 | 0.48 |
| 4:AD:3:ARG:O | 4:AD:5:ILE:HG22 | 2.12 | 0.48 |
| 5:AE:140:ARG:O | 5:AE:143:ARG:NH2 | 2.46 | 0.48 |
| 7:AG:73:MET:HG3 | 7:AG:89:MET:O | 2.14 | 0.48 |
| 8:AH:96:GLY:N | 8:AH:99:GLU:OE2 | 2.33 | 0.48 |
| 1:AA:584:G:H5' | 17:AQ:91:ARG:HH22 | 1.78 | 0.48 |
| 25:AY:35:A:H5'' | 25:AY:35:A:H8 | 1.78 | 0.48 |
| 26:BA:1204:A:N6 | 26:BA:1240:U:H2' | 2.28 | 0.48 |
| 26:BA:1798:U:OP2 | 28:BD:274:ARG:NH2 | 2.43 | 0.48 |
| 26:BA:2165:G:H1 | 26:BA:2172:U:H5 | 1.61 | 0.48 |
| 26:BA:2836:U:H2' | 26:BA:2837:G:C8 | 2.49 | 0.48 |
| 26:BA:744:G:OP1 | 29:BE:132:HIS:ND1 | 2.37 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 26:BA:1825:A:OP1 | 28:BD:249:PRO:HD3 | 2.14 | 0.48 |
| 41:BU:49:HIS:HA | 41:BU:52:ARG:HB3 | 1.94 | 0.48 |
| 1:CA:1030:C:N4 | 1:CA:1031:G:N1 | 2.58 | 0.48 |
| 1:CA:1176:A:H2' | 1:CA:1177:G:C8 | 2.49 | 0.48 |
| 1:CA:130:A:N3 | 1:CA:263:A:O2' | 2.32 | 0.48 |
| 2:CB:162:ILE:HD11 | 2:CB:184:VAL:HG22 | 1.94 | 0.48 |
| 13:CM:108:ARG:HD3 | 13:CM:108:ARG:HA | 1.74 | 0.48 |
| 13:CM:86:CYS:SG | 13:CM:87:TYR:N | 2.86 | 0.48 |
| 26:DA:597:U:H2' | 26:DA:598:G:H8 | 1.79 | 0.48 |
| 26:DA:8:A:H2' | 26:DA:9:U:C6 | 2.49 | 0.48 |
| 33:DI:128:LEU:O | 33:DI:140:LEU:N | 2.34 | 0.48 |
| 46:DZ:144:LEU:HD21 | 46:DZ:172:ALA:HB1 | 1.95 | 0.48 |
| 46:DZ:40:ASP:OD2 | 46:DZ:42:VAL:HG12 | 2.14 | 0.48 |
| 1:AA:175:C:H2' | 1:AA:176:C:C6 | 2.48 | 0.48 |
| 1:AA:390:C:H2' | 1:AA:391:G:C8 | 2.49 | 0.48 |
| 1:AA:520:A:N1 | 1:AA:536:C:H1' | 2.28 | 0.48 |
| 1:AA:688:G:H2' | 1:AA:689:C:H6 | 1.79 | 0.48 |
| 2:AB:16:HIS:HB3 | 2:AB:210:SER:CB | 2.43 | 0.48 |
| 3:AC:45:LYS:HG3 | 3:AC:46:GLU:N | 2.28 | 0.48 |
| 25:AY:58:A:O2' | 25:AY:60:U:H5 | 1.96 | 0.48 |
| 51:B4:64:GLY:C | 51:B4:66:SER:H | 2.16 | 0.48 |
| 26:BA:2292:C:P | 39:BS:17:ARG:HH12 | 2.35 | 0.48 |
| 26:BA:2820:A:OP2 | 38:BR:2:ARG:NH2 | 2.47 | 0.48 |
| 30:BF:157:VAL:HB | 30:BF:194:MET:HG2 | 1.96 | 0.48 |
| 34:BN:58:ASP:OD1 | 34:BN:58:ASP:N | 2.45 | 0.48 |
| 1:CA:1013:G:N2 | 1:CA:1015:A:H3' | 2.28 | 0.48 |
| 1:CA:1236:A:O2' | 1:CA:1304:G:H4' | 2.13 | 0.48 |
| 1:CA:524:G:H2' | 1:CA:525:C:C6 | 2.49 | 0.48 |
| 20:CT:16:HIS:O | 20:CT:19:SER:OG | 2.22 | 0.48 |
| 25:CY:64:A:C2' | 25:CY:65:G:H5' | 2.43 | 0.48 |
| 25:CY:9:A:H8 | 25:CY:11:C:N4 | 2.11 | 0.48 |
| 26:DA:1721:G:H2' | 26:DA:1740:G:O6 | 2.14 | 0.48 |
| 26:DA:2036:C:H2' | 26:DA:2037:G:C8 | 2.48 | 0.48 |
| 26:DA:2291:U:H2' | 26:DA:2292:C:C6 | 2.49 | 0.48 |
| 26:DA:752:A:P | 54:D7:3:ARG:HH22 | 2.37 | 0.48 |
| 31:DG:57:ALA:HA | 31:DG:90:LEU:HD13 | 1.94 | 0.48 |
| 36:DP:121:LYS:HG2 | 36:DP:122:PRO:HD2 | 1.96 | 0.48 |
| 46:DZ:43:GLU:O | 46:DZ:47:VAL:HG23 | 2.13 | 0.48 |
| 1:AA:1144:G:H21 | 1:AA:1146:A:H62 | 1.61 | 0.48 |
| 23:AW:2:C:H2' | 23:AW:3:C:C6 | 2.48 | 0.48 |
| 26:BA:271(H):G:H5'' | 48:B1:81:LYS:HE3 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BA:1803:A:H4' | 28:BD:259:THR:HG23 | 1.95 | 0.48 |
| 32:BH:104:GLU:HG3 | 32:BH:114:VAL:HG22 | 1.95 | 0.48 |
| 41:BU:108:GLU:O | 41:BU:112:ARG:HG2 | 2.13 | 0.48 |
| 1:CA:1268:A:N3 | 1:CA:1326:C:O2' | 2.38 | 0.48 |
| 1:CA:359:U:H2' | 1:CA:360:A:C8 | 2.49 | 0.48 |
| 1:CA:421:U:O2' | 1:CA:423:G:N7 | 2.47 | 0.48 |
| 1:CA:442:C:H42 | 1:CA:492:G:H1 | 1.61 | 0.48 |
| 1:CA:683:G:H2' | 1:CA:684:A:C8 | 2.49 | 0.48 |
| 2:CB:16:HIS:HD2 | 2:CB:204:ASN:N | 2.11 | 0.48 |
| 14:CN:24:CYS:O | 14:CN:28:GLY:N | 2.33 | 0.48 |
| 25:CY:22:G:N7 | 25:CY:46:7MG:C2 | 2.82 | 0.48 |
| 26:DA:1899:G:N3 | 26:DA:1899:G:H2' | 2.28 | 0.48 |
| 26:DA:2144:U:H1' | 26:DA:2148:G:H22 | 1.79 | 0.48 |
| 26:DA:2591:C:OP1 | 28:DD:239:ARG:HD2 | 2.14 | 0.48 |
| 26:DA:622:G:H2' | 26:DA:623:G:H8 | 1.78 | 0.48 |
| 32:DH:3:ARG:HB3 | 32:DH:3:ARG:NH1 | 2.29 | 0.48 |
| 34:DN:34:LEU:O | 34:DN:49:GLY:HA3 | 2.13 | 0.48 |
| 41:DU:108:GLU:O | 41:DU:112:ARG:HG2 | 2.14 | 0.48 |
| 43:DW:33:ARG:NE | 43:DW:52:GLU:OE1 | 2.47 | 0.48 |
| 1:AA:1066:C:O2' | 1:AA:1067:A:H5' | 2.13 | 0.48 |
| 1:AA:1162:C:H42 | 1:AA:1174:G:H1 | 1.59 | 0.48 |
| 1:AA:270:A:H2' | 1:AA:271:C:C6 | 2.49 | 0.48 |
| 1:AA:574:A:HO2' | 1:AA:882:C:HO2' | 1.60 | 0.48 |
| 9:AI:53:VAL:HG11 | 9:AI:92:TYR:CE1 | 2.49 | 0.48 |
| 51:B4:16:CYS:HB3 | 51:B4:20:ASN:HB3 | 1.96 | 0.48 |
| 26:BA:1665:A:H2' | 26:BA:1666:G:O4' | 2.13 | 0.48 |
| 1:CA:1000:U:O2 | 1:CA:1041:A:N1 | 2.47 | 0.48 |
| 7:CG:12:LEU:HD12 | 7:CG:12:LEU:H | 1.78 | 0.48 |
| 13:CM:50:GLU:O | 13:CM:54:VAL:HG22 | 2.14 | 0.48 |
| 26:DA:1466:G:O2' | 26:DA:1546:C:O2' | 2.16 | 0.48 |
| 26:DA:2483:C:H2' | 26:DA:2484:G:O4' | 2.14 | 0.48 |
| 26:DA:340:A:H2' | 26:DA:341:G:O4' | 2.14 | 0.48 |
| 30:DF:56:GLU:OE2 | 30:DF:93:LYS:NZ | 2.46 | 0.48 |
| 32:DH:122:THR:O | 32:DH:134:SER:OG | 2.29 | 0.48 |
| 32:DH:69:ARG:O | 32:DH:73:ALA:N | 2.31 | 0.48 |
| 10:AJ:55:LYS:O | 10:AJ:57:LYS:N | 2.47 | 0.48 |
| 25:AY:22:G:C8 | 25:AY:46:7MG:O6 | 2.67 | 0.48 |
| 26:BA:2336:A:H61 | 47:B0:43:THR:HG21 | 1.79 | 0.48 |
| 26:BA:1268:A:H2' | 26:BA:1269:A:O4' | 2.14 | 0.48 |
| 26:BA:2364:C:H2' | 26:BA:2365:G:O4' | 2.14 | 0.48 |
| 26:BA:774:A:N3 | 26:BA:774:A:H2' | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 26:BA:893:C:H2' | 26:BA:894:C:C6 | 2.49 | 0.48 |
| 31:BG:41:GLN:HB2 | 31:BG:90:LEU:HB2 | 1.94 | 0.48 |
| 1:CA:1434:A:H2' | 1:CA:1435:G:O4' | 2.14 | 0.48 |
| 1:CA:392:G:H2' | 1:CA:393:A:H8 | 1.78 | 0.48 |
| 1:CA:991:U:H4' | 1:CA:992:U:OP1 | 2.14 | 0.48 |
| 4:CD:53:ASP:O | 4:CD:57:ARG:HG3 | 2.13 | 0.48 |
| 8:CH:119:LEU:HB3 | 8:CH:123:GLU:HB3 | 1.94 | 0.48 |
| 11:CK:66:LEU:HB3 | 11:CK:70:LYS:NZ | 2.29 | 0.48 |
| 13:CM:4:ILE:HG22 | 13:CM:7:VAL:O | 2.13 | 0.48 |
| 13:CM:91:ARG:NE | 13:CM:97:PRO:O | 2.43 | 0.48 |
| 14:CN:12:ARG:HG2 | 14:CN:13:THR:N | 2.29 | 0.48 |
| 23:CW:9:A:O2' | 23:CW:10:G:N7 | 2.47 | 0.48 |
| 26:DA:2031:A:N3 | 26:DA:2455:G:O2' | 2.38 | 0.48 |
| 26:DA:2314:C:H2' | 26:DA:2315:G:H8 | 1.79 | 0.48 |
| 26:DA:898:C:H2' | 26:DA:899:A:C8 | 2.49 | 0.48 |
| 30:DF:116:ASP:O | 30:DF:120:GLU:HG3 | 2.14 | 0.48 |
| 35:DO:68:GLU:OE2 | 35:DO:78:ARG:NH1 | 2.47 | 0.48 |
| 43:DW:82:LEU:HB2 | 43:DW:98:LYS:HB2 | 1.95 | 0.48 |
| 3:AC:6:HIS:CD2 | 3:AC:8:ILE:H | 2.28 | 0.47 |
| 17:AQ:22:LEU:HD13 | 17:AQ:41:LYS:HG3 | 1.96 | 0.47 |
| 23:AW:29:G:H1 | 23:AW:41:C:H42 | 1.62 | 0.47 |
| 26:BA:2849:U:H4' | 26:BA:2868:A:C2 | 2.49 | 0.47 |
| 30:BF:101:LEU:HD12 | 30:BF:102:PRO:HD2 | 1.95 | 0.47 |
| 35:BO:16:ALA:HB2 | 35:BO:52:VAL:HG21 | 1.95 | 0.47 |
| 45:BY:45:VAL:HG23 | 45:BY:63:LYS:HG2 | 1.95 | 0.47 |
| 1:CA:1162:C:N4 | 1:CA:1174:G:N1 | 2.36 | 0.47 |
| 1:CA:1490:C:H2' | 1:CA:1491:G:C8 | 2.49 | 0.47 |
| 1:CA:583:A:H2' | 1:CA:584:G:O4' | 2.14 | 0.47 |
| 2:CB:153:ARG:HE | 2:CB:153:ARG:HB2 | 1.53 | 0.47 |
| 2:CB:71:VAL:CG2 | 2:CB:164:VAL:HA | 2.44 | 0.47 |
| 4:CD:57:ARG:NH2 | 5:CE:107:ARG:HD3 | 2.26 | 0.47 |
| 6:CF:69:GLU:O | 6:CF:72:VAL:HG12 | 2.14 | 0.47 |
| 10:CJ:38:ILE:HG13 | 10:CJ:71:LEU:HB3 | 1.96 | 0.47 |
| 48:D1:76:ARG:NH1 | 48:D1:97:LEU:O | 2.46 | 0.47 |
| 26:DA:1509(B):A:H2' | 26:DA:1510:G:C8 | 2.49 | 0.47 |
| 26:DA:863:A:H2' | 26:DA:864:G:H8 | 1.79 | 0.47 |
| 26:DA:947:G:H2' | 26:DA:948:G:C8 | 2.49 | 0.47 |
| 27:DB:42:C:H1' | 31:DG:68:PRO:HA | 1.96 | 0.47 |
| 26:DA:1453:U:O4 | 38:DR:67:LEU:HD21 | 2.14 | 0.47 |
| 43:DW:71:VAL:HA | 43:DW:107:LEU:HD12 | 1.96 | 0.47 |
| 45:DY:13:VAL:HB | 45:DY:72:VAL:HG13 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1104:G:O5' | 2:AB:111:ARG:HD2 | 2.14 | 0.47 |
| 1:AA:1348:U:H4' | 9:AI:120:ARG:HD2 | 1.96 | 0.47 |
| 14:AN:14:PRO:HB2 | 14:AN:16:PHE:O | 2.14 | 0.47 |
| 26:BA:1899:G:H2' | 26:BA:1899:G:N3 | 2.29 | 0.47 |
| 26:BA:2142:C:H2' | 26:BA:2143:C:C6 | 2.49 | 0.47 |
| 26:BA:218:A:C2 | 26:BA:235:U:H4' | 2.50 | 0.47 |
| 37:BQ:21:THR:HG21 | 37:BQ:101:ARG:HD3 | 1.96 | 0.47 |
| 1:CA:1017:G:H2' | 1:CA:1018:C:C6 | 2.49 | 0.47 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:N1 | 2.07 | 0.47 |
| 1:CA:59:A:H3' | 1:CA:331:G:H22 | 1.79 | 0.47 |
| 1:CA:659:U:H2' | 1:CA:660:G:O4' | 2.14 | 0.47 |
| 1:CA:811:C:N3 | 61:CA:3210:HOH:O | 2.35 | 0.47 |
| 5:CE:6:PHE:CD1 | 5:CE:36:ASP:HB3 | 2.49 | 0.47 |
| 13:CM:40:ASN:HB3 | 13:CM:43:THR:HG23 | 1.95 | 0.47 |
| 17:CQ:66:SER:OG | 17:CQ:69:LYS:HB2 | 2.14 | 0.47 |
| 48:D1:65:SER:OG | 48:D1:66:HIS:ND1 | 2.41 | 0.47 |
| 53:D6:21:TYR:CE1 | 53:D6:38:LYS:HG2 | 2.49 | 0.47 |
| 26:DA:2124:G:H1 | 26:DA:2174:C:N4 | 2.13 | 0.47 |
| 26:DA:2321:G:N3 | 26:DA:2321:G:H2' | 2.28 | 0.47 |
| 30:DF:36:VAL:HG11 | 30:DF:183:VAL:HG11 | 1.96 | 0.47 |
| 32:DH:35:VAL:HG11 | 32:DH:71:LEU:HG | 1.97 | 0.47 |
| 33:DI:102:SER:OG | 33:DI:103:ARG:N | 2.47 | 0.47 |
| 36:DP:21:ARG:HA | 36:DP:21:ARG:HD3 | 1.50 | 0.47 |
| 26:DA:863:A:P | 37:DQ:22:LYS:HG3 | 2.54 | 0.47 |
| 39:DS:77:ALA:O | 39:DS:81:GLY:N | 2.46 | 0.47 |
| 1:AA:598:U:H4' | 8:AH:94:TYR:CD2 | 2.50 | 0.47 |
| 15:AO:84:LYS:HD3 | 15:AO:84:LYS:O | 2.13 | 0.47 |
| 17:AQ:78:GLU:HG2 | 17:AQ:79:SER:N | 2.29 | 0.47 |
| 1:AA:191:G:H21 | 20:AT:103:GLY:HA2 | 1.79 | 0.47 |
| 26:BA:330:A:H2 | 26:BA:1210:A:C2' | 2.26 | 0.47 |
| 26:BA:2130:U:H1' | 26:BA:2158:A:N1 | 2.29 | 0.47 |
| 1:AA:346:G:P | 40:BT:41:ARG:HH22 | 2.36 | 0.47 |
| 45:BY:11:ASP:OD1 | 45:BY:11:ASP:N | 2.40 | 0.47 |
| 1:CA:1267:C:H6 | 1:CA:1267:C:O5' | 1.97 | 0.47 |
| 1:CA:1367:C:H4' | 10:CJ:48:THR:HG21 | 1.95 | 0.47 |
| 1:CA:235:C:H5' | 17:CQ:70:ARG:HG2 | 1.96 | 0.47 |
| 1:CA:664:G:N2 | 1:CA:741:G:H1 | 2.04 | 0.47 |
| 49:D2:16:LEU:HB2 | 49:D2:21:LEU:HD23 | 1.97 | 0.47 |
| 26:DA:885:C:H2' | 26:DA:886:C:H4' | 1.96 | 0.47 |
| 26:DA:62:C:H42 | 26:DA:93:G:H1 | 1.62 | 0.47 |
| 27:DB:24:G:H4' | 27:DB:25:A:C8 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DF:33:LEU:HD13 | 30:DF:112:MET:HE2 | 1.95 | 0.47 |
| 31:DG:111:LEU:HA | 31:DG:114:ILE:HD13 | 1.96 | 0.47 |
| 31:DG:15:VAL:HG13 | 31:DG:175:LEU:HD23 | 1.97 | 0.47 |
| 36:DP:82:GLY:HA2 | 36:DP:113:LYS:O | 2.14 | 0.47 |
| 39:DS:84:GLN:H | 39:DS:111:GLU:HB2 | 1.79 | 0.47 |
| 39:DS:30:ARG:HD3 | 39:DS:98:VAL:HG22 | 1.97 | 0.47 |
| 40:DT:99:LEU:O | 40:DT:102:ILE:HG12 | 2.14 | 0.47 |
| 1:AA:1033:G:H2' | 1:AA:1034:G:C8 | 2.45 | 0.47 |
| 1:AA:1255:G:N7 | 10:AJ:43:ARG:NH2 | 2.62 | 0.47 |
| 1:AA:1479:C:H2' | 1:AA:1480:G:C8 | 2.49 | 0.47 |
| 51:B4:18:CYS:SG | 51:B4:20:ASN:HB2 | 2.55 | 0.47 |
| 51:B4:59:PHE:C | 51:B4:61:ARG:H | 2.13 | 0.47 |
| 26:BA:826:U:H4' | 36:BP:55:ARG:HB2 | 1.96 | 0.47 |
| 45:BY:13:VAL:HB | 45:BY:72:VAL:HG13 | 1.95 | 0.47 |
| 1:CA:1004:A:H62 | 1:CA:1037:C:C2' | 2.28 | 0.47 |
| 1:CA:1179:A:H2' | 1:CA:1180:A:O4' | 2.13 | 0.47 |
| 1:CA:1225:A:OP1 | 13:CM:103:THR:OG1 | 2.30 | 0.47 |
| 1:CA:353:A:H8 | 1:CA:353:A:H5' | 1.78 | 0.47 |
| 2:CB:178:ARG:HH21 | 8:CH:74:PRO:HG3 | 1.80 | 0.47 |
| 4:CD:20:TYR:HD1 | 4:CD:26:CYS:HB3 | 1.78 | 0.47 |
| 11:CK:24:SER:OG | 11:CK:25:TYR:N | 2.45 | 0.47 |
| 25:CY:66:U:H2' | 25:CY:67:C:O4' | 2.14 | 0.47 |
| 26:DA:1029:A:N6 | 26:DA:1125:G:O2' | 2.44 | 0.47 |
| 26:DA:1639:U:C2' | 26:DA:1640:C:H5'' | 2.42 | 0.47 |
| 26:DA:212:G:H2' | 26:DA:213:A:O4' | 2.13 | 0.47 |
| 26:DA:571:A:N6 | 26:DA:2499:C:O3' | 2.46 | 0.47 |
| 26:DA:2646:C:H2' | 26:DA:2647:U:O4' | 2.15 | 0.47 |
| 31:DG:144:ILE:HG23 | 31:DG:148:MET:HE1 | 1.96 | 0.47 |
| 39:DS:53:SER:O | 39:DS:57:LYS:N | 2.47 | 0.47 |
| 1:AA:167:G:H2' | 1:AA:168:G:C8 | 2.49 | 0.47 |
| 1:AA:457:C:H2' | 1:AA:458:C:H6 | 1.79 | 0.47 |
| 1:AA:741:G:H2' | 1:AA:742:G:O4' | 2.15 | 0.47 |
| 1:AA:952:U:H2' | 1:AA:953:G:C8 | 2.50 | 0.47 |
| 2:AB:77:ALA:HB2 | 2:AB:211:ILE:HD13 | 1.96 | 0.47 |
| 1:AA:428:G:OP2 | 4:AD:10:ARG:NH1 | 2.47 | 0.47 |
| 8:AH:33:GLU:HG2 | 8:AH:48:TYR:OH | 2.14 | 0.47 |
| 24:AX:56:C:O5' | 24:AX:56:C:H6 | 1.97 | 0.47 |
| 33:BI:85:GLU:HB3 | 33:BI:86:THR:H | 1.55 | 0.47 |
| 46:BZ:108:PRO:HB3 | 46:BZ:117:LEU:HD22 | 1.97 | 0.47 |
| 2:CB:91:PRO:HG3 | 2:CB:155:LEU:HD23 | 1.95 | 0.47 |
| 5:CE:10:MET:HG3 | 5:CE:32:VAL:HG22 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CI:55:ALA:HA | 9:CI:58:HIS:CD2 | 2.50 | 0.47 |
| 18:CR:41:LYS:HB3 | 18:CR:41:LYS:NZ | 2.29 | 0.47 |
| 18:CR:73:ALA:HB3 | 18:CR:79:LEU:HG | 1.96 | 0.47 |
| 26:DA:1220:A:OP2 | 41:DU:19:LYS:NZ | 2.34 | 0.47 |
| 26:DA:1316:U:H2' | 26:DA:1317:A:C8 | 2.49 | 0.47 |
| 26:DA:1420:U:HO2' | 26:DA:1421:G:P | 2.37 | 0.47 |
| 26:DA:2136:C:H1' | 26:DA:2137:C:H5' | 1.96 | 0.47 |
| 26:DA:641:C:H42 | 26:DA:647:G:H1 | 1.62 | 0.47 |
| 26:DA:657:U:H2' | 26:DA:658:C:C6 | 2.49 | 0.47 |
| 28:DD:2:ALA:O | 28:DD:3:VAL:HB | 2.15 | 0.47 |
| 30:DF:178:PRO:HB3 | 30:DF:198:ALA:HA | 1.97 | 0.47 |
| 44:DX:35:THR:HB | 44:DX:38:GLU:HB2 | 1.97 | 0.47 |
| 4:AD:140:VAL:HG11 | 4:AD:146:ILE:HD11 | 1.96 | 0.47 |
| 4:AD:12:CYS:SG | 4:AD:19:LEU:HB2 | 2.54 | 0.47 |
| 16:AP:28:ARG:NE | 16:AP:29:ASP:OD1 | 2.29 | 0.47 |
| 16:AP:20:VAL:HG23 | 16:AP:35:LYS:HA | 1.96 | 0.47 |
| 18:AR:33:ASP:OD2 | 18:AR:36:ASN:HB2 | 2.13 | 0.47 |
| 25:AY:2:C:H42 | 25:AY:71:G:H1 | 1.63 | 0.47 |
| 25:AY:15:G:C6 | 25:AY:48:C:O2 | 2.68 | 0.47 |
| 26:BA:2181:G:HO2' | 26:BA:2182:G:P | 2.37 | 0.47 |
| 26:BA:2207:G:H2' | 26:BA:2208:A:C2 | 2.50 | 0.47 |
| 26:BA:534:U:H2' | 26:BA:535:C:C6 | 2.49 | 0.47 |
| 33:BI:48:GLU:O | 33:BI:52:ARG:HB3 | 2.14 | 0.47 |
| 1:CA:1362:C:C2' | 1:CA:1363:C:H5'' | 2.45 | 0.47 |
| 1:CA:601:C:H42 | 1:CA:637:G:H1 | 1.63 | 0.47 |
| 2:CB:17:PHE:CD2 | 2:CB:44:LEU:HD11 | 2.49 | 0.47 |
| 8:CH:84:ARG:O | 8:CH:84:ARG:HG3 | 2.14 | 0.47 |
| 20:CT:56:MET:HE2 | 20:CT:56:MET:HB2 | 1.71 | 0.47 |
| 23:CW:50:U:H2' | 23:CW:51:U:O4' | 2.15 | 0.47 |
| 24:CX:37:A:H2' | 24:CX:38:A:O4' | 2.14 | 0.47 |
| 50:D3:50:VAL:O | 50:D3:54:VAL:HB | 2.15 | 0.47 |
| 26:DA:1019:U:O2' | 26:DA:1021:A:H2 | 1.97 | 0.47 |
| 24:CX:12:G:H4' | 26:DA:1908:C:O2 | 2.14 | 0.47 |
| 28:DD:164:GLN:NE2 | 28:DD:176:ARG:HH22 | 2.12 | 0.47 |
| 35:DO:120:GLU:HG2 | 35:DO:122:LEU:HG | 1.97 | 0.47 |
| 45:DY:28:LYS:HE2 | 45:DY:28:LYS:HB3 | 1.67 | 0.47 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C6 | 2.50 | 0.47 |
| 1:AA:1513:A:H2' | 1:AA:1514:C:C6 | 2.50 | 0.47 |
| 1:AA:162:A:H3' | 1:AA:163:C:C4' | 2.45 | 0.47 |
| 1:AA:620:C:H2' | 1:AA:621:A:O4' | 2.15 | 0.47 |
| 3:AC:62:ASP:HA | 3:AC:97:LYS:HD3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 16:AP:48:TRP:HH2 | 16:AP:76:GLN:NE2 | 2.12 | 0.47 |
| 19:AS:23:ASN:HA | 19:AS:27:GLU:CD | 2.35 | 0.47 |
| 24:AX:2:G:H2' | 24:AX:2:G:N3 | 2.29 | 0.47 |
| 26:BA:2140:C:C4 | 26:BA:2151:G:N1 | 2.83 | 0.47 |
| 26:BA:2345:G:H4' | 26:BA:2346:A:H5'' | 1.97 | 0.47 |
| 30:BF:39:TRP:O | 30:BF:43:LYS:HD3 | 2.14 | 0.47 |
| 31:BG:19:LEU:HG | 31:BG:175:LEU:HD23 | 1.97 | 0.47 |
| 1:CA:1256:A:N1 | 1:CA:1278:U:H1' | 2.29 | 0.47 |
| 1:CA:1479:C:H2' | 1:CA:1480:G:H8 | 1.78 | 0.47 |
| 1:CA:24:U:OP1 | 12:CL:23:LYS:NZ | 2.47 | 0.47 |
| 13:CM:39:ILE:HG12 | 13:CM:52:GLU:HG2 | 1.96 | 0.47 |
| 14:CN:27:CYS:SG | 14:CN:29:ARG:HB2 | 2.55 | 0.47 |
| 20:CT:53:LEU:HA | 20:CT:56:MET:HG2 | 1.96 | 0.47 |
| 24:CX:8:4SU:O5' | 24:CX:8:4SU:H6 | 2.15 | 0.47 |
| 22:CV:14:A:C4 | 25:CY:34:G:C6 | 3.02 | 0.47 |
| 50:D3:8:LEU:HD13 | 50:D3:31:LEU:HD23 | 1.97 | 0.47 |
| 26:DA:1239:G:H2' | 26:DA:1240:U:O4' | 2.14 | 0.47 |
| 28:DD:134:ARG:NH1 | 28:DD:188:GLU:OE2 | 2.47 | 0.47 |
| 32:DH:98:LEU:HD13 | 32:DH:102:ALA:O | 2.13 | 0.47 |
| 26:DA:2547:U:O2 | 35:DO:23:ARG:NH2 | 2.47 | 0.47 |
| 36:DP:16:ARG:HG3 | 61:DP:305:HOH:O | 2.13 | 0.47 |
| 1:AA:1007:C:N3 | 1:AA:1022:G:C6 | 2.83 | 0.47 |
| 1:AA:1285:A:H4' | 1:AA:1286:A:O5' | 2.15 | 0.47 |
| 1:AA:1392:G:N2 | 1:AA:1502:A:C8 | 2.83 | 0.47 |
| 1:AA:1530:G:H2' | 1:AA:1531:A:O4' | 2.15 | 0.47 |
| 1:AA:564:C:O2' | 8:AH:91:ARG:NH2 | 2.38 | 0.47 |
| 26:BA:2557:G:H2' | 26:BA:2558:C:C6 | 2.50 | 0.47 |
| 26:BA:271(X):G:C2 | 26:BA:271(Y):U:O4 | 2.68 | 0.47 |
| 1:CA:1392:G:H21 | 1:CA:1502:A:H8 | 1.63 | 0.47 |
| 1:CA:643:C:H2' | 1:CA:644:G:H8 | 1.79 | 0.47 |
| 1:CA:22:G:H4' | 1:CA:885:G:C8 | 2.50 | 0.47 |
| 4:CD:22:LYS:HG3 | 58:CD:501:SF4:S4 | 2.55 | 0.47 |
| 8:CH:103:VAL:HG21 | 8:CH:109:ILE:C | 2.35 | 0.47 |
| 15:CO:69:TYR:O | 15:CO:73:GLU:HG2 | 2.14 | 0.47 |
| 17:CQ:26:GLN:HG2 | 17:CQ:37:LYS:HG2 | 1.96 | 0.47 |
| 19:CS:41:VAL:O | 19:CS:44:MET:HB2 | 2.14 | 0.47 |
| 26:DA:1270:C:H5'' | 26:DA:1271:G:O5' | 2.15 | 0.47 |
| 26:DA:1528(A):A:H2' | 26:DA:1529:G:O4' | 2.15 | 0.47 |
| 26:DA:1592:C:H2' | 26:DA:1593:G:H8 | 1.79 | 0.47 |
| 26:DA:2128:C:N4 | 26:DA:2160:G:H1 | 2.09 | 0.47 |
| 27:DB:70:C:H42 | 27:DB:107:G:H1 | 1.61 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DB:94:C:H2' | 27:DB:95:C:C6 | 2.50 | 0.47 |
| 28:DD:26:LYS:HE2 | 28:DD:28:GLU:O | 2.15 | 0.47 |
| 1:AA:1122:U:C4 | 1:AA:1123:A:N7 | 2.83 | 0.47 |
| 1:AA:346:G:OP1 | 40:BT:41:ARG:NH1 | 2.42 | 0.47 |
| 1:AA:1250:A:H4' | 9:AI:68:GLY:N | 2.30 | 0.47 |
| 9:AI:4:TYR:CE2 | 9:AI:88:TYR:HD1 | 2.33 | 0.47 |
| 26:BA:1416:G:O2' | 26:BA:1417:C:OP2 | 2.24 | 0.47 |
| 26:BA:1482:G:O6 | 26:BA:1507:A:N6 | 2.48 | 0.47 |
| 26:BA:1686:C:H2' | 26:BA:1687:G:O4' | 2.15 | 0.47 |
| 26:BA:2137:C:N3 | 26:BA:2154:G:O6 | 2.48 | 0.47 |
| 26:BA:2168:G:C6 | 26:BA:2171:A:C8 | 3.02 | 0.47 |
| 26:BA:34:C:H5'' | 26:BA:35:G:OP2 | 2.15 | 0.47 |
| 26:BA:784:A:N6 | 28:BD:229:VAL:HG11 | 2.30 | 0.47 |
| 30:BF:53:THR:HG23 | 30:BF:55:GLY:H | 1.80 | 0.47 |
| 1:CA:1360:A:O5' | 1:CA:1360:A:H8 | 1.97 | 0.47 |
| 5:CE:145:LYS:HE3 | 5:CE:149:GLU:OE2 | 2.15 | 0.47 |
| 8:CH:51:VAL:HG11 | 8:CH:60:ARG:NH1 | 2.30 | 0.47 |
| 10:CJ:62:HIS:HB3 | 14:CN:59:ALA:HB3 | 1.97 | 0.47 |
| 11:CK:65:ALA:HB3 | 11:CK:97:ALA:HB3 | 1.97 | 0.47 |
| 51:D4:16:CYS:SG | 51:D4:17:GLY:N | 2.87 | 0.47 |
| 26:DA:1127:A:H2' | 26:DA:1128:A:H5'' | 1.97 | 0.47 |
| 26:DA:2059:A:O2' | 30:DF:69:HIS:HD2 | 1.98 | 0.47 |
| 26:DA:251:A:C5 | 26:DA:252:G:H1' | 2.50 | 0.47 |
| 26:DA:2820:A:O2' | 26:DA:2821:A:OP1 | 2.29 | 0.47 |
| 26:DA:602:G:O2' | 26:DA:655:A:N6 | 2.48 | 0.47 |
| 26:DA:782:A:H5' | 26:DA:783:A:N7 | 2.30 | 0.47 |
| 27:DB:8:U:O2' | 39:DS:40:ILE:HD13 | 2.15 | 0.47 |
| 1:AA:1095:U:H5'' | 1:AA:1109:C:O2 | 2.14 | 0.47 |
| 1:AA:1353:G:OP1 | 21:AU:10:ARG:NH1 | 2.42 | 0.47 |
| 1:AA:256:U:H2' | 1:AA:257:G:C8 | 2.49 | 0.47 |
| 1:AA:413:G:N2 | 1:AA:428:G:H1' | 2.30 | 0.47 |
| 1:AA:626:U:H2' | 1:AA:627:G:H8 | 1.78 | 0.47 |
| 1:AA:743:U:H2' | 1:AA:744:C:C6 | 2.50 | 0.47 |
| 2:AB:59:GLU:O | 2:AB:63:MET:HG3 | 2.14 | 0.47 |
| 4:AD:98:GLU:HG2 | 4:AD:189:PRO:HG2 | 1.96 | 0.47 |
| 10:AJ:38:ILE:HG13 | 10:AJ:71:LEU:O | 2.15 | 0.47 |
| 1:AA:1525:G:P | 11:AK:120:ARG:HH22 | 2.37 | 0.47 |
| 18:AR:26:LEU:HD23 | 18:AR:29:PHE:CE2 | 2.50 | 0.47 |
| 33:BI:12:LEU:HD23 | 33:BI:12:LEU:HA | 1.79 | 0.47 |
| 33:BI:47:LEU:HA | 33:BI:47:LEU:HD23 | 1.75 | 0.47 |
| 26:BA:904:C:H4' | 46:BZ:169:GLU:OE2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 46:BZ:7:ALA:HB3 | 46:BZ:61:LEU:HD12 | 1.97 | 0.47 |
| 1:CA:1314:C:OP1 | 19:CS:6:LYS:NZ | 2.24 | 0.47 |
| 1:CA:258:G:OP1 | 20:CT:86:ARG:NH1 | 2.48 | 0.47 |
| 25:CY:35:A:H2' | 25:CY:36:A:O4' | 2.15 | 0.47 |
| 25:CY:50:U:H2' | 25:CY:51:U:C6 | 2.50 | 0.47 |
| 26:DA:1600:C:OP1 | 44:DX:58:HIS:NE2 | 2.37 | 0.47 |
| 26:DA:1794:U:H2' | 26:DA:1795:C:C6 | 2.50 | 0.47 |
| 26:DA:2136:C:N4 | 26:DA:2155:G:C6 | 2.82 | 0.47 |
| 26:DA:2391:G:O6 | 26:DA:2425:A:H8 | 1.98 | 0.47 |
| 26:DA:272:G:H4' | 26:DA:272(A):U:H5'' | 1.97 | 0.47 |
| 30:DF:20:LEU:HD12 | 30:DF:125:LEU:HD13 | 1.97 | 0.47 |
| 1:AA:502:G:H2' | 1:AA:503:C:O4' | 2.14 | 0.47 |
| 2:AB:80:ILE:O | 2:AB:84:GLU:HB2 | 2.15 | 0.47 |
| 13:AM:88:ARG:HG3 | 13:AM:98:VAL:CG1 | 2.45 | 0.47 |
| 19:AS:41:VAL:HG12 | 19:AS:43:GLU:H | 1.80 | 0.47 |
| 26:BA:1124:C:H1' | 56:B9:36:GLN:NE2 | 2.30 | 0.47 |
| 26:BA:1745(A):C:H5' | 26:BA:1746:G:OP2 | 2.15 | 0.47 |
| 26:BA:1778:U:H2' | 26:BA:1784:A:N6 | 2.29 | 0.47 |
| 26:BA:2163:C:H5' | 26:BA:2163:C:C6 | 2.49 | 0.47 |
| 26:BA:848:G:N9 | 26:BA:933:A:H8 | 2.11 | 0.47 |
| 26:BA:875:G:H2' | 26:BA:876:C:O4' | 2.15 | 0.47 |
| 32:BH:25:LYS:HG2 | 32:BH:34:GLU:HG2 | 1.97 | 0.47 |
| 1:CA:107:G:H2' | 1:CA:108:G:O4' | 2.15 | 0.47 |
| 1:CA:827:U:H5'' | 1:CA:828:A:OP2 | 2.15 | 0.47 |
| 2:CB:219:VAL:HA | 2:CB:222:ILE:HG12 | 1.96 | 0.47 |
| 3:CC:127:ARG:NH2 | 3:CC:192:THR:HG23 | 2.29 | 0.47 |
| 3:CC:54:ARG:H | 3:CC:69:HIS:HB2 | 1.79 | 0.47 |
| 4:CD:103:ASN:OD1 | 4:CD:114:ARG:NE | 2.39 | 0.47 |
| 6:CF:97:PHE:CE1 | 18:CR:62:GLU:HG2 | 2.50 | 0.47 |
| 1:CA:1123:A:H4' | 10:CJ:37:PRO:HD2 | 1.96 | 0.47 |
| 49:D2:29:LYS:HE2 | 49:D2:57:ILE:HG21 | 1.96 | 0.47 |
| 26:DA:1027:A:C6 | 26:DA:1126:A:C4 | 3.03 | 0.47 |
| 26:DA:2153:G:C2 | 26:DA:2154:G:C4 | 3.03 | 0.47 |
| 26:DA:2841:C:H2' | 26:DA:2842:G:C8 | 2.51 | 0.47 |
| 26:DA:613:G:O2' | 26:DA:614(C):A:N1 | 2.40 | 0.47 |
| 26:DA:900:A:C8 | 26:DA:901:A:N7 | 2.83 | 0.47 |
| 26:DA:955:C:OP1 | 37:DQ:87:LYS:HE3 | 2.15 | 0.47 |
| 34:DN:108:PRO:O | 34:DN:113:GLY:HA3 | 2.15 | 0.47 |
| 1:AA:116:A:H8 | 1:AA:116:A:O5' | 1.97 | 0.46 |
| 1:AA:664:G:N2 | 1:AA:741:G:H1 | 2.03 | 0.46 |
| 1:AA:890:G:O2' | 1:AA:906:G:O6 | 2.19 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:992:U:H4' | 1:AA:993:G:H5'' | 1.97 | 0.46 |
| 2:AB:60:ASP:OD1 | 2:AB:64:ARG:NH2 | 2.49 | 0.46 |
| 3:AC:122:GLU:O | 3:AC:126:ARG:NH1 | 2.41 | 0.46 |
| 5:AE:95:ALA:HB1 | 5:AE:96:PRO:HD2 | 1.96 | 0.46 |
| 6:AF:86:ARG:O | 6:AF:87:ARG:HG2 | 2.14 | 0.46 |
| 9:AI:79:LEU:O | 9:AI:83:ARG:HG3 | 2.15 | 0.46 |
| 1:AA:1367:C:H4' | 10:AJ:48:THR:HG21 | 1.96 | 0.46 |
| 1:AA:1458:G:H5'' | 20:AT:31:SER:HB2 | 1.96 | 0.46 |
| 24:AX:32:5MC:HM53 | 24:AX:33:U:O4 | 2.15 | 0.46 |
| 25:AY:57:G:H2' | 25:AY:58:A:H5' | 1.97 | 0.46 |
| 25:AY:58:A:N6 | 25:AY:61:C:C2 | 2.83 | 0.46 |
| 52:B5:11:THR:HG23 | 52:B5:15:ARG:HB3 | 1.96 | 0.46 |
| 26:BA:1470:G:N2 | 26:BA:1520:G:OP2 | 2.36 | 0.46 |
| 26:BA:2134:A:HO2' | 26:BA:2135:A:C5' | 2.28 | 0.46 |
| 1:CA:1129:C:H2' | 1:CA:1139:G:C5 | 2.49 | 0.46 |
| 1:CA:1323:G:H2' | 1:CA:1324:A:C8 | 2.50 | 0.46 |
| 1:CA:447:G:O6 | 1:CA:485:G:O2' | 2.23 | 0.46 |
| 2:CB:211:ILE:O | 2:CB:215:LEU:HB2 | 2.14 | 0.46 |
| 3:CC:121:ALA:HB1 | 3:CC:189:ALA:HB2 | 1.96 | 0.46 |
| 20:CT:87:LYS:O | 20:CT:91:LEU:HG | 2.15 | 0.46 |
| 26:DA:1628:G:H2' | 26:DA:1629:U:C6 | 2.50 | 0.46 |
| 26:DA:2136:C:O2' | 26:DA:2137:C:O5' | 2.22 | 0.46 |
| 26:DA:2577:A:OP2 | 52:D5:3:LYS:NZ | 2.43 | 0.46 |
| 26:DA:908:C:OP2 | 37:DQ:22:LYS:NZ | 2.48 | 0.46 |
| 31:DG:107:LEU:HD21 | 31:DG:178:PHE:CE1 | 2.50 | 0.46 |
| 31:DG:122:PRO:HG3 | 31:DG:180:PHE:HB3 | 1.96 | 0.46 |
| 31:DG:41:GLN:NE2 | 31:DG:153:ARG:HB3 | 2.30 | 0.46 |
| 34:DN:104:LYS:HA | 34:DN:107:LEU:HD12 | 1.97 | 0.46 |
| 36:DP:54:GLY:O | 61:DP:308:HOH:O | 2.20 | 0.46 |
| 39:DS:106:ARG:HG3 | 39:DS:112:PHE:CZ | 2.50 | 0.46 |
| 1:AA:405:U:H5'' | 1:AA:495:A:H2 | 1.80 | 0.46 |
| 1:AA:955:U:O2' | 19:AS:83:HIS:HD2 | 1.98 | 0.46 |
| 2:AB:10:LEU:C | 2:AB:12:GLU:H | 2.17 | 0.46 |
| 4:AD:107:ARG:NH2 | 4:AD:194:LEU:HD21 | 2.31 | 0.46 |
| 5:AE:110:LEU:HD13 | 5:AE:118:ILE:HD13 | 1.97 | 0.46 |
| 12:AL:88:GLY:O | 12:AL:99:HIS:HD2 | 1.99 | 0.46 |
| 15:AO:82:ILE:HB | 15:AO:87:ILE:HB | 1.96 | 0.46 |
| 23:AW:50:U:H2' | 23:AW:51:U:O4' | 2.14 | 0.46 |
| 31:BG:66:GLN:HG3 | 51:B4:1:MET:CE | 2.46 | 0.46 |
| 26:BA:1952:A:C6 | 26:BA:1953:A:N1 | 2.83 | 0.46 |
| 26:BA:2159:G:H2' | 26:BA:2160:G:C8 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BA:363(B):G:H2' | 26:BA:363(C):G:H5' | 1.97 | 0.46 |
| 26:BA:839:U:H2' | 26:BA:840:C:C6 | 2.51 | 0.46 |
| 27:BB:77:U:OP1 | 46:BZ:19:ARG:NH2 | 2.39 | 0.46 |
| 36:BP:135:LEU:HD23 | 36:BP:135:LEU:HA | 1.71 | 0.46 |
| 38:BR:44:LEU:HD22 | 38:BR:48:VAL:HG23 | 1.97 | 0.46 |
| 38:BR:55:ALA:HB2 | 38:BR:79:LEU:HD13 | 1.97 | 0.46 |
| 39:BS:10:ARG:O | 39:BS:14:VAL:HG13 | 2.16 | 0.46 |
| 43:BW:71:VAL:HA | 43:BW:107:LEU:HD12 | 1.96 | 0.46 |
| 44:BX:60:ARG:HA | 44:BX:75:ASP:OD2 | 2.16 | 0.46 |
| 1:CA:1256:A:C6 | 1:CA:1278:U:H1' | 2.51 | 0.46 |
| 1:CA:1279:A:O2' | 1:CA:1282:C:N4 | 2.49 | 0.46 |
| 1:CA:1291:G:O2' | 9:CI:38:GLN:HG3 | 2.14 | 0.46 |
| 1:CA:1320:C:C1' | 19:CS:73:GLU:HG2 | 2.46 | 0.46 |
| 1:CA:59:A:H5" | 1:CA:60:A:H5" | 1.96 | 0.46 |
| 25:CY:35:A:C6 | 25:CY:36:A:C2 | 3.03 | 0.46 |
| 47:D0:14:ARG:NH1 | 47:D0:14:ARG:HB2 | 2.30 | 0.46 |
| 26:DA:1430:C:H2' | 26:DA:1431:U:C6 | 2.50 | 0.46 |
| 26:DA:1916:A:H2' | 26:DA:1917:U:O4' | 2.16 | 0.46 |
| 26:DA:293:U:H5" | 26:DA:294:A:OP2 | 2.15 | 0.46 |
| 1:AA:154:C:C2' | 1:AA:155:C:H5' | 2.45 | 0.46 |
| 1:AA:65:U:H6 | 1:AA:65:U:H5' | 1.80 | 0.46 |
| 4:AD:18:LYS:HG2 | 58:AD:501:SF4:S1 | 2.55 | 0.46 |
| 10:AJ:8:LEU:N | 10:AJ:70:ARG:O | 2.33 | 0.46 |
| 26:BA:1007:C:OP1 | 34:BN:37:LYS:NZ | 2.46 | 0.46 |
| 26:BA:784:A:C6 | 28:BD:229:VAL:HG11 | 2.50 | 0.46 |
| 32:BH:69:ARG:HG3 | 32:BH:70:THR:N | 2.29 | 0.46 |
| 45:BY:28:LYS:HB3 | 45:BY:28:LYS:HE2 | 1.75 | 0.46 |
| 2:CB:71:VAL:HG12 | 2:CB:93:VAL:CG2 | 2.45 | 0.46 |
| 7:CG:72:ARG:NH2 | 7:CG:138:LYS:HZ1 | 2.12 | 0.46 |
| 13:CM:25:ILE:HG13 | 13:CM:29:ARG:HG2 | 1.97 | 0.46 |
| 26:DA:857:C:H4' | 47:D0:23:VAL:HG21 | 1.98 | 0.46 |
| 26:DA:1006:C:C2 | 26:DA:1138:G:N2 | 2.84 | 0.46 |
| 26:DA:2127:G:OP1 | 26:DA:2127:G:H4' | 2.15 | 0.46 |
| 1:AA:1002:G:N3 | 1:AA:1003:G:H1' | 2.30 | 0.46 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:C6 | 2.50 | 0.46 |
| 1:AA:1305:G:H22 | 1:AA:1331:G:H1' | 1.80 | 0.46 |
| 1:AA:316:G:OP2 | 1:AA:351:G:O2' | 2.30 | 0.46 |
| 1:AA:448:A:OP2 | 1:AA:485:G:N1 | 2.33 | 0.46 |
| 4:AD:187:ARG:HG2 | 4:AD:188:LEU:N | 2.31 | 0.46 |
| 10:AJ:31:GLY:HA2 | 10:AJ:32:ALA:HA | 1.68 | 0.46 |
| 1:AA:1296:C:H5" | 13:AM:14:ARG:HD2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AY:5:G:H2' | 25:AY:6:G:C8 | 2.51 | 0.46 |
| 26:BA:1166:C:H2' | 26:BA:1167:U:C6 | 2.51 | 0.46 |
| 26:BA:2101:G:H2' | 26:BA:2102:U:H6 | 1.80 | 0.46 |
| 26:BA:2126:A:H4' | 26:BA:2127:G:OP1 | 2.16 | 0.46 |
| 26:BA:2162:G:C3' | 26:BA:2163:C:H5'' | 2.46 | 0.46 |
| 26:BA:2562:U:O2' | 35:BO:23:ARG:HD3 | 2.15 | 0.46 |
| 26:BA:414:C:H2' | 26:BA:415:A:C8 | 2.51 | 0.46 |
| 31:BG:66:GLN:OE1 | 31:BG:98:ARG:NE | 2.43 | 0.46 |
| 1:CA:1125:U:C2 | 10:CJ:38:ILE:HD13 | 2.50 | 0.46 |
| 1:CA:1164:G:O2' | 1:CA:1165:C:H5' | 2.15 | 0.46 |
| 9:CI:18:PHE:HD2 | 9:CI:62:TYR:HD2 | 1.63 | 0.46 |
| 24:CX:47:U:N3 | 24:CX:50:U:OP1 | 2.49 | 0.46 |
| 26:DA:1199:U:H2' | 26:DA:1200:C:C6 | 2.51 | 0.46 |
| 26:DA:1789:A:H2' | 26:DA:1790:C:C6 | 2.50 | 0.46 |
| 26:DA:2296:U:OP2 | 39:DS:9:ARG:NH2 | 2.46 | 0.46 |
| 26:DA:242:G:C8 | 55:D8:5:LYS:HG2 | 2.51 | 0.46 |
| 26:DA:2689:U:P | 26:DA:2719:G:H22 | 2.39 | 0.46 |
| 31:DG:96:ARG:O | 31:DG:99:MET:HB3 | 2.15 | 0.46 |
| 36:DP:121:LYS:O | 36:DP:123:LEU:N | 2.44 | 0.46 |
| 1:AA:1118:C:H1' | 1:AA:1179:A:C4 | 2.51 | 0.46 |
| 1:AA:601:C:H2' | 1:AA:602:A:C8 | 2.50 | 0.46 |
| 1:AA:8:A:N6 | 4:AD:205:GLU:O | 2.49 | 0.46 |
| 12:AL:52:LEU:O | 12:AL:54:LYS:NZ | 2.34 | 0.46 |
| 26:BA:1766:U:H2' | 26:BA:1767:C:C6 | 2.51 | 0.46 |
| 26:BA:1769:G:O2' | 26:BA:1958:C:OP1 | 2.24 | 0.46 |
| 26:BA:1963:U:H4' | 26:BA:1964:G:OP1 | 2.15 | 0.46 |
| 26:BA:234:C:H2' | 26:BA:235:U:C6 | 2.51 | 0.46 |
| 26:BA:2871:C:N3 | 61:BA:4761:HOH:O | 2.35 | 0.46 |
| 30:BF:183:VAL:O | 30:BF:187:VAL:HG23 | 2.15 | 0.46 |
| 30:BF:33:LEU:HB3 | 36:BP:6:LEU:HD21 | 1.98 | 0.46 |
| 39:BS:110:LEU:HD12 | 39:BS:110:LEU:HA | 1.74 | 0.46 |
| 26:BA:2848:G:H8 | 40:BT:97:ALA:HB2 | 1.79 | 0.46 |
| 1:CA:1241:G:C2' | 1:CA:1242:C:H5' | 2.45 | 0.46 |
| 1:CA:1273:G:H3' | 1:CA:1274:G:C8 | 2.47 | 0.46 |
| 1:CA:1390:U:H2' | 1:CA:1391:U:C6 | 2.51 | 0.46 |
| 1:CA:390:C:H2' | 1:CA:391:G:C8 | 2.50 | 0.46 |
| 2:CB:137:ARG:HB3 | 2:CB:137:ARG:CZ | 2.45 | 0.46 |
| 2:CB:87:ARG:HD3 | 2:CB:219:VAL:HG11 | 1.98 | 0.46 |
| 23:CW:31:A:H2' | 23:CW:32:PSU:O4' | 2.16 | 0.46 |
| 24:CX:33:U:N3 | 24:CX:36:U:OP2 | 2.48 | 0.46 |
| 26:DA:2712:U:OP1 | 26:DA:2714:G:H4' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DA:852:G:H2' | 26:DA:853:G:H8 | 1.80 | 0.46 |
| 1:AA:1286:A:H3' | 1:AA:1286:A:H8 | 1.81 | 0.46 |
| 1:AA:1245:A:N6 | 1:AA:1292:U:H3 | 2.11 | 0.46 |
| 1:AA:627:G:H2' | 1:AA:628:G:H8 | 1.81 | 0.46 |
| 2:AB:67:THR:N | 2:AB:160:ASP:OD1 | 2.47 | 0.46 |
| 2:AB:80:ILE:HD11 | 2:AB:212:GLN:CA | 2.44 | 0.46 |
| 6:AF:33:TYR:CD2 | 6:AF:75:LEU:HD23 | 2.51 | 0.46 |
| 7:AG:22:LEU:HD11 | 7:AG:101:LEU:HD21 | 1.96 | 0.46 |
| 11:AK:91:ARG:NH1 | 11:AK:110:ASP:OD2 | 2.48 | 0.46 |
| 26:BA:2086:U:H2' | 26:BA:2087:G:C8 | 2.51 | 0.46 |
| 26:BA:2850:A:OP2 | 26:BA:2866:U:H5 | 1.98 | 0.46 |
| 36:BP:86:LYS:HB3 | 36:BP:118:GLY:HA3 | 1.96 | 0.46 |
| 45:BY:6:HIS:HE1 | 45:BY:72:VAL:O | 1.99 | 0.46 |
| 1:CA:841:U:H6 | 1:CA:841:U:OP1 | 1.98 | 0.46 |
| 2:CB:76:GLN:H | 2:CB:76:GLN:HG2 | 1.49 | 0.46 |
| 10:CJ:12:ASP:OD1 | 10:CJ:13:HIS:N | 2.48 | 0.46 |
| 15:CO:11:VAL:HG21 | 15:CO:34:LEU:HD22 | 1.97 | 0.46 |
| 16:CP:53:VAL:O | 16:CP:57:ARG:HB2 | 2.15 | 0.46 |
| 20:CT:26:ASN:HA | 20:CT:71:THR:HG23 | 1.97 | 0.46 |
| 26:DA:2648:C:H2' | 26:DA:2649:U:C6 | 2.50 | 0.46 |
| 27:DB:90:A:C5 | 27:DB:91:C:H1' | 2.51 | 0.46 |
| 46:DZ:141:VAL:HG12 | 46:DZ:144:LEU:HD13 | 1.98 | 0.46 |
| 46:DZ:5:LEU:O | 46:DZ:59:LEU:HA | 2.16 | 0.46 |
| 2:AB:16:HIS:C | 2:AB:18:GLY:H | 2.14 | 0.46 |
| 7:AG:138:LYS:NZ | 7:AG:142:GLU:OE2 | 2.48 | 0.46 |
| 24:AX:23:C:H2' | 24:AX:24:U:C6 | 2.51 | 0.46 |
| 25:AY:19:G:N2 | 25:AY:56:C:N3 | 2.64 | 0.46 |
| 26:BA:1047:G:H2' | 26:BA:1110:G:H1 | 1.81 | 0.46 |
| 26:BA:2359:C:H2' | 26:BA:2360:A:O4' | 2.15 | 0.46 |
| 36:BP:6:LEU:HD23 | 36:BP:6:LEU:HA | 1.71 | 0.46 |
| 41:BU:76:TYR:CZ | 41:BU:80:ILE:HG13 | 2.51 | 0.46 |
| 1:CA:296:U:O2' | 1:CA:556:C:O2 | 2.25 | 0.46 |
| 4:CD:157:LEU:HD22 | 4:CD:161:ASN:HD21 | 1.80 | 0.46 |
| 5:CE:53:LEU:HD12 | 5:CE:53:LEU:H | 1.80 | 0.46 |
| 5:CE:39:GLY:HA2 | 5:CE:71:LEU:HD13 | 1.98 | 0.46 |
| 8:CH:111:ILE:HD11 | 8:CH:118:VAL:HG12 | 1.98 | 0.46 |
| 9:CI:116:LYS:HA | 9:CI:123:PRO:HD3 | 1.97 | 0.46 |
| 11:CK:79:SER:OG | 11:CK:106:LYS:HE3 | 2.15 | 0.46 |
| 13:CM:65:LYS:N | 51:D4:50:VAL:HG21 | 2.31 | 0.46 |
| 13:CM:23:TYR:CE2 | 13:CM:70:LEU:HB3 | 2.50 | 0.46 |
| 47:D0:82:ARG:HA | 47:D0:83:PRO:HD3 | 1.67 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DA:1790:C:H5'' | 26:DA:1791:A:OP1 | 2.15 | 0.46 |
| 26:DA:1833:U:O2' | 26:DA:1969:A:N1 | 2.38 | 0.46 |
| 26:DA:2302:G:C2' | 26:DA:2303:G:H5' | 2.46 | 0.46 |
| 26:DA:1027:A:C2 | 26:DA:2488:A:H5' | 2.51 | 0.46 |
| 26:DA:699:A:H4' | 26:DA:1554:A:N6 | 2.29 | 0.46 |
| 26:DA:82:G:H5'' | 26:DA:296:C:H5' | 1.96 | 0.46 |
| 26:DA:848:G:N9 | 26:DA:933:A:H8 | 2.13 | 0.46 |
| 27:DB:20:C:C2' | 27:DB:21:G:H5' | 2.45 | 0.46 |
| 31:DG:8:LYS:HG3 | 31:DG:100:TRP:CE2 | 2.51 | 0.46 |
| 32:DH:98:LEU:HD23 | 32:DH:125:VAL:HG23 | 1.97 | 0.46 |
| 36:DP:38:GLN:O | 36:DP:39:LYS:HB3 | 2.15 | 0.46 |
| 37:DQ:108:GLY:HA3 | 46:DZ:116:VAL:HG13 | 1.96 | 0.46 |
| 46:DZ:67:LEU:HA | 46:DZ:68:PRO:HD3 | 1.83 | 0.46 |
| 1:AA:1036:G:N3 | 1:AA:1036:G:H2' | 2.31 | 0.46 |
| 1:AA:1457:G:OP1 | 20:AT:39:LYS:NZ | 2.45 | 0.46 |
| 1:AA:473:G:H2' | 1:AA:474:G:C8 | 2.50 | 0.46 |
| 1:AA:532:A:H2 | 1:AA:1206:G:H21 | 1.63 | 0.46 |
| 20:AT:45:GLN:HB2 | 20:AT:91:LEU:HD13 | 1.98 | 0.46 |
| 26:BA:1683:C:H2' | 26:BA:1684:C:C6 | 2.51 | 0.46 |
| 26:BA:2001:A:H2' | 26:BA:2002:G:C8 | 2.51 | 0.46 |
| 26:BA:45:C:OP2 | 26:BA:215:G:H2' | 2.16 | 0.46 |
| 1:CA:1135:U:H2' | 1:CA:1137:C:N3 | 2.31 | 0.46 |
| 1:CA:1251:A:N1 | 1:CA:1354:C:O2' | 2.47 | 0.46 |
| 1:CA:1392:G:N2 | 1:CA:1502:A:H8 | 2.14 | 0.46 |
| 1:CA:276:G:O3' | 17:CQ:68:ARG:NH1 | 2.48 | 0.46 |
| 12:CL:28:LYS:N | 12:CL:29:GLY:HA2 | 2.30 | 0.46 |
| 16:CP:3:LYS:O | 16:CP:21:VAL:HA | 2.15 | 0.46 |
| 1:CA:472:A:H5'' | 16:CP:80:PHE:HB3 | 1.98 | 0.46 |
| 23:CW:4:C:C4 | 23:CW:69:G:N1 | 2.84 | 0.46 |
| 26:DA:375:C:H2' | 26:DA:376:C:C6 | 2.51 | 0.46 |
| 33:DI:43:ASN:C | 33:DI:43:ASN:HD22 | 2.19 | 0.46 |
| 33:DI:66:GLU:HA | 33:DI:69:LYS:HB3 | 1.97 | 0.46 |
| 36:DP:124:LYS:HA | 36:DP:144:GLU:O | 2.16 | 0.46 |
| 1:AA:715:A:H2' | 1:AA:716:A:C8 | 2.51 | 0.46 |
| 2:AB:119:GLU:OE1 | 2:AB:153:ARG:NH2 | 2.49 | 0.46 |
| 4:AD:168:ARG:H | 4:AD:168:ARG:NH1 | 2.13 | 0.46 |
| 5:AE:105:VAL:HB | 5:AE:106:PRO:HD3 | 1.97 | 0.46 |
| 10:AJ:6:ILE:HA | 10:AJ:97:GLU:O | 2.16 | 0.46 |
| 26:BA:330:A:H2 | 26:BA:1210:A:O2' | 1.99 | 0.46 |
| 28:BD:10:THR:OG1 | 28:BD:13:ARG:HG2 | 2.16 | 0.46 |
| 37:BQ:1:MET:HB2 | 37:BQ:44:ALA:HB1 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:BS:41:ASP:OD2 | 39:BS:44:LYS:NZ | 2.42 | 0.46 |
| 1:CA:1064:G:H4' | 1:CA:1065:U:O5' | 2.16 | 0.46 |
| 1:CA:1368:G:C2' | 1:CA:1369:C:H5' | 2.46 | 0.46 |
| 1:CA:991:U:H3' | 1:CA:1212:U:C4 | 2.51 | 0.46 |
| 2:CB:23:ARG:H | 2:CB:23:ARG:HG2 | 1.53 | 0.46 |
| 1:CA:1321:C:H4' | 13:CM:87:TYR:CE2 | 2.50 | 0.46 |
| 20:CT:63:ILE:HD13 | 20:CT:80:ARG:HB3 | 1.98 | 0.46 |
| 24:CX:40:C:H2' | 24:CX:41:C:H6 | 1.81 | 0.46 |
| 55:D8:8:LYS:HB3 | 55:D8:12:LYS:HE3 | 1.98 | 0.46 |
| 26:DA:1015:G:O2' | 26:DA:1016:G:H5' | 2.15 | 0.46 |
| 26:DA:1418:G:O5' | 26:DA:1418:G:H8 | 1.99 | 0.46 |
| 26:DA:1467:C:C5 | 26:DA:1546:C:H2' | 2.51 | 0.46 |
| 26:DA:2114:A:N1 | 26:DA:2117:A:N6 | 2.64 | 0.46 |
| 26:DA:2724:C:OP1 | 29:DE:118:LYS:NZ | 2.33 | 0.46 |
| 26:DA:476:G:H4' | 26:DA:502:A:N1 | 2.31 | 0.46 |
| 28:DD:242:ARG:N | 28:DD:242:ARG:HD3 | 2.31 | 0.46 |
| 28:DD:5:LYS:HE3 | 28:DD:5:LYS:HB3 | 1.66 | 0.46 |
| 36:DP:121:LYS:HD2 | 36:DP:123:LEU:HG | 1.97 | 0.46 |
| 39:DS:62:LYS:HA | 39:DS:65:VAL:HB | 1.98 | 0.46 |
| 1:AA:99:U:H2' | 1:AA:100:C:C6 | 2.50 | 0.46 |
| 18:AR:32:ARG:HA | 18:AR:69:THR:HG21 | 1.97 | 0.46 |
| 23:AW:2:C:H2' | 23:AW:3:C:H6 | 1.81 | 0.46 |
| 48:B1:3:LYS:HB2 | 48:B1:61:ARG:HH12 | 1.81 | 0.46 |
| 26:BA:1021:A:H8 | 26:BA:1021:A:H3' | 1.79 | 0.46 |
| 26:BA:1420:U:HO2' | 26:BA:1421:G:P | 2.38 | 0.46 |
| 26:BA:879:G:O5' | 26:BA:879:G:H8 | 1.98 | 0.46 |
| 31:BG:163:ALA:HB1 | 31:BG:168:GLU:HB2 | 1.98 | 0.46 |
| 38:BR:36:THR:HG22 | 38:BR:37:THR:H | 1.81 | 0.46 |
| 46:BZ:70:LEU:HG | 46:BZ:91:LEU:HD21 | 1.98 | 0.46 |
| 1:CA:1310:G:P | 13:CM:88:ARG:HH22 | 2.39 | 0.46 |
| 1:CA:337:C:H2' | 1:CA:338:A:H8 | 1.81 | 0.46 |
| 2:CB:122:PHE:HA | 2:CB:127:ILE:HD12 | 1.98 | 0.46 |
| 5:CE:41:VAL:O | 5:CE:66:MET:HA | 2.15 | 0.46 |
| 10:CJ:7:LYS:HA | 10:CJ:71:LEU:HD12 | 1.98 | 0.46 |
| 26:DA:330:A:H2 | 26:DA:1210:A:H2' | 1.80 | 0.46 |
| 26:DA:1366:A:H2' | 26:DA:1367:A:O4' | 2.16 | 0.46 |
| 26:DA:2191:G:H2' | 26:DA:2192:G:O4' | 2.16 | 0.46 |
| 26:DA:2846:G:H2' | 26:DA:2847:U:O4' | 2.15 | 0.46 |
| 26:DA:27:G:N2 | 26:DA:512:G:H1' | 2.31 | 0.46 |
| 26:DA:855:G:H2' | 26:DA:856:C:C6 | 2.51 | 0.46 |
| 26:DA:863:A:H2' | 26:DA:864:G:C8 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DB:14:U:O3' | 27:DB:108:U:O2' | 2.33 | 0.46 |
| 29:DE:143:ASN:HD22 | 29:DE:147:PRO:HD3 | 1.80 | 0.46 |
| 39:DS:35:ILE:HD12 | 39:DS:101:LEU:HD12 | 1.98 | 0.46 |
| 40:DT:6:LEU:HA | 40:DT:6:LEU:HD12 | 1.80 | 0.46 |
| 44:DX:94:GLY:N | 44:DX:95:LEU:HA | 2.30 | 0.46 |
| 1:AA:134:A:N1 | 16:AP:25:ARG:NH1 | 2.65 | 0.45 |
| 1:AA:198:G:H2' | 1:AA:199:G:H8 | 1.81 | 0.45 |
| 1:AA:373:A:H2' | 1:AA:374:A:H8 | 1.80 | 0.45 |
| 1:AA:864:A:H2' | 1:AA:865:A:C8 | 2.51 | 0.45 |
| 21:AU:18:TYR:CD1 | 21:AU:24:ARG:HG2 | 2.51 | 0.45 |
| 26:BA:2074:U:H2' | 26:BA:2075:U:C6 | 2.51 | 0.45 |
| 26:BA:2114:A:H2' | 26:BA:2115:G:O4' | 2.16 | 0.45 |
| 26:BA:956:G:OP2 | 37:BQ:87:LYS:NZ | 2.42 | 0.45 |
| 26:BA:1814:G:H4' | 28:BD:51:VAL:HG21 | 1.99 | 0.45 |
| 28:BD:68:LYS:O | 28:BD:69:ARG:HB2 | 2.16 | 0.45 |
| 33:BI:61:ARG:HD2 | 33:BI:61:ARG:N | 2.31 | 0.45 |
| 34:BN:4:TYR:HB2 | 41:BU:101:ARG:HH12 | 1.81 | 0.45 |
| 1:CA:1126:U:C4' | 1:CA:1281:U:H1' | 2.45 | 0.45 |
| 1:CA:1260:C:O5' | 1:CA:1284:C:H4' | 2.15 | 0.45 |
| 2:CB:112:VAL:O | 2:CB:115:LEU:HD23 | 2.17 | 0.45 |
| 1:CA:532:A:N6 | 3:CC:193:TYR:HB3 | 2.25 | 0.45 |
| 3:CC:50:ALA:HB1 | 3:CC:70:VAL:HG21 | 1.98 | 0.45 |
| 1:CA:427:U:P | 4:CD:13:ARG:HH22 | 2.39 | 0.45 |
| 5:CE:110:LEU:HD13 | 5:CE:118:ILE:HD13 | 1.97 | 0.45 |
| 10:CJ:5:ARG:N | 10:CJ:72:VAL:O | 2.48 | 0.45 |
| 11:CK:20:TYR:CZ | 11:CK:83:ILE:HD12 | 2.51 | 0.45 |
| 19:CS:22:LEU:O | 19:CS:27:GLU:HG3 | 2.16 | 0.45 |
| 25:CY:33:U:H2' | 25:CY:35:A:OP2 | 2.16 | 0.45 |
| 50:D3:5:LYS:HB3 | 50:D3:57:GLU:HG2 | 1.98 | 0.45 |
| 26:DA:1913:A:H4' | 26:DA:1914:C:C5' | 2.45 | 0.45 |
| 26:DA:2378:A:H8 | 26:DA:2378:A:O5' | 1.98 | 0.45 |
| 26:DA:2507:C:H5'' | 26:DA:2573:C:N4 | 2.31 | 0.45 |
| 26:DA:992:C:OP1 | 42:DV:74:LYS:NZ | 2.33 | 0.45 |
| 29:DE:47:VAL:HG11 | 29:DE:86:PRO:HD2 | 1.98 | 0.45 |
| 40:DT:42:ILE:HG12 | 40:DT:84:GLN:NE2 | 2.31 | 0.45 |
| 1:AA:1039:C:H2' | 1:AA:1040:U:C6 | 2.51 | 0.45 |
| 1:AA:1075:C:C2' | 1:AA:1076:C:H5' | 2.46 | 0.45 |
| 1:AA:166:G:H2' | 1:AA:167:G:H8 | 1.79 | 0.45 |
| 1:AA:323:U:H5' | 20:AT:23:ARG:HB2 | 1.98 | 0.45 |
| 13:AM:3:ARG:HG2 | 13:AM:8:GLU:HA | 1.98 | 0.45 |
| 1:AA:236:G:H5'' | 17:AQ:42:TYR:OH | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:AY:48:C:OP1 | 25:AY:48:C:H2' | 2.16 | 0.45 |
| 55:B8:6:THR:HG22 | 55:B8:62:LEU:HA | 1.98 | 0.45 |
| 26:BA:2732:G:H3' | 26:BA:2733:A:O4' | 2.17 | 0.45 |
| 26:BA:2791:C:H2' | 26:BA:2792:G:H8 | 1.81 | 0.45 |
| 26:BA:740:U:H2' | 26:BA:741:G:C8 | 2.51 | 0.45 |
| 26:BA:885:C:H3' | 26:BA:886:C:C5' | 2.44 | 0.45 |
| 13:AM:68:GLY:HA3 | 31:BG:116:ASP:OD1 | 2.16 | 0.45 |
| 33:BI:130:TYR:HB3 | 33:BI:138:ILE:HB | 1.98 | 0.45 |
| 1:CA:1008:C:H2' | 1:CA:1009:G:O4' | 2.16 | 0.45 |
| 1:CA:1096:C:H2' | 1:CA:1097:C:H6 | 1.81 | 0.45 |
| 1:CA:1315:U:H2' | 1:CA:1316:G:O4' | 2.16 | 0.45 |
| 1:CA:696:A:H8 | 1:CA:696:A:O5' | 1.99 | 0.45 |
| 1:CA:727:G:P | 1:CA:742:G:H21 | 2.39 | 0.45 |
| 6:CF:87:ARG:CB | 6:CF:87:ARG:HH11 | 2.29 | 0.45 |
| 11:CK:22:HIS:HB3 | 11:CK:29:ILE:HB | 1.98 | 0.45 |
| 26:DA:2167:U:H2' | 26:DA:2167:U:O2 | 2.15 | 0.45 |
| 26:DA:288:C:H2' | 26:DA:289:A:H8 | 1.80 | 0.45 |
| 26:DA:597:U:H2' | 26:DA:598:G:C8 | 2.51 | 0.45 |
| 26:DA:921:G:C6 | 26:DA:922:U:C4 | 3.04 | 0.45 |
| 29:DE:27:LEU:HD22 | 40:DT:1:MET:CE | 2.46 | 0.45 |
| 34:DN:39:ARG:HA | 34:DN:40:PRO:HD3 | 1.88 | 0.45 |
| 35:DO:103:ALA:HB1 | 35:DO:105:GLU:OE1 | 2.16 | 0.45 |
| 1:AA:1038:C:O2' | 1:AA:1039:C:H5' | 2.17 | 0.45 |
| 1:AA:11:G:O2' | 1:AA:506:G:N2 | 2.46 | 0.45 |
| 2:AB:20:GLU:HA | 2:AB:21:ARG:NH2 | 2.30 | 0.45 |
| 2:AB:222:ILE:O | 2:AB:226:ARG:HG2 | 2.16 | 0.45 |
| 4:AD:187:ARG:HB3 | 4:AD:187:ARG:HE | 1.53 | 0.45 |
| 8:AH:51:VAL:HG21 | 8:AH:60:ARG:HB2 | 1.98 | 0.45 |
| 25:AY:2:C:N4 | 25:AY:71:G:H1 | 2.14 | 0.45 |
| 26:BA:1266:G:O5' | 43:BW:15:ARG:NH2 | 2.49 | 0.45 |
| 26:BA:141:A:H8 | 26:BA:1408:C:O2' | 1.99 | 0.45 |
| 26:BA:2010:G:H5'' | 43:BW:42:ARG:HB2 | 1.97 | 0.45 |
| 26:BA:2180:U:H2' | 26:BA:2181:G:O4' | 2.17 | 0.45 |
| 26:BA:2747:G:O6 | 26:BA:2755:C:H5'' | 2.16 | 0.45 |
| 30:BF:64:ILE:HG21 | 30:BF:78:ILE:HG23 | 1.96 | 0.45 |
| 1:CA:67:C:O2' | 1:CA:171:A:N3 | 2.37 | 0.45 |
| 1:CA:456:C:C2' | 1:CA:457:C:H5' | 2.46 | 0.45 |
| 1:CA:620:C:H2' | 1:CA:621:A:O4' | 2.17 | 0.45 |
| 9:CI:45:ALA:O | 9:CI:48:GLU:HB2 | 2.16 | 0.45 |
| 19:CS:63:THR:O | 19:CS:66:MET:HG3 | 2.16 | 0.45 |
| 23:CW:22:G:C2 | 23:CW:23:A:C5 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:CY:10:G:N2 | 25:CY:25:C:N3 | 2.54 | 0.45 |
| 25:CY:35:A:H8 | 25:CY:35:A:O5' | 1.98 | 0.45 |
| 13:CM:3:ARG:HA | 51:D4:34:GLU:HG2 | 1.99 | 0.45 |
| 26:DA:1213:A:N3 | 26:DA:1238:G:O2' | 2.46 | 0.45 |
| 26:DA:1417:C:H3' | 61:DA:4108:HOH:O | 2.16 | 0.45 |
| 26:DA:2149:G:H5'' | 26:DA:2150:U:OP2 | 2.17 | 0.45 |
| 26:DA:2543:G:H2' | 26:DA:2544:G:C8 | 2.51 | 0.45 |
| 26:DA:271(H):G:O2' | 26:DA:271(I):G:H8 | 2.00 | 0.45 |
| 29:DE:144:ARG:HB3 | 29:DE:145:LYS:H | 1.53 | 0.45 |
| 1:AA:1005:A:H1' | 1:AA:1036:G:H22 | 1.80 | 0.45 |
| 1:AA:1055:A:H2' | 3:AC:156:ARG:HD2 | 1.99 | 0.45 |
| 1:AA:163:C:H2' | 1:AA:164:U:C6 | 2.51 | 0.45 |
| 1:AA:189(D):C:O2 | 1:AA:189(H):G:C6 | 2.69 | 0.45 |
| 1:AA:735:C:H2' | 1:AA:736:C:C6 | 2.52 | 0.45 |
| 3:AC:71:ALA:HB2 | 3:AC:115:LEU:HD21 | 1.97 | 0.45 |
| 3:AC:6:HIS:HA | 3:AC:7:PRO:HD3 | 1.85 | 0.45 |
| 8:AH:49:GLU:OE2 | 8:AH:62:TYR:OH | 2.26 | 0.45 |
| 10:AJ:8:LEU:HD21 | 10:AJ:96:ILE:HG23 | 1.98 | 0.45 |
| 13:AM:113:PRO:O | 13:AM:115:LYS:NZ | 2.50 | 0.45 |
| 51:B4:41:PRO:HA | 51:B4:47:GLN:HB3 | 1.98 | 0.45 |
| 53:B6:40:CYS:HA | 53:B6:41:PRO:HD3 | 1.80 | 0.45 |
| 26:BA:2099:U:H2' | 26:BA:2100:G:C8 | 2.51 | 0.45 |
| 26:BA:2340:G:H2' | 26:BA:2341:G:H8 | 1.81 | 0.45 |
| 35:BO:98:VAL:HG13 | 35:BO:117:LEU:HB3 | 1.97 | 0.45 |
| 41:BU:76:TYR:CE1 | 41:BU:80:ILE:HG13 | 2.52 | 0.45 |
| 43:BW:88:ARG:HD2 | 43:BW:88:ARG:HA | 1.76 | 0.45 |
| 1:CA:1009:G:C2 | 1:CA:1010:G:C4 | 3.04 | 0.45 |
| 1:CA:1062:U:H2' | 1:CA:1063:C:C5 | 2.51 | 0.45 |
| 1:CA:652:U:O4 | 1:CA:752:G:O2' | 2.21 | 0.45 |
| 1:CA:859:A:H2' | 1:CA:860:A:O4' | 2.16 | 0.45 |
| 11:CK:34:ASP:OD2 | 11:CK:38:ASN:HB2 | 2.16 | 0.45 |
| 12:CL:37:CYS:SG | 12:CL:81:SER:HB2 | 2.56 | 0.45 |
| 1:CA:110:C:O2' | 16:CP:25:ARG:O | 2.27 | 0.45 |
| 49:D2:62:THR:O | 49:D2:66:GLU:HG3 | 2.16 | 0.45 |
| 51:D4:62:ARG:HB2 | 51:D4:63:TYR:CE1 | 2.51 | 0.45 |
| 56:D9:3:VAL:HA | 56:D9:35:ARG:O | 2.17 | 0.45 |
| 26:DA:1654:A:OP1 | 38:DR:1:MET:HA | 2.15 | 0.45 |
| 26:DA:2659:G:O2' | 26:DA:2661:G:N7 | 2.38 | 0.45 |
| 26:DA:536:A:H2' | 26:DA:537:C:C6 | 2.51 | 0.45 |
| 28:DD:218:ARG:HB3 | 28:DD:219:PRO:HD2 | 1.99 | 0.45 |
| 31:DG:66:GLN:HE21 | 31:DG:92:VAL:HG23 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DT:51:ARG:HG3 | 40:DT:98:LYS:NZ | 2.32 | 0.45 |
| 26:DA:996:A:H4' | 41:DU:91:ASP:OD2 | 2.16 | 0.45 |
| 46:DZ:23:LYS:NZ | 46:DZ:40:ASP:OD1 | 2.48 | 0.45 |
| 46:DZ:43:GLU:O | 46:DZ:47:VAL:N | 2.50 | 0.45 |
| 1:AA:161:A:H2' | 1:AA:162:A:C8 | 2.52 | 0.45 |
| 1:AA:811:C:O2' | 1:AA:901:A:N1 | 2.43 | 0.45 |
| 8:AH:29:SER:OG | 8:AH:32:LYS:HG3 | 2.17 | 0.45 |
| 17:AQ:78:GLU:HG2 | 17:AQ:79:SER:H | 1.81 | 0.45 |
| 24:AX:4:G:H1 | 24:AX:69:C:H42 | 1.64 | 0.45 |
| 26:BA:1045:A:H1' | 26:BA:1047:G:C2 | 2.51 | 0.45 |
| 26:BA:2191:G:C8 | 26:BA:2191:G:H5' | 2.50 | 0.45 |
| 26:BA:582:G:H2' | 26:BA:583:G:C8 | 2.52 | 0.45 |
| 28:BD:24:ILE:HD13 | 28:BD:84:TYR:HB2 | 1.99 | 0.45 |
| 43:BW:18:ARG:NH1 | 43:BW:76:VAL:O | 2.50 | 0.45 |
| 1:CA:1347:G:O2' | 1:CA:1373:G:N1 | 2.47 | 0.45 |
| 1:CA:399:G:H2' | 1:CA:400:C:C6 | 2.51 | 0.45 |
| 1:CA:920:U:H2' | 1:CA:921:U:H6 | 1.80 | 0.45 |
| 12:CL:8:ASN:O | 12:CL:12:ARG:HG3 | 2.16 | 0.45 |
| 24:CX:22:G:H8 | 24:CX:22:G:OP2 | 2.00 | 0.45 |
| 25:CY:36:A:H2' | 25:CY:37:MIA:O4' | 2.16 | 0.45 |
| 26:DA:1667:G:O2' | 26:DA:1991:U:O4 | 2.31 | 0.45 |
| 26:DA:2153:G:H3' | 26:DA:2154:G:C8 | 2.51 | 0.45 |
| 26:DA:527:C:H4' | 26:DA:528:A:O5' | 2.15 | 0.45 |
| 26:DA:652:C:C2' | 26:DA:652(A):A:H5' | 2.46 | 0.45 |
| 26:DA:71:A:H5'' | 26:DA:73:A:C8 | 2.51 | 0.45 |
| 30:DF:12:LEU:HB2 | 30:DF:124:LEU:HD11 | 1.97 | 0.45 |
| 31:DG:106:LEU:HA | 31:DG:110:ALA:CB | 2.45 | 0.45 |
| 33:DI:69:LYS:HG3 | 33:DI:73:GLU:OE1 | 2.16 | 0.45 |
| 38:DR:70:LEU:HD13 | 38:DR:75:LEU:HD13 | 1.98 | 0.45 |
| 42:DV:89:GLN:HA | 42:DV:90:PRO:HD3 | 1.83 | 0.45 |
| 1:AA:175:C:H2' | 1:AA:176:C:H6 | 1.80 | 0.45 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.52 | 0.45 |
| 1:AA:850:U:H2' | 1:AA:851:G:H5'' | 1.98 | 0.45 |
| 11:AK:20:TYR:HB2 | 11:AK:31:THR:HG23 | 1.97 | 0.45 |
| 23:AW:9:A:O2' | 23:AW:10:G:N7 | 2.49 | 0.45 |
| 26:BA:2803:C:H2' | 26:BA:2804:C:C6 | 2.51 | 0.45 |
| 26:BA:27:G:N2 | 26:BA:512:G:H1' | 2.32 | 0.45 |
| 26:BA:747:U:O2 | 26:BA:2014:A:H1' | 2.17 | 0.45 |
| 26:BA:8:A:H2' | 26:BA:9:U:C6 | 2.52 | 0.45 |
| 46:BZ:146:ILE:HA | 46:BZ:147:GLY:HA2 | 1.70 | 0.45 |
| 1:CA:1121:U:C4 | 1:CA:1122:U:C5 | 3.05 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1256:A:H61 | 1:CA:1278:U:H1' | 1.80 | 0.45 |
| 1:CA:1320:C:H2' | 1:CA:1321:C:O4' | 2.17 | 0.45 |
| 1:CA:1385:G:H2' | 1:CA:1386:G:C8 | 2.51 | 0.45 |
| 1:CA:429:U:O3' | 4:CD:22:LYS:NZ | 2.45 | 0.45 |
| 9:CI:9:ARG:HA | 9:CI:13:ALA:O | 2.17 | 0.45 |
| 13:CM:57:ARG:O | 13:CM:61:GLU:HB2 | 2.17 | 0.45 |
| 14:CN:32:SER:OG | 14:CN:32:SER:O | 2.28 | 0.45 |
| 21:CU:12:LYS:HZ2 | 21:CU:19:GLY:HA3 | 1.81 | 0.45 |
| 52:D5:40:LYS:NZ | 52:D5:44:THR:O | 2.34 | 0.45 |
| 52:D5:49:CYS:SG | 52:D5:51:TYR:HB2 | 2.57 | 0.45 |
| 54:D7:5:TRP:CD1 | 54:D7:7:PRO:HD3 | 2.50 | 0.45 |
| 26:DA:1527:G:H5'' | 26:DA:1528:A:OP1 | 2.16 | 0.45 |
| 26:DA:1876:A:H2' | 26:DA:1877:A:C8 | 2.52 | 0.45 |
| 26:DA:2120:G:O6 | 26:DA:2178:C:N3 | 2.49 | 0.45 |
| 26:DA:2207:G:H8 | 26:DA:2207:G:P | 2.40 | 0.45 |
| 26:DA:2468:G:C4 | 26:DA:2481:G:C2 | 3.05 | 0.45 |
| 26:DA:2494:G:O2' | 37:DQ:80:GLU:HA | 2.16 | 0.45 |
| 26:DA:784:A:N6 | 28:DD:229:VAL:HG11 | 2.31 | 0.45 |
| 28:DD:141:VAL:HG12 | 28:DD:164:GLN:HG3 | 1.99 | 0.45 |
| 29:DE:54:GLN:HB2 | 29:DE:76:ARG:HG2 | 1.98 | 0.45 |
| 40:DT:11:GLU:O | 40:DT:15:VAL:HG23 | 2.16 | 0.45 |
| 42:DV:12:TYR:CG | 42:DV:20:LEU:HD21 | 2.52 | 0.45 |
| 44:DX:44:GLU:OE2 | 44:DX:51:VAL:N | 2.45 | 0.45 |
| 1:AA:1504:G:OP1 | 1:AA:1507:A:H4' | 2.17 | 0.45 |
| 1:AA:445:G:H2' | 1:AA:446:G:C8 | 2.52 | 0.45 |
| 1:AA:688:G:H2' | 1:AA:689:C:C6 | 2.52 | 0.45 |
| 2:AB:19:HIS:CD2 | 2:AB:206:ASP:HB2 | 2.52 | 0.45 |
| 2:AB:48:MET:HA | 2:AB:51:LEU:HD12 | 1.97 | 0.45 |
| 1:AA:407:G:O2' | 4:AD:116:GLN:HG3 | 2.17 | 0.45 |
| 4:AD:144:ASP:N | 4:AD:144:ASP:OD1 | 2.49 | 0.45 |
| 1:AA:881:G:P | 12:AL:12:ARG:HH22 | 2.40 | 0.45 |
| 1:AA:375:U:O2' | 16:AP:6:LEU:O | 2.32 | 0.45 |
| 24:AX:4:G:H2' | 24:AX:5:G:C8 | 2.52 | 0.45 |
| 26:BA:1364:G:OP2 | 48:B1:3:LYS:HG3 | 2.17 | 0.45 |
| 26:BA:1430:C:H2' | 26:BA:1431:U:C6 | 2.51 | 0.45 |
| 26:BA:1593:G:H2' | 26:BA:1594:G:C8 | 2.52 | 0.45 |
| 26:BA:405:U:O5' | 26:BA:405:U:H6 | 1.99 | 0.45 |
| 26:BA:592:G:O6 | 61:BA:4916:HOH:O | 2.15 | 0.45 |
| 30:BF:125:LEU:HD12 | 30:BF:194:MET:HB2 | 1.98 | 0.45 |
| 1:CA:1036:G:N7 | 1:CA:1037:C:C2 | 2.85 | 0.45 |
| 1:CA:419:C:OP1 | 1:CA:513:C:O2' | 2.25 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:660:G:H1 | 1:CA:745:C:N4 | 2.12 | 0.45 |
| 1:CA:985:C:N4 | 1:CA:1220:G:N1 | 2.29 | 0.45 |
| 3:CC:8:ILE:HD13 | 3:CC:184:TYR:HB3 | 1.99 | 0.45 |
| 1:CA:411:A:OP1 | 4:CD:30:LYS:HD3 | 2.16 | 0.45 |
| 23:CW:10:G:N2 | 23:CW:11:C:C2 | 2.84 | 0.45 |
| 24:CX:5:G:H2' | 24:CX:6:G:H5' | 1.99 | 0.45 |
| 25:CY:71:G:H4' | 26:DA:1851:U:H4' | 1.99 | 0.45 |
| 26:DA:620:G:H5' | 26:DA:620:G:N3 | 2.31 | 0.45 |
| 26:DA:848:G:C2 | 26:DA:933:A:H1' | 2.52 | 0.45 |
| 32:DH:95:ARG:HG2 | 32:DH:96:ALA:N | 2.32 | 0.45 |
| 44:DX:31:HIS:CD2 | 44:DX:33:LYS:HB2 | 2.52 | 0.45 |
| 45:DY:90:LEU:HD11 | 45:DY:96:ILE:HG23 | 1.98 | 0.45 |
| 46:DZ:158:PRO:HA | 46:DZ:159:PRO:HD3 | 1.71 | 0.45 |
| 1:AA:1290:G:H2' | 1:AA:1291:G:H8 | 1.82 | 0.45 |
| 1:AA:217:C:C2' | 1:AA:218:C:H5' | 2.46 | 0.45 |
| 3:AC:8:ILE:HG23 | 3:AC:16:ARG:HG2 | 1.98 | 0.45 |
| 48:B1:3:LYS:HB3 | 48:B1:4:VAL:H | 1.50 | 0.45 |
| 26:BA:95:G:O2' | 49:B2:48:HIS:ND1 | 2.38 | 0.45 |
| 55:B8:33:ASN:HA | 55:B8:36:LYS:HD2 | 1.99 | 0.45 |
| 26:BA:2011:U:OP1 | 43:BW:42:ARG:HD3 | 2.17 | 0.45 |
| 26:BA:2168:G:O6 | 26:BA:2171:A:H2' | 2.16 | 0.45 |
| 26:BA:2199:A:OP2 | 26:BA:2200:C:H5 | 1.99 | 0.45 |
| 26:BA:2640:G:OP1 | 34:BN:97:ARG:NH2 | 2.49 | 0.45 |
| 26:BA:675:A:C8 | 26:BA:804:A:C6 | 3.05 | 0.45 |
| 28:BD:70:TRP:CE2 | 28:BD:150:LYS:HD3 | 2.52 | 0.45 |
| 28:BD:232:PRO:O | 61:BD:3103:HOH:O | 2.21 | 0.45 |
| 29:BE:31:CYS:HA | 29:BE:32:PRO:HD2 | 1.89 | 0.45 |
| 30:BF:150:GLY:HA2 | 30:BF:172:TRP:CE3 | 2.52 | 0.45 |
| 26:BA:2312:U:OP1 | 31:BG:73:ALA:HA | 2.17 | 0.45 |
| 34:BN:68:GLU:H | 34:BN:68:GLU:HG2 | 1.46 | 0.45 |
| 1:CA:1035:A:H2' | 1:CA:1036:G:H8 | 1.82 | 0.45 |
| 1:CA:1490:C:H2' | 1:CA:1491:G:O4' | 2.17 | 0.45 |
| 1:CA:826:C:H2' | 1:CA:827:U:C6 | 2.51 | 0.45 |
| 2:CB:70:PHE:HB2 | 2:CB:92:TYR:CB | 2.47 | 0.45 |
| 1:CA:1205:U:H4' | 3:CC:195:VAL:HG23 | 1.98 | 0.45 |
| 4:CD:8:VAL:O | 4:CD:11:LEU:HB2 | 2.17 | 0.45 |
| 7:CG:26:PHE:O | 7:CG:30:ILE:HG13 | 2.17 | 0.45 |
| 9:CI:17:VAL:HG11 | 9:CI:80:GLY:C | 2.37 | 0.45 |
| 48:D1:83:GLU:HA | 48:D1:84:GLY:HA2 | 1.70 | 0.45 |
| 51:D4:40:HIS:O | 51:D4:44:THR:N | 2.24 | 0.45 |
| 52:D5:33:CYS:HA | 52:D5:34:PRO:HD3 | 1.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DA:2138:C:N4 | 26:DA:2153:G:N1 | 2.32 | 0.45 |
| 26:DA:2328:A:H2' | 26:DA:2329:G:C8 | 2.52 | 0.45 |
| 26:DA:2461:C:H2' | 26:DA:2462:U:C6 | 2.52 | 0.45 |
| 26:DA:271(K):U:O2 | 33:DI:50:ARG:HG3 | 2.17 | 0.45 |
| 27:DB:34:U:O4 | 27:DB:44:G:O2' | 2.29 | 0.45 |
| 28:DD:171:ASP:O | 28:DD:187:GLY:N | 2.49 | 0.45 |
| 32:DH:148:ILE:HG12 | 32:DH:148:ILE:H | 1.54 | 0.45 |
| 1:AA:678:U:H2' | 1:AA:679:C:C6 | 2.52 | 0.45 |
| 2:AB:17:PHE:CD2 | 2:AB:44:LEU:HD21 | 2.52 | 0.45 |
| 3:AC:108:ASN:HB3 | 3:AC:111:LEU:HD12 | 1.99 | 0.45 |
| 3:AC:121:ALA:HB1 | 3:AC:189:ALA:HB2 | 1.99 | 0.45 |
| 3:AC:156:ARG:HE | 3:AC:156:ARG:HB3 | 1.50 | 0.45 |
| 26:BA:127:A:H5'' | 26:BA:128:C:C6 | 2.52 | 0.45 |
| 26:BA:1501:C:O4' | 28:BD:100:GLY:HA2 | 2.17 | 0.45 |
| 28:BD:52:ARG:NH2 | 61:BD:3112:HOH:O | 2.42 | 0.45 |
| 26:BA:245:G:O5' | 36:BP:73:GLY:HA2 | 2.16 | 0.45 |
| 1:CA:1253:G:H2' | 1:CA:1254:C:C6 | 2.52 | 0.45 |
| 1:CA:6:G:H4' | 1:CA:298:A:H4' | 1.98 | 0.45 |
| 1:CA:376:G:O2' | 16:CP:5:ARG:NH2 | 2.50 | 0.45 |
| 1:CA:982:U:H4' | 1:CA:983:A:O5' | 2.17 | 0.45 |
| 3:CC:40:ARG:NH1 | 3:CC:57:ILE:HD13 | 2.32 | 0.45 |
| 9:CI:81:ILE:O | 9:CI:85:LEU:HG | 2.17 | 0.45 |
| 19:CS:30:LEU:HA | 19:CS:48:THR:O | 2.16 | 0.45 |
| 24:CX:10:G:N2 | 24:CX:26:G:H1' | 2.31 | 0.45 |
| 26:DA:1165:U:H2' | 26:DA:1166:C:C6 | 2.51 | 0.45 |
| 26:DA:1287:A:C5 | 26:DA:1288:U:C4 | 3.05 | 0.45 |
| 26:DA:2263:C:H2' | 26:DA:2264:C:O4' | 2.17 | 0.45 |
| 26:DA:2365:G:P | 47:D0:55:ARG:HG2 | 2.57 | 0.45 |
| 26:DA:2683:C:O2 | 35:DO:70:LYS:NZ | 2.44 | 0.45 |
| 26:DA:2872:G:C2 | 26:DA:2873:A:N6 | 2.85 | 0.45 |
| 26:DA:34:C:H2' | 26:DA:34:C:O2 | 2.17 | 0.45 |
| 26:DA:862:G:H2' | 26:DA:863:A:O4' | 2.16 | 0.45 |
| 29:DE:24:THR:HG22 | 29:DE:184:VAL:HG12 | 1.98 | 0.45 |
| 30:DF:156:LEU:HD21 | 30:DF:163:VAL:HG12 | 1.98 | 0.45 |
| 31:DG:171:ALA:O | 31:DG:175:LEU:N | 2.37 | 0.45 |
| 33:DI:141:LYS:HZ2 | 33:DI:141:LYS:HB2 | 1.82 | 0.45 |
| 26:DA:297:C:OP1 | 45:DY:87:LYS:HG3 | 2.17 | 0.45 |
| 1:AA:1001(A):G:C6 | 1:AA:1002:G:C5 | 3.05 | 0.45 |
| 1:AA:1030(A):G:H2' | 1:AA:1030(C):G:OP2 | 2.17 | 0.45 |
| 1:AA:769:G:H4' | 1:AA:1513:A:H4' | 1.99 | 0.45 |
| 13:AM:108:ARG:HD3 | 13:AM:108:ARG:HA | 1.66 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:AM:15:VAL:O | 13:AM:19:LEU:HD22 | 2.17 | 0.45 |
| 20:AT:9:ASN:ND2 | 20:AT:10:LEU:H | 2.15 | 0.45 |
| 25:AY:13:C:H2' | 25:AY:14:A:H8 | 1.82 | 0.45 |
| 48:B1:67:ILE:N | 48:B1:68:PRO:HD2 | 2.31 | 0.45 |
| 26:BA:11:G:H2' | 26:BA:12:U:H5'' | 1.98 | 0.45 |
| 26:BA:2080:G:OP1 | 48:B1:35:THR:HG21 | 2.17 | 0.45 |
| 26:BA:2246:G:H2' | 26:BA:2247:A:C8 | 2.52 | 0.45 |
| 26:BA:574:C:N3 | 29:BE:145:LYS:NZ | 2.51 | 0.45 |
| 28:BD:20:ASP:OD2 | 28:BD:22:SER:HB2 | 2.17 | 0.45 |
| 30:BF:184:TYR:CE2 | 30:BF:188:ARG:HD2 | 2.52 | 0.45 |
| 31:BG:150:ASP:OD1 | 31:BG:150:ASP:N | 2.46 | 0.45 |
| 26:BA:587:C:P | 36:BP:21:ARG:HH22 | 2.40 | 0.45 |
| 37:BQ:85:LYS:HG2 | 47:B0:7:LEU:HB3 | 1.99 | 0.45 |
| 1:CA:1206:G:C6 | 1:CA:1207:G:C5 | 3.05 | 0.45 |
| 1:CA:25:C:H5' | 1:CA:524:G:H1' | 1.98 | 0.45 |
| 1:CA:502:G:C2 | 1:CA:503:C:C2 | 3.05 | 0.45 |
| 1:CA:65:U:H5' | 1:CA:65:U:H6 | 1.81 | 0.45 |
| 2:CB:71:VAL:HG23 | 2:CB:71:VAL:O | 2.17 | 0.45 |
| 4:CD:119:GLN:HG2 | 4:CD:123:HIS:CD2 | 2.52 | 0.45 |
| 17:CQ:63:ARG:HG2 | 17:CQ:64:PRO:HD2 | 1.99 | 0.45 |
| 23:CW:38:A:H5' | 26:DA:1913:A:N6 | 2.32 | 0.45 |
| 53:D6:23:THR:OG1 | 53:D6:24:GLU:N | 2.48 | 0.45 |
| 26:DA:1031:G:H21 | 56:D9:36:GLN:HE22 | 1.63 | 0.45 |
| 26:DA:1131:G:O6 | 26:DA:2040:C:H1' | 2.17 | 0.45 |
| 26:DA:1427:A:H4' | 26:DA:1428:C:O5' | 2.17 | 0.45 |
| 26:DA:1588:C:H2' | 26:DA:1589:C:H6 | 1.82 | 0.45 |
| 27:DB:73:A:C4 | 27:DB:105:A:C2 | 3.04 | 0.45 |
| 31:DG:166:ASP:O | 31:DG:170:ARG:N | 2.46 | 0.45 |
| 41:DU:85:LYS:HB2 | 41:DU:116:ALA:HB1 | 1.99 | 0.45 |
| 43:DW:2:GLU:OE2 | 43:DW:72:LYS:HE2 | 2.17 | 0.45 |
| 44:DX:31:HIS:HA | 44:DX:32:PRO:HD3 | 1.87 | 0.45 |
| 1:AA:1161:C:O2' | 1:AA:1162:C:H5' | 2.18 | 0.44 |
| 1:AA:345:C:O5' | 1:AA:345:C:H6 | 2.00 | 0.44 |
| 6:AF:55:ASP:HA | 6:AF:56:PRO:HD3 | 1.84 | 0.44 |
| 14:AN:14:PRO:HG2 | 14:AN:20:ALA:HB2 | 1.98 | 0.44 |
| 1:AA:750:G:H1' | 15:AO:22:THR:HG23 | 1.99 | 0.44 |
| 18:AR:59:SER:OG | 18:AR:62:GLU:HG2 | 2.18 | 0.44 |
| 19:AS:36:ARG:NH1 | 19:AS:52:TYR:O | 2.48 | 0.44 |
| 23:AW:61:C:H2' | 23:AW:62:C:H6 | 1.82 | 0.44 |
| 23:AW:4:C:N3 | 23:AW:69:G:O6 | 2.50 | 0.44 |
| 51:B4:48:ARG:HB3 | 51:B4:51:ASP:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BA:817:C:H4' | 26:BA:932:G:C5 | 2.52 | 0.44 |
| 36:BP:65:ARG:HG3 | 55:B8:25:MET:CG | 2.46 | 0.44 |
| 38:BR:53:HIS:O | 38:BR:56:LYS:HB2 | 2.18 | 0.44 |
| 1:CA:1084:G:C5 | 1:CA:1085:U:C4 | 3.05 | 0.44 |
| 1:CA:1120:G:N1 | 1:CA:1154:G:N3 | 2.65 | 0.44 |
| 1:CA:1258:G:O2' | 1:CA:1259:C:H5' | 2.17 | 0.44 |
| 1:CA:154:C:H2' | 1:CA:155:C:C6 | 2.52 | 0.44 |
| 1:CA:382:A:H2' | 1:CA:383:A:C8 | 2.52 | 0.44 |
| 1:CA:606:G:H5'' | 1:CA:607:A:H5' | 1.99 | 0.44 |
| 1:CA:986:A:H2' | 1:CA:987:G:O4' | 2.17 | 0.44 |
| 4:CD:173:TRP:CD1 | 4:CD:189:PRO:HG3 | 2.51 | 0.44 |
| 7:CG:155:ARG:HG2 | 7:CG:156:TRP:N | 2.32 | 0.44 |
| 1:CA:1015:A:H4' | 14:CN:15:LYS:NZ | 2.33 | 0.44 |
| 23:CW:47:U:O2' | 23:CW:48:C:OP1 | 2.29 | 0.44 |
| 26:DA:2356:C:O3' | 47:D0:20:ARG:HD3 | 2.17 | 0.44 |
| 26:DA:1913:A:H4' | 26:DA:1914:C:H5'' | 1.98 | 0.44 |
| 26:DA:751:A:H5' | 43:DW:90:ARG:HA | 1.98 | 0.44 |
| 26:DA:971:C:H2' | 26:DA:972:G:O4' | 2.17 | 0.44 |
| 31:DG:152:LEU:HD12 | 31:DG:152:LEU:H | 1.82 | 0.44 |
| 32:DH:13:LYS:HA | 32:DH:14:GLY:HA2 | 1.55 | 0.44 |
| 26:DA:2727:G:O2' | 35:DO:70:LYS:NZ | 2.51 | 0.44 |
| 36:DP:95:VAL:HG13 | 36:DP:125:VAL:HG12 | 1.98 | 0.44 |
| 41:DU:76:TYR:HH | 41:DU:92:ARG:NH1 | 2.12 | 0.44 |
| 43:DW:17:VAL:HG11 | 43:DW:103:ILE:HD11 | 1.98 | 0.44 |
| 45:DY:3:VAL:HB | 45:DY:32:PRO:HB3 | 2.00 | 0.44 |
| 1:AA:100:C:H2' | 1:AA:101:A:C8 | 2.52 | 0.44 |
| 1:AA:1027:C:H2' | 1:AA:1028:C:C6 | 2.52 | 0.44 |
| 1:AA:114:U:H1' | 1:AA:353:A:H1' | 1.99 | 0.44 |
| 1:AA:431:A:H2' | 1:AA:432:A:O4' | 2.18 | 0.44 |
| 4:AD:112:VAL:HG23 | 4:AD:116:GLN:OE1 | 2.16 | 0.44 |
| 8:AH:56:LYS:HB2 | 8:AH:58:TYR:HE1 | 1.81 | 0.44 |
| 9:AI:102:LEU:HD22 | 9:AI:102:LEU:HA | 1.85 | 0.44 |
| 9:AI:49:PRO:HG3 | 9:AI:101:PHE:CD2 | 2.51 | 0.44 |
| 17:AQ:92:ARG:HD2 | 17:AQ:92:ARG:HA | 1.92 | 0.44 |
| 19:AS:9:VAL:HG21 | 51:B4:61:ARG:HH12 | 1.82 | 0.44 |
| 25:AY:6:G:C6 | 25:AY:7:A:C5 | 3.05 | 0.44 |
| 26:BA:372:G:H8 | 48:B1:65:SER:O | 2.00 | 0.44 |
| 26:BA:686:G:H8 | 54:B7:6:GLN:O | 2.00 | 0.44 |
| 26:BA:1794:U:H2' | 26:BA:1795:C:H6 | 1.81 | 0.44 |
| 26:BA:2130:U:H2' | 26:BA:2131:G:H21 | 1.82 | 0.44 |
| 26:BA:2260:C:H2' | 26:BA:2261:C:H6 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 26:BA:971:C:O2' | 26:BA:983:A:N3 | 2.40 | 0.44 |
| 27:BB:91:C:OP1 | 37:BQ:16:ARG:HG3 | 2.18 | 0.44 |
| 29:BE:149:ARG:O | 61:BE:406:HOH:O | 2.21 | 0.44 |
| 30:BF:8:GLN:HA | 30:BF:8:GLN:NE2 | 2.32 | 0.44 |
| 32:BH:13:LYS:HA | 32:BH:14:GLY:HA2 | 1.58 | 0.44 |
| 39:BS:27:SER:HA | 39:BS:88:ASP:HB3 | 1.98 | 0.44 |
| 1:CA:683:G:H2' | 1:CA:684:A:H8 | 1.81 | 0.44 |
| 1:CA:848:C:O5' | 1:CA:848:C:H6 | 2.00 | 0.44 |
| 2:CB:68:ILE:HG12 | 2:CB:161:ALA:HB3 | 1.98 | 0.44 |
| 2:CB:162:ILE:HG13 | 2:CB:162:ILE:O | 2.15 | 0.44 |
| 2:CB:167:PRO:HG3 | 2:CB:188:ALA:HB2 | 1.98 | 0.44 |
| 3:CC:85:ARG:O | 3:CC:89:GLU:HG3 | 2.17 | 0.44 |
| 9:CI:16:ARG:HB2 | 9:CI:64:THR:HG23 | 1.99 | 0.44 |
| 12:CL:6:THR:HG23 | 12:CL:9:GLN:OE1 | 2.17 | 0.44 |
| 16:CP:40:ASP:O | 16:CP:48:TRP:HB2 | 2.18 | 0.44 |
| 6:CF:100:ASN:HD21 | 18:CR:23:LYS:HG2 | 1.83 | 0.44 |
| 26:DA:1021:A:C8 | 26:DA:1021:A:H3' | 2.52 | 0.44 |
| 26:DA:1127:A:N7 | 26:DA:2488:A:O2' | 2.50 | 0.44 |
| 26:DA:1583:A:H4' | 26:DA:1586:A:C4 | 2.52 | 0.44 |
| 26:DA:774:A:N3 | 26:DA:774:A:H2' | 2.33 | 0.44 |
| 26:DA:776:G:H4' | 26:DA:777:A:O5' | 2.17 | 0.44 |
| 26:DA:921:G:H4' | 26:DA:2269:A:C5 | 2.51 | 0.44 |
| 33:DI:77:LEU:HD11 | 33:DI:97:ILE:HG23 | 1.99 | 0.44 |
| 34:DN:73:THR:OG1 | 34:DN:82:LEU:HD11 | 2.16 | 0.44 |
| 35:DO:76:ALA:HB3 | 40:DT:75:ILE:HB | 1.99 | 0.44 |
| 46:DZ:79:ARG:HD2 | 46:DZ:80:ARG:NH2 | 2.32 | 0.44 |
| 1:AA:110:C:H2' | 1:AA:111:G:O4' | 2.18 | 0.44 |
| 2:AB:223:ILE:HD12 | 2:AB:230:VAL:HG12 | 2.00 | 0.44 |
| 2:AB:219:VAL:O | 2:AB:223:ILE:HG12 | 2.16 | 0.44 |
| 4:AD:18:LYS:HD2 | 4:AD:31:CYS:SG | 2.57 | 0.44 |
| 24:AX:46:G:H5'' | 24:AX:47:U:OP2 | 2.16 | 0.44 |
| 26:BA:226:G:N2 | 26:BA:228:A:H62 | 2.15 | 0.44 |
| 26:BA:2790:A:N3 | 26:BA:2790:A:H2' | 2.31 | 0.44 |
| 26:BA:796:C:H2' | 26:BA:797:C:C6 | 2.52 | 0.44 |
| 30:BF:165:ARG:HG2 | 30:BF:168:ARG:HH21 | 1.82 | 0.44 |
| 31:BG:43:LEU:HD12 | 31:BG:43:LEU:HA | 1.81 | 0.44 |
| 32:BH:124:GLU:OE1 | 32:BH:132:ARG:HD2 | 2.18 | 0.44 |
| 33:BI:75:LEU:HD22 | 33:BI:105:HIS:ND1 | 2.31 | 0.44 |
| 39:BS:6:ALA:O | 39:BS:10:ARG:HB2 | 2.17 | 0.44 |
| 1:CA:1001(A):G:H5'' | 1:CA:1002:G:OP2 | 2.17 | 0.44 |
| 1:CA:1131:G:H2' | 1:CA:1132:C:H6 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1132:C:H2' | 1:CA:1133:G:H8 | 1.83 | 0.44 |
| 1:CA:1239:A:H4' | 1:CA:1240:U:H5'' | 1.98 | 0.44 |
| 1:CA:543:C:O2' | 1:CA:544:G:H5' | 2.17 | 0.44 |
| 1:CA:715:A:H5'' | 1:CA:805:C:H1' | 1.99 | 0.44 |
| 1:CA:743:U:H2' | 1:CA:744:C:C6 | 2.52 | 0.44 |
| 1:CA:437:U:O2' | 4:CD:125:HIS:HE1 | 1.99 | 0.44 |
| 11:CK:66:LEU:O | 11:CK:70:LYS:HD2 | 2.18 | 0.44 |
| 14:CN:40:CYS:O | 14:CN:44:LEU:HB3 | 2.18 | 0.44 |
| 14:CN:45:ARG:O | 14:CN:49:HIS:HD2 | 1.99 | 0.44 |
| 19:CS:33:THR:HG22 | 19:CS:50:ALA:O | 2.17 | 0.44 |
| 25:CY:51:U:N3 | 25:CY:63:G:N1 | 2.41 | 0.44 |
| 25:CY:67:C:H2' | 25:CY:68:C:C6 | 2.52 | 0.44 |
| 26:DA:2355:C:H4' | 47:D0:24:LYS:HD3 | 1.99 | 0.44 |
| 26:DA:1030:G:OP2 | 37:DQ:128:LYS:HD3 | 2.17 | 0.44 |
| 26:DA:2441:C:OP2 | 26:DA:2586:C:O2' | 2.31 | 0.44 |
| 26:DA:2849:U:H4' | 26:DA:2868:A:C2 | 2.51 | 0.44 |
| 26:DA:752:A:H4' | 26:DA:753:C:H5' | 1.99 | 0.44 |
| 26:DA:902:C:H2' | 26:DA:903:C:H6 | 1.82 | 0.44 |
| 27:DB:45:A:H2' | 27:DB:46:A:H8 | 1.82 | 0.44 |
| 28:DD:96:HIS:CD2 | 28:DD:102:LYS:HG2 | 2.53 | 0.44 |
| 31:DG:3:LEU:HD23 | 31:DG:3:LEU:H | 1.81 | 0.44 |
| 36:DP:37:GLY:O | 36:DP:40:SER:OG | 2.22 | 0.44 |
| 37:DQ:29:PHE:HB2 | 37:DQ:105:GLU:OE2 | 2.18 | 0.44 |
| 37:DQ:134:ARG:CZ | 46:DZ:122:ARG:HE | 2.30 | 0.44 |
| 1:AA:1057:G:H2' | 1:AA:1058:G:O4' | 2.17 | 0.44 |
| 1:AA:1131:G:H2' | 1:AA:1132:C:H6 | 1.83 | 0.44 |
| 1:AA:217:C:O2' | 1:AA:218:C:H5' | 2.17 | 0.44 |
| 1:AA:21:G:H2' | 1:AA:22:G:C8 | 2.53 | 0.44 |
| 1:AA:435:C:H6 | 1:AA:435:C:O5' | 2.01 | 0.44 |
| 5:AE:27:ARG:HB2 | 5:AE:27:ARG:HE | 1.53 | 0.44 |
| 10:AJ:33:GLN:O | 10:AJ:75:ILE:N | 2.44 | 0.44 |
| 17:AQ:60:ILE:O | 17:AQ:62:SER:OG | 2.34 | 0.44 |
| 26:BA:1009:A:OP2 | 34:BN:37:LYS:NZ | 2.50 | 0.44 |
| 26:BA:1178:C:O5' | 26:BA:1178:C:H6 | 2.00 | 0.44 |
| 33:BI:38:LEU:H | 33:BI:38:LEU:CD1 | 2.23 | 0.44 |
| 27:BB:91:C:OP2 | 37:BQ:16:ARG:NH1 | 2.51 | 0.44 |
| 1:CA:1004:A:C2 | 1:CA:1038:C:C4 | 3.05 | 0.44 |
| 1:CA:1016:A:O2' | 1:CA:1217:C:O2' | 2.14 | 0.44 |
| 1:CA:1085:U:H3' | 1:CA:1086:U:C5 | 2.52 | 0.44 |
| 1:CA:1134:G:C6 | 1:CA:1135:U:C2 | 3.05 | 0.44 |
| 1:CA:814:A:N7 | 1:CA:816:A:C4 | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:90:U:O2' | 1:CA:91:C:H5' | 2.18 | 0.44 |
| 1:CA:994:A:C5 | 1:CA:1216:G:H4' | 2.53 | 0.44 |
| 4:CD:173:TRP:CE2 | 4:CD:189:PRO:HG3 | 2.53 | 0.44 |
| 7:CG:78:ARG:CZ | 7:CG:79:ARG:HH22 | 2.30 | 0.44 |
| 8:CH:125:ARG:HE | 8:CH:125:ARG:HB2 | 1.49 | 0.44 |
| 9:CI:24:GLY:HA2 | 9:CI:59:PHE:O | 2.17 | 0.44 |
| 13:CM:13:LYS:HA | 13:CM:44:ARG:NH1 | 2.33 | 0.44 |
| 47:D0:14:ARG:HH11 | 47:D0:14:ARG:HB2 | 1.83 | 0.44 |
| 26:DA:1129:A:N6 | 26:DA:2491:U:OP1 | 2.50 | 0.44 |
| 26:DA:1406:U:H2' | 26:DA:1407:C:C6 | 2.52 | 0.44 |
| 26:DA:1999:C:H4' | 26:DA:2723:C:O2 | 2.17 | 0.44 |
| 26:DA:2192:G:H5' | 26:DA:2193:G:OP2 | 2.17 | 0.44 |
| 26:DA:2611:U:OP2 | 26:DA:2611:U:H3' | 2.18 | 0.44 |
| 26:DA:87:C:H5'' | 26:DA:88:G:H5' | 1.99 | 0.44 |
| 27:DB:33:G:N3 | 27:DB:50:G:N2 | 2.66 | 0.44 |
| 30:DF:24:LEU:HD21 | 30:DF:114:VAL:HG12 | 1.99 | 0.44 |
| 34:DN:103:VAL:O | 34:DN:107:LEU:HG | 2.17 | 0.44 |
| 30:DF:187:VAL:HG12 | 36:DP:3:LEU:HD12 | 1.99 | 0.44 |
| 1:AA:1030(D):A:H62 | 1:AA:1031:G:H21 | 1.63 | 0.44 |
| 1:AA:1152:A:H2' | 1:AA:1153:C:H6 | 1.82 | 0.44 |
| 2:AB:107:THR:O | 2:AB:110:GLN:HB2 | 2.18 | 0.44 |
| 3:AC:156:ARG:NH2 | 3:AC:159:GLY:O | 2.48 | 0.44 |
| 11:AK:34:ASP:HB3 | 11:AK:40:ILE:HD11 | 1.99 | 0.44 |
| 25:AY:57:G:H2' | 25:AY:58:A:C5' | 2.48 | 0.44 |
| 49:B2:2:LYS:O | 49:B2:6:VAL:HG23 | 2.17 | 0.44 |
| 52:B5:16:ARG:HD2 | 52:B5:20:ARG:NH1 | 2.31 | 0.44 |
| 26:BA:187:G:OP2 | 61:BA:4447:HOH:O | 2.21 | 0.44 |
| 26:BA:2028:U:H2' | 26:BA:2029:G:O4' | 2.18 | 0.44 |
| 26:BA:2191:G:H2' | 26:BA:2192:G:O4' | 2.17 | 0.44 |
| 26:BA:2405:G:O2' | 26:BA:2411:A:N6 | 2.50 | 0.44 |
| 32:BH:125:VAL:HG12 | 32:BH:127:GLU:O | 2.18 | 0.44 |
| 33:BI:62:LYS:HE3 | 33:BI:133:HIS:CE1 | 2.53 | 0.44 |
| 26:BA:637:A:H8 | 36:BP:117:GLU:HG3 | 1.82 | 0.44 |
| 1:CA:1113:C:H42 | 1:CA:1187:G:H1 | 1.65 | 0.44 |
| 1:CA:1132:C:H2' | 1:CA:1133:G:C8 | 2.52 | 0.44 |
| 1:CA:1360:A:H2' | 1:CA:1361:G:O4' | 2.18 | 0.44 |
| 1:CA:947:G:C6 | 1:CA:948:C:C4 | 3.06 | 0.44 |
| 2:CB:36:ARG:O | 2:CB:37:ASN:HB2 | 2.17 | 0.44 |
| 3:CC:83:ARG:O | 3:CC:87:LEU:HG | 2.18 | 0.44 |
| 5:CE:6:PHE:HB3 | 5:CE:35:GLY:C | 2.37 | 0.44 |
| 5:CE:57:LYS:O | 5:CE:61:TYR:HD2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:878:G:OP1 | 8:CH:88:LYS:HB3 | 2.17 | 0.44 |
| 1:CA:1371:G:OP1 | 9:CI:12:GLU:HB2 | 2.18 | 0.44 |
| 11:CK:66:LEU:HB3 | 11:CK:70:LYS:HZ2 | 1.82 | 0.44 |
| 18:CR:33:ASP:OD2 | 18:CR:36:ASN:HB2 | 2.16 | 0.44 |
| 26:DA:1235:G:C6 | 26:DA:1236:G:N1 | 2.85 | 0.44 |
| 26:DA:2131:G:H5' | 26:DA:2131:G:N3 | 2.32 | 0.44 |
| 26:DA:2274:A:C5 | 26:DA:2276:G:C8 | 3.05 | 0.44 |
| 26:DA:2286:A:H4' | 26:DA:2287:A:O4' | 2.17 | 0.44 |
| 30:DF:140:LEU:HD13 | 30:DF:170:LEU:HD21 | 1.99 | 0.44 |
| 31:DG:161:THR:HG22 | 31:DG:163:ALA:H | 1.83 | 0.44 |
| 32:DH:137:ASP:HB3 | 32:DH:140:LYS:HB3 | 1.98 | 0.44 |
| 26:DA:2748:A:H5' | 32:DH:4:ILE:HD12 | 1.99 | 0.44 |
| 44:DX:8:ILE:O | 49:D2:36:ARG:NH2 | 2.51 | 0.44 |
| 1:AA:1479:C:H2' | 1:AA:1480:G:H8 | 1.82 | 0.44 |
| 8:AH:119:LEU:HB3 | 8:AH:123:GLU:HB3 | 1.99 | 0.44 |
| 13:AM:49:THR:OG1 | 13:AM:52:GLU:HG3 | 2.18 | 0.44 |
| 25:AY:71:G:H2' | 25:AY:72:C:C6 | 2.53 | 0.44 |
| 26:BA:1377:G:H2' | 61:BA:3925:HOH:O | 2.18 | 0.44 |
| 26:BA:1405:U:H2' | 26:BA:1406:U:H6 | 1.78 | 0.44 |
| 26:BA:2134:A:OP2 | 26:BA:2157:G:N2 | 2.50 | 0.44 |
| 26:BA:281:G:O2' | 26:BA:359:A:N6 | 2.47 | 0.44 |
| 26:BA:528:A:N1 | 26:BA:2042:A:H2' | 2.32 | 0.44 |
| 26:BA:614:U:H5' | 26:BA:614(C):A:N6 | 2.33 | 0.44 |
| 26:BA:764:A:H5' | 28:BD:210:GLY:HA2 | 1.99 | 0.44 |
| 29:BE:174:ASP:OD1 | 29:BE:175:VAL:N | 2.50 | 0.44 |
| 30:BF:24:LEU:HD23 | 30:BF:115:ALA:HA | 2.00 | 0.44 |
| 31:BG:43:LEU:HB3 | 31:BG:44:GLY:H | 1.50 | 0.44 |
| 33:BI:4:ILE:HD13 | 33:BI:47:LEU:HG | 2.00 | 0.44 |
| 26:BA:952:G:P | 37:BQ:16:ARG:HH21 | 2.40 | 0.44 |
| 26:BA:2820:A:P | 38:BR:2:ARG:HH22 | 2.41 | 0.44 |
| 1:CA:1002:G:C2 | 1:CA:1003:G:C8 | 3.06 | 0.44 |
| 1:CA:1286:A:H2' | 1:CA:1287:A:H5' | 1.99 | 0.44 |
| 1:CA:426:G:OP1 | 4:CD:38:TYR:OH | 2.30 | 0.44 |
| 1:CA:727:G:OP1 | 1:CA:742:G:N2 | 2.43 | 0.44 |
| 3:CC:98:ASN:N | 3:CC:98:ASN:OD1 | 2.49 | 0.44 |
| 5:CE:90:VAL:O | 5:CE:120:THR:HA | 2.17 | 0.44 |
| 7:CG:72:ARG:HH22 | 7:CG:138:LYS:NZ | 2.15 | 0.44 |
| 10:CJ:69:ASN:O | 10:CJ:70:ARG:HD3 | 2.18 | 0.44 |
| 13:CM:93:ARG:HD3 | 26:DA:888:C:OP1 | 2.18 | 0.44 |
| 23:CW:61:C:HO2' | 23:CW:62:C:P | 2.37 | 0.44 |
| 25:CY:8:4SU:S4 | 25:CY:14:A:N7 | 2.90 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DA:2165:G:H2' | 26:DA:2166:G:O4' | 2.17 | 0.44 |
| 26:DA:492:A:H2' | 26:DA:493:G:O4' | 2.18 | 0.44 |
| 27:DB:33:G:C6 | 27:DB:34:U:C4 | 3.06 | 0.44 |
| 1:CA:1432:G:OP2 | 40:DT:108:ARG:HD2 | 2.18 | 0.44 |
| 29:DE:27:LEU:HD22 | 40:DT:1:MET:HE1 | 1.98 | 0.44 |
| 46:DZ:120:ILE:HD13 | 46:DZ:171:ILE:HA | 1.99 | 0.44 |
| 1:AA:1223:C:H5'' | 1:AA:1224:G:H5'' | 2.00 | 0.44 |
| 1:AA:1469:G:H2' | 1:AA:1470:G:C8 | 2.53 | 0.44 |
| 1:AA:834:C:H2' | 1:AA:835:U:C6 | 2.53 | 0.44 |
| 3:AC:22:TRP:CZ2 | 14:AN:54:PRO:HG3 | 2.53 | 0.44 |
| 7:AG:72:ARG:HG3 | 7:AG:142:GLU:OE2 | 2.18 | 0.44 |
| 1:AA:589:C:H5'' | 8:AH:29:SER:HB3 | 1.99 | 0.44 |
| 1:AA:35:G:O2' | 12:AL:118:SER:O | 2.29 | 0.44 |
| 13:AM:31:LYS:O | 13:AM:35:GLU:HG3 | 2.18 | 0.44 |
| 13:AM:60:VAL:HG12 | 13:AM:66:LEU:HD11 | 2.00 | 0.44 |
| 16:AP:56:ALA:O | 16:AP:60:LEU:HB2 | 2.18 | 0.44 |
| 17:AQ:74:LEU:HD13 | 17:AQ:75:ARG:HG2 | 2.00 | 0.44 |
| 51:B4:40:HIS:HB3 | 51:B4:43:TYR:HB2 | 2.00 | 0.44 |
| 26:BA:1142(A):A:C4 | 26:BA:1144:G:C8 | 3.06 | 0.44 |
| 26:BA:1453:U:OP1 | 38:BR:77:ARG:NH1 | 2.39 | 0.44 |
| 23:AW:56:C:H5 | 26:BA:897:C:O4' | 2.00 | 0.44 |
| 31:BG:97:ASP:O | 31:BG:101:ILE:HG13 | 2.17 | 0.44 |
| 46:BZ:108:PRO:HB2 | 46:BZ:111:VAL:HG23 | 1.99 | 0.44 |
| 1:CA:1492:A:O2' | 1:CA:1493:A:O5' | 2.33 | 0.44 |
| 2:CB:16:HIS:CD2 | 2:CB:17:PHE:N | 2.85 | 0.44 |
| 7:CG:16:LEU:HD23 | 9:CI:41:VAL:HG12 | 1.99 | 0.44 |
| 26:DA:2344:U:H3' | 53:D6:37:ARG:O | 2.18 | 0.44 |
| 26:DA:1410:G:H2' | 26:DA:1411:C:H6 | 1.82 | 0.44 |
| 26:DA:2104:G:H2' | 26:DA:2105:C:C6 | 2.53 | 0.44 |
| 26:DA:2136:C:HO2' | 26:DA:2137:C:C5' | 2.27 | 0.44 |
| 26:DA:2302:G:C2 | 26:DA:2303:G:C8 | 3.06 | 0.44 |
| 26:DA:784:A:C8 | 26:DA:792:G:C5 | 3.06 | 0.44 |
| 26:DA:994:C:H1' | 42:DV:10:LYS:HE3 | 1.98 | 0.44 |
| 31:DG:129:GLY:O | 31:DG:161:THR:HB | 2.18 | 0.44 |
| 36:DP:6:LEU:HA | 36:DP:6:LEU:HD23 | 1.73 | 0.44 |
| 36:DP:83:VAL:HG11 | 36:DP:100:LEU:HD13 | 1.99 | 0.44 |
| 38:DR:28:LEU:HD12 | 38:DR:48:VAL:HG21 | 2.00 | 0.44 |
| 40:DT:50:ILE:HG22 | 40:DT:102:ILE:HD11 | 1.99 | 0.44 |
| 26:DA:483:A:H1' | 45:DY:59:GLY:O | 2.18 | 0.44 |
| 46:DZ:99:TYR:HA | 46:DZ:124:ILE:O | 2.17 | 0.44 |
| 1:AA:1025:U:O2' | 1:AA:1026:G:C8 | 2.67 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1130:A:H3' | 9:AI:18:PHE:CE2 | 2.52 | 0.44 |
| 1:AA:1261:A:H3' | 1:AA:1262:C:C6 | 2.52 | 0.44 |
| 2:AB:158:LEU:HG | 2:AB:182:ILE:HD11 | 2.00 | 0.44 |
| 2:AB:158:LEU:HA | 2:AB:159:PRO:HD3 | 1.87 | 0.44 |
| 10:AJ:69:ASN:O | 10:AJ:70:ARG:HD3 | 2.17 | 0.44 |
| 25:AY:4:C:H3' | 25:AY:5:G:H5'' | 2.00 | 0.44 |
| 26:BA:2271:G:OP1 | 47:B0:18:ALA:HB1 | 2.18 | 0.44 |
| 26:BA:1766:U:H2' | 26:BA:1767:C:H6 | 1.83 | 0.44 |
| 26:BA:2377:A:H2' | 26:BA:2378:A:C8 | 2.53 | 0.44 |
| 26:BA:2693:A:H2' | 26:BA:2694:G:C8 | 2.53 | 0.44 |
| 26:BA:892:G:N3 | 26:BA:892:G:H2' | 2.32 | 0.44 |
| 26:BA:893:C:H2' | 26:BA:894:C:H6 | 1.81 | 0.44 |
| 33:BI:103:ARG:HG3 | 33:BI:104:GLN:H | 1.82 | 0.44 |
| 33:BI:43:ASN:C | 33:BI:43:ASN:HD22 | 2.20 | 0.44 |
| 26:BA:2849:U:P | 40:BT:95:ARG:HH12 | 2.40 | 0.44 |
| 1:CA:1000:U:H2' | 1:CA:1001:A:H8 | 1.83 | 0.44 |
| 1:CA:1014:A:O2' | 1:CA:1219:U:H4' | 2.17 | 0.44 |
| 1:CA:1291:G:C6 | 1:CA:1292:U:C4 | 3.05 | 0.44 |
| 1:CA:1245:A:N1 | 1:CA:1292:U:O2 | 2.51 | 0.44 |
| 1:CA:6:G:O2' | 1:CA:7:G:H5' | 2.17 | 0.44 |
| 1:CA:570:G:H1' | 1:CA:820:U:C4 | 2.53 | 0.44 |
| 2:CB:109:SER:O | 2:CB:112:VAL:HB | 2.17 | 0.44 |
| 2:CB:15:VAL:HG21 | 2:CB:213:LEU:HD13 | 1.99 | 0.44 |
| 4:CD:111:ALA:HB1 | 4:CD:116:GLN:HB3 | 2.00 | 0.44 |
| 6:CF:37:VAL:HA | 6:CF:65:VAL:HG12 | 2.00 | 0.44 |
| 9:CI:16:ARG:CB | 9:CI:64:THR:HG23 | 2.47 | 0.44 |
| 10:CJ:43:ARG:HB2 | 10:CJ:67:THR:HG23 | 2.00 | 0.44 |
| 22:CV:14:A:C2 | 25:CY:34:G:C2 | 3.06 | 0.44 |
| 25:CY:40:C:H2' | 25:CY:41:C:C6 | 2.53 | 0.44 |
| 19:CS:67:VAL:H | 51:D4:58:ARG:HD3 | 1.82 | 0.44 |
| 26:DA:1268:A:H2' | 26:DA:1269:A:O4' | 2.17 | 0.44 |
| 26:DA:1983:C:H4' | 26:DA:2606:C:H4' | 1.99 | 0.44 |
| 26:DA:2127:G:N1 | 26:DA:2128:C:C4 | 2.85 | 0.44 |
| 26:DA:2617:C:H2' | 26:DA:2618:G:O4' | 2.17 | 0.44 |
| 26:DA:2805:G:H2' | 26:DA:2807:G:H8 | 1.79 | 0.44 |
| 26:DA:2313:C:H4' | 31:DG:91:ARG:HG3 | 2.00 | 0.44 |
| 32:DH:18:GLU:HB3 | 32:DH:25:LYS:HB2 | 2.00 | 0.44 |
| 40:DT:117:ASP:O | 40:DT:121:ILE:HG13 | 2.18 | 0.44 |
| 41:DU:66:ASN:O | 41:DU:70:ARG:HG3 | 2.18 | 0.44 |
| 1:AA:1153:C:H2' | 1:AA:1154:G:O4' | 2.18 | 0.44 |
| 1:AA:1179:A:H4' | 9:AI:103:THR:HA | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:166:G:H2' | 1:AA:167:G:C8 | 2.53 | 0.44 |
| 2:AB:51:LEU:HD23 | 2:AB:201:ILE:HD12 | 2.00 | 0.44 |
| 7:AG:16:LEU:HD23 | 9:AI:41:VAL:O | 2.18 | 0.44 |
| 12:AL:34:ARG:HG2 | 12:AL:35:GLY:N | 2.33 | 0.44 |
| 52:B5:35:GLU:HG3 | 52:B5:51:TYR:CD2 | 2.53 | 0.44 |
| 26:BA:141:A:C8 | 26:BA:1408:C:O2' | 2.68 | 0.44 |
| 26:BA:2104:G:H2' | 26:BA:2105:C:C6 | 2.53 | 0.44 |
| 26:BA:1297:C:OP1 | 26:BA:2710:C:H4' | 2.18 | 0.44 |
| 28:BD:35:LYS:HB2 | 28:BD:36:PRO:HD2 | 1.99 | 0.44 |
| 32:BH:26:VAL:HG12 | 32:BH:79:VAL:HG21 | 1.99 | 0.44 |
| 42:BV:65:GLY:HA3 | 42:BV:91:TYR:CZ | 2.53 | 0.44 |
| 1:CA:1151:A:O2' | 1:CA:1152:A:H8 | 2.00 | 0.44 |
| 1:CA:1154:G:O6 | 1:CA:1155:G:N1 | 2.51 | 0.44 |
| 1:CA:1217:C:H2' | 1:CA:1218:C:O4' | 2.18 | 0.44 |
| 1:CA:44:G:H2' | 1:CA:45:U:O4' | 2.18 | 0.44 |
| 2:CB:71:VAL:HG22 | 2:CB:163:PHE:O | 2.18 | 0.44 |
| 5:CE:96:PRO:HA | 5:CE:117:ASP:OD2 | 2.18 | 0.44 |
| 53:D6:14:THR:HG22 | 53:D6:15:GLU:HG3 | 2.00 | 0.44 |
| 26:DA:1185:C:H5'' | 26:DA:1186:G:OP1 | 2.18 | 0.44 |
| 26:DA:1308:A:H2' | 26:DA:1309:G:O4' | 2.18 | 0.44 |
| 26:DA:172:C:H2' | 26:DA:173:G:H8 | 1.83 | 0.44 |
| 26:DA:1826:G:H4' | 28:DD:242:ARG:CZ | 2.47 | 0.44 |
| 24:CX:13:C:O2' | 26:DA:1924:C:H4' | 2.17 | 0.44 |
| 26:DA:2439:A:H5' | 26:DA:2439:A:C8 | 2.52 | 0.44 |
| 26:DA:2567:G:H2' | 26:DA:2568:C:C6 | 2.53 | 0.44 |
| 26:DA:764:A:H5' | 28:DD:210:GLY:HA2 | 2.00 | 0.44 |
| 26:DA:861:A:N3 | 27:DB:79:C:O2' | 2.43 | 0.44 |
| 30:DF:39:TRP:CZ2 | 30:DF:43:LYS:HE2 | 2.52 | 0.44 |
| 27:DB:42:C:C2 | 31:DG:92:VAL:HA | 2.53 | 0.44 |
| 1:AA:1014:A:C2 | 1:AA:1219:U:H1' | 2.53 | 0.43 |
| 2:AB:21:ARG:H | 2:AB:21:ARG:HD2 | 1.83 | 0.43 |
| 4:AD:107:ARG:HD2 | 4:AD:107:ARG:HA | 1.78 | 0.43 |
| 4:AD:163:GLU:O | 4:AD:166:LYS:HG2 | 2.18 | 0.43 |
| 4:AD:19:LEU:HB3 | 4:AD:21:LEU:HD21 | 2.00 | 0.43 |
| 5:AE:131:ILE:HD13 | 5:AE:131:ILE:HA | 1.79 | 0.43 |
| 7:AG:146:GLU:OE2 | 7:AG:149:ARG:NE | 2.51 | 0.43 |
| 1:AA:973:G:OP1 | 10:AJ:57:LYS:HE3 | 2.18 | 0.43 |
| 11:AK:81:ASP:OD1 | 11:AK:81:ASP:N | 2.50 | 0.43 |
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:HE2 | 1.84 | 0.43 |
| 23:AW:19:G:N1 | 23:AW:56:C:N4 | 2.53 | 0.43 |
| 25:AY:36:A:H2' | 25:AY:37:MIA:O4' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 56:B9:32:HIS:O | 56:B9:34:GLN:HG3 | 2.18 | 0.43 |
| 26:BA:144:C:H5' | 44:BX:2:LYS:HE2 | 2.00 | 0.43 |
| 26:BA:1817:G:OP1 | 28:BD:88:ARG:NH2 | 2.43 | 0.43 |
| 26:BA:2141:G:N1 | 26:BA:2142:C:C2 | 2.86 | 0.43 |
| 26:BA:2345:G:OP2 | 53:B6:38:LYS:NZ | 2.46 | 0.43 |
| 26:BA:2561:A:H2' | 26:BA:2562:U:O4' | 2.17 | 0.43 |
| 26:BA:2749:A:P | 32:BH:3:ARG:HH21 | 2.41 | 0.43 |
| 1:CA:1177:G:H3' | 1:CA:1178:G:H8 | 1.83 | 0.43 |
| 1:CA:1278:U:H5' | 1:CA:1279:A:O4' | 2.18 | 0.43 |
| 1:CA:685:G:C2 | 1:CA:686:U:C4 | 3.06 | 0.43 |
| 1:CA:954:G:H2' | 1:CA:955:U:O4' | 2.17 | 0.43 |
| 2:CB:188:ALA:HB1 | 2:CB:192:SER:OG | 2.18 | 0.43 |
| 3:CC:111:LEU:HD11 | 3:CC:144:SER:O | 2.17 | 0.43 |
| 4:CD:20:TYR:CD1 | 4:CD:26:CYS:HB3 | 2.52 | 0.43 |
| 7:CG:22:LEU:HD13 | 7:CG:97:GLN:OE1 | 2.17 | 0.43 |
| 9:CI:4:TYR:CD2 | 9:CI:88:TYR:HB2 | 2.53 | 0.43 |
| 9:CI:89:ASN:C | 9:CI:89:ASN:HD22 | 2.22 | 0.43 |
| 10:CJ:77:PRO:O | 10:CJ:81:THR:OG1 | 2.36 | 0.43 |
| 12:CL:34:ARG:O | 12:CL:61:THR:HG23 | 2.18 | 0.43 |
| 1:CA:1226:C:C5 | 13:CM:104:ARG:HA | 2.52 | 0.43 |
| 13:CM:16:ASP:O | 13:CM:20:THR:HG23 | 2.17 | 0.43 |
| 13:CM:54:VAL:HA | 13:CM:57:ARG:HB3 | 2.00 | 0.43 |
| 15:CO:58:MET:O | 15:CO:62:GLN:N | 2.45 | 0.43 |
| 23:CW:69:G:N2 | 23:CW:70:G:C4 | 2.86 | 0.43 |
| 48:D1:91:LYS:HG2 | 48:D1:95:LEU:HD22 | 2.00 | 0.43 |
| 50:D3:10:LYS:HB3 | 50:D3:53:LEU:HA | 2.00 | 0.43 |
| 26:DA:1274:A:N3 | 26:DA:1297:C:H1' | 2.33 | 0.43 |
| 26:DA:298:G:H5'' | 26:DA:299:A:OP1 | 2.18 | 0.43 |
| 29:DE:77:ILE:CD1 | 29:DE:195:LEU:HD13 | 2.49 | 0.43 |
| 29:DE:21:VAL:HG23 | 29:DE:185:LYS:HD2 | 1.99 | 0.43 |
| 31:DG:115:ARG:NH1 | 31:DG:137:GLU:OE2 | 2.51 | 0.43 |
| 33:DI:44:LEU:HA | 33:DI:44:LEU:HD13 | 1.77 | 0.43 |
| 34:DN:88:GLU:HG2 | 34:DN:88:GLU:H | 1.56 | 0.43 |
| 26:DA:2318:G:H21 | 39:DS:3:ARG:HD2 | 1.83 | 0.43 |
| 45:DY:19:LYS:HB3 | 45:DY:19:LYS:HE2 | 1.74 | 0.43 |
| 45:DY:86:ARG:HB2 | 45:DY:98:VAL:HG23 | 1.99 | 0.43 |
| 1:AA:1131:G:H22 | 1:AA:1143:G:H21 | 1.65 | 0.43 |
| 1:AA:130:A:H5' | 17:AQ:63:ARG:HE | 1.84 | 0.43 |
| 1:AA:737:A:H2' | 1:AA:738:C:C6 | 2.53 | 0.43 |
| 2:AB:208:ILE:H | 2:AB:208:ILE:HG13 | 1.43 | 0.43 |
| 2:AB:219:VAL:HA | 2:AB:222:ILE:HD12 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1191:A:H5'' | 3:AC:4:LYS:HZ2 | 1.83 | 0.43 |
| 12:AL:92:ASP:O | 12:AL:94:PRO:HD3 | 2.18 | 0.43 |
| 21:AU:3:LYS:HB3 | 21:AU:14:TRP:CG | 2.54 | 0.43 |
| 26:BA:228:A:H8 | 26:BA:229:A:H5' | 1.83 | 0.43 |
| 45:BY:52:SER:HB2 | 45:BY:53:PRO:HD2 | 2.00 | 0.43 |
| 1:CA:1005:A:O2' | 1:CA:1006:C:OP1 | 2.32 | 0.43 |
| 1:CA:448:A:O5' | 1:CA:485:G:N2 | 2.45 | 0.43 |
| 1:CA:999:C:N4 | 1:CA:1042:G:N1 | 2.30 | 0.43 |
| 2:CB:97:TRP:HH2 | 2:CB:102:LEU:HD13 | 1.83 | 0.43 |
| 2:CB:53:ARG:HB3 | 2:CB:53:ARG:NH1 | 2.33 | 0.43 |
| 7:CG:113:GLU:O | 7:CG:119:ARG:HD3 | 2.19 | 0.43 |
| 13:CM:82:MET:HE2 | 13:CM:92:HIS:HB3 | 2.00 | 0.43 |
| 15:CO:3:ILE:O | 15:CO:3:ILE:HG12 | 2.18 | 0.43 |
| 15:CO:26:GLU:HB3 | 15:CO:81:LEU:HD13 | 1.99 | 0.43 |
| 25:CY:71:G:H2' | 25:CY:72:C:C6 | 2.53 | 0.43 |
| 51:D4:46:GLN:C | 51:D4:48:ARG:H | 2.21 | 0.43 |
| 26:DA:122:G:OP1 | 26:DA:149:A:O2' | 2.29 | 0.43 |
| 26:DA:1805:U:C2 | 26:DA:1813:G:N2 | 2.86 | 0.43 |
| 26:DA:2112:G:C4 | 26:DA:2113:U:H1' | 2.53 | 0.43 |
| 26:DA:2115:G:O2' | 26:DA:2167:U:O4 | 2.35 | 0.43 |
| 26:DA:2119:A:C2 | 26:DA:2171:A:H5' | 2.46 | 0.43 |
| 35:DO:34:THR:OG1 | 35:DO:35:VAL:N | 2.50 | 0.43 |
| 36:DP:1:MET:HG2 | 36:DP:5:ASP:HB2 | 1.99 | 0.43 |
| 36:DP:44:GLY:HA3 | 36:DP:45:LEU:HB2 | 2.00 | 0.43 |
| 1:AA:1320:C:H2' | 1:AA:1321:C:O4' | 2.19 | 0.43 |
| 2:AB:189:ASP:O | 2:AB:192:SER:OG | 2.35 | 0.43 |
| 2:AB:96:ARG:HD2 | 2:AB:98:LEU:HD23 | 2.00 | 0.43 |
| 4:AD:105:VAL:HG21 | 4:AD:126:ILE:HG13 | 2.00 | 0.43 |
| 49:B2:53:LEU:HD23 | 49:B2:53:LEU:HA | 1.83 | 0.43 |
| 55:B8:6:THR:HG23 | 55:B8:63:PRO:HD2 | 2.00 | 0.43 |
| 26:BA:1047:G:H2' | 26:BA:1110:G:N2 | 2.33 | 0.43 |
| 26:BA:1371:G:H2' | 26:BA:1372:U:H5 | 1.82 | 0.43 |
| 26:BA:1449:A:H5' | 26:BA:1450:G:OP2 | 2.18 | 0.43 |
| 26:BA:1557:C:OP2 | 26:BA:1558:A:O2' | 2.28 | 0.43 |
| 26:BA:563:G:H22 | 26:BA:578:A:H2 | 1.65 | 0.43 |
| 27:BB:29:A:H2' | 27:BB:30:C:O4' | 2.18 | 0.43 |
| 33:BI:68:LEU:HA | 33:BI:68:LEU:HD23 | 1.77 | 0.43 |
| 38:BR:54:LEU:HD12 | 38:BR:54:LEU:HA | 1.88 | 0.43 |
| 1:CA:1106:G:C6 | 1:CA:1107:C:C4 | 3.07 | 0.43 |
| 1:CA:1172:C:H2' | 1:CA:1173:G:C8 | 2.53 | 0.43 |
| 1:CA:1442:G:H8 | 1:CA:1442:G:H3' | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:16:HIS:HB3 | 2:CB:210:SER:HB3 | 1.99 | 0.43 |
| 1:CA:1106:G:OP1 | 3:CC:172:ARG:HD3 | 2.18 | 0.43 |
| 4:CD:173:TRP:CD1 | 4:CD:174:LEU:HG | 2.54 | 0.43 |
| 9:CI:23:ASN:HD22 | 9:CI:23:ASN:H | 1.66 | 0.43 |
| 10:CJ:42:THR:HG21 | 10:CJ:66:ARG:HB3 | 1.99 | 0.43 |
| 26:DA:1607:C:N4 | 26:DA:1622:G:OP2 | 2.45 | 0.43 |
| 26:DA:2512:C:H2' | 26:DA:2513:G:O4' | 2.17 | 0.43 |
| 26:DA:493:G:H2' | 26:DA:494:G:O4' | 2.17 | 0.43 |
| 26:DA:522:G:H2' | 26:DA:523:C:C6 | 2.54 | 0.43 |
| 26:DA:868:U:C4 | 26:DA:869:G:N7 | 2.87 | 0.43 |
| 26:DA:875:G:O2' | 46:DZ:151:HIS:HE1 | 2.00 | 0.43 |
| 34:DN:37:LYS:HG3 | 34:DN:42:TRP:NE1 | 2.33 | 0.43 |
| 1:AA:1032:G:H2' | 1:AA:1033:G:C8 | 2.53 | 0.43 |
| 1:AA:419:C:OP1 | 1:AA:513:C:O2' | 2.21 | 0.43 |
| 1:AA:44:G:H2' | 1:AA:45:U:O4' | 2.18 | 0.43 |
| 2:AB:87:ARG:NE | 2:AB:233:SER:HB3 | 2.33 | 0.43 |
| 9:AI:4:TYR:CD1 | 9:AI:88:TYR:HA | 2.53 | 0.43 |
| 20:AT:60:GLU:HG2 | 20:AT:81:LYS:HD3 | 2.00 | 0.43 |
| 26:BA:1001:A:H2' | 26:BA:1002:G:O4' | 2.19 | 0.43 |
| 26:BA:484:C:H2' | 26:BA:485:C:C6 | 2.53 | 0.43 |
| 26:BA:528:A:C2 | 26:BA:2043:C:H4' | 2.53 | 0.43 |
| 26:BA:813:U:H2' | 26:BA:814:C:C6 | 2.53 | 0.43 |
| 26:BA:954:G:H5'' | 37:BQ:13:GLN:HB3 | 2.00 | 0.43 |
| 28:BD:13:ARG:HD2 | 28:BD:13:ARG:HA | 1.82 | 0.43 |
| 26:BA:956:G:P | 37:BQ:14:ARG:HH22 | 2.35 | 0.43 |
| 46:BZ:104:PHE:HB3 | 46:BZ:141:VAL:HG21 | 1.99 | 0.43 |
| 1:CA:1011:G:C6 | 1:CA:1012:U:C2 | 3.06 | 0.43 |
| 1:CA:1304:G:C6 | 1:CA:1305:G:N1 | 2.86 | 0.43 |
| 1:CA:1342:C:H2' | 1:CA:1343:G:H8 | 1.83 | 0.43 |
| 1:CA:934:C:H5 | 1:CA:1344:C:H2' | 1.84 | 0.43 |
| 1:CA:404:U:H2' | 1:CA:405:U:C6 | 2.53 | 0.43 |
| 7:CG:23:VAL:HG13 | 7:CG:43:PHE:CE2 | 2.54 | 0.43 |
| 1:CA:881:G:OP2 | 12:CL:12:ARG:NH2 | 2.51 | 0.43 |
| 19:CS:65:ASN:N | 19:CS:65:ASN:OD1 | 2.51 | 0.43 |
| 23:CW:2:C:N3 | 23:CW:71:G:O6 | 2.52 | 0.43 |
| 25:CY:58:A:H4' | 25:CY:59:U:OP1 | 2.18 | 0.43 |
| 26:DA:2156:G:O5' | 26:DA:2156:G:H8 | 2.01 | 0.43 |
| 26:DA:2393:A:H2' | 26:DA:2394:C:O4' | 2.19 | 0.43 |
| 26:DA:2485:G:C2 | 26:DA:2486:G:C8 | 3.06 | 0.43 |
| 26:DA:2519:U:O4' | 26:DA:2542:A:N6 | 2.51 | 0.43 |
| 26:DA:2821:A:H2' | 26:DA:2822:G:C8 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DA:880:G:N2 | 26:DA:898:C:H1' | 2.21 | 0.43 |
| 26:DA:862:G:O2' | 27:DB:78:A:N3 | 2.51 | 0.43 |
| 29:DE:60:ASN:OD1 | 29:DE:62:PRO:HD2 | 2.18 | 0.43 |
| 37:DQ:66:ILE:HG12 | 37:DQ:104:PHE:CE1 | 2.53 | 0.43 |
| 45:DY:43:ASN:CG | 45:DY:65:ALA:HB3 | 2.39 | 0.43 |
| 1:AA:841:U:OP2 | 1:AA:841:U:H6 | 2.02 | 0.43 |
| 2:AB:211:ILE:O | 2:AB:215:LEU:HB2 | 2.19 | 0.43 |
| 9:AI:18:PHE:O | 9:AI:61:ALA:HA | 2.19 | 0.43 |
| 9:AI:55:ALA:HA | 9:AI:58:HIS:CD2 | 2.54 | 0.43 |
| 11:AK:34:ASP:OD2 | 11:AK:38:ASN:HB2 | 2.19 | 0.43 |
| 11:AK:41:THR:OG1 | 11:AK:42:TRP:N | 2.52 | 0.43 |
| 1:AA:1049:U:OP1 | 14:AN:3:ARG:HB2 | 2.19 | 0.43 |
| 26:BA:1709:U:H2' | 26:BA:1710:C:C6 | 2.54 | 0.43 |
| 26:BA:196:A:H2' | 26:BA:196:A:N3 | 2.34 | 0.43 |
| 26:BA:2121:G:N2 | 26:BA:2177:C:N3 | 2.50 | 0.43 |
| 26:BA:662:G:H5' | 36:BP:14:LYS:O | 2.18 | 0.43 |
| 32:BH:164:TYR:HB2 | 32:BH:167:GLU:HB2 | 2.00 | 0.43 |
| 39:BS:34:HIS:ND1 | 39:BS:53:SER:OG | 2.42 | 0.43 |
| 46:BZ:79:ARG:HB3 | 46:BZ:80:ARG:NH1 | 2.33 | 0.43 |
| 1:CA:731:G:H5' | 1:CA:766:A:H4' | 2.00 | 0.43 |
| 1:CA:988:G:H1' | 1:CA:1014:A:N1 | 2.32 | 0.43 |
| 5:CE:41:VAL:HG23 | 5:CE:67:VAL:HG13 | 2.01 | 0.43 |
| 1:CA:1240:U:N3 | 7:CG:30:ILE:O | 2.44 | 0.43 |
| 26:DA:1652:A:O2' | 26:DA:1653:G:H5' | 2.17 | 0.43 |
| 26:DA:1778:U:H2' | 26:DA:1784:A:N6 | 2.34 | 0.43 |
| 26:DA:1847:A:H4' | 26:DA:1848:A:OP2 | 2.18 | 0.43 |
| 26:DA:2036:C:H2' | 26:DA:2037:G:H8 | 1.83 | 0.43 |
| 26:DA:2639:A:C2 | 26:DA:2778:A:C8 | 3.07 | 0.43 |
| 26:DA:373:U:H2' | 26:DA:374:A:H8 | 1.83 | 0.43 |
| 26:DA:647:G:H8 | 26:DA:647:G:O5' | 2.02 | 0.43 |
| 26:DA:949:C:H2' | 26:DA:950:G:C8 | 2.54 | 0.43 |
| 30:DF:129:PHE:HA | 30:DF:142:TRP:NE1 | 2.33 | 0.43 |
| 31:DG:43:LEU:HB3 | 31:DG:44:GLY:H | 1.48 | 0.43 |
| 41:DU:58:ARG:HA | 41:DU:61:TRP:CE3 | 2.53 | 0.43 |
| 41:DU:43:GLY:HA3 | 42:DV:73:SER:HB3 | 2.01 | 0.43 |
| 1:AA:1277:C:O2' | 1:AA:1279:A:H1' | 2.19 | 0.43 |
| 1:AA:164:U:H2' | 1:AA:165:C:C6 | 2.54 | 0.43 |
| 1:AA:202:U:HO2' | 1:AA:203:U:P | 2.39 | 0.43 |
| 1:AA:658:G:H2' | 1:AA:659:U:C6 | 2.54 | 0.43 |
| 1:AA:71:C:N3 | 1:AA:98:G:O6 | 2.51 | 0.43 |
| 5:AE:50:GLU:HB2 | 5:AE:53:LEU:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AF:76:ALA:O | 6:AF:80:ARG:HG3 | 2.19 | 0.43 |
| 14:AN:13:THR:HA | 14:AN:14:PRO:HD3 | 1.81 | 0.43 |
| 1:AA:1217:C:OP1 | 14:AN:9:LYS:HE2 | 2.18 | 0.43 |
| 24:AX:31:G:N7 | 24:AX:32:5MC:HM52 | 2.34 | 0.43 |
| 26:BA:1654:A:OP1 | 38:BR:1:MET:HA | 2.19 | 0.43 |
| 26:BA:1712:C:H2' | 26:BA:1713:U:O4' | 2.18 | 0.43 |
| 26:BA:1669:A:H5'' | 26:BA:2550:G:OP1 | 2.18 | 0.43 |
| 26:BA:422:A:H2' | 26:BA:423:A:C8 | 2.53 | 0.43 |
| 26:BA:543:C:N3 | 26:BA:549:G:N1 | 2.49 | 0.43 |
| 46:BZ:111:VAL:CG2 | 46:BZ:117:LEU:HB2 | 2.48 | 0.43 |
| 1:CA:1187:G:OP1 | 9:CI:113:LYS:NZ | 2.50 | 0.43 |
| 1:CA:396:G:H2' | 1:CA:397:A:H5'' | 1.99 | 0.43 |
| 1:CA:553:A:H2' | 1:CA:554:C:C6 | 2.53 | 0.43 |
| 1:CA:1187:G:H5'' | 9:CI:113:LYS:HE3 | 1.99 | 0.43 |
| 1:CA:953:G:N7 | 13:CM:104:ARG:NH2 | 2.67 | 0.43 |
| 19:CS:13:ASP:HA | 19:CS:16:LEU:HB2 | 2.01 | 0.43 |
| 20:CT:59:ALA:O | 20:CT:63:ILE:HG13 | 2.19 | 0.43 |
| 26:DA:1588:C:H2' | 26:DA:1589:C:C6 | 2.53 | 0.43 |
| 26:DA:1853:A:H2' | 26:DA:1854:A:C8 | 2.54 | 0.43 |
| 26:DA:2172:U:O2' | 26:DA:2173:A:OP1 | 2.36 | 0.43 |
| 26:DA:2180:U:H2' | 26:DA:2181:G:O4' | 2.17 | 0.43 |
| 26:DA:2526:G:H2' | 26:DA:2527:C:H6 | 1.83 | 0.43 |
| 26:DA:286:C:H2' | 26:DA:287:C:C6 | 2.54 | 0.43 |
| 26:DA:910:A:C6 | 26:DA:911:A:C6 | 3.06 | 0.43 |
| 27:DB:15:A:C8 | 27:DB:110:G:C4 | 3.07 | 0.43 |
| 31:DG:150:ASP:OD1 | 31:DG:150:ASP:N | 2.44 | 0.43 |
| 37:DQ:20:ALA:HB2 | 46:DZ:79:ARG:HG2 | 2.00 | 0.43 |
| 38:DR:88:ARG:NH2 | 38:DR:89:ASP:OD1 | 2.50 | 0.43 |
| 44:DX:35:THR:HG22 | 44:DX:37:THR:N | 2.34 | 0.43 |
| 44:DX:55:ASN:O | 44:DX:79:ALA:HA | 2.19 | 0.43 |
| 1:AA:1402:C:H2' | 1:AA:1403:C:O4' | 2.18 | 0.43 |
| 1:AA:434:U:H2' | 1:AA:435:C:C6 | 2.54 | 0.43 |
| 2:AB:21:ARG:HH21 | 2:AB:21:ARG:H | 1.65 | 0.43 |
| 3:AC:78:GLY:HA3 | 3:AC:83:ARG:H | 1.84 | 0.43 |
| 11:AK:67:ASP:OD1 | 11:AK:71:LYS:HE3 | 2.18 | 0.43 |
| 13:AM:3:ARG:HG3 | 13:AM:4:ILE:H | 1.80 | 0.43 |
| 15:AO:25:THR:HG21 | 15:AO:70:LEU:HB2 | 1.99 | 0.43 |
| 31:BG:179:PRO:HG3 | 51:B4:43:TYR:OH | 2.19 | 0.43 |
| 51:B4:46:GLN:O | 51:B4:46:GLN:HG2 | 2.19 | 0.43 |
| 26:BA:1429:G:H2' | 26:BA:1430:C:C6 | 2.53 | 0.43 |
| 28:BD:20:ASP:OD1 | 28:BD:20:ASP:N | 2.39 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BP:64:LYS:HE3 | 55:B8:12:LYS:HD3 | 2.01 | 0.43 |
| 41:BU:86:ALA:O | 42:BV:49:THR:HG23 | 2.19 | 0.43 |
| 1:CA:1321:C:H3' | 1:CA:1322:C:H6 | 1.82 | 0.43 |
| 1:CA:20:U:H2' | 1:CA:21:G:O4' | 2.18 | 0.43 |
| 1:CA:21:G:H2' | 1:CA:22:G:C8 | 2.54 | 0.43 |
| 1:CA:299:G:H2' | 1:CA:300:A:C8 | 2.53 | 0.43 |
| 1:CA:427:U:H3' | 1:CA:428:G:H2' | 2.01 | 0.43 |
| 1:CA:62:U:H2' | 1:CA:63:C:C6 | 2.54 | 0.43 |
| 1:CA:707:C:H2' | 1:CA:708:C:H6 | 1.83 | 0.43 |
| 3:CC:104:GLN:NE2 | 3:CC:105:GLU:HG3 | 2.34 | 0.43 |
| 3:CC:19:GLU:HB3 | 3:CC:55:VAL:O | 2.18 | 0.43 |
| 4:CD:53:ASP:HB3 | 4:CD:57:ARG:NH1 | 2.34 | 0.43 |
| 8:CH:124:ALA:O | 8:CH:128:GLY:N | 2.52 | 0.43 |
| 8:CH:56:LYS:HB2 | 8:CH:58:TYR:HE1 | 1.83 | 0.43 |
| 9:CI:22:GLY:N | 9:CI:58:HIS:O | 2.30 | 0.43 |
| 16:CP:74:LEU:O | 16:CP:79:VAL:HG23 | 2.19 | 0.43 |
| 1:CA:719:C:N4 | 18:CR:71:LYS:NZ | 2.66 | 0.43 |
| 25:CY:19:G:C4' | 25:CY:57:G:H22 | 2.32 | 0.43 |
| 26:DA:1836:C:H2' | 26:DA:1837:C:H6 | 1.84 | 0.43 |
| 26:DA:2125:G:H1 | 26:DA:2172:U:P | 2.41 | 0.43 |
| 26:DA:2406:U:OP2 | 26:DA:2406:U:H2' | 2.19 | 0.43 |
| 26:DA:272(D):G:C2 | 26:DA:272(E):G:C8 | 3.07 | 0.43 |
| 26:DA:839:U:H2' | 26:DA:840:C:C6 | 2.53 | 0.43 |
| 34:DN:71:ILE:HG21 | 34:DN:84:LYS:HB3 | 2.01 | 0.43 |
| 40:DT:92:GLY:O | 40:DT:120:ARG:NH2 | 2.51 | 0.43 |
| 41:DU:81:HIS:HB3 | 41:DU:117:GLN:HE22 | 1.83 | 0.43 |
| 41:DU:8:VAL:O | 41:DU:12:ARG:HG3 | 2.18 | 0.43 |
| 42:DV:5:VAL:HG11 | 42:DV:57:VAL:HG21 | 2.00 | 0.43 |
| 46:DZ:4:ARG:HG3 | 46:DZ:58:VAL:HB | 2.01 | 0.43 |
| 1:AA:1030(C):G:H2' | 1:AA:1030(D):A:H8 | 1.83 | 0.43 |
| 1:AA:984:C:N4 | 1:AA:1221:G:H1 | 2.13 | 0.43 |
| 1:AA:942:G:C2 | 1:AA:1342:C:C2 | 3.06 | 0.43 |
| 1:AA:1362:C:H2' | 1:AA:1363:C:H5'' | 2.01 | 0.43 |
| 1:AA:339:C:H2' | 1:AA:340:U:C6 | 2.54 | 0.43 |
| 11:AK:62:GLN:O | 11:AK:66:LEU:HG | 2.19 | 0.43 |
| 18:AR:31:LEU:H | 18:AR:31:LEU:HD23 | 1.83 | 0.43 |
| 25:AY:23:A:H2' | 25:AY:24:G:C8 | 2.54 | 0.43 |
| 25:AY:3:C:H2' | 25:AY:4:C:O4' | 2.18 | 0.43 |
| 51:B4:68:ARG:HD2 | 51:B4:68:ARG:HA | 1.84 | 0.43 |
| 26:BA:2611:U:H2' | 52:B5:2:ALA:O | 2.19 | 0.43 |
| 26:BA:1441:G:H2' | 26:BA:1442:G:H8 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BA:700:G:O2' | 26:BA:1632:A:N3 | 2.43 | 0.43 |
| 26:BA:2037:G:H2' | 26:BA:2038:G:C8 | 2.54 | 0.43 |
| 26:BA:2335:A:C8 | 26:BA:2337:G:C5 | 3.07 | 0.43 |
| 26:BA:476:G:H4' | 26:BA:502:A:N1 | 2.34 | 0.43 |
| 30:BF:106:ARG:H | 30:BF:106:ARG:HG2 | 1.67 | 0.43 |
| 43:BW:67:ASP:N | 43:BW:67:ASP:OD1 | 2.50 | 0.43 |
| 45:BY:19:LYS:HB3 | 45:BY:19:LYS:HE2 | 1.60 | 0.43 |
| 46:BZ:151:HIS:HA | 46:BZ:169:GLU:O | 2.19 | 0.43 |
| 1:CA:988:G:O2' | 1:CA:1014:A:N6 | 2.52 | 0.43 |
| 1:CA:1051:C:H2' | 1:CA:1052:U:H6 | 1.82 | 0.43 |
| 1:CA:1119:C:C2 | 1:CA:1154:G:O6 | 2.71 | 0.43 |
| 2:CB:178:ARG:NH1 | 2:CB:196:LEU:O | 2.52 | 0.43 |
| 2:CB:73:THR:HG22 | 2:CB:95:GLN:O | 2.18 | 0.43 |
| 3:CC:20:SER:OG | 3:CC:22:TRP:NE1 | 2.52 | 0.43 |
| 7:CG:72:ARG:HH12 | 7:CG:138:LYS:NZ | 2.17 | 0.43 |
| 1:CA:1368:G:OP2 | 9:CI:112:LYS:HG3 | 2.19 | 0.43 |
| 10:CJ:99:LYS:O | 10:CJ:100:THR:OG1 | 2.32 | 0.43 |
| 13:CM:123:ALA:HB2 | 23:CW:39:PSU:H1' | 2.00 | 0.43 |
| 14:CN:37:PHE:HB2 | 14:CN:39:LEU:HB2 | 2.00 | 0.43 |
| 26:DA:1364:G:OP2 | 48:D1:3:LYS:HG3 | 2.19 | 0.43 |
| 49:D2:32:LEU:HD12 | 49:D2:57:ILE:HD12 | 2.00 | 0.43 |
| 26:DA:1652:A:C2' | 26:DA:1653:G:H5' | 2.48 | 0.43 |
| 26:DA:1720:U:H2' | 26:DA:1721:G:O4' | 2.19 | 0.43 |
| 26:DA:2031:A:C6 | 26:DA:2498:C:H1' | 2.54 | 0.43 |
| 26:DA:2152:G:H2' | 26:DA:2153:G:O4' | 2.18 | 0.43 |
| 26:DA:2526:G:H2' | 26:DA:2527:C:C6 | 2.53 | 0.43 |
| 26:DA:1999:C:H5'' | 26:DA:2723:C:O2' | 2.19 | 0.43 |
| 26:DA:2732:G:H3' | 26:DA:2733:A:O4' | 2.19 | 0.43 |
| 26:DA:2741:A:H2' | 26:DA:2742:C:O4' | 2.18 | 0.43 |
| 26:DA:289:A:H62 | 26:DA:351:G:N2 | 2.15 | 0.43 |
| 26:DA:2682:U:H5' | 29:DE:11:MET:O | 2.19 | 0.43 |
| 35:DO:69:ILE:HG12 | 35:DO:69:ILE:H | 1.61 | 0.43 |
| 36:DP:59:LEU:HD21 | 55:D8:10:ALA:HA | 2.01 | 0.43 |
| 37:DQ:16:ARG:NH2 | 37:DQ:18:LYS:HD3 | 2.33 | 0.43 |
| 37:DQ:26:TYR:O | 37:DQ:67:ARG:NH1 | 2.42 | 0.43 |
| 46:DZ:159:PRO:HA | 46:DZ:161:VAL:HG12 | 2.01 | 0.43 |
| 1:AA:438:G:H4' | 4:AD:123:HIS:CE1 | 2.54 | 0.43 |
| 1:AA:671:G:H5' | 6:AF:77:ARG:HH12 | 1.83 | 0.43 |
| 1:AA:909:A:H2' | 1:AA:910:C:O4' | 2.19 | 0.43 |
| 4:AD:33:MET:O | 4:AD:37:PRO:HB3 | 2.19 | 0.43 |
| 12:AL:117:ARG:HB3 | 12:AL:122:THR:HB | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:AO:61:GLY:O | 15:AO:65:ARG:HG3 | 2.18 | 0.43 |
| 26:BA:1394:U:H2' | 26:BA:1395:A:O4' | 2.18 | 0.43 |
| 26:BA:2100:G:H1 | 26:BA:2189:U:H3 | 1.66 | 0.43 |
| 26:BA:1783:A:H5' | 26:BA:2608:G:H4' | 2.00 | 0.43 |
| 29:BE:121:ASN:ND2 | 61:BE:411:HOH:O | 2.40 | 0.43 |
| 32:BH:117:PRO:HG3 | 32:BH:123:PHE:CD2 | 2.54 | 0.43 |
| 34:BN:9:VAL:HG11 | 34:BN:39:ARG:HH22 | 1.83 | 0.43 |
| 45:BY:54:LYS:CA | 45:BY:56:PRO:HD3 | 2.48 | 0.43 |
| 1:CA:1009:G:N2 | 1:CA:1021:G:H1' | 2.34 | 0.43 |
| 1:CA:1261:A:C6 | 1:CA:1262:C:C2 | 3.07 | 0.43 |
| 1:CA:1317:C:O2 | 19:CS:37:ARG:NH1 | 2.52 | 0.43 |
| 1:CA:776:G:HO2' | 1:CA:777:A:H8 | 1.66 | 0.43 |
| 1:CA:955:U:H2' | 1:CA:956:U:O4' | 2.19 | 0.43 |
| 4:CD:13:ARG:HD2 | 4:CD:38:TYR:O | 2.18 | 0.43 |
| 5:CE:83:GLU:HA | 5:CE:88:LYS:HA | 2.00 | 0.43 |
| 6:CF:91:VAL:HG11 | 18:CR:72:ARG:NH1 | 2.34 | 0.43 |
| 1:CA:664:G:H5'' | 18:CR:64:ARG:NH2 | 2.34 | 0.43 |
| 26:DA:1636:C:H2' | 26:DA:1637:A:C8 | 2.54 | 0.43 |
| 26:DA:2171:A:C4 | 26:DA:2172:U:C4 | 3.06 | 0.43 |
| 26:DA:2173:A:OP2 | 26:DA:2173:A:H3' | 2.18 | 0.43 |
| 26:DA:2193:G:H2' | 26:DA:2194:G:H8 | 1.84 | 0.43 |
| 25:CY:76:A:H62 | 26:DA:2422:A:C5' | 2.31 | 0.43 |
| 26:DA:2439:A:H8 | 26:DA:2439:A:H5' | 1.84 | 0.43 |
| 26:DA:2516:G:C6 | 26:DA:2517:C:C4 | 3.07 | 0.43 |
| 26:DA:2557:G:H2' | 26:DA:2558:C:H6 | 1.83 | 0.43 |
| 26:DA:2693:A:H2' | 26:DA:2694:G:C8 | 2.54 | 0.43 |
| 26:DA:322:A:C5 | 26:DA:340:A:C2 | 3.06 | 0.43 |
| 26:DA:770:G:OP2 | 61:DA:4255:HOH:O | 2.21 | 0.43 |
| 27:DB:15:A:OP2 | 27:DB:69:G:N2 | 2.49 | 0.43 |
| 30:DF:195:ASP:HB3 | 30:DF:197:ASP:OD1 | 2.18 | 0.43 |
| 31:DG:145:THR:HG23 | 31:DG:147:ASP:N | 2.23 | 0.43 |
| 31:DG:64:THR:OG1 | 31:DG:66:GLN:O | 2.37 | 0.43 |
| 45:DY:5:MET:HE1 | 45:DY:32:PRO:HA | 2.01 | 0.43 |
| 1:AA:1505:G:O2' | 22:AV:13:A:O2' | 2.33 | 0.43 |
| 1:AA:936:C:H2' | 1:AA:937:A:O4' | 2.19 | 0.43 |
| 3:AC:116:VAL:O | 3:AC:120:VAL:HG23 | 2.19 | 0.43 |
| 3:AC:6:HIS:CD2 | 3:AC:8:ILE:HB | 2.54 | 0.43 |
| 9:AI:20:ARG:HA | 9:AI:21:PRO:HD3 | 1.92 | 0.43 |
| 12:AL:110:VAL:O | 12:AL:122:THR:OG1 | 2.32 | 0.43 |
| 14:AN:23:ARG:HH11 | 14:AN:30:ALA:HB2 | 1.83 | 0.43 |
| 20:AT:29:LYS:O | 20:AT:33:ILE:HG13 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:B5:59:GLU:HG2 | 52:B5:60:VAL:H | 1.83 | 0.43 |
| 26:BA:1005:C:O2' | 34:BN:28:THR:HG21 | 2.19 | 0.43 |
| 26:BA:2154:G:C2' | 26:BA:2155:G:H5' | 2.49 | 0.43 |
| 26:BA:2712:U:OP1 | 26:BA:2714:G:H4' | 2.19 | 0.43 |
| 32:BH:11:VAL:HG13 | 32:BH:15:VAL:HG22 | 2.00 | 0.43 |
| 35:BO:98:VAL:HG22 | 35:BO:118:ALA:HA | 2.01 | 0.43 |
| 37:BQ:56:ARG:HD2 | 37:BQ:56:ARG:HA | 1.72 | 0.43 |
| 1:CA:1176:A:H2' | 1:CA:1177:G:H8 | 1.84 | 0.43 |
| 1:CA:1216:G:H5'' | 14:CN:5:ALA:CB | 2.47 | 0.43 |
| 2:CB:115:LEU:HD21 | 2:CB:153:ARG:NE | 2.34 | 0.43 |
| 1:CA:1112:C:N3 | 3:CC:177:THR:HA | 2.34 | 0.43 |
| 3:CC:42:LEU:HA | 3:CC:45:LYS:NZ | 2.33 | 0.43 |
| 5:CE:110:LEU:HD13 | 5:CE:118:ILE:HG21 | 2.00 | 0.43 |
| 13:CM:66:LEU:O | 13:CM:68:GLY:N | 2.52 | 0.43 |
| 19:CS:71:LEU:HD12 | 19:CS:71:LEU:HA | 1.91 | 0.43 |
| 25:CY:1:G:H2' | 25:CY:2:C:C6 | 2.54 | 0.43 |
| 25:CY:51:U:H2' | 25:CY:52:G:O4' | 2.18 | 0.43 |
| 50:D3:46:ASN:O | 50:D3:50:VAL:HG22 | 2.19 | 0.43 |
| 26:DA:1010:A:H1' | 26:DA:1153:C:H1' | 2.00 | 0.43 |
| 26:DA:1394:U:C4 | 26:DA:1395:A:C5 | 3.07 | 0.43 |
| 26:DA:1899:G:O2' | 26:DA:1900:A:OP2 | 2.35 | 0.43 |
| 26:DA:2019:A:H4' | 41:DU:34:LYS:HD2 | 2.01 | 0.43 |
| 26:DA:2265:U:C4 | 26:DA:2266:A:C5 | 3.07 | 0.43 |
| 26:DA:2461:C:H2' | 26:DA:2462:U:H6 | 1.84 | 0.43 |
| 26:DA:2740:A:H2' | 26:DA:2741:A:C8 | 2.54 | 0.43 |
| 26:DA:2747:G:O6 | 26:DA:2755:C:H5'' | 2.19 | 0.43 |
| 27:DB:24:G:O4' | 27:DB:26:A:N6 | 2.47 | 0.43 |
| 32:DH:124:GLU:OE1 | 32:DH:132:ARG:HD2 | 2.19 | 0.43 |
| 36:DP:99:LEU:HD23 | 36:DP:99:LEU:H | 1.83 | 0.43 |
| 37:DQ:36:ALA:HB2 | 37:DQ:103:MET:SD | 2.59 | 0.43 |
| 38:DR:2:ARG:NH1 | 38:DR:5:LYS:O | 2.52 | 0.43 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.53 | 0.42 |
| 1:AA:294:U:OP1 | 1:AA:610:G:O2' | 2.30 | 0.42 |
| 1:AA:940:C:OP1 | 7:AG:29:LYS:NZ | 2.48 | 0.42 |
| 2:AB:224:GLN:HA | 2:AB:228:GLY:O | 2.19 | 0.42 |
| 3:AC:77:ILE:HG22 | 3:AC:81:GLY:HA2 | 2.01 | 0.42 |
| 3:AC:82:GLU:HA | 3:AC:85:ARG:NE | 2.34 | 0.42 |
| 4:AD:170:VAL:HG12 | 4:AD:171:GLY:N | 2.34 | 0.42 |
| 7:AG:70:LYS:O | 7:AG:138:LYS:NZ | 2.49 | 0.42 |
| 8:AH:51:VAL:HG11 | 8:AH:60:ARG:NH1 | 2.34 | 0.42 |
| 23:AW:51:U:H2' | 23:AW:52:G:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:B1:62:VAL:HG22 | 48:B1:63:ALA:O | 2.18 | 0.42 |
| 26:BA:1354:A:H2' | 26:BA:1355:G:O4' | 2.19 | 0.42 |
| 26:BA:1504:C:H2' | 26:BA:1505:C:C6 | 2.54 | 0.42 |
| 26:BA:1794:U:H2' | 26:BA:1795:C:C6 | 2.54 | 0.42 |
| 26:BA:1882:C:H2' | 26:BA:1883:G:O4' | 2.19 | 0.42 |
| 26:BA:1913:A:H4' | 26:BA:1914:C:C5' | 2.49 | 0.42 |
| 26:BA:2199:A:H5'' | 26:BA:2200:C:OP2 | 2.19 | 0.42 |
| 33:BI:40:THR:O | 33:BI:44:LEU:HB2 | 2.19 | 0.42 |
| 36:BP:100:LEU:HD12 | 36:BP:112:LEU:HD11 | 2.01 | 0.42 |
| 43:BW:14:PRO:HG2 | 43:BW:78:GLU:CG | 2.48 | 0.42 |
| 45:BY:1:MET:HB2 | 45:BY:2:ARG:H | 1.53 | 0.42 |
| 1:CA:1025:U:H1' | 1:CA:1026:G:C8 | 2.54 | 0.42 |
| 1:CA:103:C:P | 20:CT:17:ARG:HH21 | 2.42 | 0.42 |
| 1:CA:495:A:H4' | 1:CA:496:A:OP1 | 2.18 | 0.42 |
| 1:CA:993:G:H2' | 1:CA:993:G:N3 | 2.33 | 0.42 |
| 2:CB:115:LEU:HG | 2:CB:119:GLU:OE2 | 2.19 | 0.42 |
| 2:CB:122:PHE:HE2 | 2:CB:139:LYS:HG2 | 1.84 | 0.42 |
| 10:CJ:30:SER:OG | 10:CJ:84:GLN:OE1 | 2.29 | 0.42 |
| 13:CM:4:ILE:HG23 | 13:CM:22:ILE:HD11 | 2.01 | 0.42 |
| 1:CA:228:A:H5' | 16:CP:62:VAL:HG21 | 2.01 | 0.42 |
| 18:CR:76:LEU:HA | 18:CR:76:LEU:HD12 | 1.81 | 0.42 |
| 26:DA:2529:G:O6 | 56:D9:31:LYS:NZ | 2.51 | 0.42 |
| 26:DA:1463:C:H2' | 26:DA:1464:C:C6 | 2.54 | 0.42 |
| 26:DA:150:C:H2' | 26:DA:151:C:C6 | 2.54 | 0.42 |
| 26:DA:2302:G:C6 | 26:DA:2303:G:N7 | 2.88 | 0.42 |
| 26:DA:2302:G:H1 | 26:DA:2314:C:H42 | 1.67 | 0.42 |
| 26:DA:2316:C:O2' | 31:DG:128:ARG:NH1 | 2.52 | 0.42 |
| 26:DA:2591:C:H2' | 26:DA:2592:G:C8 | 2.54 | 0.42 |
| 26:DA:2723:C:OP2 | 29:DE:109:LYS:NZ | 2.52 | 0.42 |
| 26:DA:272(E):G:C2 | 26:DA:364:C:C2 | 3.07 | 0.42 |
| 26:DA:524:U:H2' | 26:DA:525:U:C6 | 2.54 | 0.42 |
| 26:DA:563:G:OP2 | 61:DA:4169:HOH:O | 2.21 | 0.42 |
| 28:DD:75:ILE:HA | 28:DD:76:PRO:HD3 | 1.93 | 0.42 |
| 29:DE:181:LEU:HD12 | 29:DE:181:LEU:HA | 1.76 | 0.42 |
| 26:DA:660:G:H5' | 30:DF:99:TYR:CE2 | 2.53 | 0.42 |
| 31:DG:135:LEU:HD13 | 31:DG:135:LEU:HA | 1.89 | 0.42 |
| 31:DG:23:PHE:HB2 | 31:DG:25:TYR:CE1 | 2.54 | 0.42 |
| 32:DH:164:TYR:HB2 | 32:DH:167:GLU:HB2 | 2.00 | 0.42 |
| 32:DH:2:SER:O | 32:DH:3:ARG:HG2 | 2.19 | 0.42 |
| 32:DH:56:SER:HB3 | 32:DH:61:HIS:ND1 | 2.33 | 0.42 |
| 35:DO:17:ARG:HD3 | 35:DO:17:ARG:HA | 1.69 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DF:31:HIS:HB2 | 36:DP:9:ASN:OD1 | 2.19 | 0.42 |
| 38:DR:12:ARG:HG2 | 38:DR:16:HIS:ND1 | 2.34 | 0.42 |
| 41:DU:107:ALA:O | 41:DU:111:GLU:HG2 | 2.18 | 0.42 |
| 42:DV:31:ALA:O | 42:DV:61:VAL:HG12 | 2.18 | 0.42 |
| 1:AA:1286:A:H3' | 1:AA:1286:A:C8 | 2.54 | 0.42 |
| 1:AA:54:C:H2' | 1:AA:352:C:H41 | 1.84 | 0.42 |
| 1:AA:373:A:H1' | 1:AA:481:G:N3 | 2.34 | 0.42 |
| 3:AC:191:THR:OG1 | 3:AC:194:GLY:O | 2.33 | 0.42 |
| 4:AD:170:VAL:HG11 | 4:AD:174:LEU:HD12 | 2.01 | 0.42 |
| 1:AA:405:U:O4 | 4:AD:2:GLY:N | 2.53 | 0.42 |
| 5:AE:6:PHE:HB3 | 5:AE:35:GLY:C | 2.40 | 0.42 |
| 8:AH:78:GLN:HE21 | 8:AH:78:GLN:HB2 | 1.47 | 0.42 |
| 26:BA:1108:U:O2' | 26:BA:1109:C:C6 | 2.72 | 0.42 |
| 26:BA:2291:U:H2' | 26:BA:2292:C:C6 | 2.54 | 0.42 |
| 32:BH:24:VAL:HG22 | 32:BH:35:VAL:HB | 2.01 | 0.42 |
| 44:BX:64:LYS:HA | 44:BX:64:LYS:HD3 | 1.83 | 0.42 |
| 1:CA:1154:G:C8 | 1:CA:1155:G:C8 | 3.07 | 0.42 |
| 1:CA:850:U:H2' | 1:CA:851:G:H5'' | 2.01 | 0.42 |
| 4:CD:163:GLU:C | 4:CD:165:MET:H | 2.22 | 0.42 |
| 10:CJ:8:LEU:HB3 | 10:CJ:16:LEU:HD22 | 2.01 | 0.42 |
| 19:CS:41:VAL:HG13 | 19:CS:42:PRO:HD2 | 2.01 | 0.42 |
| 26:DA:1204:A:N6 | 26:DA:1240:U:H2' | 2.34 | 0.42 |
| 26:DA:1556:C:H2' | 26:DA:1557:C:H6 | 1.84 | 0.42 |
| 26:DA:1877:A:H5' | 26:DA:1878:G:OP2 | 2.19 | 0.42 |
| 26:DA:39:C:H2' | 26:DA:40:C:H6 | 1.84 | 0.42 |
| 31:DG:47:LYS:HE2 | 31:DG:47:LYS:HB3 | 1.56 | 0.42 |
| 45:DY:5:MET:HG2 | 45:DY:30:VAL:HG11 | 2.00 | 0.42 |
| 1:AA:1002:G:C6 | 1:AA:1003:G:N3 | 2.88 | 0.42 |
| 1:AA:1347:G:N2 | 1:AA:1373:G:H2' | 2.34 | 0.42 |
| 1:AA:530:G:O6 | 22:AV:21:C:H1' | 2.19 | 0.42 |
| 1:AA:539:A:H2' | 1:AA:540:G:H8 | 1.84 | 0.42 |
| 1:AA:59:A:H3' | 1:AA:331:G:H22 | 1.84 | 0.42 |
| 1:AA:78:G:C2 | 1:AA:91:C:N4 | 2.87 | 0.42 |
| 2:AB:12:GLU:HA | 2:AB:213:LEU:HD11 | 2.01 | 0.42 |
| 5:AE:103:GLY:O | 5:AE:106:PRO:HD2 | 2.19 | 0.42 |
| 6:AF:10:LEU:HD23 | 6:AF:61:LEU:HD23 | 2.02 | 0.42 |
| 9:AI:23:ASN:ND2 | 9:AI:25:LYS:HG2 | 2.34 | 0.42 |
| 13:AM:84:ILE:HG13 | 13:AM:85:GLY:CA | 2.44 | 0.42 |
| 25:AY:5:G:C2 | 25:AY:6:G:C4 | 3.07 | 0.42 |
| 25:AY:7:A:C6 | 25:AY:49:C:C4 | 3.07 | 0.42 |
| 26:BA:1177:A:H3' | 26:BA:1178:C:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BA:1252:G:OP1 | 41:BU:36:ARG:NH2 | 2.52 | 0.42 |
| 26:BA:1268:A:C2 | 26:BA:2013:A:C4 | 3.08 | 0.42 |
| 26:BA:529:A:H62 | 26:BA:2041:U:H3 | 1.67 | 0.42 |
| 26:BA:971:C:H2' | 26:BA:972:G:O4' | 2.19 | 0.42 |
| 27:BB:32:C:C2 | 27:BB:51:G:N2 | 2.86 | 0.42 |
| 31:BG:53:LEU:HD23 | 31:BG:53:LEU:HA | 1.84 | 0.42 |
| 1:CA:1122:U:H2' | 1:CA:1123:A:O4' | 2.19 | 0.42 |
| 3:CC:39:ILE:O | 3:CC:43:LEU:HG | 2.19 | 0.42 |
| 1:CA:1124:G:H5' | 10:CJ:36:GLY:H | 1.84 | 0.42 |
| 13:CM:47:ASP:O | 13:CM:48:LEU:HD23 | 2.18 | 0.42 |
| 18:CR:44:LEU:HD23 | 18:CR:50:ILE:HA | 2.02 | 0.42 |
| 23:CW:4:C:N4 | 23:CW:5:G:C6 | 2.87 | 0.42 |
| 24:CX:9:G:H21 | 24:CX:45:G:H3' | 1.84 | 0.42 |
| 26:DA:1021:A:H3' | 26:DA:1021:A:H8 | 1.84 | 0.42 |
| 26:DA:2386:C:H2' | 26:DA:2387:U:C6 | 2.54 | 0.42 |
| 26:DA:2705:A:H2' | 26:DA:2706:G:O4' | 2.20 | 0.42 |
| 26:DA:735:A:N7 | 26:DA:761:A:H2 | 2.17 | 0.42 |
| 27:DB:11:C:H3' | 27:DB:12:C:C6 | 2.55 | 0.42 |
| 29:DE:96:PHE:O | 29:DE:175:VAL:HG11 | 2.19 | 0.42 |
| 42:DV:5:VAL:CG1 | 42:DV:57:VAL:HG21 | 2.49 | 0.42 |
| 26:DA:1188:U:C4' | 42:DV:79:VAL:HG22 | 2.50 | 0.42 |
| 45:DY:7:VAL:HG21 | 45:DY:72:VAL:HG12 | 2.00 | 0.42 |
| 45:DY:83:THR:HG21 | 45:DY:99:CYS:HB2 | 2.01 | 0.42 |
| 46:DZ:100:VAL:HA | 46:DZ:101:PRO:HD3 | 1.91 | 0.42 |
| 46:DZ:28:MET:HA | 46:DZ:88:PHE:O | 2.18 | 0.42 |
| 1:AA:1004:A:N7 | 1:AA:1036:G:C2 | 2.87 | 0.42 |
| 1:AA:1241:G:H2' | 1:AA:1242:C:C6 | 2.55 | 0.42 |
| 1:AA:658:G:H2' | 1:AA:659:U:H6 | 1.85 | 0.42 |
| 4:AD:176:LEU:HD12 | 4:AD:182:LYS:O | 2.19 | 0.42 |
| 9:AI:127:LYS:O | 9:AI:128:ARG:HG2 | 2.19 | 0.42 |
| 11:AK:20:TYR:CZ | 11:AK:83:ILE:HD12 | 2.52 | 0.42 |
| 1:AA:1187:G:N3 | 14:AN:60:SER:OG | 2.53 | 0.42 |
| 17:AQ:76:LEU:HD12 | 17:AQ:77:VAL:H | 1.84 | 0.42 |
| 20:AT:13:LEU:O | 20:AT:17:ARG:HG3 | 2.19 | 0.42 |
| 49:B2:3:LEU:O | 49:B2:7:ARG:HG3 | 2.19 | 0.42 |
| 26:BA:2347:C:O2' | 53:B6:21:TYR:OH | 2.35 | 0.42 |
| 26:BA:1292:U:H2' | 26:BA:1293:C:C6 | 2.54 | 0.42 |
| 26:BA:171:G:O2' | 26:BA:172:C:H5' | 2.19 | 0.42 |
| 26:BA:2439:A:H5' | 26:BA:2439:A:H8 | 1.85 | 0.42 |
| 26:BA:2709:G:H2' | 26:BA:2710:C:C6 | 2.54 | 0.42 |
| 26:BA:489:G:N7 | 43:BW:49:LYS:NZ | 2.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BA:784:A:C8 | 26:BA:792:G:C5 | 3.07 | 0.42 |
| 26:BA:841:A:H2' | 26:BA:842:G:C8 | 2.54 | 0.42 |
| 26:BA:918:A:H5'' | 27:BB:98:G:O2' | 2.19 | 0.42 |
| 34:BN:20:GLY:HA2 | 34:BN:61:ARG:HD2 | 2.01 | 0.42 |
| 29:BE:18:ASP:HB3 | 40:BT:82:LEU:HD21 | 2.01 | 0.42 |
| 1:CA:1009:G:C4 | 1:CA:1021:G:C2 | 3.08 | 0.42 |
| 1:CA:1320:C:H5' | 1:CA:1320:C:H6 | 1.85 | 0.42 |
| 1:CA:156:G:H1 | 1:CA:165:C:H42 | 1.67 | 0.42 |
| 1:CA:933:G:C6 | 1:CA:1385:G:C6 | 3.07 | 0.42 |
| 1:CA:985:C:C2 | 1:CA:1220:G:N2 | 2.80 | 0.42 |
| 2:CB:51:LEU:HA | 2:CB:54:THR:HB | 2.01 | 0.42 |
| 3:CC:134:ILE:HG22 | 3:CC:168:ALA:HB3 | 2.01 | 0.42 |
| 5:CE:57:LYS:HG2 | 5:CE:61:TYR:HE2 | 1.84 | 0.42 |
| 7:CG:114:ARG:HB2 | 7:CG:115:ARG:NH2 | 2.35 | 0.42 |
| 7:CG:155:ARG:CZ | 7:CG:155:ARG:HB3 | 2.48 | 0.42 |
| 24:CX:21:A:H61 | 24:CX:46:G:H2' | 1.84 | 0.42 |
| 26:DA:2203:U:H2' | 26:DA:2205:C:C6 | 2.54 | 0.42 |
| 26:DA:2510:C:C4 | 26:DA:2511:U:C4 | 3.07 | 0.42 |
| 27:DB:117:G:C2 | 27:DB:118:G:C5 | 3.07 | 0.42 |
| 31:DG:43:LEU:HD11 | 31:DG:153:ARG:HG2 | 2.01 | 0.42 |
| 32:DH:89:ILE:O | 32:DH:129:THR:HG23 | 2.18 | 0.42 |
| 34:DN:123:TYR:CZ | 34:DN:129:PRO:HD2 | 2.54 | 0.42 |
| 37:DQ:73:PRO:HA | 37:DQ:93:TYR:CD1 | 2.54 | 0.42 |
| 1:AA:1029:C:N4 | 1:AA:1030(A):G:C2 | 2.88 | 0.42 |
| 1:AA:1004:A:C5 | 1:AA:1037:C:N3 | 2.87 | 0.42 |
| 1:AA:580:U:H5'' | 15:AO:58:MET:HG2 | 2.01 | 0.42 |
| 1:AA:79:G:C2 | 1:AA:90:U:C2 | 3.07 | 0.42 |
| 2:AB:18:GLY:O | 2:AB:19:HIS:HB3 | 2.19 | 0.42 |
| 3:AC:136:GLN:O | 3:AC:140:ARG:HG3 | 2.18 | 0.42 |
| 9:AI:4:TYR:CE1 | 9:AI:88:TYR:HA | 2.55 | 0.42 |
| 51:B4:28:LYS:HA | 51:B4:29:PRO:HD3 | 1.84 | 0.42 |
| 53:B6:50:ARG:HB2 | 53:B6:50:ARG:HE | 1.67 | 0.42 |
| 26:BA:1721:G:H3' | 26:BA:1722:A:H5'' | 2.01 | 0.42 |
| 26:BA:2029:G:H2' | 26:BA:2031:A:OP1 | 2.19 | 0.42 |
| 26:BA:2233:U:H2' | 26:BA:2234:G:C8 | 2.55 | 0.42 |
| 26:BA:2396:G:OP1 | 48:B1:25:LYS:NZ | 2.30 | 0.42 |
| 31:BG:28:VAL:HG23 | 31:BG:29:TRP:CD1 | 2.54 | 0.42 |
| 32:BH:170:ARG:O | 32:BH:171:LEU:HD23 | 2.19 | 0.42 |
| 35:BO:113:LYS:O | 35:BO:116:SER:OG | 2.34 | 0.42 |
| 36:BP:112:LEU:HA | 36:BP:112:LEU:HD23 | 1.85 | 0.42 |
| 1:CA:1067:A:N3 | 1:CA:1068:G:H1' | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1388:C:H2' | 1:CA:1389:C:C6 | 2.54 | 0.42 |
| 1:CA:1422:G:H5' | 35:DO:48:PRO:HB3 | 2.01 | 0.42 |
| 1:CA:357:G:O2' | 1:CA:358:U:H5' | 2.18 | 0.42 |
| 1:CA:560:U:OP2 | 61:CA:3313:HOH:O | 2.21 | 0.42 |
| 1:CA:911:U:O2' | 1:CA:912:C:H5' | 2.20 | 0.42 |
| 3:CC:69:HIS:HB3 | 3:CC:106:VAL:CG2 | 2.50 | 0.42 |
| 4:CD:150:GLU:HG3 | 4:CD:150:GLU:H | 1.68 | 0.42 |
| 12:CL:62:SER:HB2 | 12:CL:64:TYR:HD1 | 1.85 | 0.42 |
| 15:CO:18:PHE:CE2 | 15:CO:21:ASP:HB2 | 2.55 | 0.42 |
| 17:CQ:62:SER:CB | 17:CQ:72:ARG:HD3 | 2.49 | 0.42 |
| 20:CT:93:GLU:C | 20:CT:95:ALA:H | 2.23 | 0.42 |
| 48:D1:89:GLU:O | 48:D1:93:GLU:HG2 | 2.19 | 0.42 |
| 50:D3:6:VAL:HG13 | 50:D3:56:VAL:HG22 | 2.02 | 0.42 |
| 26:DA:1127:A:C2' | 26:DA:1128:A:H5'' | 2.50 | 0.42 |
| 26:DA:117:G:C6 | 26:DA:119:A:C6 | 3.07 | 0.42 |
| 26:DA:1317:A:H2' | 26:DA:1318:C:C6 | 2.55 | 0.42 |
| 26:DA:2130:U:H3 | 26:DA:2159:G:N2 | 2.17 | 0.42 |
| 26:DA:829:A:N7 | 26:DA:2248:C:H5' | 2.34 | 0.42 |
| 26:DA:954:G:O2' | 26:DA:2274:A:N1 | 2.45 | 0.42 |
| 26:DA:2408:U:H2' | 26:DA:2409:G:C8 | 2.55 | 0.42 |
| 26:DA:64:A:O3' | 44:DX:71:GLY:HA3 | 2.19 | 0.42 |
| 26:DA:764:A:H5' | 28:DD:210:GLY:CA | 2.49 | 0.42 |
| 27:DB:62:C:H2' | 27:DB:63:G:C8 | 2.55 | 0.42 |
| 27:DB:91:C:OP1 | 37:DQ:16:ARG:HG3 | 2.19 | 0.42 |
| 31:DG:53:LEU:HD23 | 31:DG:53:LEU:HA | 1.88 | 0.42 |
| 41:DU:92:ARG:H | 41:DU:92:ARG:HG2 | 1.44 | 0.42 |
| 26:DA:1341:U:O4 | 44:DX:16:LYS:HE2 | 2.19 | 0.42 |
| 1:AA:162:A:N7 | 1:AA:163:C:H1' | 2.35 | 0.42 |
| 1:AA:299:G:H2' | 1:AA:300:A:C8 | 2.55 | 0.42 |
| 1:AA:765:G:N1 | 1:AA:812:C:O2' | 2.42 | 0.42 |
| 7:AG:120:ILE:O | 7:AG:124:LEU:HB2 | 2.20 | 0.42 |
| 9:AI:20:ARG:O | 9:AI:60:ASP:N | 2.30 | 0.42 |
| 15:AO:85:LEU:HD23 | 15:AO:85:LEU:HA | 1.75 | 0.42 |
| 26:BA:2093:G:C6 | 26:BA:2225:A:C8 | 3.08 | 0.42 |
| 26:BA:2529:G:H5'' | 26:BA:2530:A:H5'' | 2.01 | 0.42 |
| 26:BA:652(C):G:H1 | 26:BA:652(V):C:N4 | 2.18 | 0.42 |
| 26:BA:775:G:C4 | 26:BA:794:G:C8 | 3.07 | 0.42 |
| 26:BA:881:G:N1 | 26:BA:897:C:N4 | 2.67 | 0.42 |
| 29:BE:12:THR:HG22 | 29:BE:13:ARG:H | 1.85 | 0.42 |
| 32:BH:98:LEU:HA | 32:BH:98:LEU:HD12 | 1.91 | 0.42 |
| 33:BI:73:GLU:HG3 | 33:BI:139:GLN:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1118:C:C2 | 1:CA:1119:C:C5 | 3.06 | 0.42 |
| 1:CA:336:C:H2' | 1:CA:337:C:C6 | 2.55 | 0.42 |
| 2:CB:107:THR:O | 2:CB:110:GLN:HB3 | 2.19 | 0.42 |
| 2:CB:82:ARG:HG3 | 2:CB:92:TYR:OH | 2.18 | 0.42 |
| 3:CC:52:LEU:HD23 | 3:CC:55:VAL:HG23 | 2.01 | 0.42 |
| 1:CA:921:U:O2 | 5:CE:19:MET:HB2 | 2.19 | 0.42 |
| 9:CI:28:VAL:HA | 9:CI:63:ILE:O | 2.20 | 0.42 |
| 11:CK:59:TYR:O | 11:CK:63:LEU:HG | 2.20 | 0.42 |
| 20:CT:56:MET:HE2 | 20:CT:88:VAL:HG21 | 2.00 | 0.42 |
| 53:D6:13:CYS:SG | 53:D6:47:THR:HG21 | 2.60 | 0.42 |
| 53:D6:18:ARG:HD2 | 53:D6:42:TRP:CG | 2.55 | 0.42 |
| 26:DA:2006:C:O5' | 26:DA:2006:C:H6 | 2.02 | 0.42 |
| 26:DA:2320:A:N3 | 26:DA:2320:A:H2' | 2.33 | 0.42 |
| 26:DA:925:C:H2' | 26:DA:926:A:H8 | 1.85 | 0.42 |
| 26:DA:935:C:C2' | 26:DA:936:C:H5' | 2.50 | 0.42 |
| 27:DB:55:U:H1' | 31:DG:29:TRP:HD1 | 1.81 | 0.42 |
| 28:DD:245:PRO:HA | 28:DD:246:PRO:HD3 | 1.91 | 0.42 |
| 26:DA:2228:G:OP1 | 28:DD:261:LYS:HE3 | 2.19 | 0.42 |
| 31:DG:121:ASN:HA | 31:DG:181:ARG:HH21 | 1.84 | 0.42 |
| 27:DB:31:C:H4' | 31:DG:29:TRP:CZ2 | 2.54 | 0.42 |
| 27:DB:57:A:N3 | 31:DG:29:TRP:HB3 | 2.33 | 0.42 |
| 32:DH:84:SER:HB3 | 32:DH:132:ARG:HH11 | 1.85 | 0.42 |
| 1:AA:171:A:H2' | 1:AA:172:A:C8 | 2.54 | 0.42 |
| 1:AA:396:G:O2' | 1:AA:398:C:OP1 | 2.23 | 0.42 |
| 2:AB:111:ARG:HG2 | 2:AB:111:ARG:HH11 | 1.84 | 0.42 |
| 8:AH:13:ILE:O | 8:AH:17:THR:HG23 | 2.20 | 0.42 |
| 20:AT:13:LEU:HD12 | 20:AT:14:LYS:N | 2.35 | 0.42 |
| 25:AY:18:G:N2 | 25:AY:58:A:C8 | 2.88 | 0.42 |
| 26:BA:1359:A:H2' | 26:BA:1360:A:H5' | 2.02 | 0.42 |
| 26:BA:1939:U:OP1 | 26:BA:2604:U:O2' | 2.33 | 0.42 |
| 26:BA:2139:C:H2' | 26:BA:2140:C:H4' | 2.01 | 0.42 |
| 26:BA:2706:G:N7 | 61:BA:4712:HOH:O | 2.37 | 0.42 |
| 26:BA:601:C:O2' | 26:BA:605:C:H5" | 2.19 | 0.42 |
| 36:BP:63:PRO:HD3 | 55:B8:27:THR:HG22 | 2.00 | 0.42 |
| 39:BS:58:LEU:HD23 | 39:BS:58:LEU:HA | 1.71 | 0.42 |
| 34:BN:4:TYR:CE2 | 41:BU:100:VAL:HG11 | 2.55 | 0.42 |
| 46:BZ:108:PRO:CB | 46:BZ:117:LEU:HD13 | 2.46 | 0.42 |
| 1:CA:1002:G:N2 | 1:CA:1038:C:N3 | 2.55 | 0.42 |
| 1:CA:1065:U:H1' | 1:CA:1066:C:OP2 | 2.20 | 0.42 |
| 1:CA:1126:U:H4' | 1:CA:1281:U:H1' | 2.01 | 0.42 |
| 1:CA:1357:A:N7 | 1:CA:1358:U:C4 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1368:G:H2' | 1:CA:1369:C:H5' | 2.01 | 0.42 |
| 1:CA:695:A:H2' | 1:CA:696:A:C8 | 2.55 | 0.42 |
| 5:CE:98:THR:HB | 5:CE:117:ASP:HB3 | 2.01 | 0.42 |
| 8:CH:51:VAL:HG12 | 8:CH:52:ASP:H | 1.84 | 0.42 |
| 1:CA:1279:A:OP2 | 10:CJ:9:ARG:NH1 | 2.53 | 0.42 |
| 1:CA:779:C:O2' | 11:CK:120:ARG:HD3 | 2.20 | 0.42 |
| 19:CS:52:TYR:HB2 | 19:CS:57:HIS:CE1 | 2.55 | 0.42 |
| 26:DA:1019:U:H3 | 26:DA:1142(A):A:N6 | 2.06 | 0.42 |
| 26:DA:108:U:H2' | 26:DA:109:G:H8 | 1.83 | 0.42 |
| 26:DA:1248:G:C5 | 41:DU:3:ARG:HB2 | 2.55 | 0.42 |
| 26:DA:1449:A:OP2 | 26:DA:1449:A:H8 | 2.02 | 0.42 |
| 26:DA:2055:C:H1' | 29:DE:145:LYS:HE2 | 2.01 | 0.42 |
| 26:DA:2187:G:C6 | 26:DA:2188:C:N3 | 2.87 | 0.42 |
| 26:DA:2262:U:H4' | 26:DA:2328:A:C2 | 2.54 | 0.42 |
| 31:DG:43:LEU:C | 31:DG:45:GLU:H | 2.21 | 0.42 |
| 33:DI:77:LEU:HG | 33:DI:101:LEU:HD12 | 2.02 | 0.42 |
| 34:DN:128:HIS:HA | 34:DN:129:PRO:HD3 | 1.81 | 0.42 |
| 26:DA:296:C:O3' | 45:DY:95:LYS:NZ | 2.52 | 0.42 |
| 46:DZ:121:HIS:HB3 | 46:DZ:123:ASP:O | 2.20 | 0.42 |
| 46:DZ:71:VAL:HG13 | 46:DZ:88:PHE:CD1 | 2.54 | 0.42 |
| 1:AA:1304:G:C6 | 1:AA:1305:G:N1 | 2.88 | 0.42 |
| 1:AA:1493:A:H5'' | 1:AA:1494:G:OP2 | 2.20 | 0.42 |
| 1:AA:457:C:H2' | 1:AA:458:C:C6 | 2.54 | 0.42 |
| 1:AA:636:U:H2' | 1:AA:637:G:H8 | 1.84 | 0.42 |
| 4:AD:36:ARG:HB3 | 4:AD:38:TYR:CZ | 2.55 | 0.42 |
| 8:AH:73:ASP:OD1 | 8:AH:75:ARG:NH1 | 2.49 | 0.42 |
| 10:AJ:8:LEU:CD2 | 10:AJ:96:ILE:HG23 | 2.50 | 0.42 |
| 16:AP:18:ARG:NH1 | 16:AP:32:TYR:OH | 2.52 | 0.42 |
| 51:B4:49:PHE:HA | 51:B4:49:PHE:HD1 | 1.72 | 0.42 |
| 53:B6:8:LYS:HD3 | 55:B8:34:TRP:CD2 | 2.55 | 0.42 |
| 26:BA:1044:G:HO2' | 26:BA:1111:A:N6 | 2.17 | 0.42 |
| 26:BA:1300:U:H4' | 26:BA:1301:A:H5'' | 2.01 | 0.42 |
| 26:BA:1470:G:H5'' | 26:BA:1471:A:OP1 | 2.20 | 0.42 |
| 26:BA:1651:G:OP1 | 38:BR:40:LYS:HE3 | 2.20 | 0.42 |
| 26:BA:1652:A:C2' | 26:BA:1653:G:H5' | 2.49 | 0.42 |
| 26:BA:2218:U:O4' | 48:B1:52:ARG:NH2 | 2.53 | 0.42 |
| 26:BA:2328:A:H2' | 26:BA:2329:G:H8 | 1.80 | 0.42 |
| 26:BA:895:U:H5' | 26:BA:896:A:OP1 | 2.20 | 0.42 |
| 26:BA:957:A:H5' | 37:BQ:76:LYS:HG2 | 2.02 | 0.42 |
| 31:BG:79:ASN:OD1 | 31:BG:79:ASN:N | 2.52 | 0.42 |
| 26:BA:2319:G:C2 | 39:BS:3:ARG:HA | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:BV:55:ALA:HB2 | 42:BV:101:GLY:HA2 | 2.02 | 0.42 |
| 46:BZ:19:ARG:HD3 | 46:BZ:25:PRO:CD | 2.50 | 0.42 |
| 1:CA:1268:A:H2 | 1:CA:1326:C:O2 | 2.02 | 0.42 |
| 1:CA:1362:C:H2' | 1:CA:1363:C:H5'' | 2.00 | 0.42 |
| 2:CB:70:PHE:HE1 | 2:CB:163:PHE:CD2 | 2.36 | 0.42 |
| 2:CB:95:GLN:HB2 | 2:CB:148:TYR:CD1 | 2.44 | 0.42 |
| 5:CE:79:GLU:HG2 | 5:CE:79:GLU:O | 2.18 | 0.42 |
| 7:CG:51:GLN:O | 7:CG:55:GLY:HA2 | 2.20 | 0.42 |
| 10:CJ:32:ALA:HB1 | 10:CJ:33:GLN:HA | 2.01 | 0.42 |
| 18:CR:73:ALA:CB | 18:CR:79:LEU:HG | 2.49 | 0.42 |
| 24:CX:21:A:H3' | 24:CX:46:G:O6 | 2.19 | 0.42 |
| 26:DA:1262:A:H2 | 52:D5:10:LYS:HD2 | 1.84 | 0.42 |
| 26:DA:11:G:H2' | 26:DA:12:U:H5'' | 2.02 | 0.42 |
| 26:DA:1242:A:N1 | 36:DP:4:SER:OG | 2.41 | 0.42 |
| 26:DA:1266:G:O5' | 43:DW:15:ARG:NH2 | 2.52 | 0.42 |
| 26:DA:1445(A):C:H2' | 26:DA:1446:C:H6 | 1.83 | 0.42 |
| 26:DA:271(K):U:H4' | 26:DA:271(L):U:OP1 | 2.20 | 0.42 |
| 26:DA:479:A:H4' | 26:DA:480:A:OP1 | 2.19 | 0.42 |
| 26:DA:740:U:H2' | 26:DA:741:G:H8 | 1.81 | 0.42 |
| 26:DA:807:U:OP2 | 36:DP:41:ARG:NH2 | 2.53 | 0.42 |
| 26:DA:820:A:N3 | 26:DA:943:U:H4' | 2.35 | 0.42 |
| 28:DD:29:PRO:HA | 28:DD:83:GLU:OE1 | 2.19 | 0.42 |
| 30:DF:117:ARG:HH12 | 36:DP:1:MET:N | 2.18 | 0.42 |
| 37:DQ:141:GLN:NE2 | 46:DZ:74:VAL:O | 2.39 | 0.42 |
| 1:AA:1262:C:H2' | 1:AA:1263:C:C6 | 2.55 | 0.42 |
| 1:AA:1267:C:H6 | 1:AA:1267:C:O5' | 2.02 | 0.42 |
| 1:AA:377:G:OP1 | 16:AP:3:LYS:HD3 | 2.20 | 0.42 |
| 1:AA:393:A:OP1 | 61:AA:4195:HOH:O | 2.21 | 0.42 |
| 1:AA:627:G:O2' | 1:AA:628:G:H5' | 2.20 | 0.42 |
| 2:AB:71:VAL:CG1 | 2:AB:170:GLU:HG2 | 2.49 | 0.42 |
| 5:AE:116:THR:HG23 | 5:AE:117:ASP:OD2 | 2.19 | 0.42 |
| 25:AY:24:G:C6 | 25:AY:25:C:C4 | 3.08 | 0.42 |
| 25:AY:53:G:N1 | 25:AY:61:C:N4 | 2.38 | 0.42 |
| 26:BA:171:G:C2' | 26:BA:172:C:H5' | 2.49 | 0.42 |
| 26:BA:185:U:H4' | 26:BA:218:A:H4' | 2.02 | 0.42 |
| 26:BA:2260:C:H2' | 26:BA:2261:C:C6 | 2.55 | 0.42 |
| 26:BA:2810:A:N6 | 26:BA:2891:G:O2' | 2.39 | 0.42 |
| 29:BE:141:ILE:HA | 29:BE:154:LYS:HE2 | 2.02 | 0.42 |
| 32:BH:56:SER:HB3 | 32:BH:61:HIS:ND1 | 2.35 | 0.42 |
| 34:BN:4:TYR:CD2 | 41:BU:100:VAL:HG11 | 2.54 | 0.42 |
| 37:BQ:37:LEU:HD21 | 37:BQ:130:LYS:HD3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BZ:24:LEU:HD21 | 46:BZ:86:VAL:HG13 | 2.01 | 0.42 |
| 1:CA:1048:G:OP1 | 14:CN:3:ARG:HD2 | 2.19 | 0.42 |
| 1:CA:1118:C:N1 | 1:CA:1119:C:H5 | 2.18 | 0.42 |
| 1:CA:255:G:C6 | 1:CA:256:U:C4 | 3.08 | 0.42 |
| 1:CA:456:C:H2' | 1:CA:457:C:H5' | 2.00 | 0.42 |
| 1:CA:586:C:O2' | 1:CA:878:G:H4' | 2.19 | 0.42 |
| 5:CE:80:ILE:HA | 5:CE:80:ILE:HD12 | 1.87 | 0.42 |
| 6:CF:2:ARG:HG3 | 6:CF:69:GLU:HG3 | 2.02 | 0.42 |
| 13:CM:3:ARG:HG2 | 13:CM:8:GLU:HA | 2.01 | 0.42 |
| 17:CQ:76:LEU:HD12 | 17:CQ:77:VAL:H | 1.84 | 0.42 |
| 6:CF:100:ASN:ND2 | 18:CR:23:LYS:HE3 | 2.34 | 0.42 |
| 25:CY:19:G:N3 | 25:CY:57:G:N1 | 2.68 | 0.42 |
| 25:CY:37:MIA:H2' | 25:CY:38:A:O4' | 2.20 | 0.42 |
| 25:CY:76:A:N6 | 26:DA:2422:A:H5' | 2.35 | 0.42 |
| 53:D6:35:GLU:HA | 53:D6:49:HIS:O | 2.20 | 0.42 |
| 26:DA:1237:A:OP1 | 61:DA:4484:HOH:O | 2.21 | 0.42 |
| 26:DA:1371:G:H2' | 26:DA:1372:U:C5 | 2.51 | 0.42 |
| 26:DA:1748:G:H2' | 26:DA:1749:A:O4' | 2.20 | 0.42 |
| 26:DA:211:A:H2' | 26:DA:212:G:O4' | 2.20 | 0.42 |
| 26:DA:2150:U:H2' | 26:DA:2151:G:C8 | 2.55 | 0.42 |
| 26:DA:2140:C:C2 | 26:DA:2152:G:C2 | 3.07 | 0.42 |
| 26:DA:644:A:C2 | 26:DA:2369:A:H1' | 2.55 | 0.42 |
| 26:DA:708:C:N4 | 26:DA:723:G:H1 | 2.18 | 0.42 |
| 26:DA:848:G:C4 | 26:DA:933:A:C8 | 3.06 | 0.42 |
| 27:DB:40:U:N3 | 27:DB:44:G:OP2 | 2.48 | 0.42 |
| 28:DD:68:LYS:O | 28:DD:69:ARG:HB2 | 2.20 | 0.42 |
| 30:DF:196:LEU:HA | 30:DF:196:LEU:HD23 | 1.86 | 0.42 |
| 35:DO:73:ASP:OD2 | 40:DT:32:TYR:OH | 2.35 | 0.42 |
| 41:DU:90:VAL:HG12 | 41:DU:95:LEU:HD12 | 2.02 | 0.42 |
| 46:DZ:97:GLU:HB2 | 46:DZ:125:LEU:HD11 | 2.02 | 0.42 |
| 1:AA:1210:C:C2' | 1:AA:1211:U:H5' | 2.50 | 0.42 |
| 1:AA:342:C:C2 | 1:AA:348:G:N2 | 2.88 | 0.42 |
| 1:AA:56:U:H2' | 1:AA:57:G:H8 | 1.79 | 0.42 |
| 1:AA:674:G:H2' | 1:AA:675:A:C8 | 2.53 | 0.42 |
| 1:AA:729:A:H2' | 1:AA:730:G:H8 | 1.84 | 0.42 |
| 1:AA:820:U:H4' | 1:AA:821:G:OP2 | 2.20 | 0.42 |
| 1:AA:16:A:O2' | 5:AE:16:THR:HB | 2.20 | 0.42 |
| 8:AH:49:GLU:HG2 | 8:AH:62:TYR:HE1 | 1.84 | 0.42 |
| 12:AL:34:ARG:HG3 | 12:AL:105:TYR:CE2 | 2.55 | 0.42 |
| 1:AA:584:G:H5' | 17:AQ:91:ARG:NH2 | 2.35 | 0.42 |
| 18:AR:25:THR:OG1 | 18:AR:25:THR:O | 2.32 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BA:1881:C:H2' | 26:BA:1882:C:C6 | 2.55 | 0.42 |
| 26:BA:2097:C:H2' | 26:BA:2098:U:O4' | 2.19 | 0.42 |
| 28:BD:242:ARG:HD3 | 28:BD:242:ARG:N | 2.34 | 0.42 |
| 29:BE:14:ILE:HD11 | 29:BE:173:VAL:HG11 | 2.01 | 0.42 |
| 31:BG:18:GLU:OE1 | 31:BG:22:ARG:HD3 | 2.20 | 0.42 |
| 32:BH:54:ARG:HD3 | 32:BH:65:HIS:ND1 | 2.35 | 0.42 |
| 32:BH:98:LEU:HD13 | 32:BH:125:VAL:HG23 | 2.00 | 0.42 |
| 35:BO:4:PRO:O | 35:BO:5:GLN:HB2 | 2.20 | 0.42 |
| 42:BV:5:VAL:HG21 | 42:BV:35:LEU:HD23 | 2.02 | 0.42 |
| 1:CA:1011:G:H21 | 1:CA:1019:C:H1' | 1.84 | 0.42 |
| 1:CA:1162:C:H2' | 1:CA:1163:C:O4' | 2.20 | 0.42 |
| 1:CA:1203:C:H2' | 1:CA:1204:A:O4' | 2.20 | 0.42 |
| 1:CA:1323:G:O2' | 1:CA:1362:C:O2' | 2.23 | 0.42 |
| 1:CA:452:A:O2' | 1:CA:453:A:OP2 | 2.34 | 0.42 |
| 2:CB:57:PHE:CE2 | 2:CB:185:ILE:HD12 | 2.50 | 0.42 |
| 2:CB:193:ASP:HA | 2:CB:194:PRO:HD2 | 1.89 | 0.42 |
| 9:CI:20:ARG:HA | 9:CI:21:PRO:HD3 | 1.92 | 0.42 |
| 11:CK:27:ASN:OD1 | 11:CK:28:THR:N | 2.46 | 0.42 |
| 14:CN:26:ARG:HD2 | 14:CN:43:CYS:HB3 | 2.01 | 0.42 |
| 14:CN:24:CYS:HA | 14:CN:38:GLY:O | 2.20 | 0.42 |
| 17:CQ:6:LEU:O | 17:CQ:58:GLU:HA | 2.20 | 0.42 |
| 17:CQ:78:GLU:OE1 | 17:CQ:81:ARG:HD3 | 2.19 | 0.42 |
| 48:D1:72:GLU:OE1 | 48:D1:76:ARG:NH2 | 2.53 | 0.42 |
| 26:DA:1221(A):C:C2 | 26:DA:1229:G:C2 | 3.08 | 0.42 |
| 26:DA:1927:A:OP1 | 26:DA:1927:A:H8 | 2.03 | 0.42 |
| 26:DA:2110:G:H4' | 26:DA:2111:C:OP2 | 2.20 | 0.42 |
| 26:DA:271(D):G:C6 | 26:DA:271(E):U:C4 | 3.08 | 0.42 |
| 26:DA:30:G:H2' | 26:DA:31:C:O4' | 2.19 | 0.42 |
| 26:DA:847:U:OP2 | 61:DA:4017:HOH:O | 2.22 | 0.42 |
| 31:DG:49:ASP:N | 31:DG:49:ASP:OD1 | 2.53 | 0.42 |
| 31:DG:72:ARG:HA | 31:DG:86:MET:O | 2.20 | 0.42 |
| 38:DR:65:LEU:HA | 38:DR:65:LEU:HD12 | 1.87 | 0.42 |
| 42:DV:21:ARG:HG2 | 42:DV:91:TYR:CE2 | 2.55 | 0.42 |
| 1:AA:1362:C:C2' | 1:AA:1363:C:H5'' | 2.49 | 0.41 |
| 1:AA:571:U:H5'' | 1:AA:819:A:C5 | 2.55 | 0.41 |
| 1:AA:841:U:C5 | 1:AA:848:C:H1' | 2.54 | 0.41 |
| 14:AN:23:ARG:NH1 | 14:AN:30:ALA:HB2 | 2.34 | 0.41 |
| 15:AO:53:HIS:O | 15:AO:56:LEU:HB3 | 2.20 | 0.41 |
| 21:AU:15:ARG:HH11 | 21:AU:15:ARG:HB2 | 1.85 | 0.41 |
| 25:AY:5:G:H2' | 25:AY:6:G:H8 | 1.85 | 0.41 |
| 26:BA:2405:G:O2' | 26:BA:2406:U:OP1 | 2.29 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:BA:26:G:H1' | 26:BA:515:A:H61 | 1.85 | 0.41 |
| 26:BA:288:C:H2' | 26:BA:289:A:C8 | 2.49 | 0.41 |
| 27:BB:40:U:H1' | 27:BB:45:A:H61 | 1.84 | 0.41 |
| 28:BD:61:LEU:O | 28:BD:63:ARG:NH1 | 2.53 | 0.41 |
| 46:BZ:104:PHE:CZ | 46:BZ:119:GLU:HG2 | 2.55 | 0.41 |
| 46:BZ:5:LEU:O | 46:BZ:59:LEU:HA | 2.20 | 0.41 |
| 1:CA:1072:G:H2' | 1:CA:1073:U:C6 | 2.55 | 0.41 |
| 1:CA:337:C:H2' | 1:CA:338:A:C8 | 2.54 | 0.41 |
| 1:CA:583:A:N6 | 1:CA:758:G:O2' | 2.53 | 0.41 |
| 1:CA:804:U:OP1 | 61:CA:3206:HOH:O | 2.21 | 0.41 |
| 1:CA:981:U:O5' | 1:CA:981:U:H6 | 2.03 | 0.41 |
| 10:CJ:16:LEU:O | 10:CJ:20:ALA:N | 2.34 | 0.41 |
| 47:D0:52:GLY:O | 47:D0:59:LEU:HA | 2.20 | 0.41 |
| 26:DA:2100:G:C6 | 26:DA:2190:G:C6 | 3.08 | 0.41 |
| 26:DA:2147:G:C4 | 26:DA:2148:G:H1' | 2.55 | 0.41 |
| 26:DA:2135:A:OP1 | 26:DA:2160:G:H1' | 2.20 | 0.41 |
| 26:DA:2093:G:C6 | 26:DA:2225:A:C8 | 3.08 | 0.41 |
| 26:DA:2370:G:C6 | 26:DA:2371:G:C6 | 3.07 | 0.41 |
| 26:DA:2483:C:O2 | 37:DQ:124:LYS:NZ | 2.52 | 0.41 |
| 26:DA:2833:G:H4' | 26:DA:2834:G:OP2 | 2.20 | 0.41 |
| 26:DA:460:A:C2 | 26:DA:470:A:C4 | 3.08 | 0.41 |
| 26:DA:812:C:H2' | 26:DA:813:U:H6 | 1.85 | 0.41 |
| 27:DB:19:G:H1 | 27:DB:64:C:H42 | 1.67 | 0.41 |
| 27:DB:80:U:H2' | 27:DB:81:G:H8 | 1.85 | 0.41 |
| 28:DD:276:LYS:H | 28:DD:276:LYS:CD | 2.15 | 0.41 |
| 29:DE:146:THR:HA | 29:DE:147:PRO:HA | 1.90 | 0.41 |
| 31:DG:137:GLU:HB3 | 31:DG:139:LEU:HG | 2.02 | 0.41 |
| 31:DG:33:ARG:O | 31:DG:34:LEU:HD23 | 2.19 | 0.41 |
| 45:DY:2:ARG:NH1 | 45:DY:4:LYS:HA | 2.35 | 0.41 |
| 45:DY:38:ILE:HD11 | 45:DY:66:PRO:HG3 | 2.01 | 0.41 |
| 45:DY:9:LYS:HA | 45:DY:10:GLY:HA2 | 1.49 | 0.41 |
| 1:AA:690:G:C6 | 1:AA:691:G:C6 | 3.08 | 0.41 |
| 1:AA:78:G:O2' | 1:AA:79:G:H8 | 2.03 | 0.41 |
| 13:AM:5:ALA:HA | 13:AM:61:GLU:OE2 | 2.18 | 0.41 |
| 1:AA:454:C:OP1 | 16:AP:75:ARG:NH2 | 2.53 | 0.41 |
| 17:AQ:87:LYS:HA | 17:AQ:87:LYS:HD3 | 1.73 | 0.41 |
| 19:AS:12:ASP:OD1 | 19:AS:35:SER:HB3 | 2.19 | 0.41 |
| 19:AS:65:ASN:N | 19:AS:65:ASN:ND2 | 2.66 | 0.41 |
| 19:AS:69:HIS:HD2 | 19:AS:73:GLU:OE1 | 2.03 | 0.41 |
| 25:AY:20:U:C4' | 25:AY:21:A:H5' | 2.50 | 0.41 |
| 25:AY:21:A:H8 | 25:AY:21:A:OP2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:B4:46:GLN:N | 51:B4:46:GLN:HE21 | 2.18 | 0.41 |
| 26:BA:1038:C:H42 | 26:BA:1117:G:H1 | 1.68 | 0.41 |
| 26:BA:1515:G:H2' | 26:BA:1516:C:C6 | 2.55 | 0.41 |
| 26:BA:1903:G:OP1 | 28:BD:241:PRO:HB2 | 2.20 | 0.41 |
| 26:BA:2150:U:H2' | 26:BA:2150:U:O2 | 2.19 | 0.41 |
| 26:BA:2135:A:N6 | 26:BA:2156:G:O2' | 2.53 | 0.41 |
| 26:BA:2418:A:H2' | 26:BA:2419:U:C6 | 2.54 | 0.41 |
| 26:BA:7:G:H2' | 26:BA:8:A:O4' | 2.20 | 0.41 |
| 26:BA:2784:C:H1' | 29:BE:37:ARG:NH1 | 2.36 | 0.41 |
| 30:BF:140:LEU:HA | 30:BF:140:LEU:HD13 | 1.86 | 0.41 |
| 32:BH:54:ARG:HA | 32:BH:55:PRO:HD3 | 1.87 | 0.41 |
| 40:BT:27:THR:HB | 40:BT:90:GLN:HB3 | 2.01 | 0.41 |
| 1:CA:1030(A):G:H2' | 1:CA:1030(B):C:H5'' | 2.02 | 0.41 |
| 1:CA:1133:G:N2 | 1:CA:1141:C:N3 | 2.61 | 0.41 |
| 1:CA:1274:G:N2 | 1:CA:1275:A:H62 | 2.17 | 0.41 |
| 1:CA:1279:A:H5'' | 1:CA:1280:A:OP1 | 2.20 | 0.41 |
| 1:CA:266:G:H8 | 1:CA:266:G:H2' | 1.68 | 0.41 |
| 1:CA:60:A:H4' | 1:CA:61:G:O5' | 2.21 | 0.41 |
| 2:CB:16:HIS:HD2 | 2:CB:204:ASN:H | 1.67 | 0.41 |
| 13:CM:72:ALA:O | 13:CM:76:ALA:N | 2.48 | 0.41 |
| 20:CT:64:ASP:OD2 | 20:CT:81:LYS:NZ | 2.44 | 0.41 |
| 24:CX:30:G:C6 | 24:CX:31:G:N7 | 2.89 | 0.41 |
| 25:CY:56:C:H2' | 25:CY:57:G:O4' | 2.20 | 0.41 |
| 49:D2:23:LYS:O | 49:D2:27:GLU:HG3 | 2.20 | 0.41 |
| 26:DA:2297:C:N3 | 26:DA:2321:G:N2 | 2.66 | 0.41 |
| 26:DA:2875:C:H2' | 26:DA:2876:G:O4' | 2.20 | 0.41 |
| 26:DA:373:U:H2' | 26:DA:374:A:C8 | 2.55 | 0.41 |
| 26:DA:382:G:OP2 | 61:DA:4359:HOH:O | 2.22 | 0.41 |
| 26:DA:732:C:H2' | 26:DA:733:G:O4' | 2.20 | 0.41 |
| 26:DA:878:A:H61 | 26:DA:899:A:HO2' | 1.59 | 0.41 |
| 36:DP:47:ASP:HA | 36:DP:48:PRO:HD3 | 1.84 | 0.41 |
| 46:DZ:96:VAL:O | 46:DZ:127:LYS:HA | 2.20 | 0.41 |
| 1:AA:1030(C):G:H2' | 1:AA:1030(D):A:C8 | 2.56 | 0.41 |
| 1:AA:114:U:H2' | 1:AA:115:G:C8 | 2.54 | 0.41 |
| 1:AA:160:A:H61 | 1:AA:345:C:H5' | 1.86 | 0.41 |
| 1:AA:456:C:H2' | 1:AA:457:C:H5' | 2.02 | 0.41 |
| 1:AA:624:C:O3' | 16:AP:10:GLY:HA2 | 2.20 | 0.41 |
| 1:AA:6:G:O2' | 1:AA:7:G:H5' | 2.20 | 0.41 |
| 1:AA:812:C:OP1 | 1:AA:903:G:H1' | 2.19 | 0.41 |
| 4:AD:194:LEU:HD12 | 4:AD:195:ALA:N | 2.36 | 0.41 |
| 10:AJ:11:PHE:CE1 | 10:AJ:67:THR:HG22 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:56:LEU:O | 13:AM:60:VAL:HG23 | 2.19 | 0.41 |
| 20:AT:48:LYS:HA | 20:AT:48:LYS:HD3 | 1.77 | 0.41 |
| 23:AW:52:G:H4' | 37:BQ:56:ARG:NH1 | 2.35 | 0.41 |
| 25:AY:22:G:N7 | 25:AY:46:7MG:C6 | 2.87 | 0.41 |
| 26:BA:2135:A:N1 | 26:BA:2156:G:O2' | 2.44 | 0.41 |
| 26:BA:2142:C:C2 | 26:BA:2143:C:C5 | 3.08 | 0.41 |
| 26:BA:652(C):G:N2 | 26:BA:652(V):C:N3 | 2.64 | 0.41 |
| 26:BA:762:U:OP1 | 61:BA:4794:HOH:O | 2.21 | 0.41 |
| 30:BF:120:GLU:HB2 | 30:BF:122:LYS:HG2 | 2.01 | 0.41 |
| 34:BN:67:LEU:HD12 | 34:BN:67:LEU:HA | 1.82 | 0.41 |
| 39:BS:59:LYS:HB2 | 39:BS:59:LYS:HE3 | 1.64 | 0.41 |
| 45:BY:9:LYS:HA | 45:BY:10:GLY:HA2 | 1.68 | 0.41 |
| 46:BZ:150:LEU:O | 46:BZ:171:ILE:HG13 | 2.19 | 0.41 |
| 1:CA:1044:A:C5 | 1:CA:1045:C:H1' | 2.55 | 0.41 |
| 1:CA:1096:C:H2' | 1:CA:1097:C:C6 | 2.55 | 0.41 |
| 1:CA:51:A:N7 | 1:CA:114:U:O2' | 2.53 | 0.41 |
| 1:CA:617:G:H4' | 16:CP:44:THR:O | 2.19 | 0.41 |
| 2:CB:70:PHE:CD1 | 2:CB:163:PHE:HB3 | 2.55 | 0.41 |
| 7:CG:65:ALA:O | 7:CG:69:VAL:HG23 | 2.20 | 0.41 |
| 8:CH:58:TYR:O | 8:CH:59:LEU:HD23 | 2.19 | 0.41 |
| 23:CW:18:G:O6 | 23:CW:55:PSU:H1' | 2.20 | 0.41 |
| 25:CY:18:G:N2 | 25:CY:55:PSU:N3 | 2.68 | 0.41 |
| 25:CY:35:A:H3' | 25:CY:36:A:C8 | 2.55 | 0.41 |
| 48:D1:86:SER:OG | 48:D1:89:GLU:OE2 | 2.19 | 0.41 |
| 49:D2:41:ILE:HG13 | 49:D2:43:GLN:HB2 | 2.02 | 0.41 |
| 26:DA:980:A:C4 | 26:DA:1136:G:O4' | 2.73 | 0.41 |
| 26:DA:1291:C:H2' | 26:DA:1292:U:C6 | 2.55 | 0.41 |
| 26:DA:1463:C:H2' | 26:DA:1464:C:H6 | 1.86 | 0.41 |
| 26:DA:1860:G:C6 | 26:DA:1883:G:N2 | 2.88 | 0.41 |
| 26:DA:2137:C:C2 | 26:DA:2138:C:C5 | 3.09 | 0.41 |
| 26:DA:2366:A:H2' | 26:DA:2367:G:O4' | 2.20 | 0.41 |
| 26:DA:38:A:H2' | 26:DA:39:C:C6 | 2.55 | 0.41 |
| 26:DA:565:C:H4' | 26:DA:1253:A:N6 | 2.35 | 0.41 |
| 26:DA:956:G:OP2 | 37:DQ:14:ARG:NH2 | 2.53 | 0.41 |
| 27:DB:32:C:H2' | 27:DB:33:G:O4' | 2.20 | 0.41 |
| 29:DE:7:VAL:HG12 | 29:DE:27:LEU:HB3 | 2.01 | 0.41 |
| 30:DF:20:LEU:HD23 | 30:DF:20:LEU:HA | 1.90 | 0.41 |
| 46:DZ:98:MET:SD | 46:DZ:100:VAL:HG23 | 2.60 | 0.41 |
| 46:DZ:159:PRO:HA | 46:DZ:161:VAL:H | 1.84 | 0.41 |
| 46:DZ:124:ILE:HD11 | 46:DZ:163:LEU:HD11 | 2.02 | 0.41 |
| 23:AW:66:U:H2' | 23:AW:67:C:C6 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:AY:68:C:C4 | 25:AY:69:G:N7 | 2.89 | 0.41 |
| 29:BE:96:PHE:O | 29:BE:175:VAL:HG11 | 2.20 | 0.41 |
| 32:BH:56:SER:OG | 32:BH:57:ASP:N | 2.54 | 0.41 |
| 34:BN:61:ARG:HE | 34:BN:61:ARG:HA | 1.85 | 0.41 |
| 1:CA:1050:G:C6 | 1:CA:1051:C:C4 | 3.09 | 0.41 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:C6 | 2.52 | 0.41 |
| 1:CA:1183:A:H5' | 1:CA:1183:A:C8 | 2.53 | 0.41 |
| 1:CA:1272:G:H2' | 1:CA:1273:G:O4' | 2.20 | 0.41 |
| 1:CA:1290:G:C4 | 1:CA:1291:G:C8 | 3.08 | 0.41 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:H8 | 1.81 | 0.41 |
| 1:CA:1468:A:H2' | 1:CA:1469:G:O4' | 2.21 | 0.41 |
| 1:CA:1496:C:H2' | 1:CA:1497:G:O4' | 2.21 | 0.41 |
| 1:CA:237:C:H5'' | 17:CQ:25:ARG:CZ | 2.49 | 0.41 |
| 1:CA:445:G:H2' | 1:CA:446:G:C8 | 2.55 | 0.41 |
| 1:CA:522:C:H41 | 12:CL:53:ARG:HH22 | 1.68 | 0.41 |
| 1:CA:607:A:H2' | 1:CA:608:A:O4' | 2.20 | 0.41 |
| 1:CA:839:U:H5'' | 1:CA:840:C:C5 | 2.56 | 0.41 |
| 1:CA:922:G:N3 | 1:CA:1398:A:H2 | 2.19 | 0.41 |
| 2:CB:32:ILE:HD13 | 2:CB:40:HIS:CG | 2.55 | 0.41 |
| 3:CC:116:VAL:O | 3:CC:120:VAL:HG23 | 2.21 | 0.41 |
| 3:CC:66:VAL:HB | 3:CC:101:LEU:HA | 2.02 | 0.41 |
| 8:CH:28:ALA:HB3 | 8:CH:57:PRO:HB2 | 2.03 | 0.41 |
| 9:CI:96:LEU:O | 9:CI:100:GLY:N | 2.54 | 0.41 |
| 13:CM:91:ARG:HH22 | 13:CM:103:THR:CG2 | 2.33 | 0.41 |
| 1:CA:1114:C:O2' | 14:CN:60:SER:O | 2.32 | 0.41 |
| 19:CS:5:LEU:HG | 19:CS:5:LEU:H | 1.48 | 0.41 |
| 26:DA:108:U:H2' | 26:DA:109:G:C8 | 2.56 | 0.41 |
| 26:DA:1638:C:H5'' | 26:DA:2710:C:O2' | 2.21 | 0.41 |
| 26:DA:859:G:O2' | 26:DA:916:G:O6 | 2.24 | 0.41 |
| 26:DA:96:G:H4' | 49:D2:48:HIS:CD2 | 2.55 | 0.41 |
| 30:DF:178:PRO:HB2 | 30:DF:201:VAL:CG2 | 2.49 | 0.41 |
| 31:DG:38:VAL:HG22 | 31:DG:93:THR:HG23 | 2.02 | 0.41 |
| 32:DH:117:PRO:HG3 | 32:DH:123:PHE:CD2 | 2.55 | 0.41 |
| 32:DH:90:LYS:HD2 | 32:DH:163:TYR:CD1 | 2.54 | 0.41 |
| 34:DN:4:TYR:HB2 | 41:DU:101:ARG:NH1 | 2.35 | 0.41 |
| 36:DP:97:PRO:HD3 | 36:DP:126:VAL:O | 2.19 | 0.41 |
| 37:DQ:18:LYS:HE3 | 37:DQ:18:LYS:HB2 | 1.68 | 0.41 |
| 37:DQ:81:VAL:HB | 47:D0:7:LEU:HD21 | 2.01 | 0.41 |
| 40:DT:65:LYS:HE2 | 40:DT:67:SER:HB2 | 2.02 | 0.41 |
| 1:AA:1152:A:H2' | 1:AA:1153:C:C6 | 2.55 | 0.41 |
| 1:AA:971:G:N2 | 1:AA:1363(A):A:OP2 | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:266:G:H4' | 1:AA:267:C:C5 | 2.55 | 0.41 |
| 1:AA:374:A:C6 | 1:AA:375:U:C4 | 3.08 | 0.41 |
| 1:AA:975:A:H4' | 1:AA:976:G:C5' | 2.46 | 0.41 |
| 2:AB:88:ALA:HB2 | 2:AB:219:VAL:HG13 | 2.03 | 0.41 |
| 4:AD:111:ALA:HB1 | 4:AD:116:GLN:HB3 | 2.03 | 0.41 |
| 11:AK:81:ASP:HB3 | 11:AK:107:SER:OG | 2.21 | 0.41 |
| 13:AM:40:ASN:HA | 13:AM:41:PRO:HD3 | 1.84 | 0.41 |
| 13:AM:54:VAL:HA | 13:AM:57:ARG:HB3 | 2.03 | 0.41 |
| 24:AX:27:U:H2' | 24:AX:28:C:C6 | 2.56 | 0.41 |
| 25:AY:62:C:H2' | 25:AY:63:G:C8 | 2.51 | 0.41 |
| 25:AY:6:G:C6 | 25:AY:7:A:C6 | 3.08 | 0.41 |
| 26:BA:1359:A:N1 | 26:BA:1372:U:O4 | 2.54 | 0.41 |
| 26:BA:2698:U:H2' | 26:BA:2699:C:C6 | 2.55 | 0.41 |
| 26:BA:493:G:H2' | 26:BA:494:G:O4' | 2.20 | 0.41 |
| 26:BA:27:G:C2 | 26:BA:512:G:N3 | 2.88 | 0.41 |
| 30:BF:143:ALA:HB1 | 30:BF:148:LEU:HB2 | 2.02 | 0.41 |
| 44:BX:12:VAL:HG21 | 44:BX:27:THR:HG22 | 2.03 | 0.41 |
| 44:BX:31:HIS:HA | 44:BX:32:PRO:HD3 | 1.96 | 0.41 |
| 46:BZ:8:TYR:HB2 | 46:BZ:38:TYR:CE2 | 2.56 | 0.41 |
| 1:CA:1030(A):G:N3 | 1:CA:1030(C):G:C8 | 2.88 | 0.41 |
| 1:CA:1128:C:H1' | 1:CA:1147:C:N4 | 2.31 | 0.41 |
| 1:CA:1373:G:H5'' | 7:CG:36:LYS:HD2 | 2.03 | 0.41 |
| 1:CA:411:A:C8 | 1:CA:413:G:C8 | 3.09 | 0.41 |
| 3:CC:11:ARG:HD3 | 3:CC:15:THR:HG21 | 2.01 | 0.41 |
| 1:CA:932:C:H4' | 7:CG:4:ARG:NH2 | 2.35 | 0.41 |
| 8:CH:6:ILE:O | 8:CH:10:LEU:HG | 2.19 | 0.41 |
| 10:CJ:6:ILE:O | 10:CJ:71:LEU:HD12 | 2.21 | 0.41 |
| 12:CL:33:ARG:O | 12:CL:85:ILE:HG12 | 2.21 | 0.41 |
| 13:CM:58:GLU:O | 13:CM:62:ASN:ND2 | 2.53 | 0.41 |
| 25:CY:38:A:C2' | 25:CY:39:PSU:H5' | 2.50 | 0.41 |
| 26:DA:443:A:H1' | 26:DA:1201:C:O4' | 2.19 | 0.41 |
| 26:DA:120:U:H5'' | 26:DA:122:G:OP2 | 2.20 | 0.41 |
| 26:DA:1857:G:C6 | 26:DA:1858:G:C6 | 3.08 | 0.41 |
| 25:CY:76:A:H62 | 26:DA:2422:A:H5' | 1.86 | 0.41 |
| 26:DA:328:U:H4' | 45:DY:68:HIS:CG | 2.56 | 0.41 |
| 26:DA:266:G:N2 | 26:DA:427:U:H1' | 2.35 | 0.41 |
| 31:DG:136:ARG:HD2 | 31:DG:137:GLU:HG3 | 2.03 | 0.41 |
| 36:DP:126:VAL:HG12 | 36:DP:148:LEU:HD22 | 2.03 | 0.41 |
| 1:AA:1002:G:H3' | 1:AA:1003:G:O4' | 2.20 | 0.41 |
| 1:AA:1241:G:O2' | 1:AA:1242:C:H5' | 2.20 | 0.41 |
| 1:AA:992:U:H4' | 1:AA:993:G:C5' | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:20:GLU:HA | 2:AB:21:ARG:HH21 | 1.86 | 0.41 |
| 2:AB:92:TYR:CE1 | 2:AB:151:GLY:HA3 | 2.55 | 0.41 |
| 3:AC:112:SER:O | 3:AC:116:VAL:HG23 | 2.20 | 0.41 |
| 3:AC:179:ARG:NH1 | 3:AC:206:GLU:OE1 | 2.54 | 0.41 |
| 5:AE:77:PRO:HG2 | 5:AE:78:HIS:HD2 | 1.85 | 0.41 |
| 1:AA:1368:G:OP2 | 9:AI:112:LYS:HG3 | 2.20 | 0.41 |
| 1:AA:130:A:H5' | 17:AQ:63:ARG:NE | 2.36 | 0.41 |
| 20:AT:59:ALA:O | 20:AT:63:ILE:HG13 | 2.21 | 0.41 |
| 48:B1:85:LEU:HB3 | 48:B1:89:GLU:HG3 | 2.03 | 0.41 |
| 26:BA:109:G:H2' | 26:BA:110:G:O4' | 2.20 | 0.41 |
| 26:BA:1518:U:H2' | 26:BA:1519:G:O4' | 2.20 | 0.41 |
| 29:BE:59:VAL:HG21 | 29:BE:74:PRO:HB3 | 2.02 | 0.41 |
| 30:BF:196:LEU:HA | 30:BF:196:LEU:HD23 | 1.91 | 0.41 |
| 31:BG:33:ARG:N | 31:BG:162:THR:OG1 | 2.52 | 0.41 |
| 32:BH:33:LEU:HD21 | 32:BH:136:ILE:HG13 | 2.02 | 0.41 |
| 38:BR:118:GLU:H | 38:BR:118:GLU:CD | 2.23 | 0.41 |
| 39:BS:83:LYS:HB2 | 39:BS:83:LYS:HE2 | 1.88 | 0.41 |
| 40:BT:42:ILE:HG12 | 40:BT:84:GLN:NE2 | 2.36 | 0.41 |
| 45:BY:55:TYR:CD1 | 45:BY:55:TYR:N | 2.88 | 0.41 |
| 1:CA:1179:A:C2 | 1:CA:1180:A:H1' | 2.55 | 0.41 |
| 1:CA:1401:G:C2 | 1:CA:1402:C:H1' | 2.55 | 0.41 |
| 1:CA:615:C:H2' | 1:CA:616:G:O4' | 2.20 | 0.41 |
| 1:CA:918:A:H2' | 1:CA:919:A:O4' | 2.21 | 0.41 |
| 13:CM:50:GLU:HG3 | 13:CM:50:GLU:O | 2.20 | 0.41 |
| 21:CU:6:ARG:HG2 | 21:CU:15:ARG:HD2 | 2.02 | 0.41 |
| 51:D4:60:GLN:O | 51:D4:63:TYR:HE2 | 2.03 | 0.41 |
| 26:DA:1153:C:H2' | 26:DA:1154:G:O4' | 2.20 | 0.41 |
| 26:DA:1446:C:N4 | 26:DA:1465:G:H1 | 2.19 | 0.41 |
| 26:DA:1754:C:OP2 | 40:DT:113:LYS:HE2 | 2.21 | 0.41 |
| 26:DA:1968:G:OP1 | 61:DA:4233:HOH:O | 2.22 | 0.41 |
| 26:DA:2238:G:N3 | 26:DA:2238:G:H2' | 2.35 | 0.41 |
| 26:DA:2507:C:H2' | 26:DA:2508:G:O4' | 2.21 | 0.41 |
| 26:DA:2751:G:C8 | 32:DH:2:SER:HA | 2.56 | 0.41 |
| 26:DA:431:U:H6 | 26:DA:431:U:O5' | 2.02 | 0.41 |
| 26:DA:79:G:H1 | 26:DA:107:C:N4 | 2.19 | 0.41 |
| 26:DA:1567:A:H2' | 28:DD:84:TYR:HE2 | 1.86 | 0.41 |
| 31:DG:68:PRO:HB3 | 31:DG:92:VAL:HB | 2.02 | 0.41 |
| 34:DN:97:ARG:HA | 34:DN:100:GLU:HB2 | 2.03 | 0.41 |
| 1:AA:1317:C:OP1 | 14:AN:17:LYS:HG2 | 2.19 | 0.41 |
| 1:AA:190:U:H3' | 1:AA:190:U:H6 | 1.85 | 0.41 |
| 2:AB:47:THR:HA | 2:AB:202:PRO:HG2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AC:19:GLU:HB3 | 3:AC:40:ARG:NH2 | 2.30 | 0.41 |
| 4:AD:57:ARG:HB3 | 4:AD:206:PHE:HB2 | 2.01 | 0.41 |
| 1:AA:4:U:O4 | 8:AH:105:ARG:HD3 | 2.20 | 0.41 |
| 8:AH:87:SER:HB2 | 8:AH:93:VAL:H | 1.85 | 0.41 |
| 26:BA:143:G:H2' | 26:BA:143(A):C:C6 | 2.55 | 0.41 |
| 26:BA:2334:G:H4' | 26:BA:2335:A:OP2 | 2.20 | 0.41 |
| 26:BA:2366:A:H2' | 26:BA:2367:G:O4' | 2.21 | 0.41 |
| 26:BA:2712:U:O2' | 26:BA:2713:A:H5' | 2.21 | 0.41 |
| 27:BB:75:G:H5'' | 27:BB:75:G:H8 | 1.85 | 0.41 |
| 32:BH:11:VAL:CG2 | 32:BH:50:VAL:HG23 | 2.50 | 0.41 |
| 26:BA:2875:C:O2' | 40:BT:4:GLY:HA3 | 2.21 | 0.41 |
| 1:CA:1070:U:O2' | 1:CA:1071:C:H5' | 2.21 | 0.41 |
| 1:CA:278:G:OP2 | 17:CQ:41:LYS:NZ | 2.36 | 0.41 |
| 1:CA:340:U:H2' | 1:CA:341:C:C6 | 2.56 | 0.41 |
| 1:CA:418:C:H2' | 1:CA:419:C:C6 | 2.56 | 0.41 |
| 3:CC:70:VAL:HG13 | 3:CC:73:PRO:HA | 2.02 | 0.41 |
| 6:CF:55:ASP:HA | 6:CF:56:PRO:HD3 | 1.83 | 0.41 |
| 9:CI:17:VAL:HG11 | 9:CI:81:ILE:N | 2.36 | 0.41 |
| 11:CK:82:VAL:HB | 11:CK:108:ILE:HG12 | 2.02 | 0.41 |
| 13:CM:3:ARG:CB | 51:D4:34:GLU:HG2 | 2.50 | 0.41 |
| 23:CW:11:C:N4 | 23:CW:24:G:H1 | 2.17 | 0.41 |
| 25:CY:27:G:N1 | 25:CY:43:C:O2 | 2.49 | 0.41 |
| 55:D8:34:TRP:CG | 55:D8:35:GLN:N | 2.89 | 0.41 |
| 26:DA:1470:G:N2 | 26:DA:1523:U:C4 | 2.88 | 0.41 |
| 26:DA:2161:C:H2' | 26:DA:2162:G:O4' | 2.20 | 0.41 |
| 26:DA:624:C:O2' | 26:DA:657:U:OP1 | 2.36 | 0.41 |
| 27:DB:118:G:C2' | 27:DB:119:G:H5' | 2.51 | 0.41 |
| 28:DD:61:LEU:HA | 28:DD:61:LEU:HD12 | 1.93 | 0.41 |
| 27:DB:57:A:C4 | 31:DG:29:TRP:HB3 | 2.55 | 0.41 |
| 32:DH:15:VAL:HG23 | 32:DH:27:LYS:O | 2.21 | 0.41 |
| 26:DA:1012:U:C4 | 34:DN:25:ARG:HG2 | 2.56 | 0.41 |
| 34:DN:26:LEU:O | 34:DN:30:ILE:HG13 | 2.21 | 0.41 |
| 46:DZ:4:ARG:HD3 | 46:DZ:60:GLU:OE1 | 2.21 | 0.41 |
| 1:AA:1418:A:H2 | 26:BA:1948:G:N3 | 2.19 | 0.41 |
| 1:AA:1469:G:H2' | 1:AA:1470:G:H8 | 1.86 | 0.41 |
| 1:AA:154:C:N3 | 1:AA:168:G:C2 | 2.88 | 0.41 |
| 1:AA:839:U:HO2' | 1:AA:840:C:P | 2.35 | 0.41 |
| 1:AA:920:U:H2' | 1:AA:921:U:C6 | 2.55 | 0.41 |
| 1:AA:938:A:C6 | 1:AA:939:G:C5 | 3.09 | 0.41 |
| 1:AA:958:A:C6 | 1:AA:959:A:N1 | 2.88 | 0.41 |
| 3:AC:32:LEU:HD13 | 3:AC:59:ARG:HD3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:AH:75:ARG:HA | 8:AH:76:PRO:HD2 | 1.87 | 0.41 |
| 14:AN:25:VAL:HG22 | 14:AN:38:GLY:O | 2.20 | 0.41 |
| 1:AA:995:C:H5' | 14:AN:8:GLU:HG2 | 2.02 | 0.41 |
| 24:AX:61:C:H2' | 24:AX:62:C:C6 | 2.56 | 0.41 |
| 50:B3:16:PRO:HB2 | 50:B3:18:ASP:OD1 | 2.20 | 0.41 |
| 51:B4:34:GLU:HG3 | 51:B4:34:GLU:H | 1.56 | 0.41 |
| 51:B4:53:GLU:HB3 | 51:B4:54:GLY:O | 2.21 | 0.41 |
| 26:BA:1179:C:H2' | 26:BA:1180:C:C6 | 2.52 | 0.41 |
| 26:BA:2070:G:C2 | 26:BA:2442:C:C2 | 3.09 | 0.41 |
| 26:BA:2131:G:H5' | 26:BA:2133:G:O4' | 2.21 | 0.41 |
| 26:BA:2287:A:H2 | 26:BA:2346:A:H62 | 1.64 | 0.41 |
| 26:BA:558:G:OP1 | 34:BN:111:PRO:HD2 | 2.21 | 0.41 |
| 26:BA:881:G:H1 | 26:BA:897:C:N4 | 2.19 | 0.41 |
| 29:BE:119:ARG:HD2 | 29:BE:120:TRP:CE2 | 2.55 | 0.41 |
| 45:BY:91:GLU:OE2 | 45:BY:91:GLU:N | 2.54 | 0.41 |
| 1:CA:1084:G:OP1 | 1:CA:1086:U:C2 | 2.73 | 0.41 |
| 1:CA:1134:G:C2 | 1:CA:1135:U:H1' | 2.56 | 0.41 |
| 1:CA:1427:U:H2' | 1:CA:1428:A:C8 | 2.55 | 0.41 |
| 1:CA:443:C:H2' | 1:CA:444:C:H6 | 1.85 | 0.41 |
| 8:CH:35:ILE:HG22 | 8:CH:39:LEU:HD23 | 2.03 | 0.41 |
| 1:CA:972:C:O2' | 10:CJ:55:LYS:O | 2.39 | 0.41 |
| 13:CM:37:THR:HG21 | 13:CM:56:LEU:HA | 2.03 | 0.41 |
| 14:CN:22:THR:HB | 14:CN:33:VAL:HG21 | 2.03 | 0.41 |
| 14:CN:45:ARG:O | 14:CN:49:HIS:CD2 | 2.74 | 0.41 |
| 1:CA:265:G:H5' | 17:CQ:64:PRO:O | 2.20 | 0.41 |
| 26:DA:1165:U:H6 | 26:DA:1165:U:O5' | 2.04 | 0.41 |
| 26:DA:1445(A):C:H2' | 26:DA:1446:C:C6 | 2.56 | 0.41 |
| 26:DA:889:C:O2' | 26:DA:890:A:O5' | 2.36 | 0.41 |
| 26:DA:899:A:C2' | 26:DA:900:A:H5'' | 2.51 | 0.41 |
| 28:DD:72:LYS:HE3 | 28:DD:72:LYS:HB3 | 1.85 | 0.41 |
| 29:DE:5:LEU:HD21 | 29:DE:79:ARG:HB2 | 2.03 | 0.41 |
| 30:DF:64:ILE:HG13 | 30:DF:65:TRP:N | 2.36 | 0.41 |
| 31:DG:122:PRO:HG2 | 31:DG:182:LYS:O | 2.20 | 0.41 |
| 31:DG:33:ARG:NH2 | 31:DG:162:THR:HG21 | 2.35 | 0.41 |
| 32:DH:86:GLU:CD | 32:DH:130:ARG:HD3 | 2.41 | 0.41 |
| 26:DA:637:A:C8 | 36:DP:117:GLU:HG3 | 2.55 | 0.41 |
| 46:DZ:50:GLN:CD | 46:DZ:50:GLN:N | 2.73 | 0.41 |
| 46:DZ:70:LEU:O | 46:DZ:89:PHE:N | 2.44 | 0.41 |
| 1:AA:1427:U:H2' | 1:AA:1428:A:C8 | 2.55 | 0.41 |
| 1:AA:925:G:H1' | 1:AA:1502:A:C4 | 2.55 | 0.41 |
| 1:AA:571:U:H5'' | 1:AA:819:A:C4 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:AA:1060:C:C4 | 3:AC:2:GLY:HA3 | 2.56 | 0.41 |
| 6:AF:9:VAL:HA | 6:AF:59:TYR:O | 2.20 | 0.41 |
| 16:AP:72:ARG:O | 16:AP:76:GLN:N | 2.30 | 0.41 |
| 17:AQ:9:VAL:CG2 | 17:AQ:84:LEU:HD13 | 2.50 | 0.41 |
| 23:AW:9:A:H1' | 23:AW:45:U:H2' | 2.03 | 0.41 |
| 50:B3:31:LEU:O | 50:B3:32:GLN:HB2 | 2.21 | 0.41 |
| 52:B5:35:GLU:HG3 | 52:B5:51:TYR:CG | 2.56 | 0.41 |
| 26:BA:1352:U:OP2 | 61:BA:4017:HOH:O | 2.22 | 0.41 |
| 26:BA:2129:C:C2 | 26:BA:2130:U:H5 | 2.39 | 0.41 |
| 26:BA:391:G:H1' | 26:BA:411:G:O4' | 2.20 | 0.41 |
| 26:BA:947:G:H2' | 26:BA:948:G:C8 | 2.56 | 0.41 |
| 33:BI:106:GLY:N | 33:BI:107:VAL:HG23 | 2.36 | 0.41 |
| 34:BN:39:ARG:HA | 34:BN:40:PRO:HD3 | 1.84 | 0.41 |
| 1:CA:1011:G:C2 | 1:CA:1019:C:C2 | 3.09 | 0.41 |
| 1:CA:1252:A:H2' | 1:CA:1253:G:O4' | 2.21 | 0.41 |
| 1:CA:1321:C:H3' | 1:CA:1322:C:C6 | 2.56 | 0.41 |
| 1:CA:1509:C:H2' | 1:CA:1510:U:O4' | 2.21 | 0.41 |
| 1:CA:1529:G:H4' | 1:CA:1530:G:OP2 | 2.21 | 0.41 |
| 1:CA:784:C:H4' | 26:DA:1837:C:OP1 | 2.20 | 0.41 |
| 1:CA:974:A:P | 14:CN:29:ARG:HH21 | 2.44 | 0.41 |
| 2:CB:48:MET:HA | 2:CB:51:LEU:CD2 | 2.51 | 0.41 |
| 4:CD:163:GLU:O | 4:CD:166:LYS:HG2 | 2.20 | 0.41 |
| 7:CG:91:VAL:HB | 7:CG:96:GLN:HG2 | 2.02 | 0.41 |
| 9:CI:7:THR:OG1 | 9:CI:83:ARG:NH1 | 2.54 | 0.41 |
| 15:CO:85:LEU:HA | 15:CO:85:LEU:HD23 | 1.82 | 0.41 |
| 19:CS:23:ASN:HA | 19:CS:27:GLU:CD | 2.41 | 0.41 |
| 9:CI:128:ARG:NH2 | 24:CX:33:U:OP2 | 2.54 | 0.41 |
| 50:D3:4:LEU:O | 50:D3:36:VAL:HA | 2.21 | 0.41 |
| 51:D4:24:THR:OG1 | 51:D4:25:TYR:N | 2.54 | 0.41 |
| 26:DA:1257:C:H2' | 26:DA:1258:C:C6 | 2.56 | 0.41 |
| 26:DA:854:G:H2' | 26:DA:855:G:C8 | 2.54 | 0.41 |
| 26:DA:899:A:O2' | 26:DA:900:A:H5'' | 2.21 | 0.41 |
| 26:DA:923:C:H2' | 26:DA:924:C:H6 | 1.84 | 0.41 |
| 29:DE:2:LYS:NZ | 29:DE:95:ILE:O | 2.40 | 0.41 |
| 32:DH:35:VAL:HA | 32:DH:36:PRO:HD2 | 1.94 | 0.41 |
| 32:DH:84:SER:CB | 32:DH:132:ARG:HH11 | 2.33 | 0.41 |
| 26:DA:2009:G:OP1 | 43:DW:41:LYS:HE2 | 2.20 | 0.41 |
| 26:DA:25:U:H5' | 43:DW:78:GLU:O | 2.21 | 0.41 |
| 46:DZ:70:LEU:HA | 46:DZ:70:LEU:HD23 | 1.80 | 0.41 |
| 1:AA:1026:G:H2' | 1:AA:1026:G:N3 | 2.35 | 0.41 |
| 1:AA:34:C:H2' | 1:AA:35:G:C8 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:953:G:H5' | 1:AA:965:A:N6 | 2.31 | 0.41 |
| 1:AA:981:U:H6 | 1:AA:981:U:O5' | 2.04 | 0.41 |
| 8:AH:118:VAL:O | 8:AH:119:LEU:HD23 | 2.21 | 0.41 |
| 13:AM:84:ILE:CG1 | 13:AM:85:GLY:HA2 | 2.44 | 0.41 |
| 13:AM:94:ARG:CZ | 19:AS:80:TYR:HD2 | 2.34 | 0.41 |
| 1:AA:1457:G:P | 20:AT:39:LYS:NZ | 2.94 | 0.41 |
| 1:AA:1305:G:OP2 | 21:AU:2:GLY:N | 2.53 | 0.41 |
| 49:B2:13:ALA:HA | 49:B2:16:LEU:HD12 | 2.03 | 0.41 |
| 50:B3:31:LEU:HD23 | 50:B3:31:LEU:HA | 1.87 | 0.41 |
| 26:BA:2138:C:C2 | 26:BA:2154:G:C2 | 3.08 | 0.41 |
| 26:BA:2156:G:H21 | 26:BA:2157:G:H22 | 1.69 | 0.41 |
| 26:BA:2641:G:H5' | 34:BN:83:LYS:HE2 | 2.03 | 0.41 |
| 26:BA:2788:C:OP1 | 29:BE:61:ARG:NH2 | 2.48 | 0.41 |
| 15:AO:56:LEU:HD21 | 26:BA:715:G:C2 | 2.56 | 0.41 |
| 28:BD:108:PRO:HB3 | 28:BD:143:HIS:HE1 | 1.84 | 0.41 |
| 31:BG:137:GLU:HG2 | 31:BG:152:LEU:HD22 | 2.03 | 0.41 |
| 35:BO:10:VAL:HG21 | 35:BO:16:ALA:HB3 | 2.03 | 0.41 |
| 35:BO:9:GLU:H | 35:BO:9:GLU:HG2 | 1.72 | 0.41 |
| 44:BX:61:GLY:HA3 | 44:BX:73:ARG:O | 2.21 | 0.41 |
| 1:CA:131:C:H2' | 1:CA:132:C:C6 | 2.55 | 0.41 |
| 1:CA:1401:G:OP1 | 22:CV:18:G:O2' | 2.28 | 0.41 |
| 1:CA:1442:G:HO2' | 1:CA:1442(A):G:P | 2.39 | 0.41 |
| 1:CA:974:A:O4' | 14:CN:31:ARG:HD3 | 2.21 | 0.41 |
| 3:CC:122:GLU:HA | 3:CC:125:GLU:OE1 | 2.21 | 0.41 |
| 4:CD:191:ARG:HD2 | 4:CD:191:ARG:HA | 1.94 | 0.41 |
| 1:CA:875:C:O2' | 8:CH:14:ARG:HD2 | 2.21 | 0.41 |
| 13:CM:24:GLY:C | 13:CM:25:ILE:HD12 | 2.41 | 0.41 |
| 13:CM:47:ASP:C | 13:CM:48:LEU:HD23 | 2.41 | 0.41 |
| 49:D2:31:GLU:O | 49:D2:35:LEU:HG | 2.21 | 0.41 |
| 31:DG:105:LYS:NZ | 51:D4:25:TYR:O | 2.53 | 0.41 |
| 53:D6:43:CYS:O | 53:D6:45:LYS:HG2 | 2.21 | 0.41 |
| 54:D7:8:ASN:HB3 | 54:D7:11:LYS:HB3 | 2.02 | 0.41 |
| 26:DA:1116:C:H2' | 26:DA:1117:G:C8 | 2.55 | 0.41 |
| 26:DA:116:C:H2' | 26:DA:117:G:O4' | 2.21 | 0.41 |
| 26:DA:793:A:OP2 | 26:DA:2072:G:H5' | 2.20 | 0.41 |
| 26:DA:2193:G:H2' | 26:DA:2194:G:C8 | 2.56 | 0.41 |
| 26:DA:819:A:C4 | 26:DA:1189:A:C2 | 3.09 | 0.41 |
| 28:DD:213:ARG:HD2 | 28:DD:213:ARG:HA | 1.86 | 0.41 |
| 33:DI:79:ILE:HA | 33:DI:80:PRO:HD2 | 1.90 | 0.41 |
| 37:DQ:79:LEU:C | 37:DQ:80:GLU:HG2 | 2.42 | 0.41 |
| 39:DS:16:ASN:O | 39:DS:19:LYS:HG2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:DS:15:ARG:HB3 | 39:DS:19:LYS:NZ | 2.36 | 0.41 |
| 44:DX:1:MET:N | 49:D2:29:LYS:HE3 | 2.36 | 0.41 |
| 1:AA:976:G:N2 | 1:AA:1363:C:OP2 | 2.45 | 0.41 |
| 1:AA:439:A:C8 | 1:AA:496:A:C6 | 3.09 | 0.41 |
| 3:AC:8:ILE:HD12 | 3:AC:8:ILE:HA | 1.94 | 0.41 |
| 4:AD:105:VAL:HG13 | 4:AD:110:PHE:HB2 | 2.02 | 0.41 |
| 6:AF:22:GLU:OE2 | 6:AF:82:ARG:HG2 | 2.21 | 0.41 |
| 6:AF:61:LEU:HD13 | 6:AF:61:LEU:HA | 1.86 | 0.41 |
| 12:AL:71:PRO:O | 12:AL:102:ARG:NH1 | 2.53 | 0.41 |
| 22:AV:16:A:H2' | 22:AV:17:U:O4' | 2.21 | 0.41 |
| 25:AY:5:G:C6 | 25:AY:6:G:C6 | 3.08 | 0.41 |
| 51:B4:53:GLU:O | 51:B4:56:VAL:HG13 | 2.21 | 0.41 |
| 26:BA:1021:A:C8 | 26:BA:1022:G:H5'' | 2.55 | 0.41 |
| 26:BA:1408:C:H2' | 26:BA:1409:C:C6 | 2.56 | 0.41 |
| 26:BA:1477:A:C2 | 26:BA:1515:G:C2 | 3.09 | 0.41 |
| 26:BA:2154:G:H2' | 26:BA:2155:G:H5' | 2.03 | 0.41 |
| 26:BA:2273:A:H2' | 26:BA:2274:A:C8 | 2.55 | 0.41 |
| 26:BA:2296:U:OP2 | 39:BS:9:ARG:NH2 | 2.49 | 0.41 |
| 26:BA:481:G:C4 | 26:BA:507:A:C2 | 3.09 | 0.41 |
| 26:BA:606:U:H4' | 26:BA:658:C:H4' | 2.03 | 0.41 |
| 30:BF:165:ARG:HG2 | 30:BF:168:ARG:NH2 | 2.36 | 0.41 |
| 31:BG:56:ALA:HA | 31:BG:153:ARG:HH21 | 1.86 | 0.41 |
| 33:BI:47:LEU:O | 33:BI:51:ILE:HG13 | 2.21 | 0.41 |
| 37:BQ:48:GLU:O | 37:BQ:52:VAL:HG23 | 2.20 | 0.41 |
| 26:BA:1649:G:O2' | 38:BR:107:ASP:OD2 | 2.32 | 0.41 |
| 27:BB:92:C:OP1 | 46:BZ:79:ARG:NH1 | 2.54 | 0.41 |
| 1:CA:61:G:C5 | 1:CA:107:G:C2 | 3.08 | 0.41 |
| 1:CA:1163:C:C2 | 1:CA:1174:G:C2 | 3.09 | 0.41 |
| 1:CA:1267:C:N4 | 1:CA:1268:A:C6 | 2.89 | 0.41 |
| 1:CA:423:G:H3' | 1:CA:423:G:N3 | 2.35 | 0.41 |
| 1:CA:757:U:O2' | 1:CA:879:C:O2 | 2.38 | 0.41 |
| 8:CH:64:LYS:HB3 | 8:CH:79:VAL:HG21 | 2.02 | 0.41 |
| 12:CL:89:ARG:HG2 | 12:CL:90:VAL:N | 2.36 | 0.41 |
| 20:CT:36:LEU:HA | 20:CT:36:LEU:HD13 | 1.90 | 0.41 |
| 24:CX:3:C:H2' | 24:CX:4:G:C8 | 2.56 | 0.41 |
| 26:DA:1005:C:H2' | 26:DA:1006:C:H6 | 1.83 | 0.41 |
| 26:DA:1518:U:H2' | 26:DA:1519:G:O4' | 2.20 | 0.41 |
| 26:DA:1575:C:H2' | 26:DA:1576:U:O4' | 2.21 | 0.41 |
| 26:DA:2135:A:H61 | 26:DA:2157:G:N2 | 2.19 | 0.41 |
| 26:DA:2669:G:C2 | 26:DA:2670:A:C8 | 3.09 | 0.41 |
| 26:DA:25:U:C4 | 26:DA:26:G:C6 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DA:642:G:H21 | 26:DA:646:A:H2 | 1.68 | 0.41 |
| 26:DA:706:A:H2' | 26:DA:707:G:O4' | 2.21 | 0.41 |
| 26:DA:77:C:O2' | 49:D2:14:ARG:NH2 | 2.52 | 0.41 |
| 28:DD:237:GLU:OE2 | 61:DD:401:HOH:O | 2.22 | 0.41 |
| 26:DA:590:A:P | 30:DF:95:ARG:HH11 | 2.44 | 0.41 |
| 31:DG:56:ALA:HA | 31:DG:153:ARG:HH21 | 1.85 | 0.41 |
| 32:DH:54:ARG:HB3 | 32:DH:65:HIS:CD2 | 2.56 | 0.41 |
| 35:DO:20:MET:HE3 | 35:DO:44:LYS:HE3 | 2.03 | 0.41 |
| 41:DU:86:ALA:O | 42:DV:49:THR:HG23 | 2.20 | 0.41 |
| 1:AA:1028:C:C2 | 1:AA:1029:C:H1' | 2.56 | 0.40 |
| 1:AA:1047:G:C2' | 1:AA:1048:G:H5' | 2.51 | 0.40 |
| 1:AA:165:C:H2' | 1:AA:166:G:C8 | 2.56 | 0.40 |
| 1:AA:183:G:H1 | 1:AA:194:C:H42 | 1.69 | 0.40 |
| 1:AA:44:G:N7 | 61:AA:4044:HOH:O | 2.37 | 0.40 |
| 2:AB:183:PRO:HA | 2:AB:198:ASP:OD2 | 2.21 | 0.40 |
| 2:AB:161:ALA:HB1 | 2:AB:185:ILE:HD11 | 2.02 | 0.40 |
| 3:AC:110:ASN:O | 3:AC:141:VAL:HG22 | 2.21 | 0.40 |
| 4:AD:178:VAL:HG12 | 4:AD:179:GLU:N | 2.35 | 0.40 |
| 14:AN:50:LYS:HB2 | 14:AN:50:LYS:HE2 | 1.76 | 0.40 |
| 19:AS:42:PRO:HD2 | 51:B4:61:ARG:HH21 | 1.86 | 0.40 |
| 26:BA:242:G:H5'' | 55:B8:64:TYR:CZ | 2.57 | 0.40 |
| 26:BA:1107:G:N2 | 26:BA:1108:U:O4 | 2.54 | 0.40 |
| 26:BA:1171:G:N7 | 26:BA:1173:G:C8 | 2.89 | 0.40 |
| 26:BA:1860:G:N2 | 26:BA:1882:C:O2 | 2.49 | 0.40 |
| 26:BA:2137:C:H2' | 26:BA:2138:C:C6 | 2.56 | 0.40 |
| 26:BA:2191:G:H8 | 26:BA:2191:G:C5' | 2.33 | 0.40 |
| 26:BA:2447:G:N2 | 26:BA:2450:A:OP2 | 2.53 | 0.40 |
| 26:BA:274:G:H2' | 26:BA:275:G:C8 | 2.56 | 0.40 |
| 29:BE:144:ARG:HB3 | 29:BE:145:LYS:H | 1.53 | 0.40 |
| 29:BE:51:PHE:CD2 | 29:BE:52:LEU:HG | 2.56 | 0.40 |
| 30:BF:177:ALA:O | 30:BF:180:GLY:N | 2.45 | 0.40 |
| 26:BA:470:A:OP1 | 30:BF:59:TYR:HE1 | 2.03 | 0.40 |
| 31:BG:64:THR:HB | 31:BG:94:LEU:HD21 | 2.03 | 0.40 |
| 32:BH:94:TYR:HA | 32:BH:106:THR:O | 2.21 | 0.40 |
| 26:BA:994:C:OP1 | 41:BU:53:ARG:NH2 | 2.54 | 0.40 |
| 46:BZ:158:PRO:HA | 46:BZ:159:PRO:HD3 | 1.90 | 0.40 |
| 46:BZ:76:LEU:HA | 46:BZ:76:LEU:HD12 | 1.87 | 0.40 |
| 46:BZ:7:ALA:O | 46:BZ:62:PRO:HD3 | 2.21 | 0.40 |
| 1:CA:130:A:H1' | 1:CA:263:A:O2' | 2.20 | 0.40 |
| 1:CA:1350:A:OP1 | 9:CI:121:ARG:HD3 | 2.22 | 0.40 |
| 1:CA:629:G:H2' | 1:CA:630:G:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:895:G:N7 | 61:CA:3246:HOH:O | 2.37 | 0.40 |
| 1:CA:9:G:H2' | 1:CA:10:A:C8 | 2.56 | 0.40 |
| 2:CB:48:MET:HA | 2:CB:51:LEU:HD21 | 2.02 | 0.40 |
| 3:CC:18:TRP:O | 3:CC:21:ARG:NH1 | 2.46 | 0.40 |
| 4:CD:179:GLU:O | 4:CD:181:MET:HE2 | 2.21 | 0.40 |
| 10:CJ:42:THR:HG23 | 10:CJ:68:HIS:HD2 | 1.86 | 0.40 |
| 12:CL:119:LYS:O | 12:CL:120:TYR:HB2 | 2.21 | 0.40 |
| 15:CO:31:LEU:HD23 | 15:CO:31:LEU:HA | 1.89 | 0.40 |
| 15:CO:3:ILE:H | 15:CO:3:ILE:HD13 | 1.86 | 0.40 |
| 16:CP:68:ASP:O | 16:CP:71:ARG:HG2 | 2.21 | 0.40 |
| 19:CS:3:ARG:NH2 | 19:CS:10:PHE:HB2 | 2.36 | 0.40 |
| 1:CA:1325:C:H4' | 21:CU:17:THR:HG21 | 2.02 | 0.40 |
| 25:CY:36:A:C2 | 25:CY:37:MIA:C4 | 3.04 | 0.40 |
| 26:DA:1479:G:C2 | 26:DA:1480:G:C4 | 3.09 | 0.40 |
| 26:DA:195:A:H2' | 26:DA:198:C:N4 | 2.36 | 0.40 |
| 26:DA:2037:G:O2' | 26:DA:2038:G:H5' | 2.22 | 0.40 |
| 26:DA:2058:A:N7 | 61:DA:3874:HOH:O | 2.37 | 0.40 |
| 26:DA:2142:C:H2' | 26:DA:2143:C:C6 | 2.56 | 0.40 |
| 26:DA:2694:G:C6 | 26:DA:2695:C:C4 | 3.08 | 0.40 |
| 26:DA:271(H):G:O2' | 26:DA:271(I):G:C8 | 2.74 | 0.40 |
| 26:DA:528:A:C2 | 26:DA:2043:C:H4' | 2.57 | 0.40 |
| 26:DA:531:C:OP1 | 26:DA:561:G:N1 | 2.50 | 0.40 |
| 26:DA:953:A:OP2 | 37:DQ:16:ARG:NE | 2.50 | 0.40 |
| 29:DE:72:VAL:HG12 | 29:DE:73:GLU:O | 2.21 | 0.40 |
| 36:DP:135:LEU:HA | 36:DP:135:LEU:HD23 | 1.79 | 0.40 |
| 26:DA:911:A:H2' | 37:DQ:9:TYR:OH | 2.22 | 0.40 |
| 26:DA:2848:G:H8 | 40:DT:97:ALA:HB2 | 1.85 | 0.40 |
| 42:DV:58:VAL:O | 42:DV:97:LYS:N | 2.45 | 0.40 |
| 45:DY:74:PRO:O | 45:DY:82:PRO:HA | 2.20 | 0.40 |
| 1:AA:993:G:N3 | 1:AA:993:G:H2' | 2.35 | 0.40 |
| 2:AB:17:PHE:HD2 | 2:AB:44:LEU:HD21 | 1.86 | 0.40 |
| 2:AB:47:THR:HG22 | 2:AB:51:LEU:HD11 | 2.03 | 0.40 |
| 3:AC:134:ILE:HD11 | 3:AC:153:VAL:HG23 | 2.04 | 0.40 |
| 3:AC:150:LYS:HB2 | 3:AC:173:VAL:HG21 | 2.02 | 0.40 |
| 8:AH:123:GLU:O | 8:AH:127:LEU:HD13 | 2.22 | 0.40 |
| 23:AW:19:G:H4' | 23:AW:20:U:OP1 | 2.20 | 0.40 |
| 25:AY:18:G:O6 | 25:AY:55:PSU:H1' | 2.21 | 0.40 |
| 52:B5:40:LYS:HE2 | 52:B5:46:CYS:HA | 2.04 | 0.40 |
| 26:BA:1022:G:C6 | 26:BA:1141:U:C5 | 3.09 | 0.40 |
| 26:BA:1421:G:C2 | 26:BA:1422:G:C8 | 3.10 | 0.40 |
| 26:BA:2138:C:C4 | 26:BA:2154:G:C6 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BB:78:A:H2' | 27:BB:79:C:O4' | 2.21 | 0.40 |
| 36:BP:88:LEU:HD22 | 36:BP:95:VAL:HG21 | 2.03 | 0.40 |
| 1:CA:1118:C:N4 | 1:CA:1119:C:H41 | 2.19 | 0.40 |
| 1:CA:1350:A:C2 | 1:CA:1351:U:C2 | 3.09 | 0.40 |
| 1:CA:981:U:H5' | 14:CN:21:TYR:CE2 | 2.56 | 0.40 |
| 2:CB:201:ILE:HA | 2:CB:202:PRO:HD2 | 1.97 | 0.40 |
| 2:CB:80:ILE:HD13 | 2:CB:211:ILE:HB | 2.02 | 0.40 |
| 2:CB:77:ALA:HB2 | 2:CB:165:VAL:HG11 | 2.03 | 0.40 |
| 3:CC:105:GLU:OE1 | 3:CC:107:GLN:N | 2.55 | 0.40 |
| 3:CC:70:VAL:HG22 | 3:CC:72:LYS:N | 2.35 | 0.40 |
| 4:CD:108:LEU:HD12 | 4:CD:108:LEU:HA | 1.74 | 0.40 |
| 4:CD:76:ARG:NE | 4:CD:80:GLU:OE1 | 2.50 | 0.40 |
| 11:CK:18:ARG:NH2 | 11:CK:35:PRO:O | 2.49 | 0.40 |
| 11:CK:87:THR:O | 11:CK:87:THR:OG1 | 2.37 | 0.40 |
| 13:CM:10:PRO:HD2 | 13:CM:18:ALA:HB1 | 2.03 | 0.40 |
| 16:CP:69:THR:O | 16:CP:72:ARG:HB2 | 2.22 | 0.40 |
| 19:CS:36:ARG:HD2 | 19:CS:52:TYR:O | 2.21 | 0.40 |
| 23:CW:23:A:H2' | 23:CW:24:G:C8 | 2.56 | 0.40 |
| 25:CY:9:A:H5' | 25:CY:46:7MG:C1' | 2.52 | 0.40 |
| 48:D1:50:ARG:NH1 | 48:D1:57:GLU:OE2 | 2.54 | 0.40 |
| 26:DA:511:U:H4' | 26:DA:1235:G:H4' | 2.03 | 0.40 |
| 26:DA:1359:A:N1 | 26:DA:1372:U:C4 | 2.89 | 0.40 |
| 26:DA:1482:G:C6 | 26:DA:1507:A:C2 | 3.08 | 0.40 |
| 26:DA:1539:G:H2' | 26:DA:1540:U:O4' | 2.20 | 0.40 |
| 26:DA:2074:U:H2' | 26:DA:2075:U:C6 | 2.56 | 0.40 |
| 26:DA:2137:C:N3 | 26:DA:2138:C:N4 | 2.68 | 0.40 |
| 26:DA:2542:A:H4' | 26:DA:2543:G:C8 | 2.56 | 0.40 |
| 26:DA:2542:A:H4' | 26:DA:2543:G:H8 | 1.87 | 0.40 |
| 26:DA:581:C:H2' | 26:DA:582:G:C8 | 2.56 | 0.40 |
| 26:DA:885:C:H2' | 26:DA:886:C:C4' | 2.51 | 0.40 |
| 29:DE:52:LEU:O | 29:DE:76:ARG:N | 2.33 | 0.40 |
| 32:DH:144:VAL:O | 32:DH:148:ILE:HG12 | 2.21 | 0.40 |
| 32:DH:9:ILE:HG12 | 32:DH:69:ARG:HD2 | 2.04 | 0.40 |
| 27:DB:50:G:OP1 | 39:DS:63:THR:HG22 | 2.21 | 0.40 |
| 1:AA:1003:G:N3 | 1:AA:1004:A:H1' | 2.36 | 0.40 |
| 1:AA:1179:A:H2' | 1:AA:1180:A:O4' | 2.21 | 0.40 |
| 1:AA:1358:U:OP2 | 1:AA:1359:C:N4 | 2.54 | 0.40 |
| 2:AB:192:SER:O | 2:AB:194:PRO:HD3 | 2.22 | 0.40 |
| 2:AB:77:ALA:O | 2:AB:81:VAL:HG22 | 2.20 | 0.40 |
| 6:AF:95:GLU:HA | 6:AF:96:PRO:HD3 | 1.98 | 0.40 |
| 7:AG:29:LYS:HD3 | 7:AG:29:LYS:HA | 1.92 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:AM:117:VAL:HG12 | 13:AM:118:ALA:O | 2.21 | 0.40 |
| 17:AQ:75:ARG:HH12 | 17:AQ:77:VAL:HA | 1.86 | 0.40 |
| 26:BA:2331:G:O2' | 47:B0:43:THR:HG22 | 2.21 | 0.40 |
| 49:B2:64:LEU:CD2 | 49:B2:68:ARG:HE | 2.34 | 0.40 |
| 26:BA:1851:U:H2' | 26:BA:1852:C:O4' | 2.21 | 0.40 |
| 26:BA:2506:U:C2 | 26:BA:2585:U:O4 | 2.75 | 0.40 |
| 35:BO:10:VAL:HG11 | 35:BO:16:ALA:HB1 | 2.04 | 0.40 |
| 36:BP:47:ASP:HA | 36:BP:48:PRO:HD3 | 1.92 | 0.40 |
| 42:BV:6:LYS:HG2 | 42:BV:11:GLN:HG2 | 2.03 | 0.40 |
| 1:CA:9:G:H2' | 1:CA:10:A:H8 | 1.85 | 0.40 |
| 1:CA:1347:G:H5'' | 9:CI:107:ARG:HB3 | 2.02 | 0.40 |
| 1:CA:300:A:H1' | 1:CA:565:U:O2 | 2.20 | 0.40 |
| 1:CA:426:G:OP1 | 4:CD:36:ARG:NH1 | 2.42 | 0.40 |
| 2:CB:197:VAL:HB | 2:CB:200:ILE:HG12 | 2.03 | 0.40 |
| 3:CC:109:PRO:HB3 | 3:CC:115:LEU:HD23 | 2.03 | 0.40 |
| 3:CC:70:VAL:N | 3:CC:106:VAL:HG23 | 2.37 | 0.40 |
| 4:CD:3:ARG:O | 4:CD:5:ILE:HG22 | 2.21 | 0.40 |
| 13:CM:95:GLY:HA2 | 13:CM:110:ARG:NH1 | 2.36 | 0.40 |
| 1:CA:255:G:P | 17:CQ:69:LYS:HZ1 | 2.42 | 0.40 |
| 24:CX:47:U:H3' | 24:CX:48:C:C5' | 2.51 | 0.40 |
| 24:CX:58:A:O2' | 24:CX:60:U:OP2 | 2.34 | 0.40 |
| 54:D7:10:ARG:O | 54:D7:14:LYS:HB2 | 2.22 | 0.40 |
| 56:D9:29:ASN:HA | 56:D9:30:PRO:HD3 | 1.88 | 0.40 |
| 26:DA:1487:G:H2' | 26:DA:1488:G:H5'' | 2.04 | 0.40 |
| 26:DA:1777:U:O2' | 26:DA:1778:U:H5' | 2.20 | 0.40 |
| 26:DA:2136:C:O2' | 26:DA:2137:C:H6 | 2.05 | 0.40 |
| 26:DA:2447:G:N2 | 26:DA:2450:A:OP2 | 2.54 | 0.40 |
| 26:DA:2689:U:C4' | 26:DA:2690:C:H5' | 2.48 | 0.40 |
| 26:DA:565:C:H2' | 26:DA:566:U:O4' | 2.21 | 0.40 |
| 26:DA:587:C:OP2 | 36:DP:21:ARG:NH2 | 2.55 | 0.40 |
| 27:DB:57:A:O4' | 31:DG:30:GLU:HG3 | 2.21 | 0.40 |
| 38:DR:78:LYS:HE2 | 38:DR:83:ILE:HD11 | 2.04 | 0.40 |
| 39:DS:36:TYR:CD2 | 39:DS:52:SER:HB3 | 2.56 | 0.40 |
| 41:DU:103:PRO:O | 41:DU:107:ALA:N | 2.50 | 0.40 |
| 46:DZ:7:ALA:HB3 | 46:DZ:61:LEU:HD12 | 2.03 | 0.40 |
| 46:DZ:79:ARG:HD2 | 46:DZ:80:ARG:CZ | 2.51 | 0.40 |
| 46:DZ:97:GLU:HA | 46:DZ:126:VAL:O | 2.21 | 0.40 |
| 1:AA:1006:C:H2' | 1:AA:1007:C:C6 | 2.56 | 0.40 |
| 1:AA:1001:A:N1 | 1:AA:1040:U:O4 | 2.54 | 0.40 |
| 1:AA:1118:C:OP1 | 9:AI:9:ARG:NH1 | 2.53 | 0.40 |
| 1:AA:1166:G:H5' | 1:AA:1168:A:OP2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1314:C:OP2 | 19:AS:4:SER:OG | 2.17 | 0.40 |
| 1:AA:1457:G:H2' | 1:AA:1458:G:C8 | 2.57 | 0.40 |
| 1:AA:201:C:H2' | 1:AA:202:U:H2' | 2.03 | 0.40 |
| 1:AA:7:G:H5'' | 1:AA:298:A:O4' | 2.22 | 0.40 |
| 1:AA:49:U:O4 | 1:AA:365:U:H5 | 2.05 | 0.40 |
| 1:AA:57:G:H2' | 1:AA:58:C:C6 | 2.57 | 0.40 |
| 1:AA:784:C:H2' | 1:AA:785:G:O4' | 2.22 | 0.40 |
| 4:AD:147:ALA:HB2 | 4:AD:182:LYS:HA | 2.04 | 0.40 |
| 1:AA:737:A:OP1 | 6:AF:92:LYS:HG3 | 2.21 | 0.40 |
| 14:AN:27:CYS:SG | 14:AN:29:ARG:HB2 | 2.61 | 0.40 |
| 1:AA:376:G:O2' | 16:AP:5:ARG:NH2 | 2.54 | 0.40 |
| 19:AS:41:VAL:O | 19:AS:44:MET:HB2 | 2.21 | 0.40 |
| 51:B4:40:HIS:HA | 51:B4:41:PRO:HD2 | 1.88 | 0.40 |
| 26:BA:1636:C:H2' | 26:BA:1637:A:C8 | 2.56 | 0.40 |
| 26:BA:2262:U:H4' | 26:BA:2328:A:C2 | 2.56 | 0.40 |
| 26:BA:286:C:H2' | 26:BA:287:C:C6 | 2.57 | 0.40 |
| 26:BA:303:U:O4 | 61:BA:4656:HOH:O | 2.22 | 0.40 |
| 26:BA:526:A:H5'' | 26:BA:527:C:OP1 | 2.21 | 0.40 |
| 26:BA:536:A:H2' | 26:BA:537:C:C6 | 2.56 | 0.40 |
| 28:BD:38:LYS:HD2 | 28:BD:38:LYS:HA | 1.98 | 0.40 |
| 30:BF:93:LYS:HA | 30:BF:93:LYS:HD3 | 1.91 | 0.40 |
| 33:BI:135:GLU:C | 33:BI:137:PRO:HD3 | 2.42 | 0.40 |
| 35:BO:23:ARG:HG3 | 35:BO:24:VAL:N | 2.36 | 0.40 |
| 40:BT:80:SER:HA | 40:BT:81:PRO:HD3 | 1.89 | 0.40 |
| 26:BA:335:C:H5' | 45:BY:73:ARG:NH2 | 2.36 | 0.40 |
| 1:CA:1442:G:C8 | 1:CA:1442:G:H3' | 2.56 | 0.40 |
| 2:CB:168:THR:OG1 | 2:CB:192:SER:HA | 2.22 | 0.40 |
| 2:CB:15:VAL:CG1 | 2:CB:209:ARG:HB3 | 2.49 | 0.40 |
| 2:CB:42:ILE:HG21 | 2:CB:202:PRO:HB2 | 2.03 | 0.40 |
| 24:CX:28:C:H2' | 24:CX:29:G:C8 | 2.56 | 0.40 |
| 24:CX:28:C:H2' | 24:CX:29:G:H8 | 1.85 | 0.40 |
| 24:CX:50:U:H3 | 24:CX:64:G:H1 | 1.68 | 0.40 |
| 48:D1:23:LYS:HB2 | 48:D1:23:LYS:HE3 | 1.79 | 0.40 |
| 52:D5:11:THR:HG22 | 52:D5:12:SER:O | 2.21 | 0.40 |
| 26:DA:1653:G:H3' | 38:DR:2:ARG:HD3 | 2.04 | 0.40 |
| 26:DA:1773:A:H5'' | 61:DA:4357:HOH:O | 2.21 | 0.40 |
| 26:DA:19:C:H2' | 26:DA:20:C:H6 | 1.86 | 0.40 |
| 26:DA:2224:G:H4' | 26:DA:2226:C:C2 | 2.56 | 0.40 |
| 26:DA:2273:A:H2' | 26:DA:2274:A:H8 | 1.85 | 0.40 |
| 26:DA:2755:C:HO2' | 26:DA:2756:U:H6 | 1.69 | 0.40 |
| 26:DA:469:G:H2' | 26:DA:470:A:H5'' | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DA:478:A:H62 | 26:DA:502:A:N6 | 2.19 | 0.40 |
| 26:DA:1501:C:O4' | 28:DD:100:GLY:HA2 | 2.21 | 0.40 |
| 29:DE:24:THR:CG2 | 29:DE:184:VAL:HG12 | 2.52 | 0.40 |
| 32:DH:77:LYS:HG3 | 32:DH:81:GLU:OE2 | 2.21 | 0.40 |
| 35:DO:9:GLU:OE2 | 35:DO:18:LYS:HE3 | 2.21 | 0.40 |
| 42:DV:39:LEU:HG | 42:DV:46:VAL:O | 2.21 | 0.40 |
| 44:DX:64:LYS:HA | 44:DX:64:LYS:HD2 | 1.88 | 0.40 |
| 44:DX:84:ALA:HB3 | 44:DX:87:GLN:NE2 | 2.37 | 0.40 |
| 1:AA:1121:U:C2' | 1:AA:1122:U:H5' | 2.52 | 0.40 |
| 1:AA:1261:A:H3' | 1:AA:1262:C:H6 | 1.87 | 0.40 |
| 1:AA:1410:G:H2' | 1:AA:1411:C:C6 | 2.57 | 0.40 |
| 1:AA:1529:G:H4' | 1:AA:1530:G:OP2 | 2.22 | 0.40 |
| 1:AA:22:G:H4' | 1:AA:885:G:C8 | 2.57 | 0.40 |
| 1:AA:38:G:O2' | 1:AA:39:G:H5'' | 2.21 | 0.40 |
| 1:AA:719:C:H1' | 18:AR:49:LYS:HB3 | 2.03 | 0.40 |
| 1:AA:881:G:H2' | 1:AA:882:C:O4' | 2.21 | 0.40 |
| 7:AG:97:GLN:HB2 | 7:AG:97:GLN:HE21 | 1.66 | 0.40 |
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:CE2 | 2.57 | 0.40 |
| 12:AL:7:ILE:O | 12:AL:11:VAL:HG23 | 2.21 | 0.40 |
| 16:AP:54:GLU:HG3 | 16:AP:55:ARG:N | 2.37 | 0.40 |
| 26:BA:125:G:N2 | 54:B7:48:LYS:HA | 2.36 | 0.40 |
| 26:BA:1022:G:N2 | 26:BA:1142(A):A:C2 | 2.80 | 0.40 |
| 26:BA:1230:C:H2' | 26:BA:1231:G:H8 | 1.86 | 0.40 |
| 26:BA:1753:G:N1 | 26:BA:1756:G:OP2 | 2.53 | 0.40 |
| 26:BA:1817:G:C6 | 26:BA:1818:U:C4 | 3.10 | 0.40 |
| 26:BA:2147:G:H2' | 26:BA:2148:G:O4' | 2.22 | 0.40 |
| 26:BA:303:U:H2' | 26:BA:304:G:C8 | 2.56 | 0.40 |
| 26:BA:484:C:H2' | 26:BA:485:C:H6 | 1.87 | 0.40 |
| 28:BD:258:LYS:HE2 | 28:BD:273:ARG:CZ | 2.51 | 0.40 |
| 31:BG:38:VAL:HG22 | 31:BG:93:THR:HG23 | 2.03 | 0.40 |
| 35:BO:79:PHE:CD2 | 40:BT:72:VAL:HG22 | 2.56 | 0.40 |
| 43:BW:13:SER:HA | 43:BW:14:PRO:HD3 | 1.82 | 0.40 |
| 43:BW:14:PRO:HG2 | 43:BW:78:GLU:CD | 2.42 | 0.40 |
| 1:CA:1028:C:O2 | 1:CA:1034:G:H1' | 2.21 | 0.40 |
| 1:CA:1065:U:P | 1:CA:1190:G:H22 | 2.45 | 0.40 |
| 1:CA:1100:C:H2' | 1:CA:1102:A:O5' | 2.22 | 0.40 |
| 1:CA:1133:G:H2' | 1:CA:1134:G:O4' | 2.22 | 0.40 |
| 1:CA:179:A:C2' | 1:CA:180:U:H5' | 2.52 | 0.40 |
| 1:CA:377:G:H5' | 16:CP:5:ARG:NH2 | 2.37 | 0.40 |
| 1:CA:407:G:H5'' | 4:CD:115:ARG:HB3 | 2.03 | 0.40 |
| 1:CA:408:A:H2' | 1:CA:409:G:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:643:C:H2' | 1:CA:644:G:C8 | 2.57 | 0.40 |
| 1:CA:785:G:C2' | 1:CA:786:G:H5' | 2.51 | 0.40 |
| 2:CB:12:GLU:C | 2:CB:14:GLY:HA3 | 2.41 | 0.40 |
| 2:CB:189:ASP:O | 2:CB:192:SER:OG | 2.40 | 0.40 |
| 6:CF:82:ARG:HD2 | 6:CF:82:ARG:HA | 1.71 | 0.40 |
| 6:CF:95:GLU:HA | 6:CF:96:PRO:HD3 | 1.85 | 0.40 |
| 8:CH:27:PRO:O | 8:CH:32:LYS:HD2 | 2.22 | 0.40 |
| 1:CA:1014:A:H4' | 19:CS:14:HIS:CE1 | 2.57 | 0.40 |
| 20:CT:24:LEU:HA | 20:CT:24:LEU:HD13 | 1.71 | 0.40 |
| 51:D4:13:ARG:O | 51:D4:30:GLU:HA | 2.20 | 0.40 |
| 53:D6:8:LYS:HD3 | 55:D8:34:TRP:CD2 | 2.56 | 0.40 |
| 56:D9:12:ASP:OD1 | 56:D9:13:LYS:HG2 | 2.21 | 0.40 |
| 26:DA:1011:G:C2 | 26:DA:1151:G:N3 | 2.90 | 0.40 |
| 26:DA:1604:C:O2' | 26:DA:1610:A:N1 | 2.38 | 0.40 |
| 26:DA:195:A:H2' | 26:DA:198:C:H41 | 1.86 | 0.40 |
| 26:DA:1935:G:H1' | 26:DA:1964:G:N2 | 2.37 | 0.40 |
| 26:DA:2625:G:H2' | 26:DA:2626:C:O4' | 2.22 | 0.40 |
| 26:DA:2734:A:H2' | 26:DA:2735:G:O4' | 2.21 | 0.40 |
| 26:DA:463:G:N2 | 26:DA:466:A:OP2 | 2.49 | 0.40 |
| 26:DA:661:C:H2' | 26:DA:662:G:C8 | 2.56 | 0.40 |
| 27:DB:5:C:N4 | 27:DB:116:G:H1 | 2.13 | 0.40 |
| 26:DA:729:G:C6 | 28:DD:208:LYS:HB2 | 2.56 | 0.40 |
| 29:DE:201:THR:OG1 | 29:DE:202:LYS:N | 2.55 | 0.40 |
| 31:DG:51:ARG:H | 31:DG:51:ARG:HG3 | 1.69 | 0.40 |
| 31:DG:97:ASP:O | 31:DG:101:ILE:HG13 | 2.21 | 0.40 |
| 33:DI:57:ARG:O | 33:DI:61:ARG:HG2 | 2.21 | 0.40 |
| 35:DO:2:ILE:HB | 35:DO:33:ALA:HB3 | 2.03 | 0.40 |
| 38:DR:1:MET:HB2 | 38:DR:2:ARG:H | 1.71 | 0.40 |
| 38:DR:96:ARG:HD3 | 38:DR:98:LEU:HD11 | 2.04 | 0.40 |
| 26:DA:2849:U:P | 40:DT:95:ARG:HH12 | 2.44 | 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%) | 208 (91%) | 13 (6%) | 8 (4%) | 3 | 5 |
| 2 | CB | 229/256 (90%) | 208 (91%) | 14 (6%) | 7 (3%) | 4 | 6 |
| 3 | AC | 204/239 (85%) | 193 (95%) | 10 (5%) | 1 (0%) | 29 | 52 |
| 3 | CC | 204/239 (85%) | 191 (94%) | 13 (6%) | 0 | 100 | 100 |
| 4 | AD | 206/209 (99%) | 197 (96%) | 9 (4%) | 0 | 100 | 100 |
| 4 | CD | 206/209 (99%) | 200 (97%) | 5 (2%) | 1 (0%) | 29 | 52 |
| 5 | AE | 146/162 (90%) | 142 (97%) | 4 (3%) | 0 | 100 | 100 |
| 5 | CE | 146/162 (90%) | 142 (97%) | 3 (2%) | 1 (1%) | 22 | 43 |
| 6 | AF | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 6 | CF | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 7 | AG | 153/156 (98%) | 149 (97%) | 3 (2%) | 1 (1%) | 22 | 43 |
| 7 | CG | 153/156 (98%) | 149 (97%) | 3 (2%) | 1 (1%) | 22 | 43 |
| 8 | AH | 135/138 (98%) | 133 (98%) | 2 (2%) | 0 | 100 | 100 |
| 8 | CH | 135/138 (98%) | 131 (97%) | 4 (3%) | 0 | 100 | 100 |
| 9 | AI | 125/128 (98%) | 119 (95%) | 5 (4%) | 1 (1%) | 19 | 39 |
| 9 | CI | 125/128 (98%) | 120 (96%) | 4 (3%) | 1 (1%) | 19 | 39 |
| 10 | AJ | 95/105 (90%) | 85 (90%) | 8 (8%) | 2 (2%) | 7 | 13 |
| 10 | CJ | 94/105 (90%) | 84 (89%) | 6 (6%) | 4 (4%) | 2 | 3 |
| 11 | AK | 112/129 (87%) | 107 (96%) | 4 (4%) | 1 (1%) | 17 | 35 |
| 11 | CK | 112/129 (87%) | 107 (96%) | 4 (4%) | 1 (1%) | 17 | 35 |
| 12 | AL | 120/132 (91%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 12 | CL | 120/132 (91%) | 117 (98%) | 2 (2%) | 1 (1%) | 19 | 39 |
| 13 | AM | 121/126 (96%) | 116 (96%) | 4 (3%) | 1 (1%) | 19 | 39 |
| 13 | CM | 120/126 (95%) | 113 (94%) | 4 (3%) | 3 (2%) | 5 | 9 |
| 14 | AN | 58/61 (95%) | 57 (98%) | 1 (2%) | 0 | 100 | 100 |
| 14 | CN | 58/61 (95%) | 57 (98%) | 1 (2%) | 0 | 100 | 100 |
| 15 | AO | 86/89 (97%) | 84 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | CO | 86/89 (97%) | 83 (96%) | 3 (4%) | 0 | 100 | 100 |
| 16 | AP | 80/88 (91%) | 78 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | CP | 80/88 (91%) | 78 (98%) | 1 (1%) | 1 (1%) | 12 | 24 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 17 | AQ | 97/105 (92%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 17 | CQ | 97/105 (92%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 18 | AR | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 18 | CR | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 19 | AS | 82/93 (88%) | 76 (93%) | 5 (6%) | 1 (1%) | 13 | 27 |
| 19 | CS | 81/93 (87%) | 75 (93%) | 6 (7%) | 0 | 100 | 100 |
| 20 | AT | 94/106 (89%) | 85 (90%) | 4 (4%) | 5 (5%) | 2 | 2 |
| 20 | CT | 94/106 (89%) | 85 (90%) | 4 (4%) | 5 (5%) | 2 | 2 |
| 21 | AU | 21/27 (78%) | 20 (95%) | 1 (5%) | 0 | 100 | 100 |
| 21 | CU | 21/27 (78%) | 21 (100%) | 0 | 0 | 100 | 100 |
| 28 | BD | 273/276 (99%) | 263 (96%) | 9 (3%) | 1 (0%) | 34 | 57 |
| 28 | DD | 273/276 (99%) | 261 (96%) | 10 (4%) | 2 (1%) | 22 | 43 |
| 29 | BE | 202/206 (98%) | 196 (97%) | 5 (2%) | 1 (0%) | 29 | 52 |
| 29 | DE | 202/206 (98%) | 196 (97%) | 5 (2%) | 1 (0%) | 29 | 52 |
| 30 | BF | 201/210 (96%) | 197 (98%) | 3 (2%) | 1 (0%) | 29 | 52 |
| 30 | DF | 201/210 (96%) | 197 (98%) | 3 (2%) | 1 (0%) | 29 | 52 |
| 31 | BG | 179/182 (98%) | 171 (96%) | 7 (4%) | 1 (1%) | 25 | 47 |
| 31 | DG | 179/182 (98%) | 168 (94%) | 8 (4%) | 3 (2%) | 9 | 18 |
| 32 | BH | 172/180 (96%) | 166 (96%) | 6 (4%) | 0 | 100 | 100 |
| 32 | DH | 172/180 (96%) | 166 (96%) | 6 (4%) | 0 | 100 | 100 |
| 33 | BI | 144/148 (97%) | 132 (92%) | 7 (5%) | 5 (4%) | 3 | 5 |
| 33 | DI | 144/148 (97%) | 135 (94%) | 8 (6%) | 1 (1%) | 22 | 43 |
| 34 | BN | 138/140 (99%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 34 | DN | 138/140 (99%) | 135 (98%) | 3 (2%) | 0 | 100 | 100 |
| 35 | BO | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 35 | DO | 120/122 (98%) | 115 (96%) | 5 (4%) | 0 | 100 | 100 |
| 36 | BP | 147/150 (98%) | 142 (97%) | 4 (3%) | 1 (1%) | 22 | 43 |
| 36 | DP | 147/150 (98%) | 139 (95%) | 6 (4%) | 2 (1%) | 11 | 22 |
| 37 | BQ | 139/141 (99%) | 135 (97%) | 4 (3%) | 0 | 100 | 100 |
| 37 | DQ | 139/141 (99%) | 134 (96%) | 4 (3%) | 1 (1%) | 22 | 43 |
| 38 | BR | 116/118 (98%) | 115 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 38 | DR | 116/118 (98%) | 114 (98%) | 2 (2%) | 0 | 100 | 100 |
| 39 | BS | 108/112 (96%) | 106 (98%) | 2 (2%) | 0 | 100 | 100 |
| 39 | DS | 108/112 (96%) | 107 (99%) | 0 | 1 (1%) | 17 | 35 |
| 40 | BT | 129/146 (88%) | 123 (95%) | 6 (5%) | 0 | 100 | 100 |
| 40 | DT | 129/146 (88%) | 126 (98%) | 3 (2%) | 0 | 100 | 100 |
| 41 | BU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 41 | DU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 42 | BV | 99/101 (98%) | 93 (94%) | 5 (5%) | 1 (1%) | 15 | 32 |
| 42 | DV | 99/101 (98%) | 96 (97%) | 2 (2%) | 1 (1%) | 15 | 32 |
| 43 | BW | 110/113 (97%) | 110 (100%) | 0 | 0 | 100 | 100 |
| 43 | DW | 110/113 (97%) | 110 (100%) | 0 | 0 | 100 | 100 |
| 44 | BX | 93/96 (97%) | 91 (98%) | 2 (2%) | 0 | 100 | 100 |
| 44 | DX | 93/96 (97%) | 91 (98%) | 1 (1%) | 1 (1%) | 14 | 30 |
| 45 | BY | 105/110 (96%) | 98 (93%) | 7 (7%) | 0 | 100 | 100 |
| 45 | DY | 105/110 (96%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 46 | BZ | 169/206 (82%) | 153 (90%) | 15 (9%) | 1 (1%) | 25 | 47 |
| 46 | DZ | 172/206 (84%) | 159 (92%) | 13 (8%) | 0 | 100 | 100 |
| 47 | B0 | 81/85 (95%) | 81 (100%) | 0 | 0 | 100 | 100 |
| 47 | D0 | 81/85 (95%) | 79 (98%) | 1 (1%) | 1 (1%) | 13 | 27 |
| 48 | B1 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 14 | 30 |
| 48 | D1 | 95/98 (97%) | 92 (97%) | 2 (2%) | 1 (1%) | 14 | 30 |
| 49 | B2 | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 49 | D2 | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 50 | B3 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 50 | D3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 51 | B4 | 67/71 (94%) | 54 (81%) | 9 (13%) | 4 (6%) | 1 | 1 |
| 51 | D4 | 67/71 (94%) | 53 (79%) | 11 (16%) | 3 (4%) | 2 | 3 |
| 52 | B5 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 52 | D5 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | B6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 53 | D6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 54 | B7 | 46/49 (94%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | D7 | 46/49 (94%) | 45 (98%) | 0 | 1 (2%) | 6 | 12 |
| 55 | B8 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 55 | D8 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 56 | B9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 56 | D9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| All | All | 11410/12128 (94%) | 10945 (96%) | 381 (3%) | 84 (1%) | 22 | 43 |

All (84) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 17 | PHE |
| 2 | AB | 19 | HIS |
| 2 | AB | 231 | GLU |
| 9 | AI | 54 | ASP |
| 10 | AJ | 56 | HIS |
| 28 | BD | 275 | LYS |
| 30 | BF | 130 | ALA |
| 33 | BI | 106 | GLY |
| 33 | BI | 107 | VAL |
| 48 | B1 | 3 | LYS |
| 51 | B4 | 53 | GLU |
| 51 | B4 | 62 | ARG |
| 2 | CB | 8 | LYS |
| 2 | CB | 16 | HIS |
| 2 | CB | 17 | PHE |
| 2 | CB | 123 | ALA |
| 2 | CB | 126 | GLU |
| 2 | CB | 231 | GLU |
| 9 | CI | 54 | ASP |
| 10 | CJ | 56 | HIS |
| 10 | CJ | 75 | ILE |
| 13 | CM | 67 | GLU |
| 13 | CM | 85 | GLY |
| 31 | DG | 14 | GLU |
| 51 | D4 | 39 | CYS |
| 51 | D4 | 45 | GLY |
| 51 | D4 | 62 | ARG |
| 54 | D7 | 46 | VAL |
| 2 | AB | 10 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 16 | HIS |
| 3 | AC | 66 | VAL |
| 7 | AG | 55 | GLY |
| 10 | AJ | 31 | GLY |
| 19 | AS | 84 | GLY |
| 20 | AT | 10 | LEU |
| 20 | AT | 47 | GLY |
| 20 | AT | 96 | GLY |
| 20 | AT | 100 | ILE |
| 33 | BI | 105 | HIS |
| 42 | BV | 79 | VAL |
| 51 | B4 | 47 | GLN |
| 2 | CB | 20 | GLU |
| 4 | CD | 46 | LYS |
| 5 | CE | 37 | ARG |
| 7 | CG | 55 | GLY |
| 10 | CJ | 78 | ASN |
| 20 | CT | 47 | GLY |
| 31 | DG | 81 | LYS |
| 42 | DV | 79 | VAL |
| 48 | D1 | 3 | LYS |
| 13 | AM | 67 | GLU |
| 29 | BE | 52 | LEU |
| 33 | BI | 10 | GLU |
| 10 | CJ | 55 | LYS |
| 20 | CT | 102 | GLY |
| 28 | DD | 239 | ARG |
| 31 | DG | 47 | LYS |
| 33 | DI | 10 | GLU |
| 39 | DS | 84 | GLN |
| 2 | AB | 125 | PRO |
| 11 | AK | 105 | VAL |
| 20 | CT | 10 | LEU |
| 28 | DD | 3 | VAL |
| 29 | DE | 52 | LEU |
| 36 | DP | 45 | LEU |
| 47 | D0 | 4 | LYS |
| 2 | AB | 11 | LEU |
| 31 | BG | 47 | LYS |
| 46 | BZ | 159 | PRO |
| 51 | B4 | 59 | PHE |
| 11 | CK | 105 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DF | 130 | ALA |
| 44 | DX | 2 | LYS |
| 33 | BI | 73 | GLU |
| 36 | BP | 29 | LYS |
| 36 | DP | 29 | LYS |
| 37 | DQ | 27 | VAL |
| 20 | AT | 102 | GLY |
| 16 | CP | 53 | VAL |
| 20 | CT | 100 | ILE |
| 13 | CM | 4 | ILE |
| 12 | CL | 30 | ALA |
| 20 | CT | 96 | GLY |
| 2 | AB | 234 | 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%) | 155 (81%) | 37 (19%) | 1 | 2 |
| 2 | CB | 187/220 (85%) | 151 (81%) | 36 (19%) | 1 | 2 |
| 3 | AC | 143/188 (76%) | 127 (89%) | 16 (11%) | 6 | 10 |
| 3 | CC | 141/188 (75%) | 116 (82%) | 25 (18%) | 2 | 3 |
| 4 | AD | 170/181 (94%) | 147 (86%) | 23 (14%) | 4 | 6 |
| 4 | CD | 174/181 (96%) | 147 (84%) | 27 (16%) | 2 | 4 |
| 5 | AE | 113/123 (92%) | 106 (94%) | 7 (6%) | 18 | 37 |
| 5 | CE | 114/123 (93%) | 99 (87%) | 15 (13%) | 4 | 7 |
| 6 | AF | 84/90 (93%) | 74 (88%) | 10 (12%) | 5 | 9 |
| 6 | CF | 86/90 (96%) | 79 (92%) | 7 (8%) | 11 | 23 |
| 7 | AG | 119/127 (94%) | 99 (83%) | 20 (17%) | 2 | 3 |
| 7 | CG | 120/127 (94%) | 106 (88%) | 14 (12%) | 5 | 10 |
| 8 | AH | 114/119 (96%) | 101 (89%) | 13 (11%) | 5 | 10 |
| 8 | CH | 114/119 (96%) | 97 (85%) | 17 (15%) | 3 | 5 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 9 | AI | 91/99 (92%) | 73 (80%) | 18 (20%) | 1 | 2 |
| 9 | CI | 89/99 (90%) | 69 (78%) | 20 (22%) | 1 | 1 |
| 10 | AJ | 66/92 (72%) | 60 (91%) | 6 (9%) | 9 | 18 |
| 10 | CJ | 69/92 (75%) | 61 (88%) | 8 (12%) | 5 | 10 |
| 11 | AK | 83/99 (84%) | 74 (89%) | 9 (11%) | 6 | 12 |
| 11 | CK | 83/99 (84%) | 72 (87%) | 11 (13%) | 4 | 7 |
| 12 | AL | 97/109 (89%) | 88 (91%) | 9 (9%) | 9 | 17 |
| 12 | CL | 97/109 (89%) | 85 (88%) | 12 (12%) | 4 | 8 |
| 13 | AM | 95/101 (94%) | 81 (85%) | 14 (15%) | 3 | 5 |
| 13 | CM | 92/101 (91%) | 74 (80%) | 18 (20%) | 1 | 2 |
| 14 | AN | 49/50 (98%) | 40 (82%) | 9 (18%) | 1 | 2 |
| 14 | CN | 49/50 (98%) | 37 (76%) | 12 (24%) | 0 | 1 |
| 15 | AO | 78/80 (98%) | 70 (90%) | 8 (10%) | 7 | 13 |
| 15 | CO | 78/80 (98%) | 67 (86%) | 11 (14%) | 3 | 6 |
| 16 | AP | 69/74 (93%) | 58 (84%) | 11 (16%) | 2 | 4 |
| 16 | CP | 68/74 (92%) | 59 (87%) | 9 (13%) | 4 | 7 |
| 17 | AQ | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 28 |
| 17 | CQ | 94/97 (97%) | 84 (89%) | 10 (11%) | 6 | 12 |
| 18 | AR | 59/77 (77%) | 50 (85%) | 9 (15%) | 2 | 4 |
| 18 | CR | 59/77 (77%) | 46 (78%) | 13 (22%) | 1 | 1 |
| 19 | AS | 70/80 (88%) | 59 (84%) | 11 (16%) | 2 | 4 |
| 19 | CS | 67/80 (84%) | 54 (81%) | 13 (19%) | 1 | 2 |
| 20 | AT | 70/82 (85%) | 60 (86%) | 10 (14%) | 3 | 5 |
| 20 | CT | 71/82 (87%) | 62 (87%) | 9 (13%) | 4 | 8 |
| 21 | AU | 18/22 (82%) | 15 (83%) | 3 (17%) | 2 | 3 |
| 21 | CU | 18/22 (82%) | 15 (83%) | 3 (17%) | 2 | 3 |
| 28 | BD | 215/218 (99%) | 196 (91%) | 19 (9%) | 10 | 19 |
| 28 | DD | 216/218 (99%) | 200 (93%) | 16 (7%) | 13 | 28 |
| 29 | BE | 164/166 (99%) | 145 (88%) | 19 (12%) | 5 | 10 |
| 29 | DE | 164/166 (99%) | 141 (86%) | 23 (14%) | 3 | 6 |
| 30 | BF | 160/166 (96%) | 142 (89%) | 18 (11%) | 6 | 10 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 30 | DF | 159/166 (96%) | 138 (87%) | 21 (13%) | 4 | 7 |
| 31 | BG | 143/156 (92%) | 127 (89%) | 16 (11%) | 6 | 10 |
| 31 | DG | 142/156 (91%) | 119 (84%) | 23 (16%) | 2 | 4 |
| 32 | BH | 144/148 (97%) | 129 (90%) | 15 (10%) | 7 | 13 |
| 32 | DH | 144/148 (97%) | 124 (86%) | 20 (14%) | 3 | 6 |
| 33 | BI | 110/124 (89%) | 88 (80%) | 22 (20%) | 1 | 2 |
| 33 | DI | 107/124 (86%) | 87 (81%) | 20 (19%) | 1 | 2 |
| 34 | BN | 118/119 (99%) | 101 (86%) | 17 (14%) | 3 | 5 |
| 34 | DN | 118/119 (99%) | 101 (86%) | 17 (14%) | 3 | 5 |
| 35 | BO | 100/100 (100%) | 92 (92%) | 8 (8%) | 12 | 24 |
| 35 | DO | 100/100 (100%) | 89 (89%) | 11 (11%) | 6 | 11 |
| 36 | BP | 116/116 (100%) | 104 (90%) | 12 (10%) | 7 | 13 |
| 36 | DP | 115/116 (99%) | 103 (90%) | 12 (10%) | 7 | 13 |
| 37 | BQ | 111/111 (100%) | 95 (86%) | 16 (14%) | 3 | 5 |
| 37 | DQ | 111/111 (100%) | 97 (87%) | 14 (13%) | 4 | 8 |
| 38 | BR | 101/101 (100%) | 83 (82%) | 18 (18%) | 2 | 3 |
| 38 | DR | 101/101 (100%) | 86 (85%) | 15 (15%) | 3 | 5 |
| 39 | BS | 87/88 (99%) | 79 (91%) | 8 (9%) | 9 | 17 |
| 39 | DS | 85/88 (97%) | 74 (87%) | 11 (13%) | 4 | 7 |
| 40 | BT | 115/127 (91%) | 107 (93%) | 8 (7%) | 15 | 30 |
| 40 | DT | 113/127 (89%) | 105 (93%) | 8 (7%) | 14 | 29 |
| 41 | BU | 93/94 (99%) | 86 (92%) | 7 (8%) | 13 | 27 |
| 41 | DU | 93/94 (99%) | 87 (94%) | 6 (6%) | 17 | 34 |
| 42 | BV | 80/82 (98%) | 70 (88%) | 10 (12%) | 4 | 8 |
| 42 | DV | 80/82 (98%) | 67 (84%) | 13 (16%) | 2 | 3 |
| 43 | BW | 90/92 (98%) | 83 (92%) | 7 (8%) | 12 | 25 |
| 43 | DW | 90/92 (98%) | 84 (93%) | 6 (7%) | 16 | 33 |
| 44 | BX | 77/78 (99%) | 72 (94%) | 5 (6%) | 17 | 34 |
| 44 | DX | 77/78 (99%) | 70 (91%) | 7 (9%) | 9 | 18 |
| 45 | BY | 85/91 (93%) | 77 (91%) | 8 (9%) | 8 | 17 |
| 45 | DY | 85/91 (93%) | 78 (92%) | 7 (8%) | 11 | 22 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 46 | BZ | 145/179 (81%) | 128 (88%) | 17 (12%) | 5 | 10 |
| 46 | DZ | 145/179 (81%) | 127 (88%) | 18 (12%) | 4 | 8 |
| 47 | B0 | 65/67 (97%) | 61 (94%) | 4 (6%) | 18 | 37 |
| 47 | D0 | 65/67 (97%) | 59 (91%) | 6 (9%) | 9 | 17 |
| 48 | B1 | 80/83 (96%) | 72 (90%) | 8 (10%) | 7 | 14 |
| 48 | D1 | 80/83 (96%) | 71 (89%) | 9 (11%) | 6 | 10 |
| 49 | B2 | 65/67 (97%) | 59 (91%) | 6 (9%) | 9 | 17 |
| 49 | D2 | 65/67 (97%) | 60 (92%) | 5 (8%) | 13 | 25 |
| 50 | B3 | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 25 |
| 50 | D3 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 39 |
| 51 | B4 | 60/63 (95%) | 51 (85%) | 9 (15%) | 3 | 5 |
| 51 | D4 | 53/63 (84%) | 38 (72%) | 15 (28%) | 0 | 1 |
| 52 | B5 | 50/52 (96%) | 46 (92%) | 4 (8%) | 12 | 24 |
| 52 | D5 | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 57 |
| 53 | B6 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 9 |
| 53 | D6 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 39 |
| 54 | B7 | 41/42 (98%) | 39 (95%) | 2 (5%) | 25 | 48 |
| 54 | D7 | 41/42 (98%) | 39 (95%) | 2 (5%) | 25 | 48 |
| 55 | B8 | 54/55 (98%) | 50 (93%) | 4 (7%) | 13 | 28 |
| 55 | D8 | 54/55 (98%) | 50 (93%) | 4 (7%) | 13 | 28 |
| 56 | B9 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 68 |
| 56 | D9 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 68 |
| All | All | 9336/10066 (93%) | 8180 (88%) | 1156 (12%) | 4 | 8 |

All (1156) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 7 | VAL |
| 2 | AB | 15 | VAL |
| 2 | AB | 17 | PHE |
| 2 | AB | 19 | HIS |
| 2 | AB | 20 | GLU |
| 2 | AB | 21 | ARG |
| 2 | AB | 24 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 35 | GLU |
| 2 | AB | 48 | MET |
| 2 | AB | 60 | ASP |
| 2 | AB | 64 | ARG |
| 2 | AB | 67 | THR |
| 2 | AB | 74 | LYS |
| 2 | AB | 76 | GLN |
| 2 | AB | 84 | GLU |
| 2 | AB | 94 | ASN |
| 2 | AB | 121 | LEU |
| 2 | AB | 127 | ILE |
| 2 | AB | 137 | ARG |
| 2 | AB | 144 | ARG |
| 2 | AB | 145 | LEU |
| 2 | AB | 153 | ARG |
| 2 | AB | 155 | LEU |
| 2 | AB | 156 | LYS |
| 2 | AB | 160 | ASP |
| 2 | AB | 170 | GLU |
| 2 | AB | 185 | ILE |
| 2 | AB | 187 | LEU |
| 2 | AB | 195 | ASP |
| 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 | 223 | ILE |
| 2 | AB | 230 | VAL |
| 3 | AC | 3 | ASN |
| 3 | AC | 8 | ILE |
| 3 | AC | 15 | THR |
| 3 | AC | 27 | LYS |
| 3 | AC | 45 | LYS |
| 3 | AC | 52 | LEU |
| 3 | AC | 77 | ILE |
| 3 | AC | 98 | ASN |
| 3 | AC | 101 | LEU |
| 3 | AC | 118 | GLN |
| 3 | AC | 131 | ARG |
| 3 | AC | 136 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 178 | LEU |
| 3 | AC | 179 | ARG |
| 3 | AC | 190 | ARG |
| 3 | AC | 195 | VAL |
| 4 | AD | 3 | ARG |
| 4 | AD | 5 | ILE |
| 4 | AD | 15 | GLU |
| 4 | AD | 19 | LEU |
| 4 | AD | 28 | SER |
| 4 | AD | 31 | CYS |
| 4 | AD | 49 | ARG |
| 4 | AD | 50 | ARG |
| 4 | AD | 58 | LEU |
| 4 | AD | 65 | ARG |
| 4 | AD | 86 | LYS |
| 4 | AD | 91 | SER |
| 4 | AD | 108 | LEU |
| 4 | AD | 112 | VAL |
| 4 | AD | 115 | ARG |
| 4 | AD | 127 | THR |
| 4 | AD | 135 | LEU |
| 4 | AD | 144 | ASP |
| 4 | AD | 155 | LEU |
| 4 | AD | 158 | ILE |
| 4 | AD | 168 | ARG |
| 4 | AD | 194 | LEU |
| 4 | AD | 196 | LEU |
| 5 | AE | 6 | PHE |
| 5 | AE | 10 | MET |
| 5 | AE | 12 | LEU |
| 5 | AE | 31 | LEU |
| 5 | AE | 41 | VAL |
| 5 | AE | 47 | LYS |
| 5 | AE | 151 | LEU |
| 6 | AF | 10 | LEU |
| 6 | AF | 17 | SER |
| 6 | AF | 28 | ARG |
| 6 | AF | 40 | VAL |
| 6 | AF | 45 | LEU |
| 6 | AF | 55 | ASP |
| 6 | AF | 61 | LEU |
| 6 | AF | 70 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | AF | 75 | LEU |
| 6 | AF | 82 | ARG |
| 7 | AG | 8 | GLU |
| 7 | AG | 12 | LEU |
| 7 | AG | 16 | LEU |
| 7 | AG | 24 | THR |
| 7 | AG | 31 | MET |
| 7 | AG | 38 | LEU |
| 7 | AG | 51 | GLN |
| 7 | AG | 61 | VAL |
| 7 | AG | 72 | ARG |
| 7 | AG | 73 | MET |
| 7 | AG | 76 | ARG |
| 7 | AG | 78 | ARG |
| 7 | AG | 79 | ARG |
| 7 | AG | 91 | VAL |
| 7 | AG | 97 | GLN |
| 7 | AG | 104 | LEU |
| 7 | AG | 113 | GLU |
| 7 | AG | 115 | ARG |
| 7 | AG | 138 | LYS |
| 7 | AG | 155 | ARG |
| 8 | AH | 25 | ASP |
| 8 | AH | 37 | ARG |
| 8 | AH | 39 | LEU |
| 8 | AH | 50 | ARG |
| 8 | AH | 52 | ASP |
| 8 | AH | 63 | LEU |
| 8 | AH | 78 | GLN |
| 8 | AH | 84 | ARG |
| 8 | AH | 91 | ARG |
| 8 | AH | 107 | LEU |
| 8 | AH | 112 | LEU |
| 8 | AH | 122 | ARG |
| 8 | AH | 137 | VAL |
| 9 | AI | 9 | ARG |
| 9 | AI | 11 | LYS |
| 9 | AI | 23 | ASN |
| 9 | AI | 42 | ARG |
| 9 | AI | 56 | LEU |
| 9 | AI | 64 | THR |
| 9 | AI | 65 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AI | 71 | SER |
| 9 | AI | 75 | ASP |
| 9 | AI | 78 | LYS |
| 9 | AI | 81 | ILE |
| 9 | AI | 89 | ASN |
| 9 | AI | 93 | ARG |
| 9 | AI | 102 | LEU |
| 9 | AI | 103 | THR |
| 9 | AI | 121 | ARG |
| 9 | AI | 127 | LYS |
| 9 | AI | 128 | ARG |
| 10 | AJ | 5 | ARG |
| 10 | AJ | 9 | ARG |
| 10 | AJ | 16 | LEU |
| 10 | AJ | 43 | ARG |
| 10 | AJ | 84 | GLN |
| 10 | AJ | 92 | THR |
| 11 | AK | 31 | THR |
| 11 | AK | 48 | ILE |
| 11 | AK | 51 | LYS |
| 11 | AK | 81 | ASP |
| 11 | AK | 87 | THR |
| 11 | AK | 91 | ARG |
| 11 | AK | 96 | ARG |
| 11 | AK | 106 | LYS |
| 11 | AK | 114 | VAL |
| 12 | AL | 16 | GLU |
| 12 | AL | 33 | ARG |
| 12 | AL | 47 | LYS |
| 12 | AL | 52 | LEU |
| 12 | AL | 54 | LYS |
| 12 | AL | 60 | LEU |
| 12 | AL | 67 | THR |
| 12 | AL | 83 | VAL |
| 12 | AL | 89 | ARG |
| 13 | AM | 3 | ARG |
| 13 | AM | 4 | ILE |
| 13 | AM | 15 | VAL |
| 13 | AM | 19 | LEU |
| 13 | AM | 43 | THR |
| 13 | AM | 46 | LYS |
| 13 | AM | 56 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | AM | 70 | LEU |
| 13 | AM | 73 | GLU |
| 13 | AM | 94 | ARG |
| 13 | AM | 98 | VAL |
| 13 | AM | 110 | ARG |
| 13 | AM | 115 | LYS |
| 13 | AM | 121 | LYS |
| 14 | AN | 3 | ARG |
| 14 | AN | 6 | LEU |
| 14 | AN | 7 | ILE |
| 14 | AN | 9 | LYS |
| 14 | AN | 12 | ARG |
| 14 | AN | 13 | THR |
| 14 | AN | 18 | VAL |
| 14 | AN | 32 | SER |
| 14 | AN | 50 | LYS |
| 15 | AO | 5 | LYS |
| 15 | AO | 7 | GLU |
| 15 | AO | 22 | THR |
| 15 | AO | 26 | GLU |
| 15 | AO | 38 | ARG |
| 15 | AO | 39 | LEU |
| 15 | AO | 76 | GLU |
| 15 | AO | 83 | GLU |
| 16 | AP | 1 | MET |
| 16 | AP | 5 | ARG |
| 16 | AP | 8 | ARG |
| 16 | AP | 19 | ILE |
| 16 | AP | 20 | VAL |
| 16 | AP | 50 | LYS |
| 16 | AP | 54 | GLU |
| 16 | AP | 60 | LEU |
| 16 | AP | 67 | THR |
| 16 | AP | 69 | THR |
| 16 | AP | 71 | ARG |
| 17 | AQ | 49 | GLU |
| 17 | AQ | 63 | ARG |
| 17 | AQ | 72 | ARG |
| 17 | AQ | 74 | LEU |
| 17 | AQ | 91 | ARG |
| 17 | AQ | 92 | ARG |
| 17 | AQ | 97 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | AR | 31 | LEU |
| 18 | AR | 35 | ARG |
| 18 | AR | 37 | VAL |
| 18 | AR | 38 | GLU |
| 18 | AR | 46 | GLU |
| 18 | AR | 55 | ARG |
| 18 | AR | 58 | LEU |
| 18 | AR | 68 | LYS |
| 18 | AR | 76 | LEU |
| 19 | AS | 5 | LEU |
| 19 | AS | 12 | ASP |
| 19 | AS | 17 | GLU |
| 19 | AS | 36 | ARG |
| 19 | AS | 37 | ARG |
| 19 | AS | 63 | THR |
| 19 | AS | 65 | ASN |
| 19 | AS | 70 | LYS |
| 19 | AS | 78 | ARG |
| 19 | AS | 81 | ARG |
| 19 | AS | 85 | LYS |
| 20 | AT | 8 | ARG |
| 20 | AT | 13 | LEU |
| 20 | AT | 19 | SER |
| 20 | AT | 24 | LEU |
| 20 | AT | 31 | SER |
| 20 | AT | 45 | GLN |
| 20 | AT | 58 | LYS |
| 20 | AT | 60 | GLU |
| 20 | AT | 62 | LEU |
| 20 | AT | 84 | LEU |
| 21 | AU | 9 | ARG |
| 21 | AU | 10 | ARG |
| 21 | AU | 24 | ARG |
| 28 | BD | 3 | VAL |
| 28 | BD | 22 | SER |
| 28 | BD | 32 | SER |
| 28 | BD | 38 | LYS |
| 28 | BD | 61 | LEU |
| 28 | BD | 71 | ASP |
| 28 | BD | 94 | LEU |
| 28 | BD | 99 | ASP |
| 28 | BD | 106 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BD | 116 | GLN |
| 28 | BD | 126 | GLN |
| 28 | BD | 211 | ARG |
| 28 | BD | 217 | ARG |
| 28 | BD | 221 | VAL |
| 28 | BD | 229 | VAL |
| 28 | BD | 242 | ARG |
| 28 | BD | 257 | LEU |
| 28 | BD | 259 | THR |
| 28 | BD | 260 | ARG |
| 29 | BE | 8 | LYS |
| 29 | BE | 9 | VAL |
| 29 | BE | 12 | THR |
| 29 | BE | 34 | VAL |
| 29 | BE | 47 | VAL |
| 29 | BE | 75 | VAL |
| 29 | BE | 77 | ILE |
| 29 | BE | 78 | LEU |
| 29 | BE | 82 | ARG |
| 29 | BE | 89 | ASP |
| 29 | BE | 116 | VAL |
| 29 | BE | 119 | ARG |
| 29 | BE | 127 | ASP |
| 29 | BE | 144 | ARG |
| 29 | BE | 154 | LYS |
| 29 | BE | 163 | GLU |
| 29 | BE | 175 | VAL |
| 29 | BE | 181 | LEU |
| 29 | BE | 184 | VAL |
| 30 | BF | 12 | LEU |
| 30 | BF | 19 | GLU |
| 30 | BF | 33 | LEU |
| 30 | BF | 43 | LYS |
| 30 | BF | 53 | THR |
| 30 | BF | 57 | VAL |
| 30 | BF | 74 | ARG |
| 30 | BF | 88 | VAL |
| 30 | BF | 106 | ARG |
| 30 | BF | 110 | LEU |
| 30 | BF | 125 | LEU |
| 30 | BF | 132 | VAL |
| 30 | BF | 140 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | BF | 162 | LEU |
| 30 | BF | 192 | LEU |
| 30 | BF | 197 | ASP |
| 30 | BF | 200 | GLU |
| 30 | BF | 201 | VAL |
| 31 | BG | 3 | LEU |
| 31 | BG | 7 | LEU |
| 31 | BG | 22 | ARG |
| 31 | BG | 43 | LEU |
| 31 | BG | 45 | GLU |
| 31 | BG | 49 | ASP |
| 31 | BG | 81 | LYS |
| 31 | BG | 82 | LEU |
| 31 | BG | 86 | MET |
| 31 | BG | 139 | LEU |
| 31 | BG | 143 | GLU |
| 31 | BG | 146 | TYR |
| 31 | BG | 159 | VAL |
| 31 | BG | 170 | ARG |
| 31 | BG | 175 | LEU |
| 31 | BG | 181 | ARG |
| 32 | BH | 2 | SER |
| 32 | BH | 6 | ARG |
| 32 | BH | 13 | LYS |
| 32 | BH | 45 | VAL |
| 32 | BH | 51 | ARG |
| 32 | BH | 69 | ARG |
| 32 | BH | 71 | LEU |
| 32 | BH | 76 | VAL |
| 32 | BH | 92 | ILE |
| 32 | BH | 98 | LEU |
| 32 | BH | 105 | LEU |
| 32 | BH | 116 | GLU |
| 32 | BH | 119 | GLU |
| 32 | BH | 122 | THR |
| 32 | BH | 124 | GLU |
| 33 | BI | 5 | LEU |
| 33 | BI | 9 | LEU |
| 33 | BI | 20 | ASP |
| 33 | BI | 38 | LEU |
| 33 | BI | 41 | GLU |
| 33 | BI | 43 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | BI | 47 | LEU |
| 33 | BI | 52 | ARG |
| 33 | BI | 58 | LEU |
| 33 | BI | 61 | ARG |
| 33 | BI | 62 | LYS |
| 33 | BI | 64 | GLU |
| 33 | BI | 66 | GLU |
| 33 | BI | 77 | LEU |
| 33 | BI | 78 | THR |
| 33 | BI | 86 | THR |
| 33 | BI | 92 | VAL |
| 33 | BI | 96 | ASP |
| 33 | BI | 101 | LEU |
| 33 | BI | 107 | VAL |
| 33 | BI | 116 | LEU |
| 33 | BI | 117 | GLU |
| 34 | BN | 1 | MET |
| 34 | BN | 5 | VAL |
| 34 | BN | 8 | GLN |
| 34 | BN | 9 | VAL |
| 34 | BN | 12 | ARG |
| 34 | BN | 28 | THR |
| 34 | BN | 33 | LEU |
| 34 | BN | 34 | LEU |
| 34 | BN | 48 | MET |
| 34 | BN | 61 | ARG |
| 34 | BN | 67 | LEU |
| 34 | BN | 68 | GLU |
| 34 | BN | 87 | LEU |
| 34 | BN | 99 | LEU |
| 34 | BN | 120 | LEU |
| 34 | BN | 138 | LEU |
| 34 | BN | 140 | VAL |
| 35 | BO | 8 | LEU |
| 35 | BO | 10 | VAL |
| 35 | BO | 18 | LYS |
| 35 | BO | 24 | VAL |
| 35 | BO | 66 | LYS |
| 35 | BO | 98 | VAL |
| 35 | BO | 105 | GLU |
| 35 | BO | 108 | GLU |
| 36 | BP | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | BP | 55 | ARG |
| 36 | BP | 59 | LEU |
| 36 | BP | 65 | ARG |
| 36 | BP | 95 | VAL |
| 36 | BP | 98 | GLU |
| 36 | BP | 101 | VAL |
| 36 | BP | 106 | LEU |
| 36 | BP | 112 | LEU |
| 36 | BP | 121 | LYS |
| 36 | BP | 144 | GLU |
| 36 | BP | 149 | GLU |
| 37 | BQ | 1 | MET |
| 37 | BQ | 7 | MET |
| 37 | BQ | 8 | LYS |
| 37 | BQ | 16 | ARG |
| 37 | BQ | 21 | THR |
| 37 | BQ | 22 | LYS |
| 37 | BQ | 45 | GLN |
| 37 | BQ | 54 | MET |
| 37 | BQ | 55 | VAL |
| 37 | BQ | 60 | ARG |
| 37 | BQ | 63 | LYS |
| 37 | BQ | 75 | THR |
| 37 | BQ | 80 | GLU |
| 37 | BQ | 85 | LYS |
| 37 | BQ | 109 | VAL |
| 37 | BQ | 110 | THR |
| 38 | BR | 1 | MET |
| 38 | BR | 18 | LEU |
| 38 | BR | 28 | LEU |
| 38 | BR | 29 | LEU |
| 38 | BR | 33 | ARG |
| 38 | BR | 36 | THR |
| 38 | BR | 44 | LEU |
| 38 | BR | 54 | LEU |
| 38 | BR | 60 | LEU |
| 38 | BR | 65 | LEU |
| 38 | BR | 67 | LEU |
| 38 | BR | 75 | LEU |
| 38 | BR | 79 | LEU |
| 38 | BR | 86 | ARG |
| 38 | BR | 100 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | BR | 102 | GLU |
| 38 | BR | 111 | LEU |
| 38 | BR | 114 | VAL |
| 39 | BS | 3 | ARG |
| 39 | BS | 20 | ARG |
| 39 | BS | 49 | VAL |
| 39 | BS | 52 | SER |
| 39 | BS | 59 | LYS |
| 39 | BS | 69 | VAL |
| 39 | BS | 73 | LEU |
| 39 | BS | 83 | LYS |
| 40 | BT | 28 | VAL |
| 40 | BT | 49 | VAL |
| 40 | BT | 53 | ARG |
| 40 | BT | 74 | ARG |
| 40 | BT | 78 | LEU |
| 40 | BT | 96 | ARG |
| 40 | BT | 118 | ARG |
| 40 | BT | 128 | GLU |
| 41 | BU | 8 | VAL |
| 41 | BU | 27 | LEU |
| 41 | BU | 31 | SER |
| 41 | BU | 74 | LEU |
| 41 | BU | 92 | ARG |
| 41 | BU | 95 | LEU |
| 41 | BU | 104 | GLN |
| 42 | BV | 21 | ARG |
| 42 | BV | 43 | GLU |
| 42 | BV | 46 | VAL |
| 42 | BV | 51 | VAL |
| 42 | BV | 52 | VAL |
| 42 | BV | 62 | LEU |
| 42 | BV | 72 | VAL |
| 42 | BV | 79 | VAL |
| 42 | BV | 95 | LEU |
| 42 | BV | 100 | ARG |
| 43 | BW | 4 | LYS |
| 43 | BW | 11 | ARG |
| 43 | BW | 15 | ARG |
| 43 | BW | 17 | VAL |
| 43 | BW | 51 | LEU |
| 43 | BW | 67 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | BW | 107 | LEU |
| 44 | BX | 2 | LYS |
| 44 | BX | 35 | THR |
| 44 | BX | 57 | LEU |
| 44 | BX | 65 | ARG |
| 44 | BX | 88 | LYS |
| 45 | BY | 1 | MET |
| 45 | BY | 7 | VAL |
| 45 | BY | 11 | ASP |
| 45 | BY | 23 | ARG |
| 45 | BY | 43 | ASN |
| 45 | BY | 55 | TYR |
| 45 | BY | 73 | ARG |
| 45 | BY | 99 | CYS |
| 46 | BZ | 5 | LEU |
| 46 | BZ | 18 | LEU |
| 46 | BZ | 19 | ARG |
| 46 | BZ | 50 | GLN |
| 46 | BZ | 76 | LEU |
| 46 | BZ | 91 | LEU |
| 46 | BZ | 102 | LEU |
| 46 | BZ | 107 | THR |
| 46 | BZ | 117 | LEU |
| 46 | BZ | 120 | ILE |
| 46 | BZ | 129 | SER |
| 46 | BZ | 131 | ARG |
| 46 | BZ | 136 | PHE |
| 46 | BZ | 153 | SER |
| 46 | BZ | 154 | ASP |
| 46 | BZ | 155 | LEU |
| 46 | BZ | 169 | GLU |
| 47 | B0 | 10 | THR |
| 47 | B0 | 20 | ARG |
| 47 | B0 | 55 | ARG |
| 47 | B0 | 74 | ARG |
| 48 | B1 | 3 | LYS |
| 48 | B1 | 21 | ARG |
| 48 | B1 | 23 | LYS |
| 48 | B1 | 35 | THR |
| 48 | B1 | 40 | ARG |
| 48 | B1 | 59 | THR |
| 48 | B1 | 78 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | B1 | 95 | LEU |
| 49 | B2 | 19 | VAL |
| 49 | B2 | 30 | ARG |
| 49 | B2 | 32 | LEU |
| 49 | B2 | 40 | SER |
| 49 | B2 | 55 | ARG |
| 49 | B2 | 70 | GLN |
| 50 | B3 | 3 | ARG |
| 50 | B3 | 8 | LEU |
| 50 | B3 | 23 | LEU |
| 50 | B3 | 54 | VAL |
| 51 | B4 | 3 | GLU |
| 51 | B4 | 34 | GLU |
| 51 | B4 | 46 | GLN |
| 51 | B4 | 49 | PHE |
| 51 | B4 | 56 | VAL |
| 51 | B4 | 58 | ARG |
| 51 | B4 | 63 | TYR |
| 51 | B4 | 66 | SER |
| 51 | B4 | 68 | ARG |
| 52 | B5 | 6 | VAL |
| 52 | B5 | 29 | THR |
| 52 | B5 | 40 | LYS |
| 52 | B5 | 55 | ARG |
| 53 | B6 | 4 | GLU |
| 53 | B6 | 6 | ARG |
| 53 | B6 | 14 | THR |
| 53 | B6 | 28 | ARG |
| 53 | B6 | 38 | LYS |
| 53 | B6 | 48 | VAL |
| 54 | B7 | 9 | ARG |
| 54 | B7 | 43 | THR |
| 55 | B8 | 6 | THR |
| 55 | B8 | 31 | HIS |
| 55 | B8 | 46 | ARG |
| 55 | B8 | 59 | LYS |
| 56 | B9 | 4 | ARG |
| 2 | CB | 8 | LYS |
| 2 | CB | 15 | VAL |
| 2 | CB | 19 | HIS |
| 2 | CB | 23 | ARG |
| 2 | CB | 24 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CB | 35 | GLU |
| 2 | CB | 50 | GLU |
| 2 | CB | 51 | LEU |
| 2 | CB | 60 | ASP |
| 2 | CB | 73 | THR |
| 2 | CB | 74 | LYS |
| 2 | CB | 76 | GLN |
| 2 | CB | 78 | GLN |
| 2 | CB | 87 | ARG |
| 2 | CB | 94 | ASN |
| 2 | CB | 97 | TRP |
| 2 | CB | 108 | ILE |
| 2 | CB | 115 | LEU |
| 2 | CB | 117 | GLU |
| 2 | CB | 119 | GLU |
| 2 | CB | 122 | PHE |
| 2 | CB | 124 | SER |
| 2 | CB | 126 | GLU |
| 2 | CB | 128 | GLU |
| 2 | CB | 139 | LYS |
| 2 | CB | 154 | LEU |
| 2 | CB | 155 | LEU |
| 2 | CB | 157 | ARG |
| 2 | CB | 158 | LEU |
| 2 | CB | 160 | ASP |
| 2 | CB | 185 | ILE |
| 2 | CB | 187 | LEU |
| 2 | CB | 200 | ILE |
| 2 | CB | 217 | ARG |
| 2 | CB | 224 | GLN |
| 2 | CB | 235 | SER |
| 3 | CC | 3 | ASN |
| 3 | CC | 15 | THR |
| 3 | CC | 17 | ASP |
| 3 | CC | 21 | ARG |
| 3 | CC | 33 | LEU |
| 3 | CC | 45 | LYS |
| 3 | CC | 47 | LEU |
| 3 | CC | 52 | LEU |
| 3 | CC | 54 | ARG |
| 3 | CC | 72 | LYS |
| 3 | CC | 85 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CC | 91 | LEU |
| 3 | CC | 98 | ASN |
| 3 | CC | 101 | LEU |
| 3 | CC | 104 | GLN |
| 3 | CC | 105 | GLU |
| 3 | CC | 115 | LEU |
| 3 | CC | 128 | PHE |
| 3 | CC | 131 | ARG |
| 3 | CC | 151 | VAL |
| 3 | CC | 152 | ILE |
| 3 | CC | 164 | ARG |
| 3 | CC | 179 | ARG |
| 3 | CC | 190 | ARG |
| 3 | CC | 195 | VAL |
| 4 | CD | 10 | ARG |
| 4 | CD | 15 | GLU |
| 4 | CD | 31 | CYS |
| 4 | CD | 34 | GLU |
| 4 | CD | 50 | ARG |
| 4 | CD | 58 | LEU |
| 4 | CD | 61 | LYS |
| 4 | CD | 65 | ARG |
| 4 | CD | 85 | LYS |
| 4 | CD | 86 | LYS |
| 4 | CD | 96 | LEU |
| 4 | CD | 107 | ARG |
| 4 | CD | 108 | LEU |
| 4 | CD | 122 | ARG |
| 4 | CD | 127 | THR |
| 4 | CD | 135 | LEU |
| 4 | CD | 145 | GLU |
| 4 | CD | 150 | GLU |
| 4 | CD | 155 | LEU |
| 4 | CD | 156 | GLU |
| 4 | CD | 169 | LYS |
| 4 | CD | 170 | VAL |
| 4 | CD | 181 | MET |
| 4 | CD | 184 | LYS |
| 4 | CD | 187 | ARG |
| 4 | CD | 194 | LEU |
| 4 | CD | 208 | SER |
| 5 | CE | 6 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CE | 10 | MET |
| 5 | CE | 12 | LEU |
| 5 | CE | 18 | ARG |
| 5 | CE | 27 | ARG |
| 5 | CE | 31 | LEU |
| 5 | CE | 41 | VAL |
| 5 | CE | 47 | LYS |
| 5 | CE | 60 | TYR |
| 5 | CE | 64 | ARG |
| 5 | CE | 78 | HIS |
| 5 | CE | 79 | GLU |
| 5 | CE | 117 | ASP |
| 5 | CE | 147 | ASP |
| 5 | CE | 150 | ARG |
| 6 | CF | 17 | SER |
| 6 | CF | 21 | LEU |
| 6 | CF | 27 | GLN |
| 6 | CF | 28 | ARG |
| 6 | CF | 45 | LEU |
| 6 | CF | 82 | ARG |
| 6 | CF | 87 | ARG |
| 7 | CG | 6 | ARG |
| 7 | CG | 12 | LEU |
| 7 | CG | 24 | THR |
| 7 | CG | 32 | ARG |
| 7 | CG | 36 | LYS |
| 7 | CG | 41 | ARG |
| 7 | CG | 51 | GLN |
| 7 | CG | 72 | ARG |
| 7 | CG | 76 | ARG |
| 7 | CG | 97 | GLN |
| 7 | CG | 104 | LEU |
| 7 | CG | 114 | ARG |
| 7 | CG | 115 | ARG |
| 7 | CG | 155 | ARG |
| 8 | CH | 3 | THR |
| 8 | CH | 25 | ASP |
| 8 | CH | 29 | SER |
| 8 | CH | 52 | ASP |
| 8 | CH | 63 | LEU |
| 8 | CH | 78 | GLN |
| 8 | CH | 84 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CH | 85 | ARG |
| 8 | CH | 91 | ARG |
| 8 | CH | 98 | LYS |
| 8 | CH | 103 | VAL |
| 8 | CH | 111 | ILE |
| 8 | CH | 112 | LEU |
| 8 | CH | 125 | ARG |
| 8 | CH | 127 | LEU |
| 8 | CH | 135 | CYS |
| 8 | CH | 137 | VAL |
| 9 | CI | 7 | THR |
| 9 | CI | 14 | VAL |
| 9 | CI | 23 | ASN |
| 9 | CI | 40 | LEU |
| 9 | CI | 51 | ARG |
| 9 | CI | 56 | LEU |
| 9 | CI | 64 | THR |
| 9 | CI | 65 | VAL |
| 9 | CI | 75 | ASP |
| 9 | CI | 81 | ILE |
| 9 | CI | 83 | ARG |
| 9 | CI | 88 | TYR |
| 9 | CI | 89 | ASN |
| 9 | CI | 102 | LEU |
| 9 | CI | 103 | THR |
| 9 | CI | 104 | ARG |
| 9 | CI | 121 | ARG |
| 9 | CI | 124 | GLN |
| 9 | CI | 125 | TYR |
| 9 | CI | 128 | ARG |
| 10 | CJ | 6 | ILE |
| 10 | CJ | 21 | GLN |
| 10 | CJ | 34 | VAL |
| 10 | CJ | 59 | SER |
| 10 | CJ | 67 | THR |
| 10 | CJ | 74 | ILE |
| 10 | CJ | 81 | THR |
| 10 | CJ | 98 | ILE |
| 11 | CK | 24 | SER |
| 11 | CK | 31 | THR |
| 11 | CK | 41 | THR |
| 11 | CK | 48 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | CK | 54 | ARG |
| 11 | CK | 92 | GLU |
| 11 | CK | 93 | GLN |
| 11 | CK | 96 | ARG |
| 11 | CK | 104 | GLN |
| 11 | CK | 123 | LYS |
| 11 | CK | 126 | ARG |
| 12 | CL | 33 | ARG |
| 12 | CL | 36 | VAL |
| 12 | CL | 39 | VAL |
| 12 | CL | 47 | LYS |
| 12 | CL | 60 | LEU |
| 12 | CL | 62 | SER |
| 12 | CL | 75 | HIS |
| 12 | CL | 83 | VAL |
| 12 | CL | 104 | VAL |
| 12 | CL | 114 | LYS |
| 12 | CL | 117 | ARG |
| 12 | CL | 124 | LYS |
| 13 | CM | 15 | VAL |
| 13 | CM | 19 | LEU |
| 13 | CM | 27 | LYS |
| 13 | CM | 29 | ARG |
| 13 | CM | 32 | GLU |
| 13 | CM | 44 | ARG |
| 13 | CM | 50 | GLU |
| 13 | CM | 52 | GLU |
| 13 | CM | 56 | LEU |
| 13 | CM | 63 | THR |
| 13 | CM | 66 | LEU |
| 13 | CM | 70 | LEU |
| 13 | CM | 71 | ARG |
| 13 | CM | 73 | GLU |
| 13 | CM | 84 | ILE |
| 13 | CM | 98 | VAL |
| 13 | CM | 105 | THR |
| 13 | CM | 121 | LYS |
| 14 | CN | 3 | ARG |
| 14 | CN | 7 | ILE |
| 14 | CN | 11 | LYS |
| 14 | CN | 13 | THR |
| 14 | CN | 15 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | CN | 17 | LYS |
| 14 | CN | 18 | VAL |
| 14 | CN | 22 | THR |
| 14 | CN | 23 | ARG |
| 14 | CN | 26 | ARG |
| 14 | CN | 32 | SER |
| 14 | CN | 46 | GLU |
| 15 | CO | 3 | ILE |
| 15 | CO | 4 | THR |
| 15 | CO | 5 | LYS |
| 15 | CO | 22 | THR |
| 15 | CO | 26 | GLU |
| 15 | CO | 38 | ARG |
| 15 | CO | 39 | LEU |
| 15 | CO | 48 | LYS |
| 15 | CO | 68 | ARG |
| 15 | CO | 83 | GLU |
| 15 | CO | 87 | ILE |
| 16 | CP | 1 | MET |
| 16 | CP | 2 | VAL |
| 16 | CP | 5 | ARG |
| 16 | CP | 20 | VAL |
| 16 | CP | 21 | VAL |
| 16 | CP | 60 | LEU |
| 16 | CP | 67 | THR |
| 16 | CP | 69 | THR |
| 16 | CP | 71 | ARG |
| 17 | CQ | 36 | ILE |
| 17 | CQ | 37 | LYS |
| 17 | CQ | 49 | GLU |
| 17 | CQ | 55 | ASP |
| 17 | CQ | 63 | ARG |
| 17 | CQ | 69 | LYS |
| 17 | CQ | 74 | LEU |
| 17 | CQ | 75 | ARG |
| 17 | CQ | 83 | ASP |
| 17 | CQ | 91 | ARG |
| 18 | CR | 25 | THR |
| 18 | CR | 26 | LEU |
| 18 | CR | 28 | GLU |
| 18 | CR | 32 | ARG |
| 18 | CR | 37 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | CR | 41 | LYS |
| 18 | CR | 42 | ARG |
| 18 | CR | 56 | THR |
| 18 | CR | 58 | LEU |
| 18 | CR | 68 | LYS |
| 18 | CR | 76 | LEU |
| 18 | CR | 84 | LYS |
| 18 | CR | 87 | ARG |
| 19 | CS | 5 | LEU |
| 19 | CS | 15 | LEU |
| 19 | CS | 22 | LEU |
| 19 | CS | 30 | LEU |
| 19 | CS | 56 | GLN |
| 19 | CS | 63 | THR |
| 19 | CS | 64 | GLU |
| 19 | CS | 65 | ASN |
| 19 | CS | 66 | MET |
| 19 | CS | 77 | THR |
| 19 | CS | 78 | ARG |
| 19 | CS | 81 | ARG |
| 19 | CS | 83 | HIS |
| 20 | CT | 8 | ARG |
| 20 | CT | 24 | LEU |
| 20 | CT | 45 | GLN |
| 20 | CT | 56 | MET |
| 20 | CT | 62 | LEU |
| 20 | CT | 71 | THR |
| 20 | CT | 80 | ARG |
| 20 | CT | 84 | LEU |
| 20 | CT | 93 | GLU |
| 21 | CU | 9 | ARG |
| 21 | CU | 10 | ARG |
| 21 | CU | 12 | LYS |
| 28 | DD | 61 | LEU |
| 28 | DD | 94 | LEU |
| 28 | DD | 99 | ASP |
| 28 | DD | 106 | ILE |
| 28 | DD | 113 | VAL |
| 28 | DD | 126 | GLN |
| 28 | DD | 134 | ARG |
| 28 | DD | 142 | VAL |
| 28 | DD | 211 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | DD | 221 | VAL |
| 28 | DD | 229 | VAL |
| 28 | DD | 242 | ARG |
| 28 | DD | 257 | LEU |
| 28 | DD | 259 | THR |
| 28 | DD | 260 | ARG |
| 28 | DD | 276 | LYS |
| 29 | DE | 7 | VAL |
| 29 | DE | 9 | VAL |
| 29 | DE | 12 | THR |
| 29 | DE | 21 | VAL |
| 29 | DE | 34 | VAL |
| 29 | DE | 38 | THR |
| 29 | DE | 40 | GLU |
| 29 | DE | 47 | VAL |
| 29 | DE | 52 | LEU |
| 29 | DE | 61 | ARG |
| 29 | DE | 73 | GLU |
| 29 | DE | 75 | VAL |
| 29 | DE | 82 | ARG |
| 29 | DE | 89 | ASP |
| 29 | DE | 116 | VAL |
| 29 | DE | 119 | ARG |
| 29 | DE | 144 | ARG |
| 29 | DE | 154 | LYS |
| 29 | DE | 163 | GLU |
| 29 | DE | 175 | VAL |
| 29 | DE | 181 | LEU |
| 29 | DE | 184 | VAL |
| 29 | DE | 195 | LEU |
| 30 | DF | 12 | LEU |
| 30 | DF | 17 | ARG |
| 30 | DF | 19 | GLU |
| 30 | DF | 20 | LEU |
| 30 | DF | 33 | LEU |
| 30 | DF | 53 | THR |
| 30 | DF | 57 | VAL |
| 30 | DF | 70 | THR |
| 30 | DF | 74 | ARG |
| 30 | DF | 88 | VAL |
| 30 | DF | 106 | ARG |
| 30 | DF | 110 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DF | 132 | VAL |
| 30 | DF | 135 | LYS |
| 30 | DF | 140 | LEU |
| 30 | DF | 152 | GLU |
| 30 | DF | 157 | VAL |
| 30 | DF | 183 | VAL |
| 30 | DF | 192 | LEU |
| 30 | DF | 201 | VAL |
| 30 | DF | 205 | ARG |
| 31 | DG | 7 | LEU |
| 31 | DG | 9 | ARG |
| 31 | DG | 16 | ARG |
| 31 | DG | 19 | LEU |
| 31 | DG | 31 | VAL |
| 31 | DG | 35 | GLU |
| 31 | DG | 43 | LEU |
| 31 | DG | 47 | LYS |
| 31 | DG | 49 | ASP |
| 31 | DG | 84 | LYS |
| 31 | DG | 97 | ASP |
| 31 | DG | 98 | ARG |
| 31 | DG | 111 | LEU |
| 31 | DG | 113 | ARG |
| 31 | DG | 115 | ARG |
| 31 | DG | 116 | ASP |
| 31 | DG | 136 | ARG |
| 31 | DG | 140 | ILE |
| 31 | DG | 143 | GLU |
| 31 | DG | 148 | MET |
| 31 | DG | 152 | LEU |
| 31 | DG | 164 | GLU |
| 31 | DG | 170 | ARG |
| 32 | DH | 3 | ARG |
| 32 | DH | 6 | ARG |
| 32 | DH | 33 | LEU |
| 32 | DH | 34 | GLU |
| 32 | DH | 41 | MET |
| 32 | DH | 42 | ARG |
| 32 | DH | 45 | VAL |
| 32 | DH | 49 | VAL |
| 32 | DH | 65 | HIS |
| 32 | DH | 69 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DH | 81 | GLU |
| 32 | DH | 95 | ARG |
| 32 | DH | 98 | LEU |
| 32 | DH | 111 | HIS |
| 32 | DH | 124 | GLU |
| 32 | DH | 136 | ILE |
| 32 | DH | 139 | GLN |
| 32 | DH | 148 | ILE |
| 32 | DH | 171 | LEU |
| 32 | DH | 172 | LYS |
| 33 | DI | 5 | LEU |
| 33 | DI | 9 | LEU |
| 33 | DI | 14 | ASP |
| 33 | DI | 15 | VAL |
| 33 | DI | 20 | ASP |
| 33 | DI | 38 | LEU |
| 33 | DI | 41 | GLU |
| 33 | DI | 43 | ASN |
| 33 | DI | 44 | LEU |
| 33 | DI | 57 | ARG |
| 33 | DI | 58 | LEU |
| 33 | DI | 75 | LEU |
| 33 | DI | 77 | LEU |
| 33 | DI | 78 | THR |
| 33 | DI | 86 | THR |
| 33 | DI | 102 | SER |
| 33 | DI | 114 | LEU |
| 33 | DI | 121 | LYS |
| 33 | DI | 135 | GLU |
| 33 | DI | 140 | LEU |
| 34 | DN | 5 | VAL |
| 34 | DN | 12 | ARG |
| 34 | DN | 28 | THR |
| 34 | DN | 33 | LEU |
| 34 | DN | 34 | LEU |
| 34 | DN | 38 | HIS |
| 34 | DN | 46 | VAL |
| 34 | DN | 48 | MET |
| 34 | DN | 62 | VAL |
| 34 | DN | 85 | ILE |
| 34 | DN | 87 | LEU |
| 34 | DN | 88 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DN | 89 | LYS |
| 34 | DN | 120 | LEU |
| 34 | DN | 137 | LYS |
| 34 | DN | 138 | LEU |
| 34 | DN | 140 | VAL |
| 35 | DO | 8 | LEU |
| 35 | DO | 9 | GLU |
| 35 | DO | 10 | VAL |
| 35 | DO | 24 | VAL |
| 35 | DO | 53 | LYS |
| 35 | DO | 66 | LYS |
| 35 | DO | 69 | ILE |
| 35 | DO | 70 | LYS |
| 35 | DO | 78 | ARG |
| 35 | DO | 92 | GLU |
| 35 | DO | 113 | LYS |
| 36 | DP | 15 | ARG |
| 36 | DP | 45 | LEU |
| 36 | DP | 55 | ARG |
| 36 | DP | 56 | SER |
| 36 | DP | 65 | ARG |
| 36 | DP | 95 | VAL |
| 36 | DP | 98 | GLU |
| 36 | DP | 106 | LEU |
| 36 | DP | 112 | LEU |
| 36 | DP | 121 | LYS |
| 36 | DP | 136 | GLU |
| 36 | DP | 144 | GLU |
| 37 | DQ | 1 | MET |
| 37 | DQ | 16 | ARG |
| 37 | DQ | 21 | THR |
| 37 | DQ | 45 | GLN |
| 37 | DQ | 48 | GLU |
| 37 | DQ | 55 | VAL |
| 37 | DQ | 56 | ARG |
| 37 | DQ | 60 | ARG |
| 37 | DQ | 75 | THR |
| 37 | DQ | 80 | GLU |
| 37 | DQ | 85 | LYS |
| 37 | DQ | 109 | VAL |
| 37 | DQ | 110 | THR |
| 37 | DQ | 133 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | DR | 1 | MET |
| 38 | DR | 18 | LEU |
| 38 | DR | 28 | LEU |
| 38 | DR | 29 | LEU |
| 38 | DR | 33 | ARG |
| 38 | DR | 36 | THR |
| 38 | DR | 44 | LEU |
| 38 | DR | 54 | LEU |
| 38 | DR | 60 | LEU |
| 38 | DR | 65 | LEU |
| 38 | DR | 75 | LEU |
| 38 | DR | 79 | LEU |
| 38 | DR | 86 | ARG |
| 38 | DR | 100 | LEU |
| 38 | DR | 111 | LEU |
| 39 | DS | 19 | LYS |
| 39 | DS | 20 | ARG |
| 39 | DS | 35 | ILE |
| 39 | DS | 44 | LYS |
| 39 | DS | 49 | VAL |
| 39 | DS | 52 | SER |
| 39 | DS | 58 | LEU |
| 39 | DS | 67 | ARG |
| 39 | DS | 73 | LEU |
| 39 | DS | 78 | LEU |
| 39 | DS | 83 | LYS |
| 40 | DT | 31 | SER |
| 40 | DT | 59 | THR |
| 40 | DT | 78 | LEU |
| 40 | DT | 85 | LYS |
| 40 | DT | 96 | ARG |
| 40 | DT | 98 | LYS |
| 40 | DT | 113 | LYS |
| 40 | DT | 118 | ARG |
| 41 | DU | 31 | SER |
| 41 | DU | 36 | ARG |
| 41 | DU | 74 | LEU |
| 41 | DU | 89 | GLU |
| 41 | DU | 92 | ARG |
| 41 | DU | 104 | GLN |
| 42 | DV | 15 | GLU |
| 42 | DV | 18 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | DV | 21 | ARG |
| 42 | DV | 24 | LYS |
| 42 | DV | 38 | LEU |
| 42 | DV | 46 | VAL |
| 42 | DV | 52 | VAL |
| 42 | DV | 57 | VAL |
| 42 | DV | 62 | LEU |
| 42 | DV | 72 | VAL |
| 42 | DV | 79 | VAL |
| 42 | DV | 95 | LEU |
| 42 | DV | 100 | ARG |
| 43 | DW | 4 | LYS |
| 43 | DW | 11 | ARG |
| 43 | DW | 17 | VAL |
| 43 | DW | 51 | LEU |
| 43 | DW | 60 | ASN |
| 43 | DW | 107 | LEU |
| 44 | DX | 44 | GLU |
| 44 | DX | 52 | VAL |
| 44 | DX | 57 | LEU |
| 44 | DX | 64 | LYS |
| 44 | DX | 66 | LEU |
| 44 | DX | 70 | LEU |
| 44 | DX | 92 | LEU |
| 45 | DY | 6 | HIS |
| 45 | DY | 23 | ARG |
| 45 | DY | 26 | LYS |
| 45 | DY | 43 | ASN |
| 45 | DY | 49 | VAL |
| 45 | DY | 91 | GLU |
| 45 | DY | 99 | CYS |
| 46 | DZ | 5 | LEU |
| 46 | DZ | 11 | GLU |
| 46 | DZ | 14 | LYS |
| 46 | DZ | 18 | LEU |
| 46 | DZ | 33 | LEU |
| 46 | DZ | 35 | ARG |
| 46 | DZ | 59 | LEU |
| 46 | DZ | 71 | VAL |
| 46 | DZ | 92 | SER |
| 46 | DZ | 97 | GLU |
| 46 | DZ | 100 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | DZ | 102 | LEU |
| 46 | DZ | 107 | THR |
| 46 | DZ | 120 | ILE |
| 46 | DZ | 131 | ARG |
| 46 | DZ | 136 | PHE |
| 46 | DZ | 154 | ASP |
| 46 | DZ | 157 | LEU |
| 47 | D0 | 19 | LYS |
| 47 | D0 | 20 | ARG |
| 47 | D0 | 24 | LYS |
| 47 | D0 | 55 | ARG |
| 47 | D0 | 68 | GLU |
| 47 | D0 | 74 | ARG |
| 48 | D1 | 3 | LYS |
| 48 | D1 | 4 | VAL |
| 48 | D1 | 21 | ARG |
| 48 | D1 | 40 | ARG |
| 48 | D1 | 59 | THR |
| 48 | D1 | 85 | LEU |
| 48 | D1 | 89 | GLU |
| 48 | D1 | 95 | LEU |
| 48 | D1 | 97 | LEU |
| 49 | D2 | 21 | LEU |
| 49 | D2 | 30 | ARG |
| 49 | D2 | 32 | LEU |
| 49 | D2 | 55 | ARG |
| 49 | D2 | 70 | GLN |
| 50 | D3 | 8 | LEU |
| 50 | D3 | 30 | ARG |
| 50 | D3 | 55 | ARG |
| 51 | D4 | 1 | MET |
| 51 | D4 | 3 | GLU |
| 51 | D4 | 5 | ILE |
| 51 | D4 | 8 | LYS |
| 51 | D4 | 10 | VAL |
| 51 | D4 | 13 | ARG |
| 51 | D4 | 14 | ILE |
| 51 | D4 | 23 | GLU |
| 51 | D4 | 31 | ILE |
| 51 | D4 | 56 | VAL |
| 51 | D4 | 58 | ARG |
| 51 | D4 | 61 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | D4 | 63 | TYR |
| 51 | D4 | 68 | ARG |
| 51 | D4 | 69 | LYS |
| 52 | D5 | 6 | VAL |
| 52 | D5 | 40 | LYS |
| 53 | D6 | 6 | ARG |
| 53 | D6 | 14 | THR |
| 53 | D6 | 38 | LYS |
| 54 | D7 | 1 | MET |
| 54 | D7 | 14 | LYS |
| 55 | D8 | 26 | LYS |
| 55 | D8 | 31 | HIS |
| 55 | D8 | 34 | TRP |
| 55 | D8 | 50 | LEU |
| 56 | D9 | 4 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 76 | GLN |
| 2 | AB | 94 | ASN |
| 3 | AC | 6 | HIS |
| 3 | AC | 28 | GLN |
| 3 | AC | 118 | GLN |
| 3 | AC | 162 | GLN |
| 3 | AC | 181 | ASN |
| 4 | AD | 42 | GLN |
| 4 | AD | 77 | ASN |
| 4 | AD | 123 | HIS |
| 5 | AE | 20 | GLN |
| 5 | AE | 38 | GLN |
| 5 | AE | 73 | ASN |
| 5 | AE | 141 | GLN |
| 6 | AF | 73 | ASN |
| 6 | AF | 94 | GLN |
| 6 | AF | 100 | ASN |
| 7 | AG | 28 | ASN |
| 7 | AG | 97 | GLN |
| 9 | AI | 23 | ASN |
| 9 | AI | 31 | GLN |
| 9 | AI | 58 | HIS |
| 9 | AI | 73 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AI | 89 | ASN |
| 9 | AI | 124 | GLN |
| 10 | AJ | 56 | HIS |
| 11 | AK | 104 | GLN |
| 12 | AL | 78 | GLN |
| 13 | AM | 92 | HIS |
| 15 | AO | 28 | GLN |
| 17 | AQ | 16 | GLN |
| 19 | AS | 23 | ASN |
| 19 | AS | 65 | ASN |
| 19 | AS | 69 | HIS |
| 20 | AT | 9 | ASN |
| 20 | AT | 26 | ASN |
| 20 | AT | 45 | GLN |
| 20 | AT | 73 | HIS |
| 28 | BD | 164 | GLN |
| 28 | BD | 166 | GLN |
| 28 | BD | 253 | GLN |
| 30 | BF | 8 | GLN |
| 30 | BF | 69 | HIS |
| 30 | BF | 169 | ASN |
| 30 | BF | 203 | GLN |
| 31 | BG | 40 | ASN |
| 33 | BI | 43 | ASN |
| 33 | BI | 105 | HIS |
| 34 | BN | 8 | GLN |
| 34 | BN | 133 | GLN |
| 36 | BP | 38 | GLN |
| 43 | BW | 60 | ASN |
| 44 | BX | 31 | HIS |
| 44 | BX | 82 | GLN |
| 45 | BY | 6 | HIS |
| 45 | BY | 92 | ASN |
| 46 | BZ | 34 | ASN |
| 51 | B4 | 46 | GLN |
| 56 | B9 | 36 | GLN |
| 2 | CB | 16 | HIS |
| 2 | CB | 40 | HIS |
| 2 | CB | 76 | GLN |
| 2 | CB | 94 | ASN |
| 2 | CB | 224 | GLN |
| 3 | CC | 3 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CC | 6 | HIS |
| 3 | CC | 28 | GLN |
| 3 | CC | 37 | GLN |
| 3 | CC | 104 | GLN |
| 3 | CC | 118 | GLN |
| 3 | CC | 123 | GLN |
| 4 | CD | 77 | ASN |
| 4 | CD | 123 | HIS |
| 4 | CD | 125 | HIS |
| 4 | CD | 161 | ASN |
| 5 | CE | 20 | GLN |
| 5 | CE | 141 | GLN |
| 6 | CF | 27 | GLN |
| 6 | CF | 73 | ASN |
| 6 | CF | 100 | ASN |
| 7 | CG | 28 | ASN |
| 8 | CH | 78 | GLN |
| 9 | CI | 23 | ASN |
| 9 | CI | 31 | GLN |
| 9 | CI | 58 | HIS |
| 9 | CI | 73 | GLN |
| 9 | CI | 89 | ASN |
| 9 | CI | 124 | GLN |
| 10 | CJ | 21 | GLN |
| 10 | CJ | 62 | HIS |
| 10 | CJ | 68 | HIS |
| 11 | CK | 93 | GLN |
| 12 | CL | 78 | GLN |
| 12 | CL | 99 | HIS |
| 13 | CM | 77 | ASN |
| 13 | CM | 92 | HIS |
| 14 | CN | 49 | HIS |
| 15 | CO | 28 | GLN |
| 16 | CP | 16 | HIS |
| 17 | CQ | 16 | GLN |
| 19 | CS | 69 | HIS |
| 20 | CT | 90 | GLN |
| 28 | DD | 164 | GLN |
| 28 | DD | 253 | GLN |
| 30 | DF | 69 | HIS |
| 30 | DF | 169 | ASN |
| 30 | DF | 203 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | DG | 40 | ASN |
| 31 | DG | 41 | GLN |
| 31 | DG | 108 | ASN |
| 33 | DI | 43 | ASN |
| 34 | DN | 8 | GLN |
| 36 | DP | 38 | GLN |
| 37 | DQ | 123 | HIS |
| 39 | DS | 68 | GLN |
| 40 | DT | 43 | GLN |
| 40 | DT | 58 | ASN |
| 42 | DV | 64 | HIS |
| 43 | DW | 60 | ASN |
| 44 | DX | 31 | HIS |
| 45 | DY | 43 | ASN |
| 46 | DZ | 55 | HIS |
| 46 | DZ | 151 | HIS |
| 47 | D0 | 35 | ASN |
| 49 | D2 | 38 | GLN |
| 50 | D3 | 32 | GLN |
| 56 | D9 | 36 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1494/1521 (98%) | 361 (24%) | 19 (1%) |
| 1 | CA | 1501/1521 (98%) | 370 (24%) | 25 (1%) |
| 22 | AV | 12/24 (50%) | 3 (25%) | 0 |
| 22 | CV | 11/24 (45%) | 3 (27%) | 0 |
| 23 | AW | 70/76 (92%) | 27 (38%) | 2 (2%) |
| 23 | CW | 67/76 (88%) | 26 (38%) | 3 (4%) |
| 24 | AX | 74/77 (96%) | 16 (21%) | 0 |
| 24 | CX | 74/77 (96%) | 23 (31%) | 0 |
| 25 | AY | 71/76 (93%) | 37 (52%) | 3 (4%) |
| 25 | CY | 69/76 (90%) | 36 (52%) | 1 (1%) |
| 26 | BA | 2812/2915 (96%) | 444 (15%) | 36 (1%) |
| 26 | DA | 2791/2915 (95%) | 563 (20%) | 24 (0%) |
| 27 | BB | 119/121 (98%) | 13 (10%) | 0 |
| 27 | DB | 119/121 (98%) | 38 (31%) | 0 |
| All | All | 9284/9620 (96%) | 1960 (21%) | 113 (1%) |

All (1960) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 5 | U |
| 1 | AA | 7 | G |
| 1 | AA | 9 | G |
| 1 | AA | 22 | G |
| 1 | AA | 29 | G |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 41 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |
| 1 | AA | 51 | A |
| 1 | AA | 55 | A |
| 1 | AA | 59 | A |
| 1 | AA | 61 | G |
| 1 | AA | 65 | U |
| 1 | AA | 77 | G |
| 1 | AA | 78 | G |
| 1 | AA | 79 | G |
| 1 | AA | 91 | C |
| 1 | AA | 96 | U |
| 1 | AA | 97 | G |
| 1 | AA | 98 | G |
| 1 | AA | 100 | C |
| 1 | AA | 101 | A |
| 1 | AA | 112 | G |
| 1 | AA | 115 | G |
| 1 | AA | 116 | A |
| 1 | AA | 121 | C |
| 1 | AA | 131 | C |
| 1 | AA | 140 | A |
| 1 | AA | 143 | A |
| 1 | AA | 154 | C |
| 1 | AA | 155 | C |
| 1 | AA | 163 | C |
| 1 | AA | 166 | G |
| 1 | AA | 169 | C |
| 1 | AA | 170 | U |
| 1 | AA | 172 | A |
| 1 | AA | 174 | C |
| 1 | AA | 180 | U |
| 1 | AA | 182 | U |
| 1 | AA | 189(C) | C |
| 1 | AA | 189(D) | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 189(F) | U |
| 1 | AA | 189(G) | G |
| 1 | AA | 189(H) | G |
| 1 | AA | 189(I) | G |
| 1 | AA | 189(K) | U |
| 1 | AA | 190 | U |
| 1 | AA | 195 | A |
| 1 | AA | 197 | A |
| 1 | AA | 202 | U |
| 1 | AA | 203 | U |
| 1 | AA | 204 | U |
| 1 | AA | 216 | G |
| 1 | AA | 243 | A |
| 1 | AA | 247 | G |
| 1 | AA | 251 | G |
| 1 | AA | 258 | G |
| 1 | AA | 266 | G |
| 1 | AA | 267 | C |
| 1 | AA | 270 | A |
| 1 | AA | 277 | C |
| 1 | AA | 289 | G |
| 1 | AA | 301 | G |
| 1 | AA | 321 | A |
| 1 | AA | 328 | C |
| 1 | AA | 332 | G |
| 1 | AA | 342 | C |
| 1 | AA | 346 | G |
| 1 | AA | 347 | G |
| 1 | AA | 348 | G |
| 1 | AA | 352 | C |
| 1 | AA | 353 | A |
| 1 | AA | 354 | G |
| 1 | AA | 355 | C |
| 1 | AA | 367 | U |
| 1 | AA | 372 | C |
| 1 | AA | 373 | A |
| 1 | AA | 396 | G |
| 1 | AA | 397 | A |
| 1 | AA | 398 | C |
| 1 | AA | 406 | G |
| 1 | AA | 409 | G |
| 1 | AA | 412 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 413 | G |
| 1 | AA | 421 | U |
| 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 | 457 | C |
| 1 | AA | 461 | A |
| 1 | AA | 470 | C |
| 1 | AA | 471 | G |
| 1 | AA | 477 | A |
| 1 | AA | 485 | G |
| 1 | AA | 496 | A |
| 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 | 544 | G |
| 1 | AA | 547 | A |
| 1 | AA | 559 | A |
| 1 | AA | 561 | U |
| 1 | AA | 564 | C |
| 1 | AA | 572 | A |
| 1 | AA | 573 | A |
| 1 | AA | 576 | G |
| 1 | AA | 581 | G |
| 1 | AA | 592 | G |
| 1 | AA | 593 | G |
| 1 | AA | 596 | C |
| 1 | AA | 617 | G |
| 1 | AA | 630 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 631 | G |
| 1 | AA | 633 | G |
| 1 | AA | 647 | C |
| 1 | AA | 653 | A |
| 1 | AA | 661 | G |
| 1 | AA | 665 | A |
| 1 | AA | 671 | G |
| 1 | AA | 673 | G |
| 1 | AA | 683 | G |
| 1 | AA | 687 | A |
| 1 | AA | 688 | G |
| 1 | AA | 693 | G |
| 1 | AA | 695 | A |
| 1 | AA | 705 | U |
| 1 | AA | 717 | C |
| 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 | 753 | A |
| 1 | AA | 755 | G |
| 1 | AA | 761 | 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 | 798 | G |
| 1 | AA | 815 | A |
| 1 | AA | 816 | A |
| 1 | AA | 817 | C |
| 1 | AA | 827 | U |
| 1 | AA | 828 | A |
| 1 | AA | 829 | G |
| 1 | AA | 832 | C |
| 1 | AA | 834 | C |
| 1 | AA | 840 | C |
| 1 | AA | 841 | U |
| 1 | AA | 848 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 851 | G |
| 1 | AA | 853 | G |
| 1 | AA | 855 | G |
| 1 | AA | 859 | A |
| 1 | AA | 874 | G |
| 1 | AA | 875 | C |
| 1 | AA | 885 | G |
| 1 | AA | 902 | G |
| 1 | AA | 914 | A |
| 1 | AA | 916 | G |
| 1 | AA | 922 | G |
| 1 | AA | 926 | G |
| 1 | AA | 927 | G |
| 1 | AA | 932 | C |
| 1 | AA | 934 | C |
| 1 | AA | 943 | U |
| 1 | AA | 957 | U |
| 1 | AA | 960 | U |
| 1 | AA | 961 | U |
| 1 | AA | 968 | A |
| 1 | AA | 969 | A |
| 1 | AA | 971 | G |
| 1 | AA | 973 | G |
| 1 | AA | 974 | A |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 979 | C |
| 1 | AA | 981 | U |
| 1 | AA | 989 | C |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 997 | U |
| 1 | AA | 1000 | U |
| 1 | AA | 1001 | A |
| 1 | AA | 1003 | G |
| 1 | AA | 1004 | A |
| 1 | AA | 1005 | A |
| 1 | AA | 1008 | C |
| 1 | AA | 1009 | G |
| 1 | AA | 1010 | G |
| 1 | AA | 1016 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1019 | C |
| 1 | AA | 1022 | G |
| 1 | AA | 1023 | G |
| 1 | AA | 1025 | U |
| 1 | AA | 1026 | G |
| 1 | AA | 1027 | C |
| 1 | AA | 1028 | C |
| 1 | AA | 1030(A) | G |
| 1 | AA | 1030(C) | G |
| 1 | AA | 1030(D) | A |
| 1 | AA | 1031 | G |
| 1 | AA | 1033 | G |
| 1 | AA | 1034 | G |
| 1 | AA | 1037 | C |
| 1 | AA | 1043 | C |
| 1 | AA | 1045 | C |
| 1 | AA | 1046 | A |
| 1 | AA | 1048 | G |
| 1 | AA | 1052 | U |
| 1 | AA | 1054 | C |
| 1 | AA | 1055 | A |
| 1 | AA | 1060 | C |
| 1 | AA | 1065 | U |
| 1 | AA | 1066 | C |
| 1 | AA | 1067 | A |
| 1 | AA | 1068 | G |
| 1 | AA | 1076 | C |
| 1 | AA | 1081 | G |
| 1 | AA | 1087 | G |
| 1 | AA | 1092 | A |
| 1 | AA | 1093 | A |
| 1 | AA | 1094 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1096 | C |
| 1 | AA | 1101 | A |
| 1 | AA | 1108 | G |
| 1 | AA | 1109 | C |
| 1 | AA | 1111 | A |
| 1 | AA | 1113 | C |
| 1 | AA | 1116 | C |
| 1 | AA | 1122 | U |
| 1 | AA | 1123 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1124 | G |
| 1 | AA | 1125 | U |
| 1 | AA | 1130 | A |
| 1 | AA | 1132 | C |
| 1 | AA | 1136 | U |
| 1 | AA | 1137 | C |
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1140 | C |
| 1 | AA | 1142 | G |
| 1 | AA | 1146 | A |
| 1 | AA | 1152 | A |
| 1 | AA | 1154 | G |
| 1 | AA | 1159 | U |
| 1 | AA | 1163 | C |
| 1 | AA | 1165 | C |
| 1 | AA | 1166 | G |
| 1 | AA | 1168 | A |
| 1 | AA | 1169 | A |
| 1 | AA | 1170 | A |
| 1 | AA | 1173 | G |
| 1 | AA | 1174 | G |
| 1 | AA | 1181 | G |
| 1 | AA | 1182 | G |
| 1 | AA | 1183 | A |
| 1 | AA | 1184 | G |
| 1 | AA | 1193 | G |
| 1 | AA | 1196 | U |
| 1 | AA | 1197 | G |
| 1 | AA | 1201 | A |
| 1 | AA | 1202 | G |
| 1 | AA | 1206 | G |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1218 | C |
| 1 | AA | 1227 | A |
| 1 | AA | 1228 | C |
| 1 | AA | 1235 | U |
| 1 | AA | 1236 | A |
| 1 | AA | 1238 | A |
| 1 | AA | 1240 | U |
| 1 | AA | 1242 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1246 | C |
| 1 | AA | 1253 | G |
| 1 | AA | 1256 | A |
| 1 | AA | 1257 | U |
| 1 | AA | 1258 | G |
| 1 | AA | 1260 | C |
| 1 | AA | 1270 | C |
| 1 | AA | 1273 | G |
| 1 | AA | 1275 | A |
| 1 | AA | 1276 | G |
| 1 | AA | 1278 | U |
| 1 | AA | 1279 | A |
| 1 | AA | 1280 | A |
| 1 | AA | 1282 | C |
| 1 | AA | 1286 | A |
| 1 | AA | 1287 | A |
| 1 | AA | 1289 | A |
| 1 | AA | 1290 | G |
| 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 | 1309 | G |
| 1 | AA | 1317 | C |
| 1 | AA | 1319 | A |
| 1 | AA | 1320 | C |
| 1 | AA | 1322 | C |
| 1 | AA | 1327 | C |
| 1 | AA | 1331 | G |
| 1 | AA | 1338 | G |
| 1 | AA | 1346 | A |
| 1 | AA | 1347 | G |
| 1 | AA | 1353 | G |
| 1 | AA | 1358 | U |
| 1 | AA | 1360 | A |
| 1 | AA | 1363 | C |
| 1 | AA | 1368 | G |
| 1 | AA | 1370 | G |
| 1 | AA | 1397 | C |
| 1 | AA | 1406 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1411 | C |
| 1 | AA | 1419 | 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 | 1475 | G |
| 1 | AA | 1487 | G |
| 1 | AA | 1491 | G |
| 1 | AA | 1492 | 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 |
| 22 | AV | 13 | A |
| 22 | AV | 19 | U |
| 22 | AV | 24 | A |
| 23 | AW | 3 | C |
| 23 | AW | 8 | 4SU |
| 23 | AW | 12 | U |
| 23 | AW | 13 | C |
| 23 | AW | 14 | A |
| 23 | AW | 15 | G |
| 23 | AW | 19 | G |
| 23 | AW | 20 | U |
| 23 | AW | 21 | A |
| 23 | AW | 23 | A |
| 23 | AW | 24 | G |
| 23 | AW | 35 | A |
| 23 | AW | 45 | U |
| 23 | AW | 46 | 7MG |
| 23 | AW | 47 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | AW | 48 | C |
| 23 | AW | 49 | C |
| 23 | AW | 50 | U |
| 23 | AW | 52 | G |
| 23 | AW | 61 | C |
| 23 | AW | 63 | G |
| 23 | AW | 64 | A |
| 23 | AW | 66 | U |
| 23 | AW | 68 | C |
| 23 | AW | 70 | G |
| 23 | AW | 73 | A |
| 23 | AW | 74 | C |
| 24 | AX | 6 | G |
| 24 | AX | 9 | G |
| 24 | AX | 14 | A |
| 24 | AX | 18 | G |
| 24 | AX | 19 | G |
| 24 | AX | 20 | U |
| 24 | AX | 21 | A |
| 24 | AX | 22 | G |
| 24 | AX | 42 | G |
| 24 | AX | 46 | G |
| 24 | AX | 47 | U |
| 24 | AX | 58 | A |
| 24 | AX | 59 | A |
| 24 | AX | 61 | C |
| 24 | AX | 67 | C |
| 24 | AX | 68 | C |
| 25 | AY | 2 | C |
| 25 | AY | 4 | C |
| 25 | AY | 5 | G |
| 25 | AY | 7 | A |
| 25 | AY | 9 | A |
| 25 | AY | 10 | G |
| 25 | AY | 11 | C |
| 25 | AY | 14 | A |
| 25 | AY | 19 | G |
| 25 | AY | 20 | U |
| 25 | AY | 21 | A |
| 25 | AY | 23 | A |
| 25 | AY | 25 | C |
| 25 | AY | 26 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | AY | 32 | PSU |
| 25 | AY | 34 | G |
| 25 | AY | 39 | PSU |
| 25 | AY | 41 | C |
| 25 | AY | 42 | C |
| 25 | AY | 44 | G |
| 25 | AY | 45 | U |
| 25 | AY | 46 | 7MG |
| 25 | AY | 47 | U |
| 25 | AY | 48 | C |
| 25 | AY | 49 | C |
| 25 | AY | 54 | 5MU |
| 25 | AY | 56 | C |
| 25 | AY | 57 | G |
| 25 | AY | 58 | A |
| 25 | AY | 59 | U |
| 25 | AY | 60 | U |
| 25 | AY | 61 | C |
| 25 | AY | 62 | C |
| 25 | AY | 67 | C |
| 25 | AY | 68 | C |
| 25 | AY | 69 | G |
| 25 | AY | 73 | A |
| 26 | BA | 10 | G |
| 26 | BA | 12 | U |
| 26 | BA | 13 | A |
| 26 | BA | 34 | C |
| 26 | BA | 45 | C |
| 26 | BA | 55 | G |
| 26 | BA | 64 | A |
| 26 | BA | 71 | A |
| 26 | BA | 72 | U |
| 26 | BA | 74 | A |
| 26 | BA | 75 | G |
| 26 | BA | 84 | A |
| 26 | BA | 100 | G |
| 26 | BA | 118 | A |
| 26 | BA | 119 | A |
| 26 | BA | 120 | U |
| 26 | BA | 149 | A |
| 26 | BA | 154 | G |
| 26 | BA | 154(A) | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | BA | 172 | C |
| 26 | BA | 182 | A |
| 26 | BA | 196 | A |
| 26 | BA | 199 | A |
| 26 | BA | 200 | U |
| 26 | BA | 205 | G |
| 26 | BA | 215 | G |
| 26 | BA | 216 | A |
| 26 | BA | 221 | A |
| 26 | BA | 222 | A |
| 26 | BA | 229 | A |
| 26 | BA | 232 | G |
| 26 | BA | 233 | A |
| 26 | BA | 248 | G |
| 26 | BA | 271(E) | U |
| 26 | BA | 271(I) | G |
| 26 | BA | 271(K) | U |
| 26 | BA | 271(L) | U |
| 26 | BA | 271(M) | G |
| 26 | BA | 271(N) | U |
| 26 | BA | 271(O) | C |
| 26 | BA | 271(S) | G |
| 26 | BA | 271(U) | G |
| 26 | BA | 272(B) | G |
| 26 | BA | 272(H) | C |
| 26 | BA | 272(I) | U |
| 26 | BA | 275 | G |
| 26 | BA | 279 | C |
| 26 | BA | 283 | A |
| 26 | BA | 294 | A |
| 26 | BA | 311 | A |
| 26 | BA | 329 | G |
| 26 | BA | 330 | A |
| 26 | BA | 352 | G |
| 26 | BA | 363 | G |
| 26 | BA | 363(B) | G |
| 26 | BA | 370 | G |
| 26 | BA | 372 | G |
| 26 | BA | 380 | U |
| 26 | BA | 386 | G |
| 26 | BA | 396 | G |
| 26 | BA | 407 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | BA | 411 | G |
| 26 | BA | 421 | U |
| 26 | BA | 428 | A |
| 26 | BA | 443 | A |
| 26 | BA | 444 | C |
| 26 | BA | 448 | U |
| 26 | BA | 451 | C |
| 26 | BA | 456 | C |
| 26 | BA | 457 | A |
| 26 | BA | 470 | A |
| 26 | BA | 481 | G |
| 26 | BA | 504 | U |
| 26 | BA | 505 | A |
| 26 | BA | 509 | C |
| 26 | BA | 512 | G |
| 26 | BA | 528 | A |
| 26 | BA | 530 | G |
| 26 | BA | 531 | C |
| 26 | BA | 532 | A |
| 26 | BA | 533 | G |
| 26 | BA | 545 | G |
| 26 | BA | 549 | G |
| 26 | BA | 563 | G |
| 26 | BA | 568 | U |
| 26 | BA | 573 | G |
| 26 | BA | 575 | A |
| 26 | BA | 586 | A |
| 26 | BA | 592 | G |
| 26 | BA | 603 | A |
| 26 | BA | 604 | G |
| 26 | BA | 607 | U |
| 26 | BA | 614(B) | G |
| 26 | BA | 615 | G |
| 26 | BA | 637 | A |
| 26 | BA | 645 | C |
| 26 | BA | 646 | A |
| 26 | BA | 652(D) | C |
| 26 | BA | 652(E) | G |
| 26 | BA | 652(T) | C |
| 26 | BA | 652(U) | G |
| 26 | BA | 669 | G |
| 26 | BA | 686 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | BA | 730 | C |
| 26 | BA | 740 | U |
| 26 | BA | 764 | A |
| 26 | BA | 775 | G |
| 26 | BA | 776 | G |
| 26 | BA | 782 | A |
| 26 | BA | 783 | A |
| 26 | BA | 784 | A |
| 26 | BA | 785 | G |
| 26 | BA | 792 | G |
| 26 | BA | 805 | G |
| 26 | BA | 812 | C |
| 26 | BA | 819 | A |
| 26 | BA | 827 | U |
| 26 | BA | 828 | U |
| 26 | BA | 830 | G |
| 26 | BA | 859 | G |
| 26 | BA | 866 | A |
| 26 | BA | 877 | U |
| 26 | BA | 880 | G |
| 26 | BA | 884 | C |
| 26 | BA | 885 | C |
| 26 | BA | 886 | C |
| 26 | BA | 887 | A |
| 26 | BA | 888 | C |
| 26 | BA | 889 | C |
| 26 | BA | 890 | A |
| 26 | BA | 892 | G |
| 26 | BA | 893 | C |
| 26 | BA | 894 | C |
| 26 | BA | 896 | A |
| 26 | BA | 897 | C |
| 26 | BA | 899 | A |
| 26 | BA | 900 | A |
| 26 | BA | 907 | U |
| 26 | BA | 910 | A |
| 26 | BA | 926 | A |
| 26 | BA | 932 | G |
| 26 | BA | 941 | A |
| 26 | BA | 945 | A |
| 26 | BA | 946 | G |
| 26 | BA | 958 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | BA | 959 | A |
| 26 | BA | 961 | C |
| 26 | BA | 974 | G |
| 26 | BA | 975 | C |
| 26 | BA | 983 | A |
| 26 | BA | 990 | A |
| 26 | BA | 996 | A |
| 26 | BA | 1012 | U |
| 26 | BA | 1013 | C |
| 26 | BA | 1022 | G |
| 26 | BA | 1025 | G |
| 26 | BA | 1026 | U |
| 26 | BA | 1033 | U |
| 26 | BA | 1038 | C |
| 26 | BA | 1045 | A |
| 26 | BA | 1046 | A |
| 26 | BA | 1047 | G |
| 26 | BA | 1048 | A |
| 26 | BA | 1051 | G |
| 26 | BA | 1107 | G |
| 26 | BA | 1110 | G |
| 26 | BA | 1112 | G |
| 26 | BA | 1128 | A |
| 26 | BA | 1130 | U |
| 26 | BA | 1135 | C |
| 26 | BA | 1136 | G |
| 26 | BA | 1139 | G |
| 26 | BA | 1170 | G |
| 26 | BA | 1171 | G |
| 26 | BA | 1173 | G |
| 26 | BA | 1174 | A |
| 26 | BA | 1175 | U |
| 26 | BA | 1176 | G |
| 26 | BA | 1177 | A |
| 26 | BA | 1210 | A |
| 26 | BA | 1211 | U |
| 26 | BA | 1220 | A |
| 26 | BA | 1244 | G |
| 26 | BA | 1253 | A |
| 26 | BA | 1256 | G |
| 26 | BA | 1271 | G |
| 26 | BA | 1272 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | BA | 1273 | U |
| 26 | BA | 1300 | U |
| 26 | BA | 1301 | A |
| 26 | BA | 1303 | G |
| 26 | BA | 1314 | C |
| 26 | BA | 1352 | U |
| 26 | BA | 1359 | A |
| 26 | BA | 1360 | A |
| 26 | BA | 1365 | A |
| 26 | BA | 1380 | G |
| 26 | BA | 1384 | A |
| 26 | BA | 1385 | G |
| 26 | BA | 1395 | A |
| 26 | BA | 1416 | G |
| 26 | BA | 1417 | C |
| 26 | BA | 1421 | G |
| 26 | BA | 1422 | G |
| 26 | BA | 1428 | C |
| 26 | BA | 1445 | A |
| 26 | BA | 1449 | A |
| 26 | BA | 1450 | G |
| 26 | BA | 1455 | G |
| 26 | BA | 1467 | C |
| 26 | BA | 1471 | A |
| 26 | BA | 1478 | G |
| 26 | BA | 1482 | G |
| 26 | BA | 1490 | A |
| 26 | BA | 1493 | C |
| 26 | BA | 1504 | C |
| 26 | BA | 1508 | A |
| 26 | BA | 1509 | C |
| 26 | BA | 1509(A) | A |
| 26 | BA | 1531 | C |
| 26 | BA | 1539 | G |
| 26 | BA | 1540 | U |
| 26 | BA | 1542 | A |
| 26 | BA | 1543 | C |
| 26 | BA | 1554 | A |
| 26 | BA | 1558 | A |
| 26 | BA | 1566 | A |
| 26 | BA | 1569 | A |
| 26 | BA | 1578 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | BA | 1580 | A |
| 26 | BA | 1581 | G |
| 26 | BA | 1584 | C |
| 26 | BA | 1586 | A |
| 26 | BA | 1608 | A |
| 26 | BA | 1610 | A |
| 26 | BA | 1648 | C |
| 26 | BA | 1654 | A |
| 26 | BA | 1674 | G |
| 26 | BA | 1696 | G |
| 26 | BA | 1700 | A |
| 26 | BA | 1701 | A |
| 26 | BA | 1703 | G |
| 26 | BA | 1722 | A |
| 26 | BA | 1739 | U |
| 26 | BA | 1746 | G |
| 26 | BA | 1756 | G |
| 26 | BA | 1762 | A |
| 26 | BA | 1763 | G |
| 26 | BA | 1764 | G |
| 26 | BA | 1773 | A |
| 26 | BA | 1780 | A |
| 26 | BA | 1791 | A |
| 26 | BA | 1800 | C |
| 26 | BA | 1816 | G |
| 26 | BA | 1828 | G |
| 26 | BA | 1839 | G |
| 26 | BA | 1847 | A |
| 26 | BA | 1858 | G |
| 26 | BA | 1861 | G |
| 26 | BA | 1878 | G |
| 26 | BA | 1889 | A |
| 26 | BA | 1900 | A |
| 26 | BA | 1906 | G |
| 26 | BA | 1919 | A |
| 26 | BA | 1927 | A |
| 26 | BA | 1929 | G |
| 26 | BA | 1930 | G |
| 26 | BA | 1937 | A |
| 26 | BA | 1938 | A |
| 26 | BA | 1955 | U |
| 26 | BA | 1963 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | BA | 1967 | C |
| 26 | BA | 1970 | A |
| 26 | BA | 1971 | A |
| 26 | BA | 1972 | A |
| 26 | BA | 1992 | G |
| 26 | BA | 1993 | U |
| 26 | BA | 1997 | G |
| 26 | BA | 2020 | A |
| 26 | BA | 2023 | G |
| 26 | BA | 2031 | A |
| 26 | BA | 2032 | G |
| 26 | BA | 2033 | A |
| 26 | BA | 2043 | C |
| 26 | BA | 2049 | G |
| 26 | BA | 2055 | C |
| 26 | BA | 2056 | G |
| 26 | BA | 2060 | A |
| 26 | BA | 2061 | G |
| 26 | BA | 2062 | A |
| 26 | BA | 2067 | G |
| 26 | BA | 2069 | G |
| 26 | BA | 2093 | G |
| 26 | BA | 2098 | U |
| 26 | BA | 2100 | G |
| 26 | BA | 2101 | G |
| 26 | BA | 2104 | G |
| 26 | BA | 2111 | C |
| 26 | BA | 2116 | G |
| 26 | BA | 2119 | A |
| 26 | BA | 2122 | U |
| 26 | BA | 2125 | G |
| 26 | BA | 2127 | G |
| 26 | BA | 2129 | C |
| 26 | BA | 2130 | U |
| 26 | BA | 2131 | G |
| 26 | BA | 2132 | U |
| 26 | BA | 2133 | G |
| 26 | BA | 2134 | A |
| 26 | BA | 2135 | A |
| 26 | BA | 2136 | C |
| 26 | BA | 2137 | C |
| 26 | BA | 2138 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | BA | 2140 | C |
| 26 | BA | 2141 | G |
| 26 | BA | 2142 | C |
| 26 | BA | 2143 | C |
| 26 | BA | 2145 | C |
| 26 | BA | 2147 | G |
| 26 | BA | 2151 | G |
| 26 | BA | 2152 | G |
| 26 | BA | 2153 | G |
| 26 | BA | 2155 | G |
| 26 | BA | 2157 | G |
| 26 | BA | 2158 | A |
| 26 | BA | 2159 | G |
| 26 | BA | 2160 | G |
| 26 | BA | 2161 | C |
| 26 | BA | 2163 | C |
| 26 | BA | 2164 | C |
| 26 | BA | 2165 | G |
| 26 | BA | 2166 | G |
| 26 | BA | 2167 | U |
| 26 | BA | 2168 | G |
| 26 | BA | 2169 | A |
| 26 | BA | 2171 | A |
| 26 | BA | 2172 | U |
| 26 | BA | 2174 | C |
| 26 | BA | 2175 | C |
| 26 | BA | 2178 | C |
| 26 | BA | 2181 | G |
| 26 | BA | 2182 | G |
| 26 | BA | 2183 | C |
| 26 | BA | 2184 | G |
| 26 | BA | 2188 | C |
| 26 | BA | 2189 | U |
| 26 | BA | 2191 | G |
| 26 | BA | 2198 | A |
| 26 | BA | 2199 | A |
| 26 | BA | 2206 | G |
| 26 | BA | 2207 | G |
| 26 | BA | 2208 | A |
| 26 | BA | 2218 | U |
| 26 | BA | 2225 | A |
| 26 | BA | 2238 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | BA | 2239 | G |
| 26 | BA | 2268 | A |
| 26 | BA | 2273 | A |
| 26 | BA | 2275 | C |
| 26 | BA | 2280 | G |
| 26 | BA | 2283 | C |
| 26 | BA | 2286 | A |
| 26 | BA | 2287 | A |
| 26 | BA | 2289 | G |
| 26 | BA | 2298 | A |
| 26 | BA | 2305 | A |
| 26 | BA | 2308 | G |
| 26 | BA | 2313 | C |
| 26 | BA | 2320 | A |
| 26 | BA | 2325 | G |
| 26 | BA | 2334 | G |
| 26 | BA | 2336 | A |
| 26 | BA | 2343 | C |
| 26 | BA | 2347 | C |
| 26 | BA | 2350 | C |
| 26 | BA | 2361 | A |
| 26 | BA | 2383 | G |
| 26 | BA | 2385 | C |
| 26 | BA | 2393 | A |
| 26 | BA | 2396 | G |
| 26 | BA | 2406 | U |
| 26 | BA | 2414 | G |
| 26 | BA | 2425 | A |
| 26 | BA | 2429 | G |
| 26 | BA | 2430 | A |
| 26 | BA | 2435 | A |
| 26 | BA | 2439 | A |
| 26 | BA | 2441 | C |
| 26 | BA | 2448 | A |
| 26 | BA | 2468 | G |
| 26 | BA | 2469 | A |
| 26 | BA | 2474 | C |
| 26 | BA | 2476 | A |
| 26 | BA | 2478 | A |
| 26 | BA | 2502 | G |
| 26 | BA | 2505 | G |
| 26 | BA | 2518 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | BA | 2529 | G |
| 26 | BA | 2554 | U |
| 26 | BA | 2566 | A |
| 26 | BA | 2567 | G |
| 26 | BA | 2573 | C |
| 26 | BA | 2582 | G |
| 26 | BA | 2602 | A |
| 26 | BA | 2609 | U |
| 26 | BA | 2611 | U |
| 26 | BA | 2612 | C |
| 26 | BA | 2629 | A |
| 26 | BA | 2630 | G |
| 26 | BA | 2654 | A |
| 26 | BA | 2689 | U |
| 26 | BA | 2690 | C |
| 26 | BA | 2691 | C |
| 26 | BA | 2703 | C |
| 26 | BA | 2712(A) | A |
| 26 | BA | 2713 | A |
| 26 | BA | 2714 | G |
| 26 | BA | 2726 | U |
| 26 | BA | 2733 | A |
| 26 | BA | 2757 | A |
| 26 | BA | 2758 | A |
| 26 | BA | 2764 | A |
| 26 | BA | 2765 | A |
| 26 | BA | 2766 | G |
| 26 | BA | 2778 | A |
| 26 | BA | 2790 | A |
| 26 | BA | 2791 | C |
| 26 | BA | 2793 | G |
| 26 | BA | 2802 | G |
| 26 | BA | 2808 | U |
| 26 | BA | 2818 | G |
| 26 | BA | 2820 | A |
| 26 | BA | 2821 | A |
| 26 | BA | 2824 | C |
| 26 | BA | 2833 | G |
| 26 | BA | 2835 | A |
| 26 | BA | 2872 | G |
| 26 | BA | 2873 | A |
| 26 | BA | 2874 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | BA | 2875 | C |
| 26 | BA | 2880 | C |
| 26 | BA | 2892 | A |
| 26 | BA | 2893 | G |
| 26 | BA | 2894 | G |
| 27 | BB | 2 | C |
| 27 | BB | 45 | A |
| 27 | BB | 52 | A |
| 27 | BB | 56 | G |
| 27 | BB | 73 | A |
| 27 | BB | 75 | G |
| 27 | BB | 85 | G |
| 27 | BB | 89 | G |
| 27 | BB | 106 | G |
| 27 | BB | 109 | C |
| 27 | BB | 110 | G |
| 27 | BB | 119 | G |
| 27 | BB | 120 | A |
| 1 | CA | 5 | U |
| 1 | CA | 6 | G |
| 1 | CA | 7 | G |
| 1 | CA | 9 | G |
| 1 | CA | 22 | G |
| 1 | CA | 29 | G |
| 1 | CA | 32 | A |
| 1 | CA | 39 | G |
| 1 | CA | 41 | G |
| 1 | CA | 47 | C |
| 1 | CA | 48 | C |
| 1 | CA | 51 | A |
| 1 | CA | 55 | A |
| 1 | CA | 59 | A |
| 1 | CA | 61 | G |
| 1 | CA | 65 | U |
| 1 | CA | 66 | G |
| 1 | CA | 70 | 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 |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 97 | G |
| 1 | CA | 98 | G |
| 1 | CA | 100 | C |
| 1 | CA | 101 | A |
| 1 | CA | 112 | G |
| 1 | CA | 116 | A |
| 1 | CA | 121 | C |
| 1 | CA | 131 | C |
| 1 | CA | 140 | A |
| 1 | CA | 142 | G |
| 1 | CA | 154 | C |
| 1 | CA | 155 | C |
| 1 | CA | 163 | C |
| 1 | CA | 166 | G |
| 1 | CA | 169 | C |
| 1 | CA | 170 | U |
| 1 | CA | 172 | A |
| 1 | CA | 174 | C |
| 1 | CA | 180 | U |
| 1 | CA | 182 | U |
| 1 | CA | 189(D) | C |
| 1 | CA | 189(F) | U |
| 1 | CA | 189(G) | G |
| 1 | CA | 189(H) | G |
| 1 | CA | 189(I) | G |
| 1 | CA | 189(K) | U |
| 1 | CA | 190 | U |
| 1 | CA | 195 | A |
| 1 | CA | 197 | A |
| 1 | CA | 201 | C |
| 1 | CA | 203 | U |
| 1 | CA | 204 | U |
| 1 | CA | 216 | G |
| 1 | CA | 243 | A |
| 1 | CA | 247 | G |
| 1 | CA | 251 | G |
| 1 | CA | 258 | G |
| 1 | CA | 266 | G |
| 1 | CA | 267 | C |
| 1 | CA | 270 | A |
| 1 | CA | 277 | C |
| 1 | CA | 289 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 301 | G |
| 1 | CA | 321 | A |
| 1 | CA | 328 | C |
| 1 | CA | 332 | G |
| 1 | CA | 342 | C |
| 1 | CA | 344 | A |
| 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 | 396 | G |
| 1 | CA | 398 | C |
| 1 | CA | 406 | G |
| 1 | CA | 409 | G |
| 1 | CA | 412 | A |
| 1 | CA | 413 | G |
| 1 | CA | 421 | U |
| 1 | CA | 424 | G |
| 1 | CA | 429 | U |
| 1 | CA | 430 | A |
| 1 | CA | 439 | A |
| 1 | CA | 442 | C |
| 1 | CA | 443 | C |
| 1 | CA | 452 | A |
| 1 | CA | 455 | C |
| 1 | CA | 457 | C |
| 1 | CA | 461 | A |
| 1 | CA | 471 | G |
| 1 | CA | 477 | A |
| 1 | CA | 485 | 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 |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 527 | G |
| 1 | CA | 531 | U |
| 1 | CA | 532 | A |
| 1 | CA | 533 | A |
| 1 | CA | 544 | G |
| 1 | CA | 547 | A |
| 1 | CA | 559 | A |
| 1 | CA | 561 | U |
| 1 | CA | 564 | C |
| 1 | CA | 572 | A |
| 1 | CA | 573 | A |
| 1 | CA | 576 | G |
| 1 | CA | 581 | G |
| 1 | CA | 592 | G |
| 1 | CA | 593 | G |
| 1 | CA | 596 | C |
| 1 | CA | 600 | C |
| 1 | CA | 617 | G |
| 1 | CA | 630 | G |
| 1 | CA | 631 | G |
| 1 | CA | 633 | G |
| 1 | CA | 647 | C |
| 1 | CA | 650 | G |
| 1 | CA | 653 | A |
| 1 | CA | 657 | G |
| 1 | CA | 661 | G |
| 1 | CA | 665 | A |
| 1 | CA | 671 | G |
| 1 | CA | 673 | G |
| 1 | CA | 683 | G |
| 1 | CA | 687 | A |
| 1 | CA | 688 | G |
| 1 | CA | 693 | G |
| 1 | CA | 695 | A |
| 1 | CA | 705 | U |
| 1 | CA | 717 | C |
| 1 | CA | 723 | U |
| 1 | CA | 724 | G |
| 1 | CA | 731 | G |
| 1 | CA | 749 | C |
| 1 | CA | 752 | G |
| 1 | CA | 753 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 755 | G |
| 1 | CA | 761 | 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 | 798 | G |
| 1 | CA | 815 | A |
| 1 | CA | 816 | A |
| 1 | CA | 817 | C |
| 1 | CA | 827 | U |
| 1 | CA | 828 | A |
| 1 | CA | 829 | G |
| 1 | CA | 833 | U |
| 1 | CA | 834 | C |
| 1 | CA | 840 | C |
| 1 | CA | 841 | U |
| 1 | CA | 848 | C |
| 1 | CA | 851 | G |
| 1 | CA | 853 | G |
| 1 | CA | 859 | A |
| 1 | CA | 874 | G |
| 1 | CA | 875 | C |
| 1 | CA | 885 | 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 | 932 | C |
| 1 | CA | 934 | C |
| 1 | CA | 943 | U |
| 1 | CA | 957 | U |
| 1 | CA | 960 | U |
| 1 | CA | 961 | U |
| 1 | CA | 968 | A |
| 1 | CA | 969 | A |
| 1 | CA | 971 | G |
| 1 | CA | 973 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 974 | A |
| 1 | CA | 975 | A |
| 1 | CA | 976 | G |
| 1 | CA | 977 | A |
| 1 | CA | 978 | A |
| 1 | CA | 979 | C |
| 1 | CA | 981 | U |
| 1 | CA | 989 | C |
| 1 | CA | 992 | U |
| 1 | CA | 993 | G |
| 1 | CA | 997 | U |
| 1 | CA | 999 | C |
| 1 | CA | 1001 | A |
| 1 | CA | 1002 | G |
| 1 | CA | 1003 | G |
| 1 | CA | 1004 | A |
| 1 | CA | 1005 | A |
| 1 | CA | 1006 | C |
| 1 | CA | 1009 | G |
| 1 | CA | 1010 | G |
| 1 | CA | 1016 | A |
| 1 | CA | 1019 | C |
| 1 | CA | 1022 | G |
| 1 | CA | 1023 | G |
| 1 | CA | 1024 | G |
| 1 | CA | 1025 | U |
| 1 | CA | 1026 | G |
| 1 | CA | 1027 | C |
| 1 | CA | 1028 | C |
| 1 | CA | 1029 | C |
| 1 | CA | 1030 | C |
| 1 | CA | 1030(A) | G |
| 1 | CA | 1030(B) | C |
| 1 | CA | 1030(C) | G |
| 1 | CA | 1031 | G |
| 1 | CA | 1033 | G |
| 1 | CA | 1034 | G |
| 1 | CA | 1037 | C |
| 1 | CA | 1038 | C |
| 1 | CA | 1039 | C |
| 1 | CA | 1041 | A |
| 1 | CA | 1043 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1045 | C |
| 1 | CA | 1046 | A |
| 1 | CA | 1050 | G |
| 1 | CA | 1052 | U |
| 1 | CA | 1053 | G |
| 1 | CA | 1054 | C |
| 1 | CA | 1060 | C |
| 1 | CA | 1065 | U |
| 1 | CA | 1066 | C |
| 1 | CA | 1068 | G |
| 1 | CA | 1076 | C |
| 1 | CA | 1081 | G |
| 1 | CA | 1087 | G |
| 1 | CA | 1092 | A |
| 1 | CA | 1093 | A |
| 1 | CA | 1094 | G |
| 1 | CA | 1095 | U |
| 1 | CA | 1096 | C |
| 1 | CA | 1100 | C |
| 1 | CA | 1101 | A |
| 1 | CA | 1108 | G |
| 1 | CA | 1109 | C |
| 1 | CA | 1111 | A |
| 1 | CA | 1116 | C |
| 1 | CA | 1122 | U |
| 1 | CA | 1124 | G |
| 1 | CA | 1125 | U |
| 1 | CA | 1127 | G |
| 1 | CA | 1129 | C |
| 1 | CA | 1130 | A |
| 1 | CA | 1132 | C |
| 1 | CA | 1136 | U |
| 1 | CA | 1137 | C |
| 1 | CA | 1138 | G |
| 1 | CA | 1139 | G |
| 1 | CA | 1140 | C |
| 1 | CA | 1142 | G |
| 1 | CA | 1146 | A |
| 1 | CA | 1147 | C |
| 1 | CA | 1152 | A |
| 1 | CA | 1154 | G |
| 1 | CA | 1159 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1163 | C |
| 1 | CA | 1165 | C |
| 1 | CA | 1166 | G |
| 1 | CA | 1168 | A |
| 1 | CA | 1169 | A |
| 1 | CA | 1170 | A |
| 1 | CA | 1174 | G |
| 1 | CA | 1176 | A |
| 1 | CA | 1182 | G |
| 1 | CA | 1183 | A |
| 1 | CA | 1184 | G |
| 1 | CA | 1193 | G |
| 1 | CA | 1196 | U |
| 1 | CA | 1197 | G |
| 1 | CA | 1202 | G |
| 1 | CA | 1206 | G |
| 1 | CA | 1211 | U |
| 1 | CA | 1212 | U |
| 1 | CA | 1213 | A |
| 1 | CA | 1218 | C |
| 1 | CA | 1227 | A |
| 1 | CA | 1228 | C |
| 1 | CA | 1235 | U |
| 1 | CA | 1236 | A |
| 1 | CA | 1238 | A |
| 1 | CA | 1240 | U |
| 1 | CA | 1242 | C |
| 1 | CA | 1246 | C |
| 1 | CA | 1253 | G |
| 1 | CA | 1256 | A |
| 1 | CA | 1257 | U |
| 1 | CA | 1258 | G |
| 1 | CA | 1260 | C |
| 1 | CA | 1262 | C |
| 1 | CA | 1273 | G |
| 1 | CA | 1275 | A |
| 1 | CA | 1276 | G |
| 1 | CA | 1278 | U |
| 1 | CA | 1279 | A |
| 1 | CA | 1280 | A |
| 1 | CA | 1281 | U |
| 1 | CA | 1282 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 1286 | A |
| 1 | CA | 1287 | A |
| 1 | CA | 1289 | A |
| 1 | CA | 1290 | G |
| 1 | CA | 1294 | G |
| 1 | CA | 1296 | C |
| 1 | CA | 1297 | C |
| 1 | CA | 1299 | A |
| 1 | CA | 1300 | G |
| 1 | CA | 1305 | G |
| 1 | CA | 1309 | G |
| 1 | CA | 1317 | C |
| 1 | CA | 1319 | A |
| 1 | CA | 1320 | C |
| 1 | CA | 1322 | C |
| 1 | CA | 1327 | C |
| 1 | CA | 1331 | G |
| 1 | CA | 1346 | A |
| 1 | CA | 1347 | G |
| 1 | CA | 1353 | G |
| 1 | CA | 1358 | U |
| 1 | CA | 1360 | A |
| 1 | CA | 1363 | C |
| 1 | CA | 1368 | G |
| 1 | CA | 1370 | G |
| 1 | CA | 1397 | C |
| 1 | CA | 1406 | U |
| 1 | CA | 1411 | C |
| 1 | CA | 1419 | G |
| 1 | CA | 1442 | G |
| 1 | CA | 1442(A) | G |
| 1 | CA | 1442(B) | A |
| 1 | CA | 1446 | U |
| 1 | CA | 1447 | A |
| 1 | CA | 1456 | G |
| 1 | CA | 1475 | G |
| 1 | CA | 1487 | G |
| 1 | CA | 1491 | G |
| 1 | CA | 1492 | A |
| 1 | CA | 1493 | A |
| 1 | CA | 1494 | G |
| 1 | CA | 1497 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1502 | A |
| 1 | CA | 1503 | A |
| 1 | CA | 1504 | G |
| 1 | CA | 1506 | U |
| 1 | CA | 1517 | G |
| 1 | CA | 1520 | G |
| 1 | CA | 1529 | G |
| 1 | CA | 1530 | G |
| 1 | CA | 1531 | A |
| 1 | CA | 1532 | U |
| 22 | CV | 14 | A |
| 22 | CV | 19 | U |
| 22 | CV | 24 | A |
| 23 | CW | 3 | C |
| 23 | CW | 8 | 4SU |
| 23 | CW | 9 | A |
| 23 | CW | 12 | U |
| 23 | CW | 13 | C |
| 23 | CW | 14 | A |
| 23 | CW | 15 | G |
| 23 | CW | 19 | G |
| 23 | CW | 22 | G |
| 23 | CW | 23 | A |
| 23 | CW | 35 | A |
| 23 | CW | 46 | 7MG |
| 23 | CW | 47 | U |
| 23 | CW | 48 | C |
| 23 | CW | 49 | C |
| 23 | CW | 50 | U |
| 23 | CW | 52 | G |
| 23 | CW | 61 | C |
| 23 | CW | 62 | C |
| 23 | CW | 63 | G |
| 23 | CW | 64 | A |
| 23 | CW | 66 | U |
| 23 | CW | 67 | C |
| 23 | CW | 68 | C |
| 23 | CW | 73 | A |
| 23 | CW | 74 | C |
| 24 | CX | 5 | G |
| 24 | CX | 6 | G |
| 24 | CX | 9 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | CX | 13 | C |
| 24 | CX | 15 | G |
| 24 | CX | 16 | C |
| 24 | CX | 18 | G |
| 24 | CX | 19 | G |
| 24 | CX | 20 | U |
| 24 | CX | 21 | A |
| 24 | CX | 22 | G |
| 24 | CX | 31 | G |
| 24 | CX | 47 | U |
| 24 | CX | 48 | C |
| 24 | CX | 52 | G |
| 24 | CX | 58 | A |
| 24 | CX | 59 | A |
| 24 | CX | 60 | U |
| 24 | CX | 62 | C |
| 24 | CX | 63 | G |
| 24 | CX | 64 | G |
| 24 | CX | 65 | C |
| 24 | CX | 68 | C |
| 25 | CY | 2 | C |
| 25 | CY | 7 | A |
| 25 | CY | 9 | A |
| 25 | CY | 10 | G |
| 25 | CY | 11 | C |
| 25 | CY | 14 | A |
| 25 | CY | 15 | G |
| 25 | CY | 19 | G |
| 25 | CY | 23 | A |
| 25 | CY | 25 | C |
| 25 | CY | 26 | A |
| 25 | CY | 32 | PSU |
| 25 | CY | 33 | U |
| 25 | CY | 34 | G |
| 25 | CY | 39 | PSU |
| 25 | CY | 41 | C |
| 25 | CY | 42 | C |
| 25 | CY | 45 | U |
| 25 | CY | 46 | 7MG |
| 25 | CY | 47 | U |
| 25 | CY | 49 | C |
| 25 | CY | 52 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | CY | 54 | 5MU |
| 25 | CY | 55 | PSU |
| 25 | CY | 56 | C |
| 25 | CY | 57 | G |
| 25 | CY | 58 | A |
| 25 | CY | 59 | U |
| 25 | CY | 61 | C |
| 25 | CY | 62 | C |
| 25 | CY | 65 | G |
| 25 | CY | 67 | C |
| 25 | CY | 68 | C |
| 25 | CY | 69 | G |
| 25 | CY | 70 | G |
| 25 | CY | 73 | A |
| 26 | DA | 10 | G |
| 26 | DA | 12 | U |
| 26 | DA | 13 | A |
| 26 | DA | 15 | G |
| 26 | DA | 34 | C |
| 26 | DA | 35 | G |
| 26 | DA | 45 | C |
| 26 | DA | 59 | U |
| 26 | DA | 71 | A |
| 26 | DA | 74 | A |
| 26 | DA | 75 | G |
| 26 | DA | 79 | G |
| 26 | DA | 83 | G |
| 26 | DA | 84 | A |
| 26 | DA | 90 | U |
| 26 | DA | 94 | C |
| 26 | DA | 100 | G |
| 26 | DA | 102 | G |
| 26 | DA | 118 | A |
| 26 | DA | 119 | A |
| 26 | DA | 120 | U |
| 26 | DA | 125 | G |
| 26 | DA | 140 | G |
| 26 | DA | 141 | A |
| 26 | DA | 154(A) | C |
| 26 | DA | 157 | U |
| 26 | DA | 173 | G |
| 26 | DA | 181 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | DA | 182 | A |
| 26 | DA | 196 | A |
| 26 | DA | 199 | A |
| 26 | DA | 205 | G |
| 26 | DA | 214 | G |
| 26 | DA | 215 | G |
| 26 | DA | 216 | A |
| 26 | DA | 221 | A |
| 26 | DA | 222 | A |
| 26 | DA | 228 | A |
| 26 | DA | 229 | A |
| 26 | DA | 232 | G |
| 26 | DA | 233 | A |
| 26 | DA | 248 | G |
| 26 | DA | 266 | G |
| 26 | DA | 271 | A |
| 26 | DA | 271(D) | G |
| 26 | DA | 271(I) | G |
| 26 | DA | 271(J) | C |
| 26 | DA | 271(L) | U |
| 26 | DA | 271(M) | G |
| 26 | DA | 271(N) | U |
| 26 | DA | 271(O) | C |
| 26 | DA | 272(A) | U |
| 26 | DA | 272(B) | G |
| 26 | DA | 274 | G |
| 26 | DA | 277 | C |
| 26 | DA | 278 | A |
| 26 | DA | 292 | C |
| 26 | DA | 293 | U |
| 26 | DA | 294 | A |
| 26 | DA | 311 | A |
| 26 | DA | 324 | A |
| 26 | DA | 327 | G |
| 26 | DA | 329 | G |
| 26 | DA | 330 | A |
| 26 | DA | 333 | G |
| 26 | DA | 338 | G |
| 26 | DA | 342 | G |
| 26 | DA | 352 | G |
| 26 | DA | 353 | G |
| 26 | DA | 354 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | DA | 362 | U |
| 26 | DA | 363 | G |
| 26 | DA | 363(A) | A |
| 26 | DA | 363(C) | G |
| 26 | DA | 364 | C |
| 26 | DA | 372 | G |
| 26 | DA | 380 | U |
| 26 | DA | 386 | G |
| 26 | DA | 389 | G |
| 26 | DA | 396 | G |
| 26 | DA | 405 | U |
| 26 | DA | 406 | G |
| 26 | DA | 411 | G |
| 26 | DA | 412 | A |
| 26 | DA | 428 | A |
| 26 | DA | 442 | G |
| 26 | DA | 443 | A |
| 26 | DA | 444 | C |
| 26 | DA | 454 | A |
| 26 | DA | 455 | C |
| 26 | DA | 457 | A |
| 26 | DA | 470 | A |
| 26 | DA | 479 | A |
| 26 | DA | 481 | G |
| 26 | DA | 504 | U |
| 26 | DA | 505 | A |
| 26 | DA | 508 | G |
| 26 | DA | 509 | C |
| 26 | DA | 512 | G |
| 26 | DA | 521 | G |
| 26 | DA | 528 | A |
| 26 | DA | 529 | A |
| 26 | DA | 530 | G |
| 26 | DA | 531 | C |
| 26 | DA | 532 | A |
| 26 | DA | 533 | G |
| 26 | DA | 545 | G |
| 26 | DA | 563 | G |
| 26 | DA | 568 | U |
| 26 | DA | 573 | G |
| 26 | DA | 575 | A |
| 26 | DA | 586 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | DA | 588 | U |
| 26 | DA | 592 | G |
| 26 | DA | 599 | G |
| 26 | DA | 603 | A |
| 26 | DA | 604 | G |
| 26 | DA | 607 | U |
| 26 | DA | 614(B) | G |
| 26 | DA | 614(C) | A |
| 26 | DA | 615 | G |
| 26 | DA | 616 | G |
| 26 | DA | 627 | A |
| 26 | DA | 637 | A |
| 26 | DA | 645 | C |
| 26 | DA | 646 | A |
| 26 | DA | 651 | G |
| 26 | DA | 652(A) | A |
| 26 | DA | 652(B) | A |
| 26 | DA | 652(C) | G |
| 26 | DA | 652(U) | G |
| 26 | DA | 669 | G |
| 26 | DA | 686 | G |
| 26 | DA | 715 | G |
| 26 | DA | 717 | G |
| 26 | DA | 726 | G |
| 26 | DA | 730 | C |
| 26 | DA | 753 | C |
| 26 | DA | 765 | G |
| 26 | DA | 774 | A |
| 26 | DA | 775 | G |
| 26 | DA | 776 | G |
| 26 | DA | 782 | A |
| 26 | DA | 783 | A |
| 26 | DA | 784 | A |
| 26 | DA | 785 | G |
| 26 | DA | 792 | G |
| 26 | DA | 805 | G |
| 26 | DA | 812 | C |
| 26 | DA | 819 | A |
| 26 | DA | 827 | U |
| 26 | DA | 828 | U |
| 26 | DA | 847 | U |
| 26 | DA | 854 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | DA | 857 | C |
| 26 | DA | 859 | G |
| 26 | DA | 866 | A |
| 26 | DA | 867 | C |
| 26 | DA | 872 | A |
| 26 | DA | 874 | G |
| 26 | DA | 879 | G |
| 26 | DA | 880 | G |
| 26 | DA | 882 | G |
| 26 | DA | 884 | C |
| 26 | DA | 886 | C |
| 26 | DA | 887 | A |
| 26 | DA | 889 | C |
| 26 | DA | 890 | A |
| 26 | DA | 893 | C |
| 26 | DA | 896 | A |
| 26 | DA | 897 | C |
| 26 | DA | 898 | C |
| 26 | DA | 900 | A |
| 26 | DA | 901 | A |
| 26 | DA | 902 | C |
| 26 | DA | 903 | C |
| 26 | DA | 910 | A |
| 26 | DA | 911 | A |
| 26 | DA | 917 | A |
| 26 | DA | 923 | C |
| 26 | DA | 932 | G |
| 26 | DA | 933 | A |
| 26 | DA | 936 | C |
| 26 | DA | 938 | G |
| 26 | DA | 941 | A |
| 26 | DA | 943 | U |
| 26 | DA | 945 | A |
| 26 | DA | 946 | G |
| 26 | DA | 953 | A |
| 26 | DA | 958 | U |
| 26 | DA | 959 | A |
| 26 | DA | 961 | C |
| 26 | DA | 974 | G |
| 26 | DA | 975 | C |
| 26 | DA | 980 | A |
| 26 | DA | 983 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | DA | 996 | A |
| 26 | DA | 1005 | C |
| 26 | DA | 1006 | C |
| 26 | DA | 1012 | U |
| 26 | DA | 1013 | C |
| 26 | DA | 1018 | C |
| 26 | DA | 1020 | A |
| 26 | DA | 1021 | A |
| 26 | DA | 1022 | G |
| 26 | DA | 1025 | G |
| 26 | DA | 1026 | U |
| 26 | DA | 1033 | U |
| 26 | DA | 1034 | G |
| 26 | DA | 1038 | C |
| 26 | DA | 1039 | G |
| 26 | DA | 1042 | G |
| 26 | DA | 1043 | C |
| 26 | DA | 1113 | U |
| 26 | DA | 1114 | G |
| 26 | DA | 1116 | C |
| 26 | DA | 1121 | C |
| 26 | DA | 1126 | A |
| 26 | DA | 1128 | A |
| 26 | DA | 1129 | A |
| 26 | DA | 1130 | U |
| 26 | DA | 1135 | C |
| 26 | DA | 1136 | G |
| 26 | DA | 1137 | G |
| 26 | DA | 1139 | G |
| 26 | DA | 1144 | G |
| 26 | DA | 1159 | U |
| 26 | DA | 1171 | G |
| 26 | DA | 1204 | A |
| 26 | DA | 1210 | A |
| 26 | DA | 1211 | U |
| 26 | DA | 1212 | G |
| 26 | DA | 1220 | A |
| 26 | DA | 1244 | G |
| 26 | DA | 1247 | A |
| 26 | DA | 1253 | A |
| 26 | DA | 1256 | G |
| 26 | DA | 1271 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | DA | 1272 | A |
| 26 | DA | 1273 | U |
| 26 | DA | 1292 | U |
| 26 | DA | 1300 | U |
| 26 | DA | 1301 | A |
| 26 | DA | 1303 | G |
| 26 | DA | 1314 | C |
| 26 | DA | 1332 | G |
| 26 | DA | 1352 | U |
| 26 | DA | 1359 | A |
| 26 | DA | 1360 | A |
| 26 | DA | 1365 | A |
| 26 | DA | 1368 | G |
| 26 | DA | 1370 | C |
| 26 | DA | 1380 | G |
| 26 | DA | 1384 | A |
| 26 | DA | 1385 | G |
| 26 | DA | 1386 | C |
| 26 | DA | 1413 | G |
| 26 | DA | 1416 | G |
| 26 | DA | 1417 | C |
| 26 | DA | 1419 | A |
| 26 | DA | 1420 | U |
| 26 | DA | 1421 | G |
| 26 | DA | 1428 | C |
| 26 | DA | 1435 | G |
| 26 | DA | 1437 | C |
| 26 | DA | 1445 | A |
| 26 | DA | 1445(A) | C |
| 26 | DA | 1449 | A |
| 26 | DA | 1450 | G |
| 26 | DA | 1459 | G |
| 26 | DA | 1461 | G |
| 26 | DA | 1467 | C |
| 26 | DA | 1471 | A |
| 26 | DA | 1474 | C |
| 26 | DA | 1482 | G |
| 26 | DA | 1488 | G |
| 26 | DA | 1489 | U |
| 26 | DA | 1490 | A |
| 26 | DA | 1493 | C |
| 26 | DA | 1496 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | DA | 1497 | U |
| 26 | DA | 1508 | A |
| 26 | DA | 1509 | C |
| 26 | DA | 1509(A) | A |
| 26 | DA | 1525 | G |
| 26 | DA | 1531 | C |
| 26 | DA | 1533 | G |
| 26 | DA | 1539 | G |
| 26 | DA | 1541 | G |
| 26 | DA | 1542 | A |
| 26 | DA | 1543 | C |
| 26 | DA | 1545 | A |
| 26 | DA | 1547 | C |
| 26 | DA | 1558 | A |
| 26 | DA | 1559 | G |
| 26 | DA | 1566 | A |
| 26 | DA | 1569 | A |
| 26 | DA | 1578 | U |
| 26 | DA | 1582 | C |
| 26 | DA | 1584 | C |
| 26 | DA | 1586 | A |
| 26 | DA | 1608 | A |
| 26 | DA | 1609 | A |
| 26 | DA | 1610 | A |
| 26 | DA | 1616 | A |
| 26 | DA | 1640 | C |
| 26 | DA | 1648 | C |
| 26 | DA | 1653 | G |
| 26 | DA | 1654 | A |
| 26 | DA | 1669 | A |
| 26 | DA | 1674 | G |
| 26 | DA | 1695 | G |
| 26 | DA | 1696 | G |
| 26 | DA | 1700 | A |
| 26 | DA | 1701 | A |
| 26 | DA | 1721 | G |
| 26 | DA | 1722 | A |
| 26 | DA | 1739 | U |
| 26 | DA | 1740 | G |
| 26 | DA | 1741 | A |
| 26 | DA | 1743 | C |
| 26 | DA | 1746 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | DA | 1750 | G |
| 26 | DA | 1756 | G |
| 26 | DA | 1758 | G |
| 26 | DA | 1762 | A |
| 26 | DA | 1763 | G |
| 26 | DA | 1764 | G |
| 26 | DA | 1773 | A |
| 26 | DA | 1780 | A |
| 26 | DA | 1782 | C |
| 26 | DA | 1791 | A |
| 26 | DA | 1800 | C |
| 26 | DA | 1801 | G |
| 26 | DA | 1812 | A |
| 26 | DA | 1816 | G |
| 26 | DA | 1828 | G |
| 26 | DA | 1829 | A |
| 26 | DA | 1835 | G |
| 26 | DA | 1847 | A |
| 26 | DA | 1848 | A |
| 26 | DA | 1877 | A |
| 26 | DA | 1878 | G |
| 26 | DA | 1889 | A |
| 26 | DA | 1900 | A |
| 26 | DA | 1906 | G |
| 26 | DA | 1913 | A |
| 26 | DA | 1914 | C |
| 26 | DA | 1927 | A |
| 26 | DA | 1929 | G |
| 26 | DA | 1930 | G |
| 26 | DA | 1931 | U |
| 26 | DA | 1937 | A |
| 26 | DA | 1938 | A |
| 26 | DA | 1955 | U |
| 26 | DA | 1963 | U |
| 26 | DA | 1967 | C |
| 26 | DA | 1970 | A |
| 26 | DA | 1971 | A |
| 26 | DA | 1972 | A |
| 26 | DA | 1984 | G |
| 26 | DA | 1993 | U |
| 26 | DA | 1997 | G |
| 26 | DA | 2020 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | DA | 2023 | G |
| 26 | DA | 2027 | G |
| 26 | DA | 2031 | A |
| 26 | DA | 2032 | G |
| 26 | DA | 2033 | A |
| 26 | DA | 2043 | C |
| 26 | DA | 2046 | G |
| 26 | DA | 2055 | C |
| 26 | DA | 2056 | G |
| 26 | DA | 2060 | A |
| 26 | DA | 2061 | G |
| 26 | DA | 2062 | A |
| 26 | DA | 2069 | G |
| 26 | DA | 2096 | U |
| 26 | DA | 2099 | U |
| 26 | DA | 2102 | U |
| 26 | DA | 2104 | G |
| 26 | DA | 2105 | C |
| 26 | DA | 2106 | G |
| 26 | DA | 2110 | G |
| 26 | DA | 2111 | C |
| 26 | DA | 2112 | G |
| 26 | DA | 2113 | U |
| 26 | DA | 2115 | G |
| 26 | DA | 2116 | G |
| 26 | DA | 2119 | A |
| 26 | DA | 2122 | U |
| 26 | DA | 2124 | G |
| 26 | DA | 2126 | A |
| 26 | DA | 2127 | G |
| 26 | DA | 2129 | C |
| 26 | DA | 2130 | U |
| 26 | DA | 2131 | G |
| 26 | DA | 2132 | U |
| 26 | DA | 2133 | G |
| 26 | DA | 2134 | A |
| 26 | DA | 2135 | A |
| 26 | DA | 2136 | C |
| 26 | DA | 2137 | C |
| 26 | DA | 2138 | C |
| 26 | DA | 2139 | C |
| 26 | DA | 2142 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | DA | 2144 | U |
| 26 | DA | 2146 | C |
| 26 | DA | 2148 | G |
| 26 | DA | 2150 | U |
| 26 | DA | 2151 | G |
| 26 | DA | 2154 | G |
| 26 | DA | 2155 | G |
| 26 | DA | 2158 | A |
| 26 | DA | 2159 | G |
| 26 | DA | 2160 | G |
| 26 | DA | 2161 | C |
| 26 | DA | 2162 | G |
| 26 | DA | 2164 | C |
| 26 | DA | 2165 | G |
| 26 | DA | 2166 | G |
| 26 | DA | 2167 | U |
| 26 | DA | 2168 | G |
| 26 | DA | 2169 | A |
| 26 | DA | 2170 | A |
| 26 | DA | 2171 | A |
| 26 | DA | 2172 | U |
| 26 | DA | 2173 | A |
| 26 | DA | 2177 | C |
| 26 | DA | 2178 | C |
| 26 | DA | 2181 | G |
| 26 | DA | 2185 | C |
| 26 | DA | 2186 | G |
| 26 | DA | 2187 | G |
| 26 | DA | 2188 | C |
| 26 | DA | 2189 | U |
| 26 | DA | 2192 | G |
| 26 | DA | 2198 | A |
| 26 | DA | 2206 | G |
| 26 | DA | 2207 | G |
| 26 | DA | 2208 | A |
| 26 | DA | 2218 | U |
| 26 | DA | 2225 | A |
| 26 | DA | 2232 | U |
| 26 | DA | 2238 | G |
| 26 | DA | 2239 | G |
| 26 | DA | 2243 | U |
| 26 | DA | 2269 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | DA | 2275 | C |
| 26 | DA | 2279 | G |
| 26 | DA | 2283 | C |
| 26 | DA | 2287 | A |
| 26 | DA | 2289 | G |
| 26 | DA | 2294 | C |
| 26 | DA | 2297 | C |
| 26 | DA | 2299 | G |
| 26 | DA | 2301 | C |
| 26 | DA | 2303 | G |
| 26 | DA | 2305 | A |
| 26 | DA | 2308 | G |
| 26 | DA | 2312 | U |
| 26 | DA | 2318 | G |
| 26 | DA | 2319 | G |
| 26 | DA | 2320 | A |
| 26 | DA | 2321 | G |
| 26 | DA | 2322 | A |
| 26 | DA | 2325 | G |
| 26 | DA | 2327 | A |
| 26 | DA | 2334 | G |
| 26 | DA | 2336 | A |
| 26 | DA | 2343 | C |
| 26 | DA | 2347 | C |
| 26 | DA | 2354 | G |
| 26 | DA | 2372 | G |
| 26 | DA | 2376 | A |
| 26 | DA | 2377 | A |
| 26 | DA | 2383 | G |
| 26 | DA | 2385 | C |
| 26 | DA | 2387 | U |
| 26 | DA | 2402 | C |
| 26 | DA | 2406 | U |
| 26 | DA | 2410 | G |
| 26 | DA | 2422 | A |
| 26 | DA | 2423 | U |
| 26 | DA | 2425 | A |
| 26 | DA | 2429 | G |
| 26 | DA | 2430 | A |
| 26 | DA | 2431 | U |
| 26 | DA | 2434 | A |
| 26 | DA | 2435 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | DA | 2439 | A |
| 26 | DA | 2441 | C |
| 26 | DA | 2445 | G |
| 26 | DA | 2448 | A |
| 26 | DA | 2465 | C |
| 26 | DA | 2474 | C |
| 26 | DA | 2476 | A |
| 26 | DA | 2490 | G |
| 26 | DA | 2494 | G |
| 26 | DA | 2502 | G |
| 26 | DA | 2505 | G |
| 26 | DA | 2506 | U |
| 26 | DA | 2518 | A |
| 26 | DA | 2520 | C |
| 26 | DA | 2525 | G |
| 26 | DA | 2532 | G |
| 26 | DA | 2549 | G |
| 26 | DA | 2554 | U |
| 26 | DA | 2555 | U |
| 26 | DA | 2566 | A |
| 26 | DA | 2567 | G |
| 26 | DA | 2569 | G |
| 26 | DA | 2573 | C |
| 26 | DA | 2578 | G |
| 26 | DA | 2602 | A |
| 26 | DA | 2603 | G |
| 26 | DA | 2609 | U |
| 26 | DA | 2611 | U |
| 26 | DA | 2612 | C |
| 26 | DA | 2629 | A |
| 26 | DA | 2630 | G |
| 26 | DA | 2634 | G |
| 26 | DA | 2652 | C |
| 26 | DA | 2654 | A |
| 26 | DA | 2663 | G |
| 26 | DA | 2673 | G |
| 26 | DA | 2689 | U |
| 26 | DA | 2690 | C |
| 26 | DA | 2691 | C |
| 26 | DA | 2703 | C |
| 26 | DA | 2712(A) | A |
| 26 | DA | 2713 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | DA | 2714 | G |
| 26 | DA | 2726 | U |
| 26 | DA | 2732 | G |
| 26 | DA | 2733 | A |
| 26 | DA | 2744 | G |
| 26 | DA | 2751 | G |
| 26 | DA | 2758 | A |
| 26 | DA | 2764 | A |
| 26 | DA | 2765 | A |
| 26 | DA | 2766 | G |
| 26 | DA | 2778 | A |
| 26 | DA | 2780 | G |
| 26 | DA | 2793 | G |
| 26 | DA | 2794 | C |
| 26 | DA | 2802 | G |
| 26 | DA | 2807 | G |
| 26 | DA | 2808 | U |
| 26 | DA | 2818 | G |
| 26 | DA | 2820 | A |
| 26 | DA | 2821 | A |
| 26 | DA | 2833 | G |
| 26 | DA | 2834 | G |
| 26 | DA | 2835 | A |
| 26 | DA | 2839 | G |
| 26 | DA | 2872 | G |
| 26 | DA | 2873 | A |
| 26 | DA | 2880 | C |
| 26 | DA | 2886 | G |
| 26 | DA | 2892 | A |
| 26 | DA | 2894 | G |
| 26 | DA | 2897 | U |
| 27 | DB | 2 | C |
| 27 | DB | 7 | G |
| 27 | DB | 8 | U |
| 27 | DB | 9 | G |
| 27 | DB | 10 | C |
| 27 | DB | 13 | A |
| 27 | DB | 15 | A |
| 27 | DB | 20 | C |
| 27 | DB | 21 | G |
| 27 | DB | 25 | A |
| 27 | DB | 28 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | DB | 30 | C |
| 27 | DB | 32 | C |
| 27 | DB | 34 | U |
| 27 | DB | 38 | C |
| 27 | DB | 41 | U |
| 27 | DB | 42 | C |
| 27 | DB | 44 | G |
| 27 | DB | 52 | A |
| 27 | DB | 53 | A |
| 27 | DB | 56 | G |
| 27 | DB | 58 | A |
| 27 | DB | 59 | A |
| 27 | DB | 63 | G |
| 27 | DB | 64 | C |
| 27 | DB | 65 | C |
| 27 | DB | 66 | A |
| 27 | DB | 73 | A |
| 27 | DB | 85 | G |
| 27 | DB | 93 | G |
| 27 | DB | 94 | C |
| 27 | DB | 106 | G |
| 27 | DB | 108 | U |
| 27 | DB | 110 | G |
| 27 | DB | 111 | G |
| 27 | DB | 112 | U |
| 27 | DB | 119 | G |
| 27 | DB | 120 | A |

All (113) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 115 | G |
| 1 | AA | 266 | G |
| 1 | AA | 347 | G |
| 1 | AA | 429 | U |
| 1 | AA | 509 | A |
| 1 | AA | 560 | U |
| 1 | AA | 687 | A |
| 1 | AA | 748 | C |
| 1 | AA | 793 | U |
| 1 | AA | 839 | U |
| 1 | AA | 913 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 991 | U |
| 1 | AA | 1065 | U |
| 1 | AA | 1067 | A |
| 1 | AA | 1165 | C |
| 1 | AA | 1201 | A |
| 1 | AA | 1256 | A |
| 1 | AA | 1285 | A |
| 1 | AA | 1442 | G |
| 23 | AW | 13 | C |
| 23 | AW | 45 | U |
| 25 | AY | 19 | G |
| 25 | AY | 44 | G |
| 25 | AY | 58 | A |
| 26 | BA | 71 | A |
| 26 | BA | 196 | A |
| 26 | BA | 271(M) | G |
| 26 | BA | 278 | A |
| 26 | BA | 548 | A |
| 26 | BA | 746 | A |
| 26 | BA | 774 | A |
| 26 | BA | 827 | U |
| 26 | BA | 899 | A |
| 26 | BA | 958 | U |
| 26 | BA | 960 | A |
| 26 | BA | 974 | G |
| 26 | BA | 1047 | G |
| 26 | BA | 1174 | A |
| 26 | BA | 1175 | U |
| 26 | BA | 1176 | G |
| 26 | BA | 1210 | A |
| 26 | BA | 1300 | U |
| 26 | BA | 1301 | A |
| 26 | BA | 1420 | U |
| 26 | BA | 1530 | C |
| 26 | BA | 1608 | A |
| 26 | BA | 1653 | G |
| 26 | BA | 1992 | G |
| 26 | BA | 2126 | A |
| 26 | BA | 2134 | A |
| 26 | BA | 2163 | C |
| 26 | BA | 2181 | G |
| 26 | BA | 2183 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | BA | 2187 | G |
| 26 | BA | 2238 | G |
| 26 | BA | 2406 | U |
| 26 | BA | 2430 | A |
| 26 | BA | 2689 | U |
| 26 | BA | 2756 | U |
| 26 | BA | 2893 | G |
| 1 | CA | 60 | A |
| 1 | CA | 65 | U |
| 1 | CA | 115 | G |
| 1 | CA | 266 | G |
| 1 | CA | 429 | U |
| 1 | CA | 509 | A |
| 1 | CA | 560 | U |
| 1 | CA | 687 | A |
| 1 | CA | 748 | C |
| 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 | 1064 | G |
| 1 | CA | 1065 | U |
| 1 | CA | 1129 | C |
| 1 | CA | 1183 | A |
| 1 | CA | 1201 | A |
| 1 | CA | 1212 | U |
| 1 | CA | 1256 | A |
| 1 | CA | 1331 | G |
| 1 | CA | 1442 | G |
| 1 | CA | 1492 | A |
| 23 | CW | 13 | C |
| 23 | CW | 14 | A |
| 23 | CW | 66 | U |
| 25 | CY | 46 | 7MG |
| 26 | DA | 196 | A |
| 26 | DA | 271(M) | G |
| 26 | DA | 277 | C |
| 26 | DA | 614(B) | G |
| 26 | DA | 752 | A |
| 26 | DA | 774 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | DA | 856 | C |
| 26 | DA | 888 | C |
| 26 | DA | 900 | A |
| 26 | DA | 1210 | A |
| 26 | DA | 1300 | U |
| 26 | DA | 1379 | A |
| 26 | DA | 1420 | U |
| 26 | DA | 1427 | A |
| 26 | DA | 1558 | A |
| 26 | DA | 1653 | G |
| 26 | DA | 1913 | A |
| 26 | DA | 1992 | G |
| 26 | DA | 2110 | G |
| 26 | DA | 2126 | A |
| 26 | DA | 2318 | G |
| 26 | DA | 2422 | A |
| 26 | DA | 2430 | A |
| 26 | DA | 2689 | U |

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

40 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 |
| 23 | PSU | AW | 32 | 57,23 | 17,21,22 | 1.51 | 2 (11%) | 20,30,33 | 3.11 | 6 (30%) |
| 23 | MIA | AW | 37 | 23 | 24,31,32 | 2.20 | 4 (16%) | 26,44,47 | 2.40 | 9 (34%) |
| 23 | MIA | CW | 37 | 23 | 18,24,32 | 1.12 | 2 (11%) | 18,35,47 | 1.23 | 2 (11%) |
| 24 | 31H | AX | 76 | 24,57 | 28,34,35 | 1.20 | 4 (14%) | 23,47,50 | 1.61 | 4 (17%) |
| 23 | 7MG | AW | 46 | 23 | 22,26,27 | 1.79 | 4 (18%) | 28,39,42 | 2.72 | 9 (32%) |
| 25 | 7MG | AY | 46 | 25 | 22,26,27 | 1.70 | 4 (18%) | 28,39,42 | 3.20 | 12 (42%) |
| 24 | 4SU | CX | 8 | 24 | 14,21,22 | 1.24 | 2 (14%) | 15,30,33 | 2.35 | 2 (13%) |
| 25 | PSU | CY | 32 | 25 | 17,21,22 | 1.47 | 3 (17%) | 20,30,33 | 3.26 | 7 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | PSU | CW | 32 | 23 | 17,21,22 | 1.53 | 2 (11%) | 20,30,33 | 3.20 | 6 (30%) |
| 23 | PSU | AW | 55 | 23 | 17,21,22 | 1.59 | 2 (11%) | 20,30,33 | 3.39 | 6 (30%) |
| 25 | PSU | CY | 55 | 25 | 17,21,22 | 1.39 | 3 (17%) | 20,30,33 | 3.23 | 6 (30%) |
| 25 | PSU | AY | 55 | 25 | 17,21,22 | 1.63 | 3 (17%) | 20,30,33 | 3.02 | 6 (30%) |
| 23 | 5MU | AW | 54 | 23 | 15,22,23 | 1.06 | 1 (6%) | 16,32,35 | 1.99 | 1 (6%) |
| 24 | 5MC | AX | 32 | 24 | 15,22,23 | 1.33 | 1 (6%) | 19,32,35 | 1.30 | 3 (15%) |
| 23 | 4SU | AW | 8 | 23 | 14,21,22 | 1.31 | 1 (7%) | 15,30,33 | 1.54 | 2 (13%) |
| 23 | PSU | AW | 39 | 23 | 17,21,22 | 1.53 | 2 (11%) | 20,30,33 | 3.15 | 6 (30%) |
| 25 | MIA | AY | 37 | 25 | 18,24,32 | 1.15 | 2 (11%) | 18,35,47 | 1.24 | 2 (11%) |
| 24 | 5MU | CX | 54 | 24 | 15,22,23 | 1.10 | 1 (6%) | 16,32,35 | 1.74 | 2 (12%) |
| 24 | 5MC | CX | 32 | 24 | 15,22,23 | 1.23 | 1 (6%) | 19,32,35 | 1.39 | 2 (10%) |
| 23 | F3N | CW | 76 | 23 | 30,36,37 | 1.50 | 6 (20%) | 29,51,54 | 1.19 | 1 (3%) |
| 25 | PSU | AY | 32 | 25 | 17,21,22 | 1.45 | 2 (11%) | 20,30,33 | 3.18 | 6 (30%) |
| 24 | PSU | CX | 55 | 24 | 17,21,22 | 1.58 | 2 (11%) | 20,30,33 | 3.10 | 6 (30%) |
| 23 | 5MU | CW | 54 | 23 | 15,22,23 | 1.10 | 1 (6%) | 16,32,35 | 2.11 | 1 (6%) |
| 23 | PSU | CW | 55 | 23 | 17,21,22 | 1.50 | 2 (11%) | 20,30,33 | 3.19 | 6 (30%) |
| 25 | 4SU | CY | 8 | 25 | 14,21,22 | 1.38 | 1 (7%) | 15,30,33 | 1.44 | 2 (13%) |
| 23 | F3N | AW | 76 | 23 | 30,36,37 | 1.49 | 5 (16%) | 29,51,54 | 1.21 | 1 (3%) |
| 24 | PSU | AX | 55 | 24 | 17,21,22 | 1.78 | 3 (17%) | 20,30,33 | 3.16 | 7 (35%) |
| 25 | 4SU | AY | 8 | 25 | 14,21,22 | 1.31 | 1 (7%) | 15,30,33 | 1.40 | 2 (13%) |
| 25 | 5MU | CY | 54 | 25 | 15,22,23 | 1.05 | 1 (6%) | 16,32,35 | 1.86 | 2 (12%) |
| 23 | 4SU | CW | 8 | 23 | 14,21,22 | 1.27 | 1 (7%) | 15,30,33 | 1.30 | 2 (13%) |
| 25 | PSU | CY | 39 | 25 | 17,21,22 | 1.85 | 4 (23%) | 20,30,33 | 2.88 | 7 (35%) |
| 25 | MIA | CY | 37 | 25 | 18,24,32 | 1.17 | 2 (11%) | 18,35,47 | 1.27 | 2 (11%) |
| 25 | 5MU | AY | 54 | 25 | 15,22,23 | 1.12 | 1 (6%) | 16,32,35 | 1.99 | 2 (12%) |
| 24 | 4SU | AX | 8 | 24 | 14,21,22 | 1.46 | 2 (14%) | 15,30,33 | 2.69 | 2 (13%) |
| 23 | 7MG | CW | 46 | 23 | 22,26,27 | 1.84 | 4 (18%) | 28,39,42 | 2.56 | 10 (35%) |
| 25 | 7MG | CY | 46 | 25 | 22,26,27 | 1.80 | 4 (18%) | 28,39,42 | 2.81 | 12 (42%) |
| 23 | PSU | CW | 39 | 23 | 17,21,22 | 1.55 | 2 (11%) | 20,30,33 | 3.51 | 6 (30%) |
| 24 | 5MU | AX | 54 | 24,57 | 15,22,23 | 1.08 | 1 (6%) | 16,32,35 | 1.88 | 2 (12%) |
| 25 | PSU | AY | 39 | 25 | 17,21,22 | 1.51 | 2 (11%) | 20,30,33 | 3.30 | 7 (35%) |
| 24 | 31H | CX | 76 | 24,57 | 28,34,35 | 1.21 | 3 (10%) | 23,47,50 | 1.51 | 2 (8%) |

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 |
|-----|------|-------|-----|-------|---------|------------|---------|
| 23 | PSU | AW | 32 | 57,23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | MIA | AW | 37 | 23 | - | 1/11/33/34 | 0/3/3/3 |
| 23 | MIA | CW | 37 | 23 | - | 0/3/25/34 | 0/3/3/3 |
| 24 | 31H | AX | 76 | 24,57 | - | 7/18/40/41 | 0/3/3/3 |
| 23 | 7MG | AW | 46 | 23 | - | 3/7/37/38 | 0/3/3/3 |
| 25 | 7MG | AY | 46 | 25 | - | 4/7/37/38 | 0/3/3/3 |
| 24 | 4SU | CX | 8 | 24 | - | 0/5/25/26 | 0/2/2/2 |
| 25 | PSU | CY | 32 | 25 | - | 3/7/25/26 | 0/2/2/2 |
| 23 | PSU | CW | 32 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | PSU | AW | 55 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 25 | PSU | CY | 55 | 25 | - | 6/7/25/26 | 0/2/2/2 |
| 25 | PSU | AY | 55 | 25 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 5MU | AW | 54 | 23 | - | 0/5/25/26 | 0/2/2/2 |
| 24 | 5MC | AX | 32 | 24 | - | 0/5/25/26 | 0/2/2/2 |
| 23 | 4SU | AW | 8 | 23 | - | 0/5/25/26 | 0/2/2/2 |
| 23 | PSU | AW | 39 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 25 | MIA | AY | 37 | 25 | - | 3/3/25/34 | 0/3/3/3 |
| 24 | 5MU | CX | 54 | 24 | - | 0/5/25/26 | 0/2/2/2 |
| 24 | 5MC | CX | 32 | 24 | - | 0/5/25/26 | 0/2/2/2 |
| 23 | F3N | CW | 76 | 23 | - | 5/15/37/38 | 0/4/4/4 |
| 25 | PSU | AY | 32 | 25 | - | 2/7/25/26 | 0/2/2/2 |
| 24 | PSU | CX | 55 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 5MU | CW | 54 | 23 | - | 0/5/25/26 | 0/2/2/2 |
| 23 | PSU | CW | 55 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 25 | 4SU | CY | 8 | 25 | - | 1/5/25/26 | 0/2/2/2 |
| 23 | F3N | AW | 76 | 23 | - | 0/15/37/38 | 0/4/4/4 |
| 24 | PSU | AX | 55 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 25 | 4SU | AY | 8 | 25 | - | 0/5/25/26 | 0/2/2/2 |
| 25 | 5MU | CY | 54 | 25 | - | 2/5/25/26 | 0/2/2/2 |
| 23 | 4SU | CW | 8 | 23 | - | 0/5/25/26 | 0/2/2/2 |
| 25 | PSU | CY | 39 | 25 | - | 2/7/25/26 | 0/2/2/2 |
| 25 | MIA | CY | 37 | 25 | - | 3/3/25/34 | 0/3/3/3 |
| 25 | 5MU | AY | 54 | 25 | - | 3/5/25/26 | 0/2/2/2 |
| 24 | 4SU | AX | 8 | 24 | - | 0/5/25/26 | 0/2/2/2 |
| 23 | 7MG | CW | 46 | 23 | - | 3/7/37/38 | 0/3/3/3 |
| 25 | 7MG | CY | 46 | 25 | - | 2/7/37/38 | 0/3/3/3 |
| 23 | PSU | CW | 39 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 5MU | AX | 54 | 24,57 | - | 0/5/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|-------------|---------|
| 25 | PSU | AY | 39 | 25 | - | 2/7/25/26 | 0/2/2/2 |
| 24 | 31H | CX | 76 | 24,57 | - | 12/18/40/41 | 0/3/3/3 |

All (94) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | AW | 37 | MIA | C13-C14 | 7.34 | 1.53 | 1.32 |
| 23 | AW | 37 | MIA | C2-S10 | -6.22 | 1.70 | 1.75 |
| 23 | CW | 46 | 7MG | C6-C5 | 5.71 | 1.49 | 1.41 |
| 24 | AX | 55 | PSU | C5-C1' | -5.39 | 1.47 | 1.52 |
| 25 | CY | 39 | PSU | C5-C1' | -5.30 | 1.47 | 1.52 |
| 23 | AW | 76 | F3N | CB-CG | -4.99 | 1.39 | 1.51 |
| 25 | CY | 46 | 7MG | C6-C5 | 4.94 | 1.48 | 1.41 |
| 23 | AW | 46 | 7MG | C6-C5 | 4.86 | 1.48 | 1.41 |
| 25 | AY | 55 | PSU | C5-C1' | -4.82 | 1.48 | 1.52 |
| 24 | AX | 32 | 5MC | C5-C4 | 4.71 | 1.48 | 1.41 |
| 25 | CY | 46 | 7MG | C5-C4 | 4.63 | 1.48 | 1.39 |
| 23 | AW | 46 | 7MG | C5-C4 | 4.57 | 1.48 | 1.39 |
| 23 | CW | 76 | F3N | CB-CG | -4.53 | 1.40 | 1.51 |
| 25 | AY | 46 | 7MG | C5-C4 | 4.48 | 1.47 | 1.39 |
| 23 | AW | 55 | PSU | C5-C1' | -4.46 | 1.48 | 1.52 |
| 23 | CW | 39 | PSU | C5-C1' | -4.44 | 1.48 | 1.52 |
| 24 | CX | 32 | 5MC | C5-C4 | 4.39 | 1.48 | 1.41 |
| 24 | CX | 55 | PSU | C5-C1' | -4.39 | 1.48 | 1.52 |
| 25 | CY | 8 | 4SU | C4-S4 | -4.25 | 1.59 | 1.67 |
| 23 | AW | 8 | 4SU | C4-S4 | -4.18 | 1.59 | 1.67 |
| 23 | CW | 55 | PSU | C5-C1' | -4.13 | 1.48 | 1.52 |
| 23 | CW | 32 | PSU | C5-C1' | -4.13 | 1.48 | 1.52 |
| 25 | AY | 8 | 4SU | C4-S4 | -4.10 | 1.60 | 1.67 |
| 23 | AW | 32 | PSU | C5-C1' | -4.05 | 1.48 | 1.52 |
| 25 | AY | 46 | 7MG | C6-C5 | 4.04 | 1.47 | 1.41 |
| 23 | CW | 46 | 7MG | C5-C4 | 4.01 | 1.47 | 1.39 |
| 25 | AY | 39 | PSU | C5-C1' | -3.93 | 1.48 | 1.52 |
| 24 | AX | 8 | 4SU | C4-S4 | -3.91 | 1.60 | 1.67 |
| 23 | CW | 8 | 4SU | C4-S4 | -3.88 | 1.60 | 1.67 |
| 23 | AW | 39 | PSU | C5-C1' | -3.88 | 1.48 | 1.52 |
| 25 | AY | 32 | PSU | C4-C5 | 3.83 | 1.49 | 1.41 |
| 24 | CX | 8 | 4SU | C4-S4 | -3.80 | 1.60 | 1.67 |
| 25 | AY | 46 | 7MG | C5-N7 | -3.63 | 1.33 | 1.39 |
| 25 | CY | 32 | PSU | C4-C5 | 3.58 | 1.49 | 1.41 |
| 24 | CX | 54 | 5MU | C4-C5 | 3.49 | 1.48 | 1.41 |
| 25 | CY | 32 | PSU | C5-C1' | -3.47 | 1.49 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | CW | 54 | 5MU | C4-C5 | 3.46 | 1.48 | 1.41 |
| 25 | AY | 54 | 5MU | C4-C5 | 3.46 | 1.48 | 1.41 |
| 23 | AW | 39 | PSU | C4-C5 | 3.45 | 1.48 | 1.41 |
| 23 | CW | 76 | F3N | O4'-C1' | 3.44 | 1.45 | 1.41 |
| 25 | AY | 39 | PSU | C4-C5 | 3.44 | 1.48 | 1.41 |
| 23 | CW | 32 | PSU | C4-C5 | 3.43 | 1.48 | 1.41 |
| 23 | AW | 54 | 5MU | C4-C5 | 3.42 | 1.48 | 1.41 |
| 25 | CY | 39 | PSU | C4-C5 | 3.41 | 1.48 | 1.41 |
| 23 | AW | 55 | PSU | C4-C5 | 3.41 | 1.48 | 1.41 |
| 24 | AX | 8 | 4SU | C2-N3 | -3.40 | 1.31 | 1.38 |
| 23 | AW | 32 | PSU | C4-C5 | 3.40 | 1.48 | 1.41 |
| 24 | CX | 55 | PSU | C4-C5 | 3.37 | 1.48 | 1.41 |
| 23 | AW | 76 | F3N | O4'-C1' | 3.33 | 1.45 | 1.41 |
| 25 | AY | 55 | PSU | C4-C5 | 3.33 | 1.48 | 1.41 |
| 24 | AX | 54 | 5MU | C4-C5 | 3.32 | 1.48 | 1.41 |
| 25 | CY | 54 | 5MU | C4-C5 | 3.30 | 1.48 | 1.41 |
| 23 | CW | 55 | PSU | C4-C5 | 3.28 | 1.48 | 1.41 |
| 24 | CX | 76 | 31H | C5-C4 | -3.27 | 1.32 | 1.40 |
| 23 | CW | 46 | 7MG | C5-N7 | -3.25 | 1.34 | 1.39 |
| 23 | AW | 46 | 7MG | C5-N7 | -3.22 | 1.34 | 1.39 |
| 24 | AX | 55 | PSU | C4-C5 | 3.21 | 1.48 | 1.41 |
| 25 | CY | 55 | PSU | C5-C1' | -3.21 | 1.49 | 1.52 |
| 25 | AY | 32 | PSU | C5-C1' | -3.17 | 1.49 | 1.52 |
| 25 | CY | 55 | PSU | C4-C5 | 3.16 | 1.48 | 1.41 |
| 23 | CW | 76 | F3N | C5-C4 | -3.12 | 1.32 | 1.40 |
| 23 | CW | 39 | PSU | C4-C5 | 3.06 | 1.48 | 1.41 |
| 25 | CY | 46 | 7MG | C5-N7 | -3.01 | 1.34 | 1.39 |
| 23 | AW | 76 | F3N | C5-C4 | -2.84 | 1.33 | 1.40 |
| 25 | CY | 37 | MIA | C5-C4 | 2.84 | 1.48 | 1.40 |
| 24 | AX | 76 | 31H | C5-C4 | -2.83 | 1.33 | 1.40 |
| 25 | AY | 37 | MIA | C5-C4 | 2.80 | 1.48 | 1.40 |
| 25 | AY | 37 | MIA | C2-N3 | 2.76 | 1.36 | 1.32 |
| 25 | CY | 37 | MIA | C2-N3 | 2.73 | 1.36 | 1.32 |
| 23 | CW | 37 | MIA | C5-C4 | 2.68 | 1.48 | 1.40 |
| 23 | CW | 37 | MIA | C2-N3 | 2.67 | 1.36 | 1.32 |
| 23 | AW | 37 | MIA | C5-C4 | 2.54 | 1.47 | 1.40 |
| 23 | CW | 76 | F3N | C6-C5 | -2.54 | 1.33 | 1.43 |
| 23 | AW | 76 | F3N | C6-C5 | -2.52 | 1.33 | 1.43 |
| 25 | CY | 39 | PSU | O4'-C1' | -2.51 | 1.40 | 1.44 |
| 25 | CY | 46 | 7MG | C4-N9 | -2.47 | 1.33 | 1.38 |
| 23 | AW | 46 | 7MG | C4-N9 | -2.46 | 1.33 | 1.38 |
| 23 | CW | 46 | 7MG | C4-N9 | -2.43 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | AX | 76 | 31H | C5-N7 | -2.42 | 1.31 | 1.39 |
| 24 | CX | 76 | 31H | C6-C5 | -2.41 | 1.34 | 1.43 |
| 24 | AX | 76 | 31H | C6-C5 | -2.38 | 1.34 | 1.43 |
| 24 | CX | 76 | 31H | C3'-N3' | 2.34 | 1.49 | 1.45 |
| 24 | AX | 55 | PSU | O4'-C1' | -2.28 | 1.41 | 1.44 |
| 23 | AW | 76 | F3N | C5-N7 | -2.26 | 1.31 | 1.39 |
| 24 | CX | 8 | 4SU | C2-N3 | -2.23 | 1.33 | 1.38 |
| 25 | CY | 39 | PSU | C2-N1 | -2.17 | 1.33 | 1.38 |
| 23 | AW | 37 | MIA | C6-N1 | 2.11 | 1.35 | 1.32 |
| 25 | CY | 32 | PSU | O4'-C1' | -2.10 | 1.41 | 1.44 |
| 23 | CW | 76 | F3N | C3'-N3' | 2.07 | 1.49 | 1.45 |
| 24 | AX | 76 | 31H | C3'-N3' | 2.07 | 1.49 | 1.45 |
| 25 | AY | 46 | 7MG | C4-N3 | 2.05 | 1.36 | 1.34 |
| 23 | CW | 76 | F3N | C5-N7 | -2.01 | 1.32 | 1.39 |
| 25 | AY | 55 | PSU | O4'-C1' | -2.00 | 1.41 | 1.44 |
| 25 | CY | 55 | PSU | C2-N1 | -2.00 | 1.34 | 1.38 |

All (181) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 25 | AY | 46 | 7MG | N3-C4-N9 | 11.30 | 141.42 | 126.91 |
| 23 | CW | 39 | PSU | N1-C2-N3 | -9.66 | 120.75 | 128.43 |
| 25 | CY | 55 | PSU | N1-C2-N3 | -9.28 | 121.06 | 128.43 |
| 24 | AX | 8 | 4SU | C2-N3-C4 | 9.19 | 128.48 | 115.15 |
| 25 | AY | 39 | PSU | N1-C2-N3 | -9.08 | 121.21 | 128.43 |
| 25 | AY | 32 | PSU | N1-C2-N3 | -8.82 | 121.42 | 128.43 |
| 25 | CY | 32 | PSU | N1-C2-N3 | -8.79 | 121.44 | 128.43 |
| 23 | CW | 32 | PSU | N1-C2-N3 | -8.65 | 121.56 | 128.43 |
| 23 | AW | 46 | 7MG | N3-C4-N9 | 8.61 | 137.97 | 126.91 |
| 23 | AW | 39 | PSU | N1-C2-N3 | -8.49 | 121.68 | 128.43 |
| 23 | AW | 32 | PSU | N1-C2-N3 | -8.46 | 121.70 | 128.43 |
| 23 | CW | 55 | PSU | N1-C2-N3 | -8.38 | 121.77 | 128.43 |
| 25 | CY | 46 | 7MG | N3-C4-N9 | 8.37 | 137.66 | 126.91 |
| 24 | CX | 55 | PSU | N1-C2-N3 | -8.24 | 121.88 | 128.43 |
| 23 | AW | 55 | PSU | N1-C2-N3 | -8.21 | 121.91 | 128.43 |
| 24 | AX | 55 | PSU | N1-C2-N3 | -8.15 | 121.95 | 128.43 |
| 23 | CW | 39 | PSU | C4-N3-C2 | 8.02 | 121.92 | 115.14 |
| 23 | CW | 54 | 5MU | C4-N3-C2 | 7.93 | 121.84 | 115.14 |
| 25 | AY | 55 | PSU | N1-C2-N3 | -7.87 | 122.18 | 128.43 |
| 24 | CX | 8 | 4SU | C2-N3-C4 | 7.74 | 126.37 | 115.15 |
| 23 | AW | 55 | PSU | C4-N3-C2 | 7.57 | 121.53 | 115.14 |
| 23 | AW | 54 | 5MU | C4-N3-C2 | 7.45 | 121.44 | 115.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | CY | 32 | PSU | C4-N3-C2 | 7.45 | 121.43 | 115.14 |
| 25 | AY | 39 | PSU | C4-N3-C2 | 7.28 | 121.28 | 115.14 |
| 25 | CY | 55 | PSU | C4-N3-C2 | 7.18 | 121.20 | 115.14 |
| 25 | AY | 54 | 5MU | C4-N3-C2 | 7.13 | 121.17 | 115.14 |
| 23 | CW | 46 | 7MG | N3-C4-N9 | 7.12 | 136.05 | 126.91 |
| 23 | AW | 37 | MIA | C12-C13-C14 | -7.05 | 113.42 | 127.14 |
| 23 | AW | 39 | PSU | C4-N3-C2 | 6.97 | 121.03 | 115.14 |
| 24 | AX | 54 | 5MU | C4-N3-C2 | 6.82 | 120.90 | 115.14 |
| 23 | AW | 32 | PSU | C4-N3-C2 | 6.77 | 120.86 | 115.14 |
| 24 | AX | 55 | PSU | C4-N3-C2 | 6.76 | 120.85 | 115.14 |
| 24 | CX | 55 | PSU | C4-N3-C2 | 6.68 | 120.78 | 115.14 |
| 25 | AY | 32 | PSU | C4-N3-C2 | 6.64 | 120.75 | 115.14 |
| 25 | AY | 55 | PSU | C4-N3-C2 | 6.63 | 120.74 | 115.14 |
| 23 | CW | 32 | PSU | C4-N3-C2 | 6.36 | 120.51 | 115.14 |
| 25 | AY | 46 | 7MG | C5-C4-N3 | -6.29 | 116.23 | 126.49 |
| 24 | CX | 54 | 5MU | C4-N3-C2 | 6.24 | 120.41 | 115.14 |
| 23 | AW | 55 | PSU | C5-C4-N3 | -6.23 | 117.33 | 125.36 |
| 23 | CW | 55 | PSU | C4-N3-C2 | 6.17 | 120.36 | 115.14 |
| 24 | AX | 55 | PSU | C5-C4-N3 | -6.03 | 117.59 | 125.36 |
| 25 | CY | 39 | PSU | C5-C4-N3 | -6.01 | 117.62 | 125.36 |
| 25 | CY | 54 | 5MU | C4-N3-C2 | 5.98 | 120.19 | 115.14 |
| 25 | AY | 55 | PSU | C5-C4-N3 | -5.92 | 117.73 | 125.36 |
| 25 | CY | 32 | PSU | C5-C4-N3 | -5.67 | 118.06 | 125.36 |
| 25 | CY | 39 | PSU | N1-C2-N3 | -5.61 | 123.97 | 128.43 |
| 24 | CX | 76 | 31H | N3-C2-N1 | -5.53 | 120.04 | 128.68 |
| 23 | CW | 76 | F3N | N3-C2-N1 | -5.52 | 120.06 | 128.68 |
| 24 | CX | 55 | PSU | C5-C4-N3 | -5.48 | 118.29 | 125.36 |
| 23 | CW | 39 | PSU | C5-C4-N3 | -5.47 | 118.31 | 125.36 |
| 23 | CW | 46 | 7MG | N7-C8-N9 | -5.46 | 95.56 | 103.38 |
| 23 | AW | 76 | F3N | N3-C2-N1 | -5.44 | 120.18 | 128.68 |
| 23 | AW | 32 | PSU | C5-C4-N3 | -5.44 | 118.36 | 125.36 |
| 23 | AW | 39 | PSU | C5-C4-N3 | -5.43 | 118.36 | 125.36 |
| 24 | AX | 76 | 31H | N3-C2-N1 | -5.42 | 120.20 | 128.68 |
| 25 | CY | 39 | PSU | C4-N3-C2 | 5.40 | 119.70 | 115.14 |
| 23 | AW | 46 | 7MG | N7-C8-N9 | -5.39 | 95.67 | 103.38 |
| 23 | AW | 55 | PSU | C5-C1'-C2' | -5.38 | 105.73 | 115.32 |
| 25 | CY | 46 | 7MG | C6-N1-C2 | 5.37 | 124.47 | 115.93 |
| 25 | CY | 46 | 7MG | N7-C8-N9 | -5.29 | 95.81 | 103.38 |
| 23 | AW | 46 | 7MG | C6-N1-C2 | 5.20 | 124.19 | 115.93 |
| 23 | CW | 55 | PSU | C5-C4-N3 | -5.13 | 118.75 | 125.36 |
| 25 | AY | 46 | 7MG | C6-C5-C4 | 5.12 | 120.69 | 115.20 |
| 25 | AY | 39 | PSU | C5-C4-N3 | -5.11 | 118.77 | 125.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | CW | 46 | 7MG | C5-C4-N3 | -5.11 | 118.15 | 126.49 |
| 23 | CW | 32 | PSU | C5-C4-N3 | -5.04 | 118.86 | 125.36 |
| 25 | AY | 32 | PSU | C5-C4-N3 | -4.96 | 118.97 | 125.36 |
| 25 | AY | 46 | 7MG | N7-C8-N9 | -4.91 | 96.35 | 103.38 |
| 25 | CY | 55 | PSU | C5-C4-N3 | -4.81 | 119.16 | 125.36 |
| 23 | AW | 8 | 4SU | C2-N3-C4 | 4.81 | 122.12 | 115.15 |
| 23 | CW | 55 | PSU | C5-C6-N1 | -4.73 | 118.63 | 124.44 |
| 25 | CY | 39 | PSU | C5-C1'-C2' | -4.68 | 106.96 | 115.32 |
| 23 | AW | 37 | MIA | C2-N3-C4 | 4.65 | 121.73 | 115.32 |
| 23 | CW | 32 | PSU | C5-C6-N1 | -4.58 | 118.81 | 124.44 |
| 24 | CX | 55 | PSU | C5-C6-N1 | -4.46 | 118.96 | 124.44 |
| 23 | AW | 46 | 7MG | C5-C4-N3 | -4.46 | 119.21 | 126.49 |
| 25 | CY | 46 | 7MG | C5-C4-N3 | -4.45 | 119.22 | 126.49 |
| 24 | AX | 55 | PSU | C5-C6-N1 | -4.42 | 119.00 | 124.44 |
| 25 | AY | 32 | PSU | C6-N1-C2 | 4.41 | 122.63 | 115.36 |
| 23 | CW | 32 | PSU | C6-N1-C2 | 4.38 | 122.59 | 115.36 |
| 23 | CW | 55 | PSU | C6-N1-C2 | 4.34 | 122.53 | 115.36 |
| 25 | AY | 39 | PSU | C5-C6-N1 | -4.33 | 119.12 | 124.44 |
| 25 | AY | 55 | PSU | C5-C6-N1 | -4.32 | 119.13 | 124.44 |
| 24 | CX | 8 | 4SU | C5-C4-N3 | -4.27 | 118.12 | 123.83 |
| 25 | AY | 32 | PSU | C5-C6-N1 | -4.25 | 119.21 | 124.44 |
| 24 | AX | 8 | 4SU | C5-C4-N3 | -4.25 | 118.14 | 123.83 |
| 25 | AY | 39 | PSU | C6-N1-C2 | 4.24 | 122.36 | 115.36 |
| 23 | AW | 37 | MIA | C15-C14-C13 | -4.18 | 110.58 | 122.65 |
| 24 | CX | 55 | PSU | C6-N1-C2 | 4.12 | 122.15 | 115.36 |
| 23 | AW | 39 | PSU | C6-N1-C2 | 4.08 | 122.09 | 115.36 |
| 23 | CW | 39 | PSU | C5-C1'-C2' | -4.07 | 108.06 | 115.32 |
| 23 | CW | 39 | PSU | C6-N1-C2 | 4.06 | 122.06 | 115.36 |
| 23 | AW | 32 | PSU | C6-N1-C2 | 4.03 | 122.01 | 115.36 |
| 23 | AW | 39 | PSU | C5-C6-N1 | -4.03 | 119.49 | 124.44 |
| 24 | AX | 55 | PSU | C6-N1-C2 | 4.02 | 122.00 | 115.36 |
| 23 | CW | 46 | 7MG | C6-N1-C2 | 4.02 | 122.32 | 115.93 |
| 25 | AY | 46 | 7MG | C6-N1-C2 | 3.99 | 122.28 | 115.93 |
| 23 | AW | 46 | 7MG | C5-C6-N1 | -3.95 | 115.03 | 123.14 |
| 23 | CW | 39 | PSU | C5-C6-N1 | -3.94 | 119.60 | 124.44 |
| 25 | CY | 8 | 4SU | C2-N3-C4 | 3.93 | 120.85 | 115.15 |
| 23 | AW | 37 | MIA | C5-C6-N1 | -3.90 | 117.57 | 120.81 |
| 23 | AW | 32 | PSU | C5-C6-N1 | -3.87 | 119.69 | 124.44 |
| 25 | AY | 55 | PSU | C6-N1-C2 | 3.86 | 121.72 | 115.36 |
| 25 | CY | 55 | PSU | C6-N1-C2 | 3.84 | 121.70 | 115.36 |
| 25 | AY | 8 | 4SU | C2-N3-C4 | 3.83 | 120.70 | 115.15 |
| 25 | CY | 32 | PSU | C6-N1-C2 | 3.81 | 121.65 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | CY | 46 | 7MG | C5-C6-N1 | -3.80 | 115.33 | 123.14 |
| 23 | AW | 46 | 7MG | C6-C5-C4 | 3.71 | 119.18 | 115.20 |
| 25 | CY | 39 | PSU | O4'-C1'-C5 | -3.69 | 104.22 | 109.93 |
| 23 | AW | 55 | PSU | C6-N1-C2 | 3.68 | 121.42 | 115.36 |
| 23 | AW | 55 | PSU | C5-C6-N1 | -3.67 | 119.92 | 124.44 |
| 24 | CX | 32 | 5MC | C2-N3-C4 | 3.67 | 120.45 | 116.02 |
| 23 | CW | 32 | PSU | C5-C1'-C2' | -3.67 | 108.77 | 115.32 |
| 25 | CY | 39 | PSU | C5-C6-N1 | -3.66 | 119.94 | 124.44 |
| 23 | CW | 55 | PSU | C5-C1'-C2' | -3.63 | 108.85 | 115.32 |
| 23 | CW | 8 | 4SU | C2-N3-C4 | 3.59 | 120.35 | 115.15 |
| 23 | AW | 37 | MIA | C16-C14-C13 | -3.54 | 112.43 | 122.65 |
| 25 | CY | 55 | PSU | C5-C1'-C2' | -3.53 | 109.03 | 115.32 |
| 23 | CW | 37 | MIA | N3-C2-N1 | -3.38 | 123.39 | 128.68 |
| 23 | CW | 46 | 7MG | C5-C6-N1 | -3.34 | 116.28 | 123.14 |
| 23 | CW | 46 | 7MG | C6-C5-C4 | 3.32 | 118.76 | 115.20 |
| 25 | AY | 37 | MIA | N3-C2-N1 | -3.25 | 123.60 | 128.68 |
| 25 | CY | 32 | PSU | C5-C6-N1 | -3.23 | 120.47 | 124.44 |
| 25 | CY | 46 | 7MG | C6-C5-C4 | 3.22 | 118.66 | 115.20 |
| 25 | AY | 46 | 7MG | C5-C6-N1 | -3.21 | 116.54 | 123.14 |
| 25 | CY | 39 | PSU | C6-N1-C2 | 3.20 | 120.64 | 115.36 |
| 24 | AX | 32 | 5MC | C2-N3-C4 | 3.20 | 119.88 | 116.02 |
| 23 | AW | 37 | MIA | C4-C5-N7 | -3.18 | 106.08 | 109.40 |
| 25 | CY | 37 | MIA | N3-C2-N1 | -3.16 | 123.73 | 128.68 |
| 25 | CY | 32 | PSU | O4'-C1'-C5 | -3.11 | 105.12 | 109.93 |
| 24 | AX | 76 | 31H | O4'-C1'-C2' | -3.05 | 102.47 | 106.93 |
| 25 | CY | 54 | 5MU | C5-C6-N1 | -2.97 | 118.99 | 122.19 |
| 25 | CY | 37 | MIA | C4-C5-N7 | -2.94 | 106.34 | 109.40 |
| 25 | AY | 46 | 7MG | C5-C4-N9 | -2.92 | 102.35 | 106.44 |
| 23 | CW | 46 | 7MG | C8-N7-C5 | 2.91 | 116.52 | 108.94 |
| 24 | CX | 32 | 5MC | N4-C4-N3 | 2.88 | 121.10 | 117.03 |
| 23 | CW | 8 | 4SU | C5-C4-N3 | -2.86 | 120.01 | 123.83 |
| 25 | AY | 8 | 4SU | C5-C4-N3 | -2.83 | 120.05 | 123.83 |
| 23 | AW | 37 | MIA | C2-N1-C6 | 2.81 | 122.22 | 117.19 |
| 25 | AY | 37 | MIA | C4-C5-N7 | -2.81 | 106.47 | 109.40 |
| 24 | AX | 32 | 5MC | C5-C6-N1 | -2.77 | 119.20 | 122.19 |
| 23 | AW | 8 | 4SU | C5-C4-N3 | -2.77 | 120.13 | 123.83 |
| 23 | CW | 37 | MIA | C4-C5-N7 | -2.75 | 106.54 | 109.40 |
| 23 | AW | 39 | PSU | C5-C1'-C2' | -2.68 | 110.53 | 115.32 |
| 25 | AY | 32 | PSU | O4'-C1'-C5 | 2.68 | 114.08 | 109.93 |
| 23 | CW | 46 | 7MG | C2-N3-C4 | 2.66 | 121.25 | 113.89 |
| 24 | CX | 76 | 31H | O4'-C1'-C2' | -2.65 | 103.06 | 106.93 |
| 25 | CY | 55 | PSU | C5-C6-N1 | -2.62 | 121.22 | 124.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | AY | 46 | 7MG | C8-N7-C5 | 2.61 | 115.73 | 108.94 |
| 23 | AW | 46 | 7MG | C8-N7-C5 | 2.60 | 115.70 | 108.94 |
| 23 | AW | 46 | 7MG | C5-C4-N9 | -2.59 | 102.81 | 106.44 |
| 25 | CY | 46 | 7MG | C8-N7-C5 | 2.54 | 115.55 | 108.94 |
| 23 | AW | 37 | MIA | N3-C2-N1 | -2.51 | 122.37 | 126.98 |
| 25 | CY | 8 | 4SU | C5-C4-N3 | -2.47 | 120.52 | 123.83 |
| 25 | AY | 46 | 7MG | C2-N3-C4 | 2.44 | 120.64 | 113.89 |
| 25 | CY | 46 | 7MG | N2-C2-N1 | 2.44 | 121.04 | 117.25 |
| 24 | AX | 55 | PSU | C5-C1'-C2' | -2.44 | 110.97 | 115.32 |
| 24 | AX | 54 | 5MU | C5-C6-N1 | -2.40 | 119.61 | 122.19 |
| 24 | CX | 54 | 5MU | C5-C6-N1 | -2.38 | 119.62 | 122.19 |
| 25 | CY | 46 | 7MG | C5-C4-N9 | -2.38 | 103.10 | 106.44 |
| 23 | AW | 32 | PSU | C5-C1'-C2' | -2.35 | 111.12 | 115.32 |
| 25 | CY | 46 | 7MG | O4'-C1'-N9 | -2.35 | 106.17 | 109.35 |
| 25 | AY | 54 | 5MU | C5-C6-N1 | -2.29 | 119.73 | 122.19 |
| 25 | AY | 39 | PSU | C5-C1'-C2' | -2.28 | 111.26 | 115.32 |
| 25 | AY | 46 | 7MG | C4-N9-C1' | 2.24 | 131.90 | 126.60 |
| 24 | AX | 32 | 5MC | N4-C4-N3 | 2.20 | 120.14 | 117.03 |
| 25 | CY | 46 | 7MG | C2-N3-C4 | 2.16 | 119.87 | 113.89 |
| 24 | AX | 76 | 31H | O2'-C2'-C3' | 2.16 | 116.46 | 111.16 |
| 23 | CW | 46 | 7MG | N2-C2-N1 | 2.16 | 120.61 | 117.25 |
| 25 | AY | 46 | 7MG | N2-C2-N3 | 2.16 | 120.61 | 117.25 |
| 25 | CY | 32 | PSU | O4'-C1'-C2' | 2.11 | 108.08 | 104.66 |
| 23 | CW | 46 | 7MG | O4'-C1'-N9 | 2.11 | 112.19 | 109.35 |
| 25 | AY | 46 | 7MG | CM7-N7-C5 | 2.09 | 132.04 | 124.01 |
| 24 | AX | 76 | 31H | CA-N-CN | -2.08 | 119.62 | 122.82 |
| 25 | CY | 46 | 7MG | CM7-N7-C5 | 2.08 | 132.01 | 124.01 |
| 23 | AW | 37 | MIA | C16-C14-C15 | -2.04 | 110.09 | 114.60 |
| 25 | AY | 55 | PSU | O4'-C1'-C2' | 2.02 | 107.94 | 104.66 |
| 24 | CX | 55 | PSU | C5-C1'-C2' | -2.01 | 111.73 | 115.32 |
| 24 | AX | 55 | PSU | O4'-C1'-C2' | 2.01 | 107.92 | 104.66 |
| 25 | AY | 39 | PSU | O4'-C1'-C5 | 2.01 | 113.04 | 109.93 |
| 23 | AW | 46 | 7MG | CM7-N7-C5 | 2.00 | 131.71 | 124.01 |

There are no chirality outliers.

All (64) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | AW | 37 | MIA | C12-C13-C14-C16 |
| 24 | AX | 76 | 31H | OCN-CN-N-CA |
| 25 | AY | 46 | 7MG | C4'-C5'-O5'-P |
| 25 | CY | 55 | PSU | C2'-C1'-C5-C4 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | CY | 55 | PSU | C2'-C1'-C5-C6 |
| 25 | AY | 37 | MIA | C3'-C4'-C5'-O5' |
| 25 | AY | 32 | PSU | O4'-C4'-C5'-O5' |
| 25 | CY | 8 | 4SU | C2'-C1'-N1-C6 |
| 25 | CY | 54 | 5MU | C3'-C4'-C5'-O5' |
| 25 | CY | 54 | 5MU | O4'-C4'-C5'-O5' |
| 25 | CY | 37 | MIA | C3'-C4'-C5'-O5' |
| 25 | AY | 54 | 5MU | C2'-C1'-N1-C6 |
| 25 | AY | 54 | 5MU | C3'-C4'-C5'-O5' |
| 25 | CY | 46 | 7MG | O4'-C4'-C5'-O5' |
| 24 | CX | 76 | 31H | C4'-C5'-O5'-P |
| 24 | CX | 76 | 31H | CB-CA-N-CN |
| 24 | CX | 76 | 31H | OCN-CN-N-CA |
| 24 | CX | 76 | 31H | O-C-N3'-C3' |
| 25 | CY | 32 | PSU | O4'-C4'-C5'-O5' |
| 25 | CY | 55 | PSU | O4'-C4'-C5'-O5' |
| 25 | AY | 54 | 5MU | O4'-C4'-C5'-O5' |
| 25 | CY | 46 | 7MG | C3'-C4'-C5'-O5' |
| 23 | AW | 46 | 7MG | O4'-C4'-C5'-O5' |
| 25 | CY | 32 | PSU | C3'-C4'-C5'-O5' |
| 25 | AY | 32 | PSU | C3'-C4'-C5'-O5' |
| 24 | AX | 76 | 31H | C4'-C5'-O5'-P |
| 24 | AX | 76 | 31H | C3'-C4'-C5'-O5' |
| 23 | CW | 76 | F3N | C3'-C4'-C5'-O5' |
| 24 | CX | 76 | 31H | CB-CG-SD-CE |
| 24 | CX | 76 | 31H | C3'-C4'-C5'-O5' |
| 23 | AW | 46 | 7MG | C3'-C4'-C5'-O5' |
| 25 | AY | 39 | PSU | C3'-C4'-C5'-O5' |
| 25 | AY | 37 | MIA | O4'-C4'-C5'-O5' |
| 25 | CY | 37 | MIA | O4'-C4'-C5'-O5' |
| 25 | AY | 39 | PSU | O4'-C4'-C5'-O5' |
| 24 | AX | 76 | 31H | O4'-C4'-C5'-O5' |
| 24 | CX | 76 | 31H | O4'-C4'-C5'-O5' |
| 24 | CX | 76 | 31H | N3'-C-CA-N |
| 23 | CW | 76 | F3N | C-CA-CB-CG |
| 23 | CW | 76 | F3N | O4'-C4'-C5'-O5' |
| 25 | AY | 46 | 7MG | C2'-C1'-N9-C8 |
| 23 | CW | 46 | 7MG | C2'-C1'-N9-C8 |
| 23 | CW | 76 | F3N | C4'-C5'-O5'-P |
| 25 | CY | 37 | MIA | C4'-C5'-O5'-P |
| 25 | CY | 55 | PSU | C3'-C4'-C5'-O5' |
| 23 | CW | 76 | F3N | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | CX | 76 | 31H | O-C-CA-N |
| 23 | AW | 46 | 7MG | C4'-C5'-O5'-P |
| 23 | CW | 46 | 7MG | C4'-C5'-O5'-P |
| 24 | AX | 76 | 31H | N3'-C-CA-N |
| 25 | CY | 55 | PSU | O4'-C1'-C5-C6 |
| 24 | CX | 76 | 31H | C-CA-CB-CG |
| 25 | CY | 55 | PSU | O4'-C1'-C5-C4 |
| 24 | AX | 76 | 31H | O-C-CA-N |
| 25 | CY | 39 | PSU | C4'-C5'-O5'-P |
| 24 | CX | 76 | 31H | N-CA-CB-CG |
| 25 | CY | 32 | PSU | C2'-C1'-C5-C6 |
| 25 | AY | 46 | 7MG | O4'-C1'-N9-C8 |
| 23 | CW | 46 | 7MG | O4'-C1'-N9-C8 |
| 25 | AY | 37 | MIA | C4'-C5'-O5'-P |
| 25 | AY | 46 | 7MG | C3'-C4'-C5'-O5' |
| 25 | CY | 39 | PSU | O4'-C4'-C5'-O5' |
| 24 | AX | 76 | 31H | CB-CA-N-CN |
| 24 | CX | 76 | 31H | N3'-C-CA-CB |

There are no ring outliers.

26 monomers are involved in 48 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | AX | 76 | 31H | 1 | 0 |
| 25 | AY | 46 | 7MG | 3 | 0 |
| 24 | CX | 8 | 4SU | 3 | 0 |
| 23 | CW | 32 | PSU | 1 | 0 |
| 23 | AW | 55 | PSU | 1 | 0 |
| 25 | CY | 55 | PSU | 2 | 0 |
| 25 | AY | 55 | PSU | 1 | 0 |
| 24 | AX | 32 | 5MC | 2 | 0 |
| 23 | AW | 39 | PSU | 1 | 0 |
| 25 | AY | 37 | MIA | 1 | 0 |
| 24 | CX | 32 | 5MC | 1 | 0 |
| 23 | CW | 76 | F3N | 3 | 0 |
| 24 | CX | 55 | PSU | 1 | 0 |
| 23 | CW | 55 | PSU | 1 | 0 |
| 25 | CY | 8 | 4SU | 2 | 0 |
| 23 | AW | 76 | F3N | 1 | 0 |
| 25 | AY | 8 | 4SU | 1 | 0 |
| 23 | CW | 8 | 4SU | 2 | 0 |
| 25 | CY | 39 | PSU | 8 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25 | CY | 37 | MIA | 3 | 0 |
| 24 | AX | 8 | 4SU | 1 | 0 |
| 23 | CW | 46 | 7MG | 2 | 0 |
| 25 | CY | 46 | 7MG | 4 | 0 |
| 23 | CW | 39 | PSU | 1 | 0 |
| 25 | AY | 39 | PSU | 2 | 0 |
| 24 | CX | 76 | 31H | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2063 ligands modelled in this entry, 2061 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 58 | SF4 | CD | 501 | 4 | 0,12,12 | 0.00 | - | - | | |
| 58 | SF4 | AD | 501 | 4 | 0,12,12 | 0.00 | - | - | | |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 58 | SF4 | CD | 501 | 4 | - | - | 0/6/5/5 |
| 58 | SF4 | AD | 501 | 4 | - | - | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 58 | CD | 501 | SF4 | 1 | 0 |
| 58 | 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 | 1497/1521 (98%) | 0.04 | 16 (1%) 80 78 | 41, 72, 93, 106 | 0 |
| 1 | CA | 1503/1521 (98%) | 0.06 | 62 (4%) 37 30 | 43, 75, 94, 106 | 0 |
| 2 | AB | 231/256 (90%) | 0.69 | 29 (12%) 3 2 | 68, 82, 89, 95 | 0 |
| 2 | CB | 231/256 (90%) | 1.72 | 85 (36%) 0 0 | 68, 83, 90, 96 | 0 |
| 3 | AC | 206/239 (86%) | 0.79 | 24 (11%) 4 3 | 69, 79, 87, 94 | 0 |
| 3 | CC | 206/239 (86%) | 1.62 | 73 (35%) 0 0 | 70, 82, 90, 94 | 0 |
| 4 | AD | 208/209 (99%) | 1.04 | 38 (18%) 1 0 | 57, 72, 81, 87 | 0 |
| 4 | CD | 208/209 (99%) | 0.96 | 25 (12%) 4 2 | 60, 72, 81, 89 | 0 |
| 5 | AE | 148/162 (91%) | 0.74 | 12 (8%) 12 8 | 58, 71, 81, 85 | 0 |
| 5 | CE | 148/162 (91%) | 1.07 | 21 (14%) 2 1 | 60, 74, 83, 86 | 0 |
| 6 | AF | 100/101 (99%) | 0.41 | 1 (1%) 82 80 | 52, 67, 75, 85 | 0 |
| 6 | CF | 100/101 (99%) | 0.38 | 3 (3%) 50 43 | 57, 71, 81, 85 | 0 |
| 7 | AG | 155/156 (99%) | 0.42 | 9 (5%) 23 17 | 66, 76, 85, 96 | 0 |
| 7 | CG | 155/156 (99%) | 1.29 | 47 (30%) 0 0 | 68, 77, 86, 97 | 0 |
| 8 | AH | 137/138 (99%) | 0.32 | 2 (1%) 73 70 | 62, 72, 79, 83 | 0 |
| 8 | CH | 137/138 (99%) | 1.22 | 35 (25%) 0 0 | 64, 74, 80, 85 | 0 |
| 9 | AI | 127/128 (99%) | 0.99 | 19 (14%) 2 1 | 62, 80, 87, 89 | 0 |
| 9 | CI | 127/128 (99%) | 2.96 | 83 (65%) 0 0 | 69, 82, 89, 91 | 0 |
| 10 | AJ | 97/105 (92%) | 0.82 | 13 (13%) 3 2 | 66, 83, 91, 92 | 0 |
| 10 | CJ | 96/105 (91%) | 2.14 | 43 (44%) 0 0 | 68, 84, 91, 93 | 0 |
| 11 | AK | 114/129 (88%) | 0.86 | 10 (8%) 10 7 | 51, 70, 80, 84 | 0 |
| 11 | CK | 114/129 (88%) | 0.93 | 13 (11%) 5 3 | 52, 72, 81, 85 | 0 |
| 12 | AL | 122/132 (92%) | 0.24 | 1 (0%) 86 84 | 41, 56, 71, 75 | 0 |
| 12 | CL | 122/132 (92%) | 0.85 | 23 (18%) 1 0 | 58, 73, 82, 87 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AM | 123/126 (97%) | 0.46 | 7 (5%) 23 18 | 57, 72, 83, 88 | 0 |
| 13 | CM | 122/126 (96%) | 1.98 | 51 (41%) 0 0 | 69, 85, 92, 97 | 0 |
| 14 | AN | 60/61 (98%) | 1.05 | 8 (13%) 3 2 | 70, 76, 83, 84 | 0 |
| 14 | CN | 60/61 (98%) | 3.05 | 42 (70%) 0 0 | 73, 79, 85, 87 | 0 |
| 15 | AO | 88/89 (98%) | 0.53 | 5 (5%) 23 18 | 54, 68, 79, 83 | 0 |
| 15 | CO | 88/89 (98%) | 0.55 | 6 (6%) 17 12 | 56, 70, 81, 84 | 0 |
| 16 | AP | 82/88 (93%) | 1.40 | 22 (26%) 0 0 | 59, 71, 79, 84 | 0 |
| 16 | CP | 82/88 (93%) | 0.65 | 3 (3%) 41 34 | 59, 70, 79, 83 | 0 |
| 17 | AQ | 99/105 (94%) | 0.61 | 8 (8%) 12 8 | 57, 70, 79, 84 | 0 |
| 17 | CQ | 99/105 (94%) | 1.09 | 21 (21%) 0 0 | 60, 71, 79, 84 | 0 |
| 18 | AR | 68/88 (77%) | 0.76 | 9 (13%) 3 2 | 59, 69, 81, 84 | 0 |
| 18 | CR | 68/88 (77%) | 0.90 | 11 (16%) 1 1 | 58, 70, 81, 85 | 0 |
| 19 | AS | 84/93 (90%) | 0.31 | 2 (2%) 59 53 | 70, 81, 87, 92 | 0 |
| 19 | CS | 83/93 (89%) | 2.05 | 38 (45%) 0 0 | 74, 83, 90, 94 | 0 |
| 20 | AT | 96/106 (90%) | 0.37 | 5 (5%) 27 21 | 59, 71, 80, 83 | 0 |
| 20 | CT | 96/106 (90%) | 0.58 | 8 (8%) 11 8 | 59, 71, 80, 83 | 0 |
| 21 | AU | 23/27 (85%) | 1.17 | 5 (21%) 0 0 | 70, 75, 78, 82 | 0 |
| 21 | CU | 23/27 (85%) | 2.81 | 15 (65%) 0 0 | 71, 78, 81, 82 | 0 |
| 22 | AV | 13/24 (54%) | 1.83 | 5 (38%) 0 0 | 58, 77, 95, 100 | 0 |
| 22 | CV | 12/24 (50%) | 2.36 | 7 (58%) 0 0 | 64, 81, 93, 95 | 0 |
| 23 | AW | 66/76 (86%) | 1.04 | 10 (15%) 2 1 | 66, 95, 102, 105 | 0 |
| 23 | CW | 64/76 (84%) | 3.10 | 47 (73%) 0 0 | 70, 96, 101, 106 | 0 |
| 24 | AX | 71/77 (92%) | -0.01 | 0 100 100 | 42, 73, 90, 96 | 0 |
| 24 | CX | 71/77 (92%) | 0.11 | 2 (2%) 53 46 | 55, 86, 95, 98 | 0 |
| 25 | AY | 67/76 (88%) | 0.49 | 8 (11%) 4 3 | 44, 97, 101, 105 | 0 |
| 25 | CY | 66/76 (86%) | 1.70 | 27 (40%) 0 0 | 48, 98, 102, 103 | 0 |
| 26 | BA | 2819/2915 (96%) | 0.52 | 17 (0%) 89 88 | 23, 43, 87, 106 | 0 |
| 26 | DA | 2800/2915 (96%) | -0.10 | 60 (2%) 63 58 | 27, 48, 90, 108 | 0 |
| 27 | BB | 120/121 (99%) | 0.49 | 0 100 100 | 41, 64, 76, 88 | 0 |
| 27 | DB | 120/121 (99%) | -0.08 | 2 (1%) 70 66 | 48, 70, 80, 91 | 0 |
| 28 | BD | 275/276 (99%) | 0.46 | 3 (1%) 80 78 | 24, 41, 58, 79 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28 | DD | 275/276 (99%) | 0.40 | 8 (2%) 51 45 | 28, 44, 61, 79 | 0 |
| 29 | BE | 204/206 (99%) | 0.59 | 1 (0%) 91 89 | 23, 46, 65, 83 | 0 |
| 29 | DE | 204/206 (99%) | 0.25 | 1 (0%) 91 89 | 26, 50, 67, 84 | 0 |
| 30 | BF | 203/210 (96%) | 0.61 | 1 (0%) 91 89 | 25, 51, 76, 86 | 0 |
| 30 | DF | 203/210 (96%) | 0.43 | 7 (3%) 45 38 | 28, 56, 78, 88 | 0 |
| 31 | BG | 181/182 (99%) | 0.51 | 3 (1%) 70 66 | 55, 72, 83, 93 | 0 |
| 31 | DG | 181/182 (99%) | 1.53 | 58 (32%) 0 0 | 64, 76, 85, 93 | 0 |
| 32 | BH | 174/180 (96%) | 0.51 | 1 (0%) 89 88 | 50, 66, 75, 82 | 0 |
| 32 | DH | 174/180 (96%) | 1.74 | 72 (41%) 0 0 | 56, 71, 79, 83 | 0 |
| 33 | BI | 146/148 (98%) | 0.33 | 1 (0%) 87 86 | 49, 74, 83, 87 | 0 |
| 33 | DI | 146/148 (98%) | 0.12 | 2 (1%) 75 71 | 50, 74, 83, 87 | 0 |
| 34 | BN | 140/140 (100%) | 0.67 | 0 100 100 | 29, 48, 67, 79 | 0 |
| 34 | DN | 140/140 (100%) | 0.80 | 13 (9%) 8 6 | 35, 53, 70, 82 | 0 |
| 35 | BO | 122/122 (100%) | 0.28 | 0 100 100 | 25, 40, 57, 67 | 0 |
| 35 | DO | 122/122 (100%) | 0.47 | 2 (1%) 72 68 | 44, 58, 74, 79 | 0 |
| 36 | BP | 149/150 (99%) | 0.55 | 0 100 100 | 25, 55, 75, 80 | 0 |
| 36 | DP | 149/150 (99%) | 0.59 | 6 (4%) 38 31 | 28, 58, 78, 83 | 0 |
| 37 | BQ | 141/141 (100%) | 0.76 | 2 (1%) 75 71 | 37, 52, 68, 77 | 0 |
| 37 | DQ | 141/141 (100%) | 1.22 | 27 (19%) 1 0 | 41, 58, 72, 79 | 0 |
| 38 | BR | 118/118 (100%) | 0.42 | 0 100 100 | 22, 34, 50, 59 | 0 |
| 38 | DR | 118/118 (100%) | 0.65 | 6 (5%) 28 22 | 38, 53, 64, 75 | 0 |
| 39 | BS | 110/112 (98%) | 0.33 | 0 100 100 | 34, 50, 64, 70 | 0 |
| 39 | DS | 110/112 (98%) | 1.42 | 29 (26%) 0 0 | 70, 79, 87, 91 | 0 |
| 40 | BT | 131/146 (89%) | 0.38 | 0 100 100 | 38, 51, 73, 82 | 0 |
| 40 | DT | 131/146 (89%) | 0.23 | 2 (1%) 73 70 | 40, 54, 75, 81 | 0 |
| 41 | BU | 116/118 (98%) | 0.44 | 0 100 100 | 17, 30, 50, 63 | 0 |
| 41 | DU | 116/118 (98%) | 0.54 | 5 (4%) 35 28 | 40, 59, 79, 85 | 0 |
| 42 | BV | 101/101 (100%) | 0.28 | 0 100 100 | 16, 38, 58, 68 | 0 |
| 42 | DV | 101/101 (100%) | 0.33 | 4 (3%) 38 31 | 44, 73, 81, 92 | 0 |
| 43 | BW | 112/113 (99%) | 0.38 | 0 100 100 | 22, 30, 49, 83 | 0 |
| 43 | DW | 112/113 (99%) | 0.71 | 4 (3%) 42 35 | 35, 50, 66, 86 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | BX | 95/96 (98%) | 0.64 | 0 100 100 | 31, 46, 67, 83 | 0 |
| 44 | DX | 95/96 (98%) | 0.70 | 10 (10%) 6 4 | 36, 50, 68, 83 | 0 |
| 45 | BY | 107/110 (97%) | 0.47 | 1 (0%) 84 82 | 42, 59, 73, 84 | 0 |
| 45 | DY | 107/110 (97%) | 0.77 | 12 (11%) 5 3 | 47, 61, 75, 84 | 0 |
| 46 | BZ | 171/206 (83%) | 0.95 | 30 (17%) 1 0 | 40, 66, 91, 95 | 0 |
| 46 | DZ | 174/206 (84%) | 1.90 | 67 (38%) 0 0 | 69, 85, 94, 101 | 0 |
| 47 | B0 | 83/85 (97%) | 0.96 | 6 (7%) 15 11 | 34, 50, 67, 75 | 0 |
| 47 | D0 | 83/85 (97%) | 1.15 | 10 (12%) 4 2 | 40, 56, 71, 76 | 0 |
| 48 | B1 | 97/98 (98%) | 0.47 | 2 (2%) 63 58 | 31, 49, 72, 76 | 0 |
| 48 | D1 | 97/98 (98%) | 0.54 | 5 (5%) 27 21 | 34, 53, 73, 78 | 0 |
| 49 | B2 | 70/72 (97%) | 0.42 | 0 100 100 | 33, 49, 64, 82 | 0 |
| 49 | D2 | 70/72 (97%) | 0.38 | 1 (1%) 75 71 | 58, 69, 78, 82 | 0 |
| 50 | B3 | 59/60 (98%) | 0.22 | 0 100 100 | 24, 37, 63, 74 | 0 |
| 50 | D3 | 59/60 (98%) | 0.92 | 8 (13%) 3 1 | 52, 65, 79, 87 | 0 |
| 51 | B4 | 69/71 (97%) | 0.46 | 4 (5%) 23 17 | 49, 76, 89, 91 | 0 |
| 51 | D4 | 69/71 (97%) | 1.72 | 27 (39%) 0 0 | 74, 89, 95, 99 | 0 |
| 52 | B5 | 59/60 (98%) | 0.42 | 1 (1%) 70 66 | 16, 30, 46, 68 | 0 |
| 52 | D5 | 59/60 (98%) | 0.30 | 1 (1%) 70 66 | 35, 49, 65, 77 | 0 |
| 53 | B6 | 53/54 (98%) | 0.31 | 0 100 100 | 32, 44, 57, 72 | 0 |
| 53 | D6 | 53/54 (98%) | 0.70 | 3 (5%) 23 18 | 49, 64, 74, 79 | 0 |
| 54 | B7 | 48/49 (97%) | 0.77 | 3 (6%) 20 15 | 23, 32, 58, 70 | 0 |
| 54 | D7 | 48/49 (97%) | 0.98 | 5 (10%) 6 4 | 26, 35, 61, 70 | 0 |
| 55 | B8 | 64/65 (98%) | 0.62 | 0 100 100 | 34, 42, 50, 65 | 0 |
| 55 | D8 | 64/65 (98%) | 0.55 | 1 (1%) 72 68 | 37, 46, 54, 65 | 0 |
| 56 | B9 | 37/37 (100%) | 0.94 | 1 (2%) 54 48 | 36, 51, 65, 73 | 0 |
| 56 | D9 | 37/37 (100%) | 0.71 | 4 (10%) 5 3 | 43, 55, 68, 76 | 0 |
| All | All | 20895/21748 (96%) | 0.54 | 1598 (7%) 13 10 | 16, 64, 89, 108 | 0 |

All (1598) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | CB | 165 | VAL | 12.1 |
| 46 | DZ | 155 | LEU | 10.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | CM | 124 | PRO | 10.0 |
| 46 | DZ | 107 | THR | 9.1 |
| 46 | DZ | 171 | ILE | 8.6 |
| 46 | DZ | 114 | GLY | 8.5 |
| 9 | CI | 14 | VAL | 8.1 |
| 13 | CM | 123 | ALA | 8.0 |
| 2 | CB | 200 | ILE | 8.0 |
| 9 | CI | 7 | THR | 7.9 |
| 10 | CJ | 47 | PHE | 7.9 |
| 10 | CJ | 63 | PHE | 7.8 |
| 7 | CG | 83 | ALA | 7.7 |
| 46 | DZ | 108 | PRO | 7.6 |
| 9 | CI | 36 | TYR | 7.6 |
| 9 | CI | 76 | ALA | 7.5 |
| 46 | BZ | 106 | GLY | 7.3 |
| 9 | CI | 106 | ALA | 7.3 |
| 23 | CW | 31 | A | 7.3 |
| 13 | AM | 124 | PRO | 7.1 |
| 14 | CN | 25 | VAL | 7.0 |
| 14 | CN | 53 | LEU | 6.9 |
| 14 | CN | 38 | GLY | 6.9 |
| 46 | BZ | 107 | THR | 6.9 |
| 46 | DZ | 113 | ALA | 6.9 |
| 28 | DD | 2 | ALA | 6.7 |
| 14 | CN | 59 | ALA | 6.7 |
| 1 | CA | 1030(B) | C | 6.7 |
| 13 | CM | 95 | GLY | 6.6 |
| 9 | CI | 79 | LEU | 6.6 |
| 39 | DS | 32 | LEU | 6.6 |
| 10 | CJ | 71 | LEU | 6.5 |
| 13 | CM | 122 | LYS | 6.5 |
| 46 | DZ | 149 | SER | 6.5 |
| 23 | CW | 71 | G | 6.4 |
| 13 | CM | 102 | ARG | 6.4 |
| 46 | BZ | 108 | PRO | 6.3 |
| 10 | CJ | 46 | ARG | 6.3 |
| 2 | CB | 92 | TYR | 6.3 |
| 51 | D4 | 49 | PHE | 6.3 |
| 46 | BZ | 120 | ILE | 6.2 |
| 7 | CG | 82 | GLY | 6.2 |
| 14 | CN | 39 | LEU | 6.2 |
| 13 | CM | 90 | LEU | 6.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | CI | 9 | ARG | 6.2 |
| 3 | CC | 13 | GLY | 6.1 |
| 14 | CN | 44 | LEU | 6.1 |
| 47 | B0 | 7 | LEU | 6.0 |
| 3 | CC | 53 | ALA | 6.0 |
| 19 | CS | 80 | TYR | 6.0 |
| 9 | CI | 80 | GLY | 6.0 |
| 13 | CM | 94 | ARG | 6.0 |
| 9 | CI | 123 | PRO | 6.0 |
| 25 | AY | 36 | A | 6.0 |
| 47 | D0 | 2 | ALA | 5.9 |
| 14 | CN | 34 | TYR | 5.9 |
| 2 | CB | 81 | VAL | 5.9 |
| 3 | CC | 184 | TYR | 5.9 |
| 46 | DZ | 116 | VAL | 5.9 |
| 44 | DX | 92 | LEU | 5.9 |
| 46 | BZ | 144 | LEU | 5.9 |
| 21 | CU | 6 | ARG | 5.9 |
| 51 | D4 | 57 | GLU | 5.9 |
| 3 | CC | 145 | GLY | 5.9 |
| 9 | CI | 115 | GLY | 5.9 |
| 8 | CH | 2 | LEU | 5.8 |
| 13 | AM | 123 | ALA | 5.8 |
| 5 | CE | 94 | ALA | 5.8 |
| 9 | AI | 19 | LEU | 5.8 |
| 23 | CW | 3 | C | 5.8 |
| 26 | DA | 229 | A | 5.7 |
| 2 | CB | 214 | ILE | 5.7 |
| 31 | DG | 140 | ILE | 5.7 |
| 7 | AG | 82 | GLY | 5.7 |
| 13 | CM | 60 | VAL | 5.6 |
| 48 | D1 | 2 | SER | 5.6 |
| 14 | CN | 35 | ARG | 5.5 |
| 3 | CC | 182 | ILE | 5.5 |
| 13 | CM | 92 | HIS | 5.5 |
| 9 | CI | 109 | VAL | 5.5 |
| 23 | AW | 71 | G | 5.5 |
| 9 | CI | 15 | ALA | 5.5 |
| 51 | D4 | 40 | HIS | 5.5 |
| 46 | DZ | 115 | GLY | 5.5 |
| 26 | DA | 2127 | G | 5.4 |
| 3 | CC | 206 | GLU | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 14 | CN | 29 | ARG | 5.4 |
| 26 | DA | 2132 | U | 5.4 |
| 46 | DZ | 170 | THR | 5.4 |
| 2 | CB | 211 | ILE | 5.4 |
| 14 | AN | 2 | ALA | 5.4 |
| 46 | DZ | 172 | ALA | 5.4 |
| 2 | CB | 70 | PHE | 5.4 |
| 23 | CW | 4 | C | 5.4 |
| 23 | CW | 30 | G | 5.4 |
| 2 | CB | 187 | LEU | 5.4 |
| 32 | DH | 115 | VAL | 5.4 |
| 32 | DH | 113 | VAL | 5.4 |
| 46 | BZ | 118 | GLN | 5.4 |
| 23 | CW | 72 | C | 5.4 |
| 13 | AM | 2 | ALA | 5.4 |
| 32 | DH | 94 | TYR | 5.4 |
| 3 | CC | 8 | ILE | 5.3 |
| 9 | AI | 106 | ALA | 5.3 |
| 54 | B7 | 48 | LYS | 5.3 |
| 17 | CQ | 80 | GLY | 5.3 |
| 32 | DH | 102 | ALA | 5.3 |
| 54 | D7 | 48 | LYS | 5.3 |
| 7 | CG | 4 | ARG | 5.3 |
| 51 | D4 | 54 | GLY | 5.3 |
| 46 | BZ | 141 | VAL | 5.3 |
| 37 | DQ | 104 | PHE | 5.3 |
| 9 | CI | 5 | TYR | 5.3 |
| 21 | CU | 14 | TRP | 5.3 |
| 7 | CG | 81 | GLY | 5.3 |
| 23 | CW | 56 | C | 5.2 |
| 9 | CI | 17 | VAL | 5.2 |
| 25 | CY | 36 | A | 5.2 |
| 32 | DH | 107 | VAL | 5.2 |
| 23 | CW | 70 | G | 5.2 |
| 46 | DZ | 143 | GLY | 5.2 |
| 31 | DG | 142 | PRO | 5.2 |
| 47 | B0 | 6 | GLY | 5.1 |
| 19 | CS | 82 | GLY | 5.1 |
| 3 | CC | 71 | ALA | 5.1 |
| 7 | AG | 83 | ALA | 5.1 |
| 7 | AG | 85 | TYR | 5.1 |
| 26 | DA | 896 | A | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 19 | CS | 41 | VAL | 5.1 |
| 51 | D4 | 44 | THR | 5.0 |
| 21 | CU | 11 | GLY | 5.0 |
| 9 | CI | 110 | GLU | 5.0 |
| 3 | CC | 12 | LEU | 5.0 |
| 19 | CS | 79 | THR | 5.0 |
| 46 | DZ | 141 | VAL | 5.0 |
| 31 | DG | 29 | TRP | 5.0 |
| 10 | CJ | 67 | THR | 5.0 |
| 21 | CU | 15 | ARG | 5.0 |
| 14 | CN | 42 | ILE | 5.0 |
| 2 | CB | 77 | ALA | 5.0 |
| 26 | DA | 2155 | G | 5.0 |
| 26 | DA | 2128 | C | 5.0 |
| 26 | DA | 2146 | C | 5.0 |
| 46 | DZ | 52 | SER | 5.0 |
| 14 | CN | 57 | ARG | 5.0 |
| 19 | CS | 49 | ILE | 4.9 |
| 23 | CW | 73 | A | 4.9 |
| 26 | DA | 883 | G | 4.9 |
| 14 | CN | 61 | TRP | 4.9 |
| 10 | CJ | 49 | VAL | 4.9 |
| 23 | CW | 23 | A | 4.9 |
| 9 | CI | 66 | ARG | 4.9 |
| 2 | CB | 164 | VAL | 4.9 |
| 46 | BZ | 111 | VAL | 4.9 |
| 2 | CB | 196 | LEU | 4.9 |
| 39 | DS | 58 | LEU | 4.9 |
| 14 | CN | 31 | ARG | 4.9 |
| 47 | D0 | 7 | LEU | 4.9 |
| 46 | DZ | 125 | LEU | 4.9 |
| 9 | CI | 126 | SER | 4.9 |
| 9 | CI | 114 | TYR | 4.8 |
| 13 | CM | 4 | ILE | 4.8 |
| 53 | D6 | 54 | ILE | 4.8 |
| 3 | CC | 21 | ARG | 4.8 |
| 2 | CB | 31 | TYR | 4.8 |
| 7 | CG | 156 | TRP | 4.8 |
| 19 | CS | 30 | LEU | 4.8 |
| 47 | B0 | 2 | ALA | 4.8 |
| 10 | CJ | 65 | LEU | 4.8 |
| 10 | CJ | 62 | HIS | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | CW | 45 | U | 4.8 |
| 25 | CY | 62 | C | 4.8 |
| 13 | CM | 82 | MET | 4.8 |
| 9 | CI | 107 | ARG | 4.8 |
| 54 | D7 | 46 | VAL | 4.8 |
| 46 | BZ | 113 | ALA | 4.8 |
| 25 | CY | 35 | A | 4.7 |
| 46 | DZ | 111 | VAL | 4.7 |
| 46 | DZ | 139 | VAL | 4.7 |
| 46 | DZ | 144 | LEU | 4.7 |
| 51 | D4 | 52 | THR | 4.7 |
| 26 | DA | 2160 | G | 4.7 |
| 2 | CB | 207 | ALA | 4.7 |
| 22 | CV | 24 | A | 4.7 |
| 5 | CE | 8 | GLU | 4.7 |
| 9 | CI | 75 | ASP | 4.7 |
| 46 | BZ | 114 | GLY | 4.7 |
| 46 | DZ | 156 | LYS | 4.6 |
| 1 | CA | 1532 | U | 4.6 |
| 32 | DH | 106 | THR | 4.6 |
| 31 | DG | 149 | VAL | 4.6 |
| 23 | CW | 44 | G | 4.6 |
| 9 | CI | 62 | TYR | 4.6 |
| 9 | CI | 61 | ALA | 4.6 |
| 9 | CI | 19 | LEU | 4.6 |
| 26 | BA | 896 | A | 4.6 |
| 22 | CV | 22 | U | 4.6 |
| 4 | AD | 138 | TYR | 4.6 |
| 31 | DG | 146 | TYR | 4.6 |
| 2 | CB | 203 | GLY | 4.6 |
| 19 | CS | 52 | TYR | 4.6 |
| 32 | DH | 105 | LEU | 4.6 |
| 10 | CJ | 38 | ILE | 4.6 |
| 21 | CU | 2 | GLY | 4.6 |
| 13 | CM | 120 | LYS | 4.6 |
| 2 | CB | 152 | PHE | 4.5 |
| 9 | CI | 4 | TYR | 4.5 |
| 22 | AV | 13 | A | 4.5 |
| 2 | CB | 122 | PHE | 4.5 |
| 1 | CA | 1115 | C | 4.5 |
| 13 | CM | 121 | LYS | 4.5 |
| 13 | CM | 78 | ILE | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 14 | CN | 37 | PHE | 4.5 |
| 9 | CI | 108 | VAL | 4.5 |
| 31 | DG | 41 | GLN | 4.5 |
| 1 | AA | 1030(B) | C | 4.5 |
| 9 | CI | 116 | LYS | 4.5 |
| 26 | DA | 2173 | A | 4.5 |
| 31 | DG | 11 | TYR | 4.5 |
| 31 | DG | 35 | GLU | 4.5 |
| 2 | CB | 118 | LEU | 4.4 |
| 48 | B1 | 98 | LEU | 4.4 |
| 17 | AQ | 27 | PHE | 4.4 |
| 51 | D4 | 51 | ASP | 4.4 |
| 1 | AA | 1001(A) | G | 4.4 |
| 23 | CW | 57 | G | 4.4 |
| 13 | CM | 66 | LEU | 4.4 |
| 14 | CN | 58 | LYS | 4.4 |
| 2 | CB | 228 | GLY | 4.4 |
| 1 | AA | 1002 | G | 4.4 |
| 3 | CC | 6 | HIS | 4.4 |
| 10 | CJ | 48 | THR | 4.4 |
| 10 | CJ | 50 | ILE | 4.4 |
| 25 | CY | 18 | G | 4.4 |
| 52 | B5 | 60 | VAL | 4.4 |
| 10 | CJ | 10 | GLY | 4.4 |
| 39 | DS | 56 | LEU | 4.4 |
| 7 | CG | 80 | VAL | 4.4 |
| 31 | BG | 146 | TYR | 4.4 |
| 50 | D3 | 26 | LEU | 4.4 |
| 7 | CG | 154 | TYR | 4.3 |
| 2 | CB | 201 | ILE | 4.3 |
| 9 | CI | 27 | THR | 4.3 |
| 9 | CI | 33 | PHE | 4.3 |
| 23 | AW | 73 | A | 4.3 |
| 13 | CM | 7 | VAL | 4.3 |
| 23 | AW | 20 | U | 4.3 |
| 26 | DA | 2144 | U | 4.3 |
| 9 | CI | 125 | TYR | 4.3 |
| 25 | CY | 61 | C | 4.3 |
| 46 | DZ | 119 | GLU | 4.3 |
| 9 | CI | 81 | ILE | 4.3 |
| 3 | CC | 80 | GLY | 4.3 |
| 3 | CC | 181 | ASN | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | CB | 163 | PHE | 4.3 |
| 1 | CA | 1220 | G | 4.3 |
| 9 | CI | 127 | LYS | 4.3 |
| 26 | DA | 2154 | G | 4.3 |
| 7 | AG | 153 | HIS | 4.3 |
| 46 | DZ | 96 | VAL | 4.3 |
| 10 | CJ | 60 | ARG | 4.3 |
| 44 | DX | 68 | ARG | 4.3 |
| 3 | CC | 159 | GLY | 4.3 |
| 19 | CS | 35 | SER | 4.3 |
| 3 | CC | 207 | VAL | 4.2 |
| 5 | CE | 109 | ILE | 4.2 |
| 25 | CY | 63 | G | 4.2 |
| 7 | CG | 79 | ARG | 4.2 |
| 7 | CG | 84 | ASN | 4.2 |
| 26 | BA | 2145 | C | 4.2 |
| 26 | DA | 885 | C | 4.2 |
| 19 | CS | 14 | HIS | 4.2 |
| 23 | CW | 5 | G | 4.2 |
| 3 | CC | 204 | LEU | 4.2 |
| 32 | DH | 166 | GLY | 4.2 |
| 21 | CU | 8 | THR | 4.2 |
| 9 | AI | 8 | GLY | 4.2 |
| 25 | CY | 34 | G | 4.2 |
| 3 | CC | 60 | ALA | 4.2 |
| 7 | CG | 2 | ALA | 4.2 |
| 39 | DS | 5 | THR | 4.2 |
| 39 | DS | 40 | ILE | 4.2 |
| 16 | AP | 19 | ILE | 4.2 |
| 13 | CM | 87 | TYR | 4.2 |
| 9 | CI | 105 | ASP | 4.2 |
| 46 | BZ | 112 | ARG | 4.2 |
| 1 | CA | 1030(A) | G | 4.1 |
| 13 | CM | 6 | GLY | 4.1 |
| 10 | CJ | 55 | LYS | 4.1 |
| 51 | D4 | 50 | VAL | 4.1 |
| 2 | CB | 48 | MET | 4.1 |
| 13 | CM | 15 | VAL | 4.1 |
| 32 | DH | 48 | GLY | 4.1 |
| 47 | D0 | 45 | PHE | 4.1 |
| 1 | CA | 1114 | C | 4.1 |
| 51 | D4 | 32 | TYR | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | CW | 28 | G | 4.1 |
| 13 | CM | 5 | ALA | 4.1 |
| 14 | CN | 41 | ARG | 4.0 |
| 19 | CS | 69 | HIS | 4.0 |
| 23 | CW | 13 | C | 4.0 |
| 9 | CI | 74 | ILE | 4.0 |
| 2 | AB | 165 | VAL | 4.0 |
| 22 | AV | 12 | A | 4.0 |
| 22 | AV | 24 | A | 4.0 |
| 3 | CC | 189 | ALA | 4.0 |
| 14 | CN | 50 | LYS | 4.0 |
| 46 | BZ | 146 | ILE | 4.0 |
| 9 | CI | 26 | VAL | 4.0 |
| 12 | CL | 32 | PHE | 4.0 |
| 14 | CN | 47 | LEU | 4.0 |
| 10 | CJ | 66 | ARG | 4.0 |
| 34 | DN | 140 | VAL | 4.0 |
| 46 | DZ | 106 | GLY | 4.0 |
| 32 | DH | 97 | ARG | 4.0 |
| 25 | CY | 53 | G | 4.0 |
| 3 | CC | 65 | ALA | 4.0 |
| 46 | DZ | 147 | GLY | 4.0 |
| 22 | CV | 23 | A | 4.0 |
| 16 | AP | 2 | VAL | 4.0 |
| 1 | CA | 1150 | U | 4.0 |
| 46 | DZ | 152 | ALA | 4.0 |
| 8 | CH | 135 | CYS | 4.0 |
| 2 | CB | 132 | LYS | 4.0 |
| 26 | DA | 2145 | C | 4.0 |
| 3 | CC | 14 | ILE | 4.0 |
| 19 | CS | 40 | ILE | 4.0 |
| 31 | DG | 39 | ILE | 4.0 |
| 9 | CI | 124 | GLN | 4.0 |
| 14 | CN | 30 | ALA | 4.0 |
| 4 | AD | 135 | LEU | 3.9 |
| 14 | CN | 36 | PHE | 3.9 |
| 2 | CB | 101 | MET | 3.9 |
| 10 | CJ | 12 | ASP | 3.9 |
| 9 | CI | 67 | GLY | 3.9 |
| 23 | CW | 69 | G | 3.9 |
| 27 | DB | 119 | G | 3.9 |
| 3 | AC | 15 | THR | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | DH | 98 | LEU | 3.9 |
| 12 | CL | 28 | LYS | 3.9 |
| 13 | CM | 119 | GLY | 3.9 |
| 32 | DH | 114 | VAL | 3.9 |
| 9 | CI | 120 | ARG | 3.9 |
| 18 | CR | 87 | ARG | 3.9 |
| 31 | DG | 102 | PHE | 3.9 |
| 9 | CI | 28 | VAL | 3.9 |
| 23 | AW | 70 | G | 3.9 |
| 5 | CE | 90 | VAL | 3.9 |
| 13 | CM | 98 | VAL | 3.9 |
| 1 | AA | 1257 | U | 3.9 |
| 3 | CC | 134 | ILE | 3.9 |
| 51 | D4 | 59 | PHE | 3.9 |
| 26 | DA | 2153 | G | 3.9 |
| 9 | AI | 113 | LYS | 3.9 |
| 31 | DG | 136 | ARG | 3.8 |
| 23 | AW | 44 | G | 3.8 |
| 31 | DG | 17 | PRO | 3.8 |
| 13 | CM | 64 | TRP | 3.8 |
| 19 | CS | 10 | PHE | 3.8 |
| 46 | DZ | 137 | ILE | 3.8 |
| 7 | CG | 109 | ASN | 3.8 |
| 44 | DX | 89 | ILE | 3.8 |
| 31 | DG | 19 | LEU | 3.8 |
| 9 | CI | 18 | PHE | 3.8 |
| 26 | DA | 2156 | G | 3.8 |
| 22 | CV | 21 | C | 3.8 |
| 14 | CN | 46 | GLU | 3.8 |
| 51 | B4 | 50 | VAL | 3.8 |
| 45 | DY | 1 | MET | 3.8 |
| 23 | CW | 2 | C | 3.8 |
| 46 | BZ | 104 | PHE | 3.8 |
| 31 | DG | 173 | LEU | 3.8 |
| 3 | CC | 179 | ARG | 3.8 |
| 25 | CY | 57 | G | 3.8 |
| 10 | CJ | 85 | LEU | 3.8 |
| 26 | BA | 885 | C | 3.8 |
| 37 | DQ | 33 | GLY | 3.8 |
| 21 | CU | 16 | GLY | 3.8 |
| 37 | DQ | 32 | TYR | 3.7 |
| 9 | CI | 112 | LYS | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | CA | 1219 | U | 3.7 |
| 23 | CW | 14 | A | 3.7 |
| 7 | AG | 79 | ARG | 3.7 |
| 31 | DG | 182 | LYS | 3.7 |
| 1 | AA | 163 | C | 3.7 |
| 23 | AW | 72 | C | 3.7 |
| 19 | CS | 32 | LYS | 3.7 |
| 47 | D0 | 3 | HIS | 3.7 |
| 12 | CL | 39 | VAL | 3.7 |
| 47 | B0 | 4 | LYS | 3.7 |
| 9 | CI | 101 | PHE | 3.7 |
| 25 | CY | 64 | A | 3.7 |
| 26 | DA | 2158 | A | 3.7 |
| 46 | DZ | 121 | HIS | 3.7 |
| 39 | DS | 82 | ILE | 3.7 |
| 10 | CJ | 72 | VAL | 3.7 |
| 30 | DF | 12 | LEU | 3.7 |
| 31 | DG | 133 | LEU | 3.7 |
| 1 | AA | 1036 | G | 3.7 |
| 31 | DG | 139 | LEU | 3.7 |
| 32 | DH | 101 | ARG | 3.7 |
| 26 | DA | 2131 | G | 3.7 |
| 21 | CU | 17 | THR | 3.7 |
| 32 | BH | 2 | SER | 3.7 |
| 2 | CB | 188 | ALA | 3.7 |
| 16 | AP | 59 | TRP | 3.7 |
| 19 | CS | 31 | ILE | 3.7 |
| 26 | BA | 2146 | C | 3.7 |
| 2 | AB | 221 | LEU | 3.6 |
| 32 | DH | 111 | HIS | 3.6 |
| 14 | CN | 2 | ALA | 3.6 |
| 2 | CB | 72 | GLY | 3.6 |
| 3 | CC | 155 | GLY | 3.6 |
| 37 | DQ | 5 | ARG | 3.6 |
| 54 | D7 | 47 | ARG | 3.6 |
| 2 | CB | 215 | LEU | 3.6 |
| 1 | CA | 1036 | G | 3.6 |
| 9 | CI | 122 | ALA | 3.6 |
| 45 | DY | 65 | ALA | 3.6 |
| 9 | CI | 6 | GLY | 3.6 |
| 31 | DG | 115 | ARG | 3.6 |
| 31 | DG | 181 | ARG | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | CJ | 54 | PHE | 3.6 |
| 18 | AR | 85 | LEU | 3.6 |
| 31 | DG | 34 | LEU | 3.6 |
| 39 | DS | 54 | LEU | 3.6 |
| 2 | CB | 177 | ALA | 3.6 |
| 9 | CI | 64 | THR | 3.6 |
| 20 | CT | 24 | LEU | 3.6 |
| 23 | CW | 36 | A | 3.6 |
| 9 | AI | 15 | ALA | 3.6 |
| 3 | CC | 16 | ARG | 3.6 |
| 1 | CA | 1116 | C | 3.6 |
| 32 | DH | 36 | PRO | 3.6 |
| 10 | CJ | 15 | THR | 3.6 |
| 1 | CA | 1257 | U | 3.6 |
| 5 | CE | 10 | MET | 3.6 |
| 45 | DY | 5 | MET | 3.6 |
| 46 | DZ | 150 | LEU | 3.6 |
| 46 | DZ | 122 | ARG | 3.6 |
| 9 | CI | 54 | ASP | 3.6 |
| 19 | CS | 13 | ASP | 3.6 |
| 12 | CL | 18 | VAL | 3.6 |
| 46 | DZ | 118 | GLN | 3.6 |
| 4 | AD | 70 | ILE | 3.6 |
| 7 | CG | 9 | VAL | 3.6 |
| 31 | DG | 157 | ILE | 3.6 |
| 1 | CA | 1321 | C | 3.6 |
| 9 | CI | 128 | ARG | 3.5 |
| 14 | AN | 16 | PHE | 3.5 |
| 1 | CA | 1186 | G | 3.5 |
| 3 | CC | 178 | LEU | 3.5 |
| 3 | CC | 17 | ASP | 3.5 |
| 2 | CB | 131 | PRO | 3.5 |
| 2 | CB | 202 | PRO | 3.5 |
| 22 | CV | 14 | A | 3.5 |
| 26 | DA | 888 | C | 3.5 |
| 18 | CR | 85 | LEU | 3.5 |
| 32 | DH | 159 | GLU | 3.5 |
| 3 | AC | 128 | PHE | 3.5 |
| 1 | CA | 1112 | C | 3.5 |
| 26 | DA | 884 | C | 3.5 |
| 14 | CN | 56 | VAL | 3.5 |
| 19 | CS | 53 | ASN | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 46 | DZ | 174 | VAL | 3.5 |
| 17 | CQ | 91 | ARG | 3.5 |
| 32 | DH | 96 | ALA | 3.5 |
| 46 | DZ | 51 | ALA | 3.5 |
| 3 | CC | 198 | VAL | 3.5 |
| 1 | CA | 1001 | A | 3.5 |
| 5 | AE | 6 | PHE | 3.5 |
| 23 | AW | 3 | C | 3.5 |
| 23 | CW | 10 | G | 3.5 |
| 23 | CW | 38 | A | 3.5 |
| 31 | DG | 48 | GLU | 3.5 |
| 43 | DW | 112 | GLY | 3.5 |
| 2 | CB | 232 | PRO | 3.5 |
| 3 | AC | 91 | LEU | 3.5 |
| 32 | DH | 72 | ILE | 3.5 |
| 2 | AB | 227 | GLY | 3.4 |
| 3 | CC | 23 | TYR | 3.4 |
| 12 | CL | 64 | TYR | 3.4 |
| 26 | DA | 2159 | G | 3.4 |
| 9 | CI | 83 | ARG | 3.4 |
| 4 | AD | 2 | GLY | 3.4 |
| 47 | D0 | 76 | GLY | 3.4 |
| 46 | DZ | 153 | SER | 3.4 |
| 10 | CJ | 41 | PRO | 3.4 |
| 23 | CW | 41 | C | 3.4 |
| 21 | CU | 10 | ARG | 3.4 |
| 4 | CD | 135 | LEU | 3.4 |
| 21 | CU | 13 | ILE | 3.4 |
| 46 | DZ | 146 | ILE | 3.4 |
| 32 | DH | 145 | ALA | 3.4 |
| 4 | AD | 120 | LEU | 3.4 |
| 27 | DB | 118 | G | 3.4 |
| 13 | AM | 87 | TYR | 3.4 |
| 38 | DR | 69 | ASP | 3.4 |
| 5 | CE | 33 | VAL | 3.4 |
| 7 | CG | 12 | LEU | 3.4 |
| 3 | CC | 158 | GLY | 3.4 |
| 38 | DR | 68 | ARG | 3.4 |
| 46 | DZ | 142 | SER | 3.4 |
| 19 | CS | 75 | ALA | 3.4 |
| 25 | AY | 34 | G | 3.4 |
| 3 | AC | 201 | TYR | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | AB | 118 | LEU | 3.4 |
| 8 | CH | 95 | VAL | 3.4 |
| 9 | CI | 50 | LEU | 3.4 |
| 17 | CQ | 36 | ILE | 3.4 |
| 13 | CM | 72 | ALA | 3.4 |
| 46 | BZ | 109 | ALA | 3.4 |
| 5 | CE | 12 | LEU | 3.4 |
| 45 | DY | 106 | LEU | 3.4 |
| 13 | CM | 103 | THR | 3.4 |
| 2 | CB | 162 | ILE | 3.4 |
| 14 | CN | 60 | SER | 3.4 |
| 26 | BA | 888 | C | 3.4 |
| 10 | CJ | 64 | GLU | 3.4 |
| 10 | CJ | 88 | LEU | 3.4 |
| 12 | CL | 27 | LEU | 3.4 |
| 48 | D1 | 22 | GLY | 3.4 |
| 2 | AB | 230 | VAL | 3.4 |
| 8 | CH | 122 | ARG | 3.4 |
| 31 | DG | 28 | VAL | 3.4 |
| 32 | DH | 76 | VAL | 3.4 |
| 32 | DH | 95 | ARG | 3.4 |
| 36 | DP | 125 | VAL | 3.4 |
| 1 | CA | 1187 | G | 3.3 |
| 7 | CG | 40 | ALA | 3.3 |
| 4 | AD | 180 | GLY | 3.3 |
| 32 | DH | 35 | VAL | 3.3 |
| 31 | DG | 141 | PHE | 3.3 |
| 10 | CJ | 61 | GLU | 3.3 |
| 16 | AP | 38 | TYR | 3.3 |
| 4 | AD | 112 | VAL | 3.3 |
| 7 | AG | 84 | ASN | 3.3 |
| 2 | AB | 228 | GLY | 3.3 |
| 13 | CM | 93 | ARG | 3.3 |
| 3 | AC | 8 | ILE | 3.3 |
| 26 | DA | 2174 | C | 3.3 |
| 13 | CM | 110 | ARG | 3.3 |
| 31 | DG | 6 | ALA | 3.3 |
| 32 | DH | 124 | GLU | 3.3 |
| 10 | CJ | 27 | ALA | 3.3 |
| 23 | CW | 47 | U | 3.3 |
| 9 | CI | 92 | TYR | 3.3 |
| 25 | AY | 35 | A | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 51 | D4 | 42 | PHE | 3.3 |
| 3 | AC | 39 | ILE | 3.3 |
| 25 | CY | 52 | G | 3.3 |
| 2 | CB | 83 | MET | 3.3 |
| 4 | AD | 21 | LEU | 3.3 |
| 7 | CG | 16 | LEU | 3.3 |
| 47 | D0 | 5 | LYS | 3.3 |
| 9 | AI | 114 | TYR | 3.3 |
| 4 | CD | 146 | ILE | 3.3 |
| 19 | AS | 71 | LEU | 3.3 |
| 23 | CW | 22 | G | 3.3 |
| 9 | CI | 42 | ARG | 3.3 |
| 32 | DH | 125 | VAL | 3.2 |
| 28 | BD | 276 | LYS | 3.2 |
| 46 | BZ | 149 | SER | 3.2 |
| 31 | DG | 15 | VAL | 3.2 |
| 8 | CH | 94 | TYR | 3.2 |
| 26 | BA | 2140 | C | 3.2 |
| 2 | CB | 223 | ILE | 3.2 |
| 4 | AD | 102 | ASP | 3.2 |
| 10 | AJ | 46 | ARG | 3.2 |
| 9 | AI | 47 | LEU | 3.2 |
| 37 | DQ | 37 | LEU | 3.2 |
| 9 | CI | 88 | TYR | 3.2 |
| 1 | CA | 1224 | G | 3.2 |
| 26 | DA | 2139 | C | 3.2 |
| 4 | CD | 134 | ASP | 3.2 |
| 16 | AP | 7 | ALA | 3.2 |
| 51 | D4 | 68 | ARG | 3.2 |
| 32 | DH | 112 | PRO | 3.2 |
| 8 | CH | 61 | VAL | 3.2 |
| 2 | CB | 193 | ASP | 3.2 |
| 2 | CB | 197 | VAL | 3.2 |
| 32 | DH | 144 | VAL | 3.2 |
| 2 | AB | 68 | ILE | 3.2 |
| 1 | CA | 1035 | A | 3.2 |
| 18 | CR | 26 | LEU | 3.2 |
| 46 | BZ | 143 | GLY | 3.2 |
| 4 | AD | 169 | LYS | 3.2 |
| 23 | CW | 18 | G | 3.2 |
| 26 | DA | 2125 | G | 3.2 |
| 46 | DZ | 99 | TYR | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CB | 62 | ALA | 3.2 |
| 31 | DG | 60 | LEU | 3.2 |
| 31 | DG | 108 | ASN | 3.2 |
| 19 | CS | 56 | GLN | 3.2 |
| 25 | AY | 20 | U | 3.2 |
| 14 | AN | 7 | ILE | 3.2 |
| 23 | CW | 29 | G | 3.2 |
| 26 | DA | 2157 | G | 3.2 |
| 46 | BZ | 164 | ALA | 3.2 |
| 2 | AB | 215 | LEU | 3.2 |
| 37 | DQ | 63 | LYS | 3.2 |
| 2 | AB | 126 | GLU | 3.1 |
| 19 | CS | 83 | HIS | 3.1 |
| 22 | AV | 23 | A | 3.1 |
| 23 | CW | 75 | C | 3.1 |
| 2 | CB | 222 | ILE | 3.1 |
| 39 | DS | 83 | LYS | 3.1 |
| 3 | CC | 9 | GLY | 3.1 |
| 44 | DX | 69 | TYR | 3.1 |
| 2 | CB | 220 | ASP | 3.1 |
| 31 | DG | 156 | ASP | 3.1 |
| 7 | CG | 62 | PHE | 3.1 |
| 46 | DZ | 161 | VAL | 3.1 |
| 8 | CH | 131 | GLY | 3.1 |
| 3 | CC | 91 | LEU | 3.1 |
| 10 | CJ | 8 | LEU | 3.1 |
| 23 | CW | 40 | C | 3.1 |
| 26 | DA | 2161 | C | 3.1 |
| 42 | DV | 73 | SER | 3.1 |
| 1 | CA | 1202 | G | 3.1 |
| 10 | CJ | 13 | HIS | 3.1 |
| 32 | DH | 13 | LYS | 3.1 |
| 34 | DN | 9 | VAL | 3.1 |
| 25 | CY | 47 | U | 3.1 |
| 10 | CJ | 40 | LEU | 3.1 |
| 14 | AN | 59 | ALA | 3.1 |
| 23 | AW | 2 | C | 3.1 |
| 9 | CI | 37 | PHE | 3.1 |
| 7 | CG | 32 | ARG | 3.1 |
| 46 | DZ | 4 | ARG | 3.1 |
| 7 | AG | 81 | GLY | 3.1 |
| 14 | CN | 55 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 16 | AP | 35 | LYS | 3.1 |
| 26 | DA | 1026 | U | 3.1 |
| 46 | DZ | 124 | ILE | 3.1 |
| 1 | CA | 1531 | A | 3.1 |
| 10 | CJ | 56 | HIS | 3.1 |
| 23 | CW | 58 | A | 3.1 |
| 3 | CC | 19 | GLU | 3.1 |
| 17 | CQ | 9 | VAL | 3.1 |
| 17 | CQ | 11 | VAL | 3.1 |
| 39 | DS | 35 | ILE | 3.1 |
| 56 | B9 | 17 | ILE | 3.1 |
| 3 | AC | 126 | ARG | 3.1 |
| 32 | DH | 30 | LYS | 3.1 |
| 13 | AM | 56 | LEU | 3.1 |
| 37 | DQ | 114 | ALA | 3.1 |
| 25 | CY | 12 | U | 3.1 |
| 39 | DS | 57 | LYS | 3.1 |
| 30 | DF | 131 | GLY | 3.1 |
| 37 | DQ | 65 | PHE | 3.1 |
| 23 | CW | 74 | C | 3.1 |
| 33 | DI | 12 | LEU | 3.1 |
| 5 | CE | 81 | GLU | 3.1 |
| 19 | CS | 70 | LYS | 3.1 |
| 32 | DH | 133 | VAL | 3.0 |
| 51 | D4 | 56 | VAL | 3.0 |
| 8 | CH | 133 | LEU | 3.0 |
| 13 | CM | 42 | ALA | 3.0 |
| 21 | CU | 5 | ASP | 3.0 |
| 3 | CC | 124 | ILE | 3.0 |
| 11 | CK | 31 | THR | 3.0 |
| 28 | BD | 275 | LYS | 3.0 |
| 2 | CB | 29 | ALA | 3.0 |
| 4 | AD | 176 | LEU | 3.0 |
| 15 | AO | 87 | ILE | 3.0 |
| 44 | DX | 94 | GLY | 3.0 |
| 32 | DH | 128 | PRO | 3.0 |
| 9 | CI | 63 | ILE | 3.0 |
| 14 | CN | 45 | ARG | 3.0 |
| 21 | CU | 9 | ARG | 3.0 |
| 3 | AC | 204 | LEU | 3.0 |
| 12 | CL | 60 | LEU | 3.0 |
| 46 | DZ | 163 | LEU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | CW | 9 | A | 3.0 |
| 26 | DA | 887 | A | 3.0 |
| 45 | DY | 44 | ILE | 3.0 |
| 10 | CJ | 92 | THR | 3.0 |
| 18 | AR | 79 | LEU | 3.0 |
| 32 | DH | 45 | VAL | 3.0 |
| 17 | AQ | 28 | PRO | 3.0 |
| 23 | CW | 15 | G | 3.0 |
| 26 | BA | 1509 | C | 3.0 |
| 26 | DA | 886 | C | 3.0 |
| 8 | CH | 86 | ILE | 3.0 |
| 9 | CI | 10 | ARG | 3.0 |
| 1 | CA | 1286 | A | 3.0 |
| 3 | CC | 10 | PHE | 3.0 |
| 4 | AD | 20 | TYR | 3.0 |
| 19 | CS | 38 | SER | 3.0 |
| 7 | CG | 22 | LEU | 3.0 |
| 8 | CH | 93 | VAL | 3.0 |
| 17 | AQ | 98 | LEU | 3.0 |
| 31 | DG | 3 | LEU | 3.0 |
| 8 | CH | 128 | GLY | 3.0 |
| 9 | CI | 69 | GLY | 3.0 |
| 4 | AD | 3 | ARG | 3.0 |
| 2 | AB | 214 | ILE | 2.9 |
| 1 | CA | 204 | U | 2.9 |
| 23 | CW | 24 | G | 2.9 |
| 25 | AY | 24 | G | 2.9 |
| 26 | DA | 2110 | G | 2.9 |
| 46 | DZ | 104 | PHE | 2.9 |
| 9 | CI | 65 | VAL | 2.9 |
| 10 | AJ | 10 | GLY | 2.9 |
| 4 | CD | 168 | ARG | 2.9 |
| 45 | DY | 45 | VAL | 2.9 |
| 26 | DA | 2896 | C | 2.9 |
| 31 | DG | 137 | GLU | 2.9 |
| 50 | D3 | 60 | GLU | 2.9 |
| 3 | AC | 193 | TYR | 2.9 |
| 4 | AD | 11 | LEU | 2.9 |
| 17 | AQ | 31 | LEU | 2.9 |
| 32 | DH | 103 | LEU | 2.9 |
| 51 | D4 | 43 | TYR | 2.9 |
| 37 | DQ | 97 | VAL | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 46 | DZ | 173 | ALA | 2.9 |
| 3 | CC | 157 | ILE | 2.9 |
| 32 | DH | 32 | GLU | 2.9 |
| 10 | CJ | 19 | SER | 2.9 |
| 3 | AC | 87 | LEU | 2.9 |
| 4 | AD | 165 | MET | 2.9 |
| 4 | CD | 188 | LEU | 2.9 |
| 32 | DH | 37 | VAL | 2.9 |
| 37 | DQ | 103 | MET | 2.9 |
| 7 | CG | 78 | ARG | 2.9 |
| 14 | CN | 27 | CYS | 2.9 |
| 39 | DS | 11 | LYS | 2.9 |
| 39 | DS | 12 | PHE | 2.9 |
| 9 | AI | 109 | VAL | 2.9 |
| 23 | CW | 42 | C | 2.9 |
| 26 | DA | 2140 | C | 2.9 |
| 56 | D9 | 25 | VAL | 2.9 |
| 7 | CG | 39 | ALA | 2.9 |
| 3 | AC | 72 | LYS | 2.9 |
| 2 | CB | 185 | ILE | 2.9 |
| 46 | DZ | 55 | HIS | 2.9 |
| 47 | B0 | 3 | HIS | 2.9 |
| 1 | AA | 1035 | A | 2.9 |
| 3 | AC | 78 | GLY | 2.9 |
| 4 | AD | 110 | PHE | 2.9 |
| 2 | CB | 71 | VAL | 2.9 |
| 4 | CD | 148 | VAL | 2.9 |
| 19 | CS | 66 | MET | 2.9 |
| 37 | DQ | 106 | VAL | 2.9 |
| 45 | DY | 29 | GLU | 2.9 |
| 3 | AC | 65 | ALA | 2.9 |
| 32 | DH | 8 | PRO | 2.9 |
| 2 | CB | 66 | GLY | 2.9 |
| 32 | DH | 148 | ILE | 2.9 |
| 46 | BZ | 169 | GLU | 2.9 |
| 3 | CC | 4 | LYS | 2.9 |
| 44 | DX | 1 | MET | 2.9 |
| 13 | CM | 76 | ALA | 2.9 |
| 46 | DZ | 3 | TYR | 2.9 |
| 1 | CA | 1348 | U | 2.9 |
| 9 | CI | 29 | ASN | 2.9 |
| 12 | CL | 62 | SER | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | DA | 1509 | C | 2.9 |
| 14 | CN | 15 | LYS | 2.9 |
| 1 | CA | 1131 | G | 2.9 |
| 2 | AB | 188 | ALA | 2.9 |
| 4 | AD | 33 | MET | 2.9 |
| 7 | CG | 91 | VAL | 2.9 |
| 9 | CI | 121 | ARG | 2.9 |
| 13 | CM | 88 | ARG | 2.9 |
| 23 | CW | 27 | G | 2.9 |
| 26 | DA | 2133 | G | 2.9 |
| 50 | D3 | 29 | ARG | 2.9 |
| 2 | CB | 39 | ILE | 2.8 |
| 2 | CB | 41 | ILE | 2.8 |
| 32 | DH | 151 | ILE | 2.8 |
| 3 | CC | 113 | ALA | 2.8 |
| 7 | CG | 145 | ALA | 2.8 |
| 20 | CT | 44 | ALA | 2.8 |
| 31 | DG | 5 | VAL | 2.8 |
| 13 | CM | 21 | TYR | 2.8 |
| 14 | CN | 24 | CYS | 2.8 |
| 17 | CQ | 54 | GLY | 2.8 |
| 1 | AA | 1031 | G | 2.8 |
| 26 | DA | 2112 | G | 2.8 |
| 1 | CA | 975 | A | 2.8 |
| 1 | CA | 1111 | A | 2.8 |
| 1 | CA | 1250 | A | 2.8 |
| 9 | CI | 32 | ASP | 2.8 |
| 31 | DG | 61 | ALA | 2.8 |
| 46 | DZ | 98 | MET | 2.8 |
| 4 | AD | 167 | GLY | 2.8 |
| 2 | AB | 222 | ILE | 2.8 |
| 7 | CG | 30 | ILE | 2.8 |
| 32 | DH | 123 | PHE | 2.8 |
| 4 | CD | 108 | LEU | 2.8 |
| 8 | CH | 99 | GLU | 2.8 |
| 13 | CM | 67 | GLU | 2.8 |
| 14 | AN | 15 | LYS | 2.8 |
| 1 | CA | 1322 | C | 2.8 |
| 5 | AE | 134 | ALA | 2.8 |
| 18 | CR | 86 | VAL | 2.8 |
| 26 | BA | 884 | C | 2.8 |
| 2 | CB | 233 | SER | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | DH | 6 | ARG | 2.8 |
| 4 | AD | 157 | LEU | 2.8 |
| 38 | DR | 29 | LEU | 2.8 |
| 49 | D2 | 60 | LEU | 2.8 |
| 9 | CI | 103 | THR | 2.8 |
| 2 | AB | 15 | VAL | 2.8 |
| 9 | CI | 45 | ALA | 2.8 |
| 10 | AJ | 20 | ALA | 2.8 |
| 23 | CW | 61 | C | 2.8 |
| 7 | AG | 156 | TRP | 2.8 |
| 2 | CB | 76 | GLN | 2.8 |
| 2 | CB | 170 | GLU | 2.8 |
| 31 | DG | 178 | PHE | 2.8 |
| 33 | DI | 85 | GLU | 2.8 |
| 9 | CI | 40 | LEU | 2.8 |
| 46 | DZ | 5 | LEU | 2.8 |
| 47 | D0 | 75 | LEU | 2.8 |
| 9 | CI | 68 | GLY | 2.8 |
| 20 | CT | 9 | ASN | 2.8 |
| 9 | CI | 82 | ALA | 2.8 |
| 10 | CJ | 26 | ALA | 2.8 |
| 46 | DZ | 164 | ALA | 2.8 |
| 54 | B7 | 46 | VAL | 2.8 |
| 9 | AI | 112 | LYS | 2.8 |
| 1 | CA | 1033 | G | 2.8 |
| 25 | CY | 6 | G | 2.8 |
| 26 | DA | 645 | C | 2.8 |
| 4 | CD | 186 | LEU | 2.8 |
| 15 | AO | 57 | LEU | 2.8 |
| 7 | CG | 147 | ALA | 2.8 |
| 9 | CI | 71 | SER | 2.8 |
| 39 | DS | 52 | SER | 2.8 |
| 2 | AB | 200 | ILE | 2.8 |
| 12 | CL | 10 | LEU | 2.8 |
| 25 | CY | 22 | G | 2.8 |
| 31 | BG | 139 | LEU | 2.8 |
| 31 | DG | 152 | LEU | 2.8 |
| 39 | DS | 3 | ARG | 2.8 |
| 31 | DG | 2 | PRO | 2.7 |
| 40 | DT | 1 | MET | 2.7 |
| 9 | AI | 117 | HIS | 2.7 |
| 3 | CC | 101 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | CJ | 74 | ILE | 2.7 |
| 32 | DH | 89 | ILE | 2.7 |
| 13 | CM | 80 | ARG | 2.7 |
| 51 | D4 | 48 | ARG | 2.7 |
| 1 | CA | 1151 | A | 2.7 |
| 1 | AA | 1028 | C | 2.7 |
| 1 | CA | 973 | G | 2.7 |
| 34 | DN | 43 | THR | 2.7 |
| 23 | AW | 56 | C | 2.7 |
| 4 | CD | 105 | VAL | 2.7 |
| 17 | CQ | 23 | VAL | 2.7 |
| 41 | DU | 2 | PRO | 2.7 |
| 2 | CB | 90 | MET | 2.7 |
| 3 | CC | 147 | LYS | 2.7 |
| 18 | AR | 31 | LEU | 2.7 |
| 54 | B7 | 47 | ARG | 2.7 |
| 21 | AU | 17 | THR | 2.7 |
| 10 | AJ | 18 | ALA | 2.7 |
| 39 | DS | 79 | ALA | 2.7 |
| 2 | CB | 231 | GLU | 2.7 |
| 3 | CC | 197 | GLY | 2.7 |
| 8 | CH | 96 | GLY | 2.7 |
| 14 | CN | 12 | ARG | 2.7 |
| 17 | CQ | 84 | LEU | 2.7 |
| 34 | DN | 45 | ASN | 2.7 |
| 38 | DR | 70 | LEU | 2.7 |
| 53 | D6 | 50 | ARG | 2.7 |
| 45 | DY | 55 | TYR | 2.7 |
| 13 | AM | 25 | ILE | 2.7 |
| 46 | DZ | 120 | ILE | 2.7 |
| 51 | B4 | 46 | GLN | 2.7 |
| 37 | DQ | 18 | LYS | 2.7 |
| 2 | AB | 229 | VAL | 2.7 |
| 3 | CC | 180 | ALA | 2.7 |
| 7 | CG | 7 | ALA | 2.7 |
| 37 | DQ | 109 | VAL | 2.7 |
| 39 | DS | 34 | HIS | 2.7 |
| 13 | CM | 104 | ARG | 2.7 |
| 32 | DH | 116 | GLU | 2.7 |
| 36 | DP | 15 | ARG | 2.7 |
| 26 | DA | 2175 | C | 2.7 |
| 46 | BZ | 115 | GLY | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 18 | AR | 78 | LEU | 2.7 |
| 25 | CY | 65 | G | 2.7 |
| 50 | D3 | 53 | LEU | 2.7 |
| 34 | DN | 85 | ILE | 2.7 |
| 3 | CC | 15 | THR | 2.7 |
| 3 | CC | 177 | THR | 2.7 |
| 19 | CS | 77 | THR | 2.7 |
| 10 | CJ | 59 | SER | 2.7 |
| 2 | CB | 112 | VAL | 2.7 |
| 14 | CN | 26 | ARG | 2.7 |
| 4 | CD | 183 | GLY | 2.7 |
| 51 | D4 | 45 | GLY | 2.7 |
| 8 | CH | 112 | LEU | 2.7 |
| 9 | AI | 59 | PHE | 2.7 |
| 9 | CI | 113 | LYS | 2.7 |
| 20 | AT | 55 | ILE | 2.7 |
| 22 | CV | 15 | A | 2.7 |
| 2 | AB | 78 | GLN | 2.7 |
| 46 | DZ | 46 | LYS | 2.7 |
| 47 | B0 | 5 | LYS | 2.7 |
| 34 | DN | 23 | LEU | 2.7 |
| 39 | DS | 26 | LEU | 2.7 |
| 13 | CM | 23 | TYR | 2.7 |
| 14 | AN | 61 | TRP | 2.7 |
| 43 | DW | 9 | TYR | 2.7 |
| 8 | CH | 134 | ILE | 2.7 |
| 9 | AI | 121 | ARG | 2.7 |
| 3 | CC | 146 | ALA | 2.7 |
| 51 | D4 | 7 | PRO | 2.7 |
| 1 | CA | 1002 | G | 2.7 |
| 1 | CA | 1034 | G | 2.7 |
| 26 | DA | 2147 | G | 2.7 |
| 35 | DO | 1 | MET | 2.7 |
| 19 | CS | 71 | LEU | 2.7 |
| 43 | DW | 82 | LEU | 2.7 |
| 9 | CI | 93 | ARG | 2.7 |
| 13 | CM | 97 | PRO | 2.6 |
| 31 | DG | 138 | GLN | 2.6 |
| 1 | AA | 162 | A | 2.6 |
| 14 | CN | 6 | LEU | 2.6 |
| 13 | CM | 50 | GLU | 2.6 |
| 8 | CH | 104 | ARG | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 12 | CL | 13 | LYS | 2.6 |
| 46 | DZ | 47 | VAL | 2.6 |
| 26 | DA | 2138 | C | 2.6 |
| 2 | AB | 163 | PHE | 2.6 |
| 3 | CC | 190 | ARG | 2.6 |
| 38 | DR | 71 | GLN | 2.6 |
| 8 | CH | 83 | ILE | 2.6 |
| 9 | CI | 8 | GLY | 2.6 |
| 9 | CI | 77 | ILE | 2.6 |
| 16 | AP | 4 | ILE | 2.6 |
| 26 | DA | 614(B) | G | 2.6 |
| 9 | AI | 49 | PRO | 2.6 |
| 32 | DH | 126 | PRO | 2.6 |
| 14 | CN | 23 | ARG | 2.6 |
| 19 | CS | 37 | ARG | 2.6 |
| 26 | BA | 897 | C | 2.6 |
| 22 | CV | 13 | A | 2.6 |
| 20 | AT | 20 | LEU | 2.6 |
| 37 | DQ | 17 | LEU | 2.6 |
| 45 | BY | 1 | MET | 2.6 |
| 6 | CF | 55 | ASP | 2.6 |
| 11 | CK | 13 | GLN | 2.6 |
| 26 | BA | 1026 | U | 2.6 |
| 19 | CS | 43 | GLU | 2.6 |
| 11 | AK | 87 | THR | 2.6 |
| 5 | CE | 130 | ASN | 2.6 |
| 23 | CW | 35 | A | 2.6 |
| 2 | CB | 93 | VAL | 2.6 |
| 3 | CC | 64 | VAL | 2.6 |
| 37 | DQ | 2 | LEU | 2.6 |
| 1 | CA | 1001(A) | G | 2.6 |
| 19 | CS | 12 | ASP | 2.6 |
| 23 | CW | 19 | G | 2.6 |
| 26 | DA | 2803 | C | 2.6 |
| 47 | D0 | 74 | ARG | 2.6 |
| 4 | CD | 161 | ASN | 2.6 |
| 9 | CI | 11 | LYS | 2.6 |
| 26 | DA | 2134 | A | 2.6 |
| 18 | AR | 29 | PHE | 2.6 |
| 39 | DS | 20 | ARG | 2.6 |
| 3 | AC | 124 | ILE | 2.6 |
| 16 | AP | 33 | ILE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | AK | 19 | ALA | 2.6 |
| 21 | AU | 14 | TRP | 2.6 |
| 11 | CK | 59 | TYR | 2.6 |
| 4 | AD | 133 | VAL | 2.6 |
| 16 | CP | 20 | VAL | 2.6 |
| 25 | AY | 13 | C | 2.6 |
| 25 | CY | 48 | C | 2.6 |
| 10 | CJ | 89 | ASP | 2.6 |
| 32 | DH | 43 | VAL | 2.6 |
| 13 | CM | 85 | GLY | 2.6 |
| 2 | CB | 144 | ARG | 2.6 |
| 5 | CE | 131 | ILE | 2.5 |
| 10 | CJ | 96 | ILE | 2.5 |
| 16 | AP | 36 | ILE | 2.5 |
| 4 | AD | 147 | ALA | 2.5 |
| 16 | AP | 48 | TRP | 2.5 |
| 23 | CW | 34 | G | 2.5 |
| 26 | DA | 2162 | G | 2.5 |
| 3 | CC | 183 | ASP | 2.5 |
| 46 | DZ | 97 | GLU | 2.5 |
| 4 | AD | 148 | VAL | 2.5 |
| 17 | CQ | 6 | LEU | 2.5 |
| 51 | D4 | 35 | VAL | 2.5 |
| 51 | D4 | 19 | GLY | 2.5 |
| 9 | CI | 119 | ALA | 2.5 |
| 14 | CN | 49 | HIS | 2.5 |
| 32 | DH | 165 | ALA | 2.5 |
| 45 | DY | 35 | TYR | 2.5 |
| 2 | CB | 136 | VAL | 2.5 |
| 4 | AD | 17 | VAL | 2.5 |
| 4 | AD | 170 | VAL | 2.5 |
| 11 | CK | 14 | VAL | 2.5 |
| 17 | CQ | 98 | LEU | 2.5 |
| 7 | CG | 6 | ARG | 2.5 |
| 7 | CG | 26 | PHE | 2.5 |
| 23 | CW | 11 | C | 2.5 |
| 2 | CB | 16 | HIS | 2.5 |
| 2 | CB | 127 | ILE | 2.5 |
| 3 | CC | 202 | ILE | 2.5 |
| 15 | CO | 87 | ILE | 2.5 |
| 1 | CA | 1092 | A | 2.5 |
| 2 | CB | 115 | LEU | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CB | 148 | TYR | 2.5 |
| 4 | CD | 49 | ARG | 2.5 |
| 7 | CG | 85 | TYR | 2.5 |
| 28 | DD | 217 | ARG | 2.5 |
| 47 | D0 | 44 | ARG | 2.5 |
| 56 | D9 | 13 | LYS | 2.5 |
| 2 | CB | 216 | SER | 2.5 |
| 46 | DZ | 65 | GLN | 2.5 |
| 1 | CA | 1149 | C | 2.5 |
| 31 | DG | 88 | ILE | 2.5 |
| 31 | DG | 151 | ALA | 2.5 |
| 46 | DZ | 112 | ARG | 2.5 |
| 13 | AM | 98 | VAL | 2.5 |
| 37 | DQ | 79 | LEU | 2.5 |
| 44 | DX | 49 | VAL | 2.5 |
| 18 | CR | 43 | PHE | 2.5 |
| 26 | BA | 229 | A | 2.5 |
| 2 | AB | 67 | THR | 2.5 |
| 10 | CJ | 53 | PRO | 2.5 |
| 47 | D0 | 4 | LYS | 2.5 |
| 18 | CR | 47 | THR | 2.5 |
| 34 | DN | 57 | ALA | 2.5 |
| 41 | DU | 73 | GLY | 2.5 |
| 14 | CN | 40 | CYS | 2.5 |
| 2 | CB | 78 | GLN | 2.5 |
| 31 | BG | 137 | GLU | 2.5 |
| 28 | DD | 276 | LYS | 2.5 |
| 31 | DG | 27 | ASN | 2.5 |
| 1 | AA | 161 | A | 2.5 |
| 3 | CC | 149 | ALA | 2.5 |
| 12 | CL | 56 | ALA | 2.5 |
| 31 | DG | 85 | GLY | 2.5 |
| 3 | CC | 167 | TRP | 2.5 |
| 18 | CR | 46 | GLU | 2.5 |
| 31 | DG | 62 | LEU | 2.5 |
| 4 | AD | 140 | VAL | 2.5 |
| 7 | AG | 80 | VAL | 2.5 |
| 53 | D6 | 52 | VAL | 2.5 |
| 8 | CH | 65 | TYR | 2.5 |
| 1 | CA | 961 | U | 2.5 |
| 7 | CG | 33 | ASP | 2.5 |
| 9 | CI | 20 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CB | 34 | ALA | 2.5 |
| 3 | CC | 200 | ALA | 2.5 |
| 19 | CS | 50 | ALA | 2.5 |
| 32 | DH | 18 | GLU | 2.5 |
| 8 | CH | 138 | TRP | 2.5 |
| 19 | CS | 6 | LYS | 2.5 |
| 4 | AD | 105 | VAL | 2.5 |
| 16 | AP | 39 | TYR | 2.5 |
| 1 | CA | 979 | C | 2.5 |
| 1 | CA | 1221 | G | 2.5 |
| 1 | CA | 1368 | G | 2.5 |
| 46 | BZ | 121 | HIS | 2.4 |
| 5 | CE | 123 | LEU | 2.4 |
| 10 | AJ | 23 | ILE | 2.4 |
| 17 | AQ | 36 | ILE | 2.4 |
| 32 | DH | 121 | ILE | 2.4 |
| 37 | DQ | 66 | ILE | 2.4 |
| 16 | CP | 51 | VAL | 2.4 |
| 2 | CB | 96 | ARG | 2.4 |
| 3 | CC | 30 | ARG | 2.4 |
| 8 | CH | 91 | ARG | 2.4 |
| 21 | AU | 15 | ARG | 2.4 |
| 46 | BZ | 148 | ASP | 2.4 |
| 4 | AD | 150 | GLU | 2.4 |
| 42 | DV | 30 | GLY | 2.4 |
| 18 | AR | 25 | THR | 2.4 |
| 2 | CB | 69 | LEU | 2.4 |
| 10 | AJ | 16 | LEU | 2.4 |
| 5 | CE | 148 | VAL | 2.4 |
| 7 | CG | 155 | ARG | 2.4 |
| 11 | AK | 82 | VAL | 2.4 |
| 3 | CC | 122 | GLU | 2.4 |
| 32 | DH | 34 | GLU | 2.4 |
| 2 | CB | 133 | LYS | 2.4 |
| 11 | CK | 25 | TYR | 2.4 |
| 3 | AC | 168 | ALA | 2.4 |
| 4 | CD | 89 | THR | 2.4 |
| 7 | CG | 152 | ALA | 2.4 |
| 16 | AP | 24 | ALA | 2.4 |
| 23 | AW | 4 | C | 2.4 |
| 31 | DG | 73 | ALA | 2.4 |
| 4 | AD | 174 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 7 | CG | 10 | ARG | 2.4 |
| 11 | CK | 96 | ARG | 2.4 |
| 13 | CM | 3 | ARG | 2.4 |
| 46 | BZ | 155 | LEU | 2.4 |
| 2 | CB | 150 | SER | 2.4 |
| 48 | B1 | 2 | SER | 2.4 |
| 1 | AA | 1030(A) | G | 2.4 |
| 11 | AK | 84 | VAL | 2.4 |
| 11 | CK | 114 | VAL | 2.4 |
| 24 | CX | 4 | G | 2.4 |
| 32 | DH | 49 | VAL | 2.4 |
| 4 | CD | 185 | PHE | 2.4 |
| 32 | DH | 74 | ASN | 2.4 |
| 9 | CI | 30 | GLY | 2.4 |
| 16 | AP | 32 | TYR | 2.4 |
| 1 | CA | 978 | A | 2.4 |
| 18 | AR | 42 | ARG | 2.4 |
| 22 | AV | 14 | A | 2.4 |
| 46 | DZ | 151 | HIS | 2.4 |
| 11 | AK | 57 | THR | 2.4 |
| 18 | AR | 40 | LEU | 2.4 |
| 20 | CT | 59 | ALA | 2.4 |
| 31 | DG | 161 | THR | 2.4 |
| 7 | CG | 27 | ILE | 2.4 |
| 7 | CG | 42 | ILE | 2.4 |
| 16 | CP | 19 | ILE | 2.4 |
| 25 | CY | 13 | C | 2.4 |
| 26 | DA | 2111 | C | 2.4 |
| 29 | BE | 87 | GLU | 2.4 |
| 3 | CC | 37 | GLN | 2.4 |
| 7 | CG | 37 | ASN | 2.4 |
| 15 | AO | 89 | GLY | 2.4 |
| 6 | CF | 89 | MET | 2.4 |
| 9 | CI | 49 | PRO | 2.4 |
| 9 | CI | 117 | HIS | 2.4 |
| 51 | D4 | 41 | PRO | 2.4 |
| 39 | DS | 51 | ALA | 2.4 |
| 3 | AC | 154 | SER | 2.4 |
| 17 | CQ | 12 | SER | 2.4 |
| 46 | DZ | 148 | ASP | 2.4 |
| 1 | CA | 1223 | C | 2.4 |
| 8 | CH | 108 | GLY | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | BA | 2142 | C | 2.4 |
| 50 | D3 | 9 | VAL | 2.4 |
| 2 | CB | 53 | ARG | 2.4 |
| 7 | CG | 3 | ARG | 2.4 |
| 19 | CS | 36 | ARG | 2.4 |
| 12 | CL | 48 | PRO | 2.4 |
| 8 | CH | 124 | ALA | 2.4 |
| 17 | CQ | 44 | ALA | 2.4 |
| 26 | BA | 1176 | G | 2.4 |
| 32 | DH | 71 | LEU | 2.4 |
| 38 | DR | 65 | LEU | 2.4 |
| 3 | AC | 14 | ILE | 2.4 |
| 3 | CC | 22 | TRP | 2.4 |
| 10 | CJ | 11 | PHE | 2.4 |
| 17 | CQ | 56 | VAL | 2.4 |
| 9 | CI | 70 | LYS | 2.4 |
| 25 | CY | 51 | U | 2.4 |
| 2 | AB | 77 | ALA | 2.4 |
| 8 | CH | 36 | LEU | 2.4 |
| 9 | CI | 46 | ALA | 2.4 |
| 2 | CB | 206 | ASP | 2.4 |
| 3 | AC | 134 | ILE | 2.4 |
| 25 | CY | 28 | G | 2.4 |
| 26 | BA | 2141 | G | 2.4 |
| 37 | DQ | 62 | GLY | 2.4 |
| 3 | AC | 203 | PHE | 2.4 |
| 9 | AI | 111 | ARG | 2.4 |
| 13 | CM | 73 | GLU | 2.4 |
| 14 | CN | 8 | GLU | 2.4 |
| 30 | DF | 139 | PHE | 2.4 |
| 45 | DY | 50 | ARG | 2.4 |
| 56 | D9 | 16 | VAL | 2.4 |
| 5 | AE | 10 | MET | 2.3 |
| 1 | CA | 1030 | C | 2.3 |
| 11 | AK | 25 | TYR | 2.3 |
| 21 | CU | 21 | TYR | 2.3 |
| 26 | DA | 2129 | C | 2.3 |
| 51 | B4 | 60 | GLN | 2.3 |
| 2 | CB | 51 | LEU | 2.3 |
| 4 | AD | 97 | LEU | 2.3 |
| 5 | AE | 132 | ALA | 2.3 |
| 2 | CB | 37 | ASN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | CD | 158 | ILE | 2.3 |
| 5 | CE | 14 | ARG | 2.3 |
| 7 | CG | 13 | GLN | 2.3 |
| 23 | CW | 6 | G | 2.3 |
| 24 | CX | 70 | G | 2.3 |
| 3 | CC | 142 | MET | 2.3 |
| 12 | CL | 94 | PRO | 2.3 |
| 31 | DG | 86 | MET | 2.3 |
| 3 | CC | 188 | LEU | 2.3 |
| 1 | CA | 1251 | A | 2.3 |
| 9 | AI | 110 | GLU | 2.3 |
| 11 | AK | 126 | ARG | 2.3 |
| 11 | CK | 117 | ASN | 2.3 |
| 15 | AO | 88 | ARG | 2.3 |
| 15 | CO | 68 | ARG | 2.3 |
| 17 | CQ | 90 | ILE | 2.3 |
| 5 | AE | 90 | VAL | 2.3 |
| 9 | AI | 108 | VAL | 2.3 |
| 10 | CJ | 94 | VAL | 2.3 |
| 14 | CN | 18 | VAL | 2.3 |
| 14 | CN | 11 | LYS | 2.3 |
| 37 | DQ | 1 | MET | 2.3 |
| 8 | AH | 133 | LEU | 2.3 |
| 19 | CS | 68 | GLY | 2.3 |
| 20 | CT | 20 | LEU | 2.3 |
| 23 | CW | 12 | U | 2.3 |
| 30 | DF | 15 | SER | 2.3 |
| 44 | DX | 91 | ALA | 2.3 |
| 1 | CA | 1357 | A | 2.3 |
| 8 | CH | 111 | ILE | 2.3 |
| 20 | CT | 41 | ILE | 2.3 |
| 23 | CW | 43 | C | 2.3 |
| 2 | CB | 139 | LYS | 2.3 |
| 4 | AD | 8 | VAL | 2.3 |
| 4 | CD | 160 | GLN | 2.3 |
| 4 | CD | 184 | LYS | 2.3 |
| 17 | CQ | 73 | VAL | 2.3 |
| 17 | CQ | 87 | LYS | 2.3 |
| 39 | DS | 46 | VAL | 2.3 |
| 41 | DU | 40 | PHE | 2.3 |
| 51 | D4 | 21 | VAL | 2.3 |
| 19 | CS | 81 | ARG | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | DH | 12 | PRO | 2.3 |
| 11 | CK | 89 | ALA | 2.3 |
| 15 | AO | 69 | TYR | 2.3 |
| 46 | DZ | 157 | LEU | 2.3 |
| 20 | CT | 32 | ALA | 2.3 |
| 30 | DF | 166 | ALA | 2.3 |
| 52 | D5 | 29 | THR | 2.3 |
| 4 | CD | 140 | VAL | 2.3 |
| 25 | CY | 2 | C | 2.3 |
| 2 | AB | 160 | ASP | 2.3 |
| 9 | AI | 120 | ARG | 2.3 |
| 12 | CL | 19 | ARG | 2.3 |
| 31 | DG | 154 | GLY | 2.3 |
| 15 | CO | 57 | LEU | 2.3 |
| 20 | AT | 24 | LEU | 2.3 |
| 20 | CT | 26 | ASN | 2.3 |
| 32 | DH | 171 | LEU | 2.3 |
| 32 | DH | 164 | TYR | 2.3 |
| 3 | CC | 5 | ILE | 2.3 |
| 31 | DG | 77 | ILE | 2.3 |
| 31 | DG | 114 | ILE | 2.3 |
| 2 | AB | 231 | GLU | 2.3 |
| 3 | AC | 206 | GLU | 2.3 |
| 3 | CC | 173 | VAL | 2.3 |
| 8 | CH | 136 | GLU | 2.3 |
| 10 | CJ | 58 | ASP | 2.3 |
| 1 | CA | 1118 | C | 2.3 |
| 7 | CG | 132 | GLY | 2.3 |
| 2 | AB | 101 | MET | 2.3 |
| 7 | CG | 14 | PRO | 2.3 |
| 32 | DH | 147 | ASN | 2.3 |
| 35 | DO | 41 | ALA | 2.3 |
| 16 | AP | 34 | GLU | 2.3 |
| 31 | DG | 104 | GLU | 2.3 |
| 2 | CB | 58 | ILE | 2.3 |
| 19 | AS | 81 | ARG | 2.3 |
| 37 | DQ | 102 | VAL | 2.3 |
| 42 | DV | 72 | VAL | 2.3 |
| 46 | DZ | 105 | VAL | 2.3 |
| 18 | CR | 84 | LYS | 2.3 |
| 14 | AN | 14 | PRO | 2.3 |
| 16 | AP | 60 | LEU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 10 | AJ | 64 | GLU | 2.3 |
| 1 | CA | 958 | A | 2.3 |
| 1 | CA | 1041 | A | 2.3 |
| 25 | CY | 21 | A | 2.3 |
| 26 | DA | 2119 | A | 2.3 |
| 5 | CE | 150 | ARG | 2.3 |
| 3 | AC | 182 | ILE | 2.3 |
| 12 | CL | 7 | ILE | 2.3 |
| 19 | CS | 60 | VAL | 2.3 |
| 46 | DZ | 140 | ASP | 2.3 |
| 4 | AD | 155 | LEU | 2.2 |
| 2 | CB | 116 | GLU | 2.2 |
| 3 | AC | 89 | GLU | 2.2 |
| 4 | CD | 164 | ALA | 2.2 |
| 31 | DG | 110 | ALA | 2.2 |
| 37 | DQ | 110 | THR | 2.2 |
| 1 | AA | 1030 | C | 2.2 |
| 5 | AE | 133 | TYR | 2.2 |
| 7 | CG | 18 | TYR | 2.2 |
| 51 | D4 | 67 | TYR | 2.2 |
| 1 | CA | 1363(A) | A | 2.2 |
| 3 | CC | 66 | VAL | 2.2 |
| 5 | CE | 105 | VAL | 2.2 |
| 32 | DH | 24 | VAL | 2.2 |
| 32 | DH | 82 | GLY | 2.2 |
| 34 | DN | 10 | GLU | 2.2 |
| 3 | CC | 61 | ALA | 2.2 |
| 7 | CG | 31 | MET | 2.2 |
| 13 | CM | 65 | LYS | 2.2 |
| 13 | CM | 75 | ALA | 2.2 |
| 14 | CN | 10 | ALA | 2.2 |
| 17 | AQ | 37 | LYS | 2.2 |
| 46 | DZ | 69 | THR | 2.2 |
| 11 | AK | 81 | ASP | 2.2 |
| 3 | AC | 81 | GLY | 2.2 |
| 26 | BA | 2161 | C | 2.2 |
| 36 | DP | 20 | GLY | 2.2 |
| 46 | BZ | 119 | GLU | 2.2 |
| 46 | DZ | 169 | GLU | 2.2 |
| 2 | CB | 210 | SER | 2.2 |
| 15 | CO | 31 | LEU | 2.2 |
| 31 | DG | 106 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | DG | 120 | LEU | 2.2 |
| 2 | CB | 209 | ARG | 2.2 |
| 14 | CN | 19 | ARG | 2.2 |
| 16 | AP | 57 | ARG | 2.2 |
| 5 | CE | 84 | PHE | 2.2 |
| 9 | CI | 73 | GLN | 2.2 |
| 31 | DG | 134 | GLY | 2.2 |
| 48 | D1 | 28 | GLY | 2.2 |
| 2 | CB | 32 | ILE | 2.2 |
| 10 | AJ | 98 | ILE | 2.2 |
| 10 | CJ | 6 | ILE | 2.2 |
| 12 | CL | 70 | ILE | 2.2 |
| 51 | D4 | 34 | GLU | 2.2 |
| 4 | AD | 166 | LYS | 2.2 |
| 17 | AQ | 35 | VAL | 2.2 |
| 46 | BZ | 116 | VAL | 2.2 |
| 46 | BZ | 165 | VAL | 2.2 |
| 3 | CC | 59 | ARG | 2.2 |
| 6 | AF | 98 | LEU | 2.2 |
| 10 | CJ | 39 | PRO | 2.2 |
| 21 | CU | 23 | PRO | 2.2 |
| 54 | D7 | 23 | ARG | 2.2 |
| 55 | D8 | 2 | PRO | 2.2 |
| 1 | CA | 4 | U | 2.2 |
| 13 | CM | 107 | ALA | 2.2 |
| 26 | BA | 2132 | U | 2.2 |
| 37 | DQ | 136 | ALA | 2.2 |
| 32 | DH | 47 | GLU | 2.2 |
| 34 | DN | 69 | GLN | 2.2 |
| 46 | DZ | 50 | GLN | 2.2 |
| 8 | CH | 35 | ILE | 2.2 |
| 12 | CL | 100 | ILE | 2.2 |
| 46 | DZ | 128 | VAL | 2.2 |
| 4 | AD | 50 | ARG | 2.2 |
| 32 | DH | 132 | ARG | 2.2 |
| 5 | AE | 128 | PRO | 2.2 |
| 8 | CH | 10 | LEU | 2.2 |
| 12 | CL | 93 | LEU | 2.2 |
| 34 | DN | 91 | LEU | 2.2 |
| 26 | DA | 2142 | C | 2.2 |
| 11 | AK | 60 | ALA | 2.2 |
| 32 | DH | 73 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | CA | 1308 | U | 2.2 |
| 3 | CC | 205 | GLY | 2.2 |
| 42 | DV | 42 | GLY | 2.2 |
| 46 | DZ | 154 | ASP | 2.2 |
| 1 | CA | 1287 | A | 2.2 |
| 3 | CC | 186 | PHE | 2.2 |
| 4 | AD | 158 | ILE | 2.2 |
| 10 | AJ | 43 | ARG | 2.2 |
| 19 | CS | 4 | SER | 2.2 |
| 32 | DH | 99 | VAL | 2.2 |
| 39 | DS | 39 | ILE | 2.2 |
| 3 | AC | 196 | LEU | 2.2 |
| 20 | AT | 72 | LEU | 2.2 |
| 32 | DH | 29 | PRO | 2.2 |
| 2 | CB | 97 | TRP | 2.2 |
| 19 | CS | 73 | GLU | 2.2 |
| 4 | AD | 69 | GLY | 2.2 |
| 1 | CA | 1040 | U | 2.2 |
| 2 | CB | 111 | ARG | 2.2 |
| 39 | DS | 29 | PHE | 2.2 |
| 1 | CA | 1061 | G | 2.2 |
| 13 | CM | 17 | VAL | 2.2 |
| 18 | AR | 37 | VAL | 2.2 |
| 43 | DW | 17 | VAL | 2.2 |
| 10 | AJ | 71 | LEU | 2.2 |
| 2 | AB | 66 | GLY | 2.2 |
| 2 | AB | 48 | MET | 2.2 |
| 3 | CC | 129 | ALA | 2.2 |
| 12 | CL | 95 | GLY | 2.2 |
| 21 | AU | 11 | GLY | 2.2 |
| 31 | DG | 116 | ASP | 2.2 |
| 39 | DS | 104 | GLY | 2.2 |
| 44 | DX | 42 | ALA | 2.2 |
| 9 | CI | 16 | ARG | 2.2 |
| 36 | DP | 18 | ARG | 2.2 |
| 50 | D3 | 35 | ARG | 2.2 |
| 2 | CB | 55 | PHE | 2.2 |
| 26 | BA | 2143 | C | 2.2 |
| 7 | CG | 151 | TYR | 2.1 |
| 14 | CN | 4 | LYS | 2.1 |
| 23 | CW | 50 | U | 2.1 |
| 10 | AJ | 49 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 14 | AN | 56 | VAL | 2.1 |
| 29 | DE | 196 | VAL | 2.1 |
| 32 | DH | 17 | VAL | 2.1 |
| 32 | DH | 52 | VAL | 2.1 |
| 37 | DQ | 125 | LEU | 2.1 |
| 26 | DA | 2141 | G | 2.1 |
| 1 | AA | 1030(D) | A | 2.1 |
| 12 | CL | 14 | GLY | 2.1 |
| 12 | CL | 30 | ALA | 2.1 |
| 10 | CJ | 87 | THR | 2.1 |
| 31 | DG | 51 | ARG | 2.1 |
| 36 | DP | 79 | ARG | 2.1 |
| 48 | D1 | 26 | ARG | 2.1 |
| 4 | CD | 110 | PHE | 2.1 |
| 37 | BQ | 112 | GLU | 2.1 |
| 51 | D4 | 30 | GLU | 2.1 |
| 18 | CR | 66 | LEU | 2.1 |
| 25 | CY | 33 | U | 2.1 |
| 26 | DA | 958 | U | 2.1 |
| 28 | DD | 18 | VAL | 2.1 |
| 36 | DP | 123 | LEU | 2.1 |
| 39 | DS | 91 | PRO | 2.1 |
| 1 | CA | 1117 | G | 2.1 |
| 4 | CD | 34 | GLU | 2.1 |
| 39 | DS | 111 | GLU | 2.1 |
| 3 | CC | 20 | SER | 2.1 |
| 5 | CE | 13 | ILE | 2.1 |
| 28 | BD | 142 | VAL | 2.1 |
| 31 | DG | 144 | ILE | 2.1 |
| 31 | DG | 159 | VAL | 2.1 |
| 41 | DU | 90 | VAL | 2.1 |
| 16 | AP | 6 | LEU | 2.1 |
| 33 | BI | 75 | LEU | 2.1 |
| 39 | DS | 24 | LEU | 2.1 |
| 46 | BZ | 102 | LEU | 2.1 |
| 46 | DZ | 102 | LEU | 2.1 |
| 46 | DZ | 133 | ILE | 2.1 |
| 4 | AD | 23 | GLY | 2.1 |
| 19 | CS | 57 | HIS | 2.1 |
| 8 | CH | 116 | LYS | 2.1 |
| 44 | DX | 60 | ARG | 2.1 |
| 2 | CB | 123 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 51 | D4 | 53 | GLU | 2.1 |
| 8 | CH | 24 | THR | 2.1 |
| 13 | CM | 105 | THR | 2.1 |
| 51 | D4 | 27 | THR | 2.1 |
| 4 | AD | 116 | GLN | 2.1 |
| 1 | CA | 983 | A | 2.1 |
| 1 | CA | 1093 | A | 2.1 |
| 1 | CA | 1343 | G | 2.1 |
| 2 | CB | 98 | LEU | 2.1 |
| 3 | CC | 57 | ILE | 2.1 |
| 3 | CC | 201 | TYR | 2.1 |
| 5 | AE | 12 | LEU | 2.1 |
| 7 | CG | 105 | VAL | 2.1 |
| 8 | CH | 53 | VAL | 2.1 |
| 19 | CS | 78 | ARG | 2.1 |
| 21 | AU | 2 | GLY | 2.1 |
| 28 | DD | 275 | LYS | 2.1 |
| 34 | DN | 84 | LYS | 2.1 |
| 37 | BQ | 97 | VAL | 2.1 |
| 56 | D9 | 9 | ARG | 2.1 |
| 1 | CA | 1397 | C | 2.1 |
| 23 | CW | 33 | U | 2.1 |
| 37 | DQ | 105 | GLU | 2.1 |
| 4 | CD | 48 | ALA | 2.1 |
| 32 | DH | 75 | ALA | 2.1 |
| 2 | CB | 67 | THR | 2.1 |
| 46 | BZ | 170 | THR | 2.1 |
| 14 | CN | 16 | PHE | 2.1 |
| 32 | DH | 109 | PHE | 2.1 |
| 3 | CC | 33 | LEU | 2.1 |
| 4 | CD | 101 | LEU | 2.1 |
| 11 | AK | 63 | LEU | 2.1 |
| 13 | CM | 70 | LEU | 2.1 |
| 41 | DU | 17 | ILE | 2.1 |
| 2 | CB | 183 | PRO | 2.1 |
| 17 | CQ | 24 | GLU | 2.1 |
| 25 | AY | 23 | A | 2.1 |
| 26 | DA | 652(B) | A | 2.1 |
| 26 | DA | 2123 | G | 2.1 |
| 26 | DA | 2310 | A | 2.1 |
| 2 | CB | 85 | ALA | 2.1 |
| 26 | DA | 2113 | U | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | CA | 962 | C | 2.1 |
| 13 | CM | 106 | ASN | 2.1 |
| 26 | DA | 2164 | C | 2.1 |
| 37 | DQ | 3 | MET | 2.1 |
| 45 | DY | 43 | ASN | 2.1 |
| 32 | DH | 110 | SER | 2.1 |
| 3 | CC | 185 | GLY | 2.1 |
| 12 | AL | 29 | GLY | 2.1 |
| 39 | DS | 60 | GLY | 2.1 |
| 51 | B4 | 54 | GLY | 2.1 |
| 2 | AB | 80 | ILE | 2.1 |
| 2 | AB | 136 | VAL | 2.1 |
| 3 | CC | 152 | ILE | 2.1 |
| 4 | CD | 121 | VAL | 2.1 |
| 5 | AE | 55 | VAL | 2.1 |
| 8 | CH | 119 | LEU | 2.1 |
| 5 | AE | 129 | ILE | 2.1 |
| 46 | DZ | 42 | VAL | 2.1 |
| 13 | CM | 113 | PRO | 2.1 |
| 17 | AQ | 95 | TYR | 2.1 |
| 48 | D1 | 71 | TYR | 2.1 |
| 9 | CI | 31 | GLN | 2.1 |
| 1 | CA | 1190 | G | 2.1 |
| 5 | CE | 9 | LYS | 2.1 |
| 7 | CG | 117 | ALA | 2.1 |
| 26 | DA | 2166 | G | 2.1 |
| 30 | DF | 80 | ALA | 2.1 |
| 7 | CG | 149 | ARG | 2.1 |
| 11 | CK | 87 | THR | 2.1 |
| 25 | AY | 47 | U | 2.1 |
| 25 | CY | 60 | U | 2.1 |
| 26 | DA | 2897 | U | 2.1 |
| 30 | BF | 34 | TRP | 2.1 |
| 2 | CB | 43 | ASP | 2.1 |
| 3 | CC | 58 | GLU | 2.1 |
| 7 | CG | 34 | GLY | 2.1 |
| 32 | DH | 119 | GLU | 2.1 |
| 5 | CE | 82 | VAL | 2.1 |
| 8 | CH | 63 | LEU | 2.1 |
| 16 | AP | 20 | VAL | 2.1 |
| 20 | AT | 13 | LEU | 2.1 |
| 32 | DH | 88 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | CK | 108 | ILE | 2.1 |
| 28 | DD | 204 | ILE | 2.1 |
| 17 | CQ | 100 | LYS | 2.1 |
| 30 | DF | 81 | PRO | 2.1 |
| 34 | DN | 11 | PRO | 2.1 |
| 21 | CU | 22 | ARG | 2.1 |
| 17 | CQ | 7 | THR | 2.1 |
| 32 | DH | 129 | THR | 2.1 |
| 8 | CH | 31 | PHE | 2.1 |
| 11 | CK | 90 | GLY | 2.1 |
| 16 | AP | 68 | ASP | 2.1 |
| 25 | CY | 58 | A | 2.1 |
| 46 | BZ | 147 | GLY | 2.1 |
| 9 | CI | 87 | GLN | 2.0 |
| 15 | CO | 60 | VAL | 2.0 |
| 26 | DA | 889 | C | 2.0 |
| 34 | DN | 26 | LEU | 2.0 |
| 13 | CM | 84 | ILE | 2.0 |
| 46 | BZ | 122 | ARG | 2.0 |
| 6 | CF | 73 | ASN | 2.0 |
| 3 | CC | 56 | ASP | 2.0 |
| 7 | CG | 15 | ASP | 2.0 |
| 13 | CM | 63 | THR | 2.0 |
| 32 | DH | 122 | THR | 2.0 |
| 32 | DH | 25 | LYS | 2.0 |
| 9 | CI | 56 | LEU | 2.0 |
| 15 | CO | 56 | LEU | 2.0 |
| 25 | CY | 66 | U | 2.0 |
| 50 | D3 | 23 | LEU | 2.0 |
| 1 | AA | 1034 | G | 2.0 |
| 2 | CB | 19 | HIS | 2.0 |
| 11 | CK | 109 | VAL | 2.0 |
| 23 | CW | 65 | G | 2.0 |
| 26 | DA | 2148 | G | 2.0 |
| 26 | DA | 2319 | G | 2.0 |
| 39 | DS | 14 | VAL | 2.0 |
| 5 | AE | 131 | ILE | 2.0 |
| 1 | CA | 1320 | C | 2.0 |
| 13 | CM | 71 | ARG | 2.0 |
| 18 | CR | 42 | ARG | 2.0 |
| 51 | D4 | 58 | ARG | 2.0 |
| 4 | CD | 68 | TYR | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 17 | CQ | 32 | TYR | 2.0 |
| 4 | AD | 111 | ALA | 2.0 |
| 12 | CL | 26 | ALA | 2.0 |
| 19 | CS | 24 | ALA | 2.0 |
| 8 | CH | 4 | ASP | 2.0 |
| 16 | AP | 37 | GLY | 2.0 |
| 8 | AH | 112 | LEU | 2.0 |
| 9 | CI | 47 | LEU | 2.0 |
| 28 | DD | 37 | LEU | 2.0 |
| 8 | CH | 84 | ARG | 2.0 |
| 9 | AI | 28 | VAL | 2.0 |
| 10 | AJ | 5 | ARG | 2.0 |
| 10 | AJ | 60 | ARG | 2.0 |
| 17 | CQ | 86 | GLU | 2.0 |
| 31 | DG | 109 | VAL | 2.0 |
| 5 | AE | 118 | ILE | 2.0 |
| 37 | DQ | 91 | GLU | 2.0 |
| 45 | DY | 64 | GLU | 2.0 |
| 46 | BZ | 124 | ILE | 2.0 |
| 1 | AA | 1026 | G | 2.0 |
| 18 | CR | 34 | TYR | 2.0 |
| 16 | AP | 29 | ASP | 2.0 |
| 25 | CY | 56 | C | 2.0 |
| 26 | DA | 2100 | G | 2.0 |
| 32 | DH | 157 | TYR | 2.0 |
| 40 | DT | 126 | ALA | 2.0 |
| 46 | DZ | 21 | ALA | 2.0 |
| 2 | AB | 73 | THR | 2.0 |
| 2 | CB | 181 | PHE | 2.0 |
| 37 | DQ | 58 | PHE | 2.0 |
| 54 | D7 | 1 | MET | 2.0 |
| 2 | AB | 213 | LEU | 2.0 |
| 5 | CE | 142 | LEU | 2.0 |
| 39 | DS | 110 | LEU | 2.0 |
| 46 | DZ | 145 | GLU | 2.0 |
| 2 | AB | 75 | LYS | 2.0 |
| 5 | CE | 100 | VAL | 2.0 |
| 9 | AI | 98 | PRO | 2.0 |
| 12 | CL | 96 | VAL | 2.0 |
| 16 | AP | 53 | VAL | 2.0 |
| 28 | DD | 38 | LYS | 2.0 |
| 50 | D3 | 6 | VAL | 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 25 | 7MG | CY | 46 | 24/25 | 0.71 | 0.25 | 87,101,108,135 | 0 |
| 23 | 7MG | CW | 46 | 24/25 | 0.73 | 0.33 | 81,97,101,125 | 0 |
| 25 | 5MU | CY | 54 | 21/22 | 0.74 | 0.49 | 89,99,105,136 | 0 |
| 25 | PSU | CY | 55 | 20/21 | 0.75 | 0.41 | 86,100,107,118 | 0 |
| 23 | 4SU | CW | 8 | 20/21 | 0.77 | 0.29 | 85,96,117,121 | 0 |
| 25 | 4SU | CY | 8 | 20/21 | 0.79 | 0.16 | 88,102,112,128 | 0 |
| 25 | MIA | CY | 37 | 22/30 | 0.79 | 0.30 | 79,95,102,124 | 0 |
| 24 | 4SU | CX | 8 | 20/21 | 0.80 | 0.13 | 84,92,105,111 | 0 |
| 23 | 7MG | AW | 46 | 24/25 | 0.80 | 0.21 | 80,97,112,135 | 0 |
| 25 | PSU | CY | 39 | 20/21 | 0.81 | 0.27 | 86,91,104,110 | 0 |
| 25 | PSU | AY | 55 | 20/21 | 0.81 | 0.20 | 85,96,106,117 | 0 |
| 25 | 7MG | AY | 46 | 24/25 | 0.82 | 0.18 | 80,99,107,116 | 0 |
| 25 | PSU | CY | 32 | 20/21 | 0.83 | 0.26 | 77,91,109,114 | 0 |
| 25 | 4SU | AY | 8 | 20/21 | 0.83 | 0.13 | 83,95,104,129 | 0 |
| 23 | PSU | AW | 55 | 20/21 | 0.83 | 0.27 | 76,88,103,105 | 0 |
| 25 | PSU | AY | 32 | 20/21 | 0.83 | 0.26 | 76,92,107,110 | 0 |
| 23 | 4SU | AW | 8 | 20/21 | 0.84 | 0.17 | 83,89,107,110 | 0 |
| 23 | PSU | CW | 55 | 20/21 | 0.84 | 0.34 | 76,90,103,106 | 0 |
| 25 | 5MU | AY | 54 | 21/22 | 0.85 | 0.20 | 81,89,99,128 | 0 |
| 23 | PSU | AW | 32 | 20/21 | 0.86 | 0.26 | 77,84,98,106 | 0 |
| 23 | 5MU | CW | 54 | 21/22 | 0.86 | 0.23 | 76,87,97,99 | 0 |
| 25 | MIA | AY | 37 | 22/30 | 0.86 | 0.22 | 79,89,101,116 | 0 |
| 25 | PSU | AY | 39 | 20/21 | 0.86 | 0.25 | 84,90,102,107 | 0 |
| 23 | MIA | CW | 37 | 22/30 | 0.87 | 0.30 | 72,86,92,96 | 0 |
| 23 | PSU | CW | 32 | 20/21 | 0.87 | 0.48 | 77,86,95,106 | 0 |
| 23 | PSU | CW | 39 | 20/21 | 0.89 | 0.43 | 76,85,92,95 | 0 |
| 24 | 31H | CX | 76 | 32/33 | 0.90 | 0.35 | 48,68,88,99 | 0 |
| 23 | 5MU | AW | 54 | 21/22 | 0.91 | 0.21 | 66,80,87,93 | 0 |
| 24 | PSU | CX | 55 | 20/21 | 0.92 | 0.15 | 81,87,92,97 | 0 |
| 23 | PSU | AW | 39 | 20/21 | 0.93 | 0.24 | 71,82,92,93 | 0 |
| 23 | MIA | AW | 37 | 29/30 | 0.93 | 0.25 | 56,65,80,82 | 0 |
| 24 | 4SU | AX | 8 | 20/21 | 0.93 | 0.17 | 59,69,79,85 | 0 |
| 23 | F3N | CW | 76 | 33/34 | 0.93 | 0.44 | 53,69,79,80 | 0 |
| 24 | 31H | AX | 76 | 32/33 | 0.94 | 0.33 | 31,57,76,77 | 10 |
| 24 | 5MU | CX | 54 | 21/22 | 0.94 | 0.21 | 71,85,94,104 | 0 |
| 23 | F3N | AW | 76 | 33/34 | 0.94 | 0.38 | 44,58,72,77 | 0 |
| 24 | PSU | AX | 55 | 20/21 | 0.94 | 0.16 | 52,69,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 24 | 5MC | CX | 32 | 21/22 | 0.95 | 0.18 | 63,77,85,87 | 0 |
| 24 | 5MU | AX | 54 | 21/22 | 0.96 | 0.16 | 46,72,77,86 | 0 |
| 24 | 5MC | AX | 32 | 21/22 | 0.97 | 0.20 | 50,57,69,76 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | CE | 202 | 1/1 | 0.26 | 0.19 | 95,95,95,95 | 0 |
| 59 | ZN | D4 | 501 | 1/1 | 0.33 | 0.12 | 162,162,162,162 | 0 |
| 57 | MG | AA | 1784 | 1/1 | 0.34 | 0.29 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3254 | 1/1 | 0.43 | 0.15 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3327 | 1/1 | 0.47 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3086 | 1/1 | 0.48 | 0.13 | 93,93,93,93 | 0 |
| 57 | MG | BA | 3702 | 1/1 | 0.49 | 0.12 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3135 | 1/1 | 0.49 | 0.18 | 63,63,63,63 | 0 |
| 57 | MG | AA | 1618 | 1/1 | 0.55 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3628 | 1/1 | 0.57 | 0.19 | 77,77,77,77 | 0 |
| 57 | MG | BA | 3734 | 1/1 | 0.57 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | CA | 3115 | 1/1 | 0.58 | 0.34 | 82,82,82,82 | 0 |
| 57 | MG | DA | 3070 | 1/1 | 0.59 | 0.19 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3033 | 1/1 | 0.60 | 0.49 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3463 | 1/1 | 0.60 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3204 | 1/1 | 0.60 | 0.21 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3439 | 1/1 | 0.61 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3318 | 1/1 | 0.62 | 0.10 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3057 | 1/1 | 0.63 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | AX | 3007 | 1/1 | 0.63 | 0.30 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3154 | 1/1 | 0.63 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3693 | 1/1 | 0.64 | 0.16 | 77,77,77,77 | 0 |
| 57 | MG | CA | 3003 | 1/1 | 0.64 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3516 | 1/1 | 0.65 | 0.21 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3272 | 1/1 | 0.66 | 0.26 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3710 | 1/1 | 0.66 | 0.79 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3116 | 1/1 | 0.67 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | AA | 1743 | 1/1 | 0.67 | 0.17 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3099 | 1/1 | 0.68 | 0.18 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3487 | 1/1 | 0.68 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3655 | 1/1 | 0.69 | 0.13 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3569 | 1/1 | 0.69 | 0.22 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3122 | 1/1 | 0.69 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | AA | 1713 | 1/1 | 0.69 | 0.11 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3652 | 1/1 | 0.69 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3199 | 1/1 | 0.69 | 0.25 | 62,62,62,62 | 0 |
| 57 | MG | AA | 1679 | 1/1 | 0.69 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3313 | 1/1 | 0.70 | 0.11 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3545 | 1/1 | 0.70 | 0.12 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3288 | 1/1 | 0.70 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3041 | 1/1 | 0.71 | 0.29 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3068 | 1/1 | 0.71 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3712 | 1/1 | 0.71 | 0.22 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3727 | 1/1 | 0.71 | 0.24 | 53,53,53,53 | 0 |
| 57 | MG | CA | 3006 | 1/1 | 0.71 | 0.11 | 68,68,68,68 | 0 |
| 57 | MG | AA | 1669 | 1/1 | 0.72 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | AL | 201 | 1/1 | 0.72 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3058 | 1/1 | 0.72 | 0.19 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3667 | 1/1 | 0.72 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | AA | 1701 | 1/1 | 0.72 | 0.27 | 73,73,73,73 | 0 |
| 57 | MG | BA | 3688 | 1/1 | 0.72 | 0.27 | 61,61,61,61 | 0 |
| 57 | MG | DQ | 3003 | 1/1 | 0.73 | 0.64 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3176 | 1/1 | 0.73 | 0.26 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3071 | 1/1 | 0.73 | 0.23 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3680 | 1/1 | 0.73 | 0.32 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3634 | 1/1 | 0.73 | 0.14 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3332 | 1/1 | 0.73 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | CA | 3059 | 1/1 | 0.73 | 0.16 | 75,75,75,75 | 0 |
| 57 | MG | DA | 3596 | 1/1 | 0.73 | 0.19 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3538 | 1/1 | 0.74 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3487 | 1/1 | 0.74 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3376 | 1/1 | 0.74 | 0.11 | 51,51,51,51 | 0 |
| 57 | MG | BB | 3004 | 1/1 | 0.74 | 0.21 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3265 | 1/1 | 0.74 | 0.29 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3097 | 1/1 | 0.74 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | BB | 3020 | 1/1 | 0.75 | 0.16 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3016 | 1/1 | 0.75 | 0.28 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1684 | 1/1 | 0.75 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | CA | 3130 | 1/1 | 0.75 | 0.28 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3502 | 1/1 | 0.75 | 0.24 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3624 | 1/1 | 0.75 | 0.48 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1686 | 1/1 | 0.75 | 0.14 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3253 | 1/1 | 0.75 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3340 | 1/1 | 0.75 | 0.18 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3121 | 1/1 | 0.75 | 0.29 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3086 | 1/1 | 0.76 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3279 | 1/1 | 0.76 | 0.14 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3032 | 1/1 | 0.76 | 0.21 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3579 | 1/1 | 0.76 | 0.11 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3005 | 1/1 | 0.76 | 0.20 | 73,73,73,73 | 0 |
| 57 | MG | CA | 3014 | 1/1 | 0.76 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3122 | 1/1 | 0.76 | 0.13 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3061 | 1/1 | 0.76 | 0.21 | 60,60,60,60 | 0 |
| 57 | MG | CA | 3154 | 1/1 | 0.76 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3174 | 1/1 | 0.76 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3400 | 1/1 | 0.76 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | AA | 1689 | 1/1 | 0.77 | 0.29 | 71,71,71,71 | 0 |
| 57 | MG | BA | 3224 | 1/1 | 0.77 | 0.30 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3108 | 1/1 | 0.77 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3032 | 1/1 | 0.77 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3066 | 1/1 | 0.77 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3015 | 1/1 | 0.77 | 0.18 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3164 | 1/1 | 0.77 | 0.22 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3637 | 1/1 | 0.77 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3015 | 1/1 | 0.77 | 0.23 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3079 | 1/1 | 0.77 | 0.11 | 72,72,72,72 | 0 |
| 57 | MG | BG | 202 | 1/1 | 0.78 | 0.15 | 52,52,52,52 | 0 |
| 57 | MG | AA | 1620 | 1/1 | 0.78 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3074 | 1/1 | 0.78 | 0.23 | 69,69,69,69 | 0 |
| 57 | MG | AA | 1631 | 1/1 | 0.78 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3676 | 1/1 | 0.78 | 0.17 | 70,70,70,70 | 0 |
| 57 | MG | DA | 3016 | 1/1 | 0.78 | 0.09 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3730 | 1/1 | 0.78 | 0.17 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3369 | 1/1 | 0.78 | 0.28 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3114 | 1/1 | 0.78 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3611 | 1/1 | 0.78 | 0.18 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3284 | 1/1 | 0.78 | 0.14 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3026 | 1/1 | 0.78 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3314 | 1/1 | 0.78 | 0.12 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3041 | 1/1 | 0.78 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3520 | 1/1 | 0.79 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3715 | 1/1 | 0.79 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3229 | 1/1 | 0.79 | 0.24 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3498 | 1/1 | 0.79 | 0.21 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3320 | 1/1 | 0.79 | 0.09 | 49,49,49,49 | 0 |
| 57 | MG | AA | 1625 | 1/1 | 0.79 | 0.17 | 73,73,73,73 | 0 |
| 57 | MG | DA | 3024 | 1/1 | 0.79 | 0.41 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3191 | 1/1 | 0.79 | 0.30 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3052 | 1/1 | 0.79 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | AA | 1655 | 1/1 | 0.79 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3542 | 1/1 | 0.79 | 0.17 | 60,60,60,60 | 0 |
| 57 | MG | DB | 3007 | 1/1 | 0.79 | 0.12 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3657 | 1/1 | 0.79 | 0.45 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3002 | 1/1 | 0.79 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | CA | 3019 | 1/1 | 0.79 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | AA | 1610 | 1/1 | 0.79 | 0.18 | 81,81,81,81 | 0 |
| 57 | MG | BA | 3759 | 1/1 | 0.79 | 0.13 | 70,70,70,70 | 0 |
| 57 | MG | AA | 1711 | 1/1 | 0.79 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3160 | 1/1 | 0.79 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3006 | 1/1 | 0.79 | 0.24 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3231 | 1/1 | 0.79 | 0.17 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3420 | 1/1 | 0.80 | 0.11 | 49,49,49,49 | 0 |
| 57 | MG | CA | 3013 | 1/1 | 0.80 | 0.14 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3696 | 1/1 | 0.80 | 0.10 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3612 | 1/1 | 0.80 | 0.08 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3091 | 1/1 | 0.80 | 0.15 | 69,69,69,69 | 0 |
| 57 | MG | AA | 1604 | 1/1 | 0.80 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3700 | 1/1 | 0.80 | 0.24 | 36,36,36,36 | 0 |
| 57 | MG | CA | 3061 | 1/1 | 0.80 | 0.21 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3356 | 1/1 | 0.80 | 0.16 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3713 | 1/1 | 0.80 | 0.28 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3089 | 1/1 | 0.80 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3721 | 1/1 | 0.80 | 0.10 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3557 | 1/1 | 0.80 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3678 | 1/1 | 0.80 | 0.10 | 67,67,67,67 | 0 |
| 57 | MG | AA | 1622 | 1/1 | 0.80 | 0.21 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3650 | 1/1 | 0.80 | 0.14 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3649 | 1/1 | 0.80 | 0.13 | 71,71,71,71 | 0 |
| 57 | MG | DA | 3056 | 1/1 | 0.80 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3257 | 1/1 | 0.81 | 0.18 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3648 | 1/1 | 0.81 | 0.07 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3281 | 1/1 | 0.81 | 0.28 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3458 | 1/1 | 0.81 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1697 | 1/1 | 0.81 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3411 | 1/1 | 0.81 | 0.24 | 50,50,50,50 | 0 |
| 57 | MG | AA | 1741 | 1/1 | 0.81 | 0.12 | 86,86,86,86 | 0 |
| 57 | MG | DA | 3351 | 1/1 | 0.81 | 0.08 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3644 | 1/1 | 0.81 | 0.18 | 64,64,64,64 | 0 |
| 57 | MG | CA | 3049 | 1/1 | 0.81 | 0.21 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3453 | 1/1 | 0.81 | 0.28 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3670 | 1/1 | 0.81 | 0.18 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3513 | 1/1 | 0.81 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | AA | 1710 | 1/1 | 0.81 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3442 | 1/1 | 0.81 | 0.19 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3395 | 1/1 | 0.81 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3270 | 1/1 | 0.81 | 0.22 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3625 | 1/1 | 0.81 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3197 | 1/1 | 0.81 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | AA | 1623 | 1/1 | 0.81 | 0.24 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3301 | 1/1 | 0.81 | 0.11 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3094 | 1/1 | 0.81 | 0.08 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3475 | 1/1 | 0.81 | 0.09 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3591 | 1/1 | 0.81 | 0.06 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3205 | 1/1 | 0.82 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | AA | 1616 | 1/1 | 0.82 | 0.09 | 73,73,73,73 | 0 |
| 57 | MG | BB | 3001 | 1/1 | 0.82 | 0.29 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3233 | 1/1 | 0.82 | 0.13 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3101 | 1/1 | 0.82 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | BN | 3002 | 1/1 | 0.82 | 0.20 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3755 | 1/1 | 0.82 | 0.24 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3183 | 1/1 | 0.82 | 0.48 | 49,49,49,49 | 0 |
| 57 | MG | BE | 301 | 1/1 | 0.82 | 0.20 | 31,31,31,31 | 0 |
| 57 | MG | AA | 1810 | 1/1 | 0.82 | 0.09 | 86,86,86,86 | 0 |
| 57 | MG | CA | 3102 | 1/1 | 0.82 | 0.16 | 71,71,71,71 | 0 |
| 57 | MG | AA | 1644 | 1/1 | 0.82 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3343 | 1/1 | 0.82 | 0.18 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3257 | 1/1 | 0.82 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3058 | 1/1 | 0.82 | 0.19 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3514 | 1/1 | 0.82 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3468 | 1/1 | 0.82 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | BF | 310 | 1/1 | 0.82 | 0.23 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3497 | 1/1 | 0.82 | 0.19 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3162 | 1/1 | 0.82 | 0.07 | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DB | 3003 | 1/1 | 0.82 | 0.10 | 78,78,78,78 | 0 |
| 57 | MG | BA | 3347 | 1/1 | 0.82 | 0.19 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3619 | 1/1 | 0.82 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3530 | 1/1 | 0.82 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | BZ | 301 | 1/1 | 0.82 | 0.18 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3627 | 1/1 | 0.82 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | CA | 3146 | 1/1 | 0.82 | 0.18 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3592 | 1/1 | 0.82 | 0.14 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3035 | 1/1 | 0.82 | 0.12 | 37,37,37,37 | 0 |
| 57 | MG | AA | 1660 | 1/1 | 0.82 | 0.24 | 51,51,51,51 | 0 |
| 57 | MG | AX | 3016 | 1/1 | 0.82 | 0.61 | 86,86,86,86 | 0 |
| 57 | MG | DA | 3143 | 1/1 | 0.82 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3560 | 1/1 | 0.82 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3717 | 1/1 | 0.82 | 0.15 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3607 | 1/1 | 0.82 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | CA | 3050 | 1/1 | 0.82 | 0.19 | 73,73,73,73 | 0 |
| 57 | MG | DA | 3549 | 1/1 | 0.82 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3807 | 1/1 | 0.82 | 0.24 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3200 | 1/1 | 0.83 | 0.25 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3004 | 1/1 | 0.83 | 0.09 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3397 | 1/1 | 0.83 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3060 | 1/1 | 0.83 | 0.22 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3394 | 1/1 | 0.83 | 0.05 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3423 | 1/1 | 0.83 | 0.16 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3233 | 1/1 | 0.83 | 0.28 | 40,40,40,40 | 0 |
| 57 | MG | CA | 3143 | 1/1 | 0.83 | 0.20 | 74,74,74,74 | 0 |
| 57 | MG | BA | 3593 | 1/1 | 0.83 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1766 | 1/1 | 0.83 | 0.19 | 71,71,71,71 | 0 |
| 57 | MG | BA | 3235 | 1/1 | 0.83 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | CE | 201 | 1/1 | 0.83 | 0.18 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3618 | 1/1 | 0.83 | 0.10 | 46,46,46,46 | 0 |
| 57 | MG | AW | 3001 | 1/1 | 0.83 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | DB | 3001 | 1/1 | 0.83 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | AA | 1664 | 1/1 | 0.83 | 0.22 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3002 | 1/1 | 0.83 | 0.14 | 77,77,77,77 | 0 |
| 57 | MG | DA | 3238 | 1/1 | 0.83 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3111 | 1/1 | 0.83 | 0.32 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3600 | 1/1 | 0.83 | 0.28 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3608 | 1/1 | 0.83 | 0.29 | 58,58,58,58 | 0 |
| 57 | MG | AA | 1650 | 1/1 | 0.83 | 0.15 | 74,74,74,74 | 0 |
| 57 | MG | CA | 3070 | 1/1 | 0.83 | 0.15 | 69,69,69,69 | 0 |
| 57 | MG | BB | 3019 | 1/1 | 0.83 | 0.20 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3606 | 1/1 | 0.83 | 0.20 | 74,74,74,74 | 0 |
| 57 | MG | DA | 3369 | 1/1 | 0.83 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3031 | 1/1 | 0.83 | 0.14 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3227 | 1/1 | 0.83 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3240 | 1/1 | 0.83 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3738 | 1/1 | 0.83 | 0.13 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3090 | 1/1 | 0.83 | 0.17 | 76,76,76,76 | 0 |
| 57 | MG | CA | 3017 | 1/1 | 0.83 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | CA | 3012 | 1/1 | 0.83 | 0.32 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3002 | 1/1 | 0.83 | 0.28 | 53,53,53,53 | 0 |
| 57 | MG | CA | 3016 | 1/1 | 0.83 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | DB | 3010 | 1/1 | 0.83 | 0.13 | 75,75,75,75 | 0 |
| 57 | MG | AX | 3005 | 1/1 | 0.84 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3140 | 1/1 | 0.84 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | AA | 1696 | 1/1 | 0.84 | 0.10 | 83,83,83,83 | 0 |
| 57 | MG | CA | 3112 | 1/1 | 0.84 | 0.10 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3568 | 1/1 | 0.84 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3411 | 1/1 | 0.84 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3426 | 1/1 | 0.84 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3598 | 1/1 | 0.84 | 0.15 | 33,33,33,33 | 0 |
| 57 | MG | B7 | 104 | 1/1 | 0.84 | 0.27 | 62,62,62,62 | 0 |
| 57 | MG | DF | 303 | 1/1 | 0.84 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3039 | 1/1 | 0.84 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3379 | 1/1 | 0.84 | 0.09 | 46,46,46,46 | 0 |
| 57 | MG | CA | 3108 | 1/1 | 0.84 | 0.11 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3065 | 1/1 | 0.84 | 0.10 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3155 | 1/1 | 0.84 | 0.19 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3087 | 1/1 | 0.84 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3456 | 1/1 | 0.84 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | AA | 1695 | 1/1 | 0.84 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1723 | 1/1 | 0.84 | 0.15 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3123 | 1/1 | 0.84 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3049 | 1/1 | 0.84 | 0.19 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3687 | 1/1 | 0.84 | 0.18 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3604 | 1/1 | 0.84 | 0.15 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3145 | 1/1 | 0.84 | 0.25 | 48,48,48,48 | 0 |
| 57 | MG | DF | 302 | 1/1 | 0.84 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3778 | 1/1 | 0.84 | 0.08 | 40,40,40,40 | 0 |
| 57 | MG | CA | 3009 | 1/1 | 0.84 | 0.12 | 73,73,73,73 | 0 |
| 57 | MG | CA | 3001 | 1/1 | 0.84 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3809 | 1/1 | 0.84 | 0.37 | 61,61,61,61 | 0 |
| 57 | MG | AA | 1613 | 1/1 | 0.84 | 0.18 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3505 | 1/1 | 0.84 | 0.22 | 53,53,53,53 | 0 |
| 57 | MG | AA | 1789 | 1/1 | 0.85 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3234 | 1/1 | 0.85 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | CA | 3164 | 1/1 | 0.85 | 0.33 | 76,76,76,76 | 0 |
| 57 | MG | DA | 3111 | 1/1 | 0.85 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3281 | 1/1 | 0.85 | 0.11 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3491 | 1/1 | 0.85 | 0.25 | 43,43,43,43 | 0 |
| 57 | MG | AA | 1663 | 1/1 | 0.85 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3196 | 1/1 | 0.85 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3571 | 1/1 | 0.85 | 0.24 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3092 | 1/1 | 0.85 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | AA | 1612 | 1/1 | 0.85 | 0.16 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3477 | 1/1 | 0.85 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3620 | 1/1 | 0.85 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3078 | 1/1 | 0.85 | 0.32 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3637 | 1/1 | 0.85 | 0.14 | 72,72,72,72 | 0 |
| 57 | MG | BA | 3656 | 1/1 | 0.85 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3139 | 1/1 | 0.85 | 0.36 | 81,81,81,81 | 0 |
| 57 | MG | AA | 1699 | 1/1 | 0.85 | 0.32 | 58,58,58,58 | 0 |
| 57 | MG | AX | 3012 | 1/1 | 0.85 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | AX | 3013 | 1/1 | 0.85 | 0.20 | 70,70,70,70 | 0 |
| 57 | MG | DA | 3317 | 1/1 | 0.85 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3636 | 1/1 | 0.85 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3175 | 1/1 | 0.85 | 0.29 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3574 | 1/1 | 0.85 | 0.07 | 61,61,61,61 | 0 |
| 57 | MG | AA | 1682 | 1/1 | 0.85 | 0.26 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3225 | 1/1 | 0.85 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | CA | 3161 | 1/1 | 0.85 | 0.13 | 76,76,76,76 | 0 |
| 57 | MG | BA | 3570 | 1/1 | 0.85 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3056 | 1/1 | 0.85 | 0.31 | 46,46,46,46 | 0 |
| 57 | MG | CA | 3068 | 1/1 | 0.85 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | AA | 1764 | 1/1 | 0.85 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | AA | 1667 | 1/1 | 0.85 | 0.19 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3125 | 1/1 | 0.85 | 0.21 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3632 | 1/1 | 0.85 | 0.26 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3107 | 1/1 | 0.85 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | CA | 3041 | 1/1 | 0.85 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3283 | 1/1 | 0.85 | 0.40 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3173 | 1/1 | 0.85 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3046 | 1/1 | 0.85 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3280 | 1/1 | 0.85 | 0.09 | 48,48,48,48 | 0 |
| 57 | MG | AA | 1601 | 1/1 | 0.85 | 0.12 | 81,81,81,81 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1787 | 1/1 | 0.85 | 0.15 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3462 | 1/1 | 0.85 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3062 | 1/1 | 0.85 | 0.30 | 59,59,59,59 | 0 |
| 57 | MG | D8 | 5001 | 1/1 | 0.85 | 0.22 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3103 | 1/1 | 0.85 | 0.35 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3011 | 1/1 | 0.85 | 0.25 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3057 | 1/1 | 0.85 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3485 | 1/1 | 0.85 | 0.24 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3263 | 1/1 | 0.85 | 0.28 | 60,60,60,60 | 0 |
| 57 | MG | AA | 1602 | 1/1 | 0.85 | 0.10 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3008 | 1/1 | 0.85 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3488 | 1/1 | 0.86 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3456 | 1/1 | 0.86 | 0.30 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3338 | 1/1 | 0.86 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3415 | 1/1 | 0.86 | 0.18 | 43,43,43,43 | 0 |
| 57 | MG | AA | 1738 | 1/1 | 0.86 | 0.22 | 68,68,68,68 | 0 |
| 57 | MG | AA | 1777 | 1/1 | 0.86 | 0.09 | 71,71,71,71 | 0 |
| 57 | MG | BA | 3318 | 1/1 | 0.86 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | B8 | 5002 | 1/1 | 0.86 | 0.31 | 53,53,53,53 | 0 |
| 57 | MG | CA | 3109 | 1/1 | 0.86 | 0.15 | 74,74,74,74 | 0 |
| 57 | MG | DA | 3170 | 1/1 | 0.86 | 0.10 | 35,35,35,35 | 0 |
| 57 | MG | CA | 3052 | 1/1 | 0.86 | 0.12 | 71,71,71,71 | 0 |
| 57 | MG | DA | 3136 | 1/1 | 0.86 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3617 | 1/1 | 0.86 | 0.25 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3102 | 1/1 | 0.86 | 0.31 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3088 | 1/1 | 0.86 | 0.26 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3029 | 1/1 | 0.86 | 0.27 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3525 | 1/1 | 0.86 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3052 | 1/1 | 0.86 | 0.27 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3418 | 1/1 | 0.86 | 0.07 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3346 | 1/1 | 0.86 | 0.10 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3232 | 1/1 | 0.86 | 0.24 | 49,49,49,49 | 0 |
| 57 | MG | AA | 1606 | 1/1 | 0.86 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3417 | 1/1 | 0.86 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3161 | 1/1 | 0.86 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3253 | 1/1 | 0.86 | 0.20 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3099 | 1/1 | 0.86 | 0.24 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3018 | 1/1 | 0.86 | 0.40 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3243 | 1/1 | 0.86 | 0.67 | 44,44,44,44 | 0 |
| 57 | MG | AX | 3003 | 1/1 | 0.86 | 0.23 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3250 | 1/1 | 0.86 | 0.21 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3118 | 1/1 | 0.86 | 0.16 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3107 | 1/1 | 0.86 | 0.33 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3005 | 1/1 | 0.86 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3130 | 1/1 | 0.86 | 0.15 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3172 | 1/1 | 0.86 | 0.21 | 61,61,61,61 | 0 |
| 57 | MG | AA | 1763 | 1/1 | 0.86 | 0.07 | 79,79,79,79 | 0 |
| 57 | MG | DA | 3390 | 1/1 | 0.86 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | BW | 3001 | 1/1 | 0.86 | 0.35 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3094 | 1/1 | 0.86 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3726 | 1/1 | 0.86 | 0.20 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3538 | 1/1 | 0.86 | 0.12 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3577 | 1/1 | 0.86 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3112 | 1/1 | 0.86 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3275 | 1/1 | 0.86 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3330 | 1/1 | 0.86 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3333 | 1/1 | 0.86 | 0.17 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3723 | 1/1 | 0.86 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | AA | 1658 | 1/1 | 0.86 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3416 | 1/1 | 0.86 | 0.26 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3424 | 1/1 | 0.86 | 0.18 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3633 | 1/1 | 0.86 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3435 | 1/1 | 0.86 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | DG | 3001 | 1/1 | 0.86 | 0.14 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3530 | 1/1 | 0.86 | 0.25 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3519 | 1/1 | 0.86 | 0.14 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3365 | 1/1 | 0.86 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3286 | 1/1 | 0.86 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3592 | 1/1 | 0.86 | 0.09 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3611 | 1/1 | 0.86 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3141 | 1/1 | 0.86 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3512 | 1/1 | 0.86 | 0.12 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3153 | 1/1 | 0.86 | 0.15 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3157 | 1/1 | 0.86 | 0.12 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3681 | 1/1 | 0.86 | 0.23 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3271 | 1/1 | 0.86 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3235 | 1/1 | 0.86 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3109 | 1/1 | 0.86 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3523 | 1/1 | 0.86 | 0.21 | 41,41,41,41 | 0 |
| 57 | MG | AA | 1628 | 1/1 | 0.86 | 0.10 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3668 | 1/1 | 0.86 | 0.15 | 75,75,75,75 | 0 |
| 57 | MG | BA | 3360 | 1/1 | 0.86 | 0.23 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3747 | 1/1 | 0.86 | 0.24 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3377 | 1/1 | 0.86 | 0.21 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3286 | 1/1 | 0.86 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3653 | 1/1 | 0.86 | 0.17 | 33,33,33,33 | 0 |
| 57 | MG | AA | 1812 | 1/1 | 0.86 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3614 | 1/1 | 0.86 | 0.17 | 53,53,53,53 | 0 |
| 60 | K | AX | 3001 | 1/1 | 0.87 | 0.13 | 77,77,77,77 | 0 |
| 57 | MG | BA | 3732 | 1/1 | 0.87 | 0.24 | 33,33,33,33 | 0 |
| 57 | MG | DP | 201 | 1/1 | 0.87 | 0.21 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3504 | 1/1 | 0.87 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3484 | 1/1 | 0.87 | 0.13 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3452 | 1/1 | 0.87 | 0.11 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3192 | 1/1 | 0.87 | 0.32 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3604 | 1/1 | 0.87 | 0.20 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3745 | 1/1 | 0.87 | 0.24 | 61,61,61,61 | 0 |
| 57 | MG | CA | 3110 | 1/1 | 0.87 | 0.12 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3230 | 1/1 | 0.87 | 0.33 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3149 | 1/1 | 0.87 | 0.19 | 42,42,42,42 | 0 |
| 57 | MG | AA | 1632 | 1/1 | 0.87 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3442 | 1/1 | 0.87 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3493 | 1/1 | 0.87 | 0.08 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3600 | 1/1 | 0.87 | 0.13 | 72,72,72,72 | 0 |
| 57 | MG | CA | 3051 | 1/1 | 0.87 | 0.11 | 77,77,77,77 | 0 |
| 57 | MG | BA | 3588 | 1/1 | 0.87 | 0.09 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3106 | 1/1 | 0.87 | 0.25 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3023 | 1/1 | 0.87 | 0.14 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3597 | 1/1 | 0.87 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3127 | 1/1 | 0.87 | 0.30 | 45,45,45,45 | 0 |
| 57 | MG | AA | 1614 | 1/1 | 0.87 | 0.19 | 75,75,75,75 | 0 |
| 57 | MG | B2 | 3001 | 1/1 | 0.87 | 0.25 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3042 | 1/1 | 0.87 | 0.29 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3338 | 1/1 | 0.87 | 0.07 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3805 | 1/1 | 0.87 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3653 | 1/1 | 0.87 | 0.21 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3564 | 1/1 | 0.87 | 0.09 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3792 | 1/1 | 0.87 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | AA | 1788 | 1/1 | 0.87 | 0.09 | 75,75,75,75 | 0 |
| 57 | MG | BA | 3441 | 1/1 | 0.87 | 0.20 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3623 | 1/1 | 0.87 | 0.10 | 45,45,45,45 | 0 |
| 57 | MG | AA | 1634 | 1/1 | 0.87 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | AA | 1630 | 1/1 | 0.87 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3603 | 1/1 | 0.87 | 0.06 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3190 | 1/1 | 0.87 | 0.20 | 63,63,63,63 | 0 |
| 57 | MG | AA | 1651 | 1/1 | 0.87 | 0.25 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3106 | 1/1 | 0.87 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3010 | 1/1 | 0.87 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3150 | 1/1 | 0.87 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3549 | 1/1 | 0.87 | 0.11 | 66,66,66,66 | 0 |
| 57 | MG | AA | 1771 | 1/1 | 0.87 | 0.15 | 75,75,75,75 | 0 |
| 57 | MG | AA | 1755 | 1/1 | 0.87 | 0.09 | 80,80,80,80 | 0 |
| 57 | MG | DA | 3067 | 1/1 | 0.87 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3045 | 1/1 | 0.87 | 0.22 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3561 | 1/1 | 0.87 | 0.26 | 34,34,34,34 | 0 |
| 57 | MG | DD | 302 | 1/1 | 0.87 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3239 | 1/1 | 0.87 | 0.22 | 47,47,47,47 | 0 |
| 57 | MG | AA | 1680 | 1/1 | 0.87 | 0.17 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3510 | 1/1 | 0.87 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3087 | 1/1 | 0.87 | 0.07 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3660 | 1/1 | 0.87 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | CA | 3111 | 1/1 | 0.87 | 0.15 | 72,72,72,72 | 0 |
| 57 | MG | AA | 1666 | 1/1 | 0.87 | 0.33 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3140 | 1/1 | 0.87 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3024 | 1/1 | 0.87 | 0.23 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3212 | 1/1 | 0.87 | 0.21 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3626 | 1/1 | 0.87 | 0.11 | 81,81,81,81 | 0 |
| 57 | MG | BA | 3245 | 1/1 | 0.87 | 0.32 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3500 | 1/1 | 0.87 | 0.35 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1629 | 1/1 | 0.87 | 0.35 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3508 | 1/1 | 0.88 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | CA | 3007 | 1/1 | 0.88 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3201 | 1/1 | 0.88 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3017 | 1/1 | 0.88 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | CA | 3030 | 1/1 | 0.88 | 0.07 | 74,74,74,74 | 0 |
| 57 | MG | DA | 3577 | 1/1 | 0.88 | 0.07 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3418 | 1/1 | 0.88 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | CA | 3022 | 1/1 | 0.88 | 0.23 | 76,76,76,76 | 0 |
| 57 | MG | BA | 3254 | 1/1 | 0.88 | 0.16 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3445 | 1/1 | 0.88 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3088 | 1/1 | 0.88 | 0.17 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3139 | 1/1 | 0.88 | 0.22 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3541 | 1/1 | 0.88 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | CA | 3153 | 1/1 | 0.88 | 0.11 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3051 | 1/1 | 0.88 | 0.13 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3508 | 1/1 | 0.88 | 0.21 | 20,20,20,20 | 0 |
| 57 | MG | AA | 1633 | 1/1 | 0.88 | 0.27 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3129 | 1/1 | 0.88 | 0.16 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1747 | 1/1 | 0.88 | 0.15 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3324 | 1/1 | 0.88 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3633 | 1/1 | 0.88 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3200 | 1/1 | 0.88 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3347 | 1/1 | 0.88 | 0.14 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3494 | 1/1 | 0.88 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3275 | 1/1 | 0.88 | 0.16 | 66,66,66,66 | 0 |
| 57 | MG | BB | 3006 | 1/1 | 0.88 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3663 | 1/1 | 0.88 | 0.15 | 73,73,73,73 | 0 |
| 57 | MG | AX | 3010 | 1/1 | 0.88 | 0.40 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3794 | 1/1 | 0.88 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | AA | 1640 | 1/1 | 0.88 | 0.22 | 54,54,54,54 | 0 |
| 57 | MG | B0 | 3002 | 1/1 | 0.88 | 0.21 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3311 | 1/1 | 0.88 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3250 | 1/1 | 0.88 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3341 | 1/1 | 0.88 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3313 | 1/1 | 0.88 | 0.19 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3381 | 1/1 | 0.88 | 0.11 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3642 | 1/1 | 0.88 | 0.18 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3375 | 1/1 | 0.88 | 0.10 | 57,57,57,57 | 0 |
| 57 | MG | DB | 3005 | 1/1 | 0.88 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | AN | 503 | 1/1 | 0.88 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3271 | 1/1 | 0.88 | 0.16 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3187 | 1/1 | 0.88 | 0.20 | 47,47,47,47 | 0 |
| 57 | MG | AA | 1707 | 1/1 | 0.88 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3506 | 1/1 | 0.88 | 0.22 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3131 | 1/1 | 0.88 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3444 | 1/1 | 0.88 | 0.21 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3020 | 1/1 | 0.88 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3065 | 1/1 | 0.88 | 0.31 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3289 | 1/1 | 0.88 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3014 | 1/1 | 0.88 | 0.14 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3073 | 1/1 | 0.88 | 0.16 | 32,32,32,32 | 0 |
| 57 | MG | AA | 1603 | 1/1 | 0.88 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3383 | 1/1 | 0.88 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3515 | 1/1 | 0.88 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | DA | 3427 | 1/1 | 0.88 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3578 | 1/1 | 0.88 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3767 | 1/1 | 0.88 | 0.23 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3208 | 1/1 | 0.88 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3194 | 1/1 | 0.88 | 0.16 | 48,48,48,48 | 0 |
| 57 | MG | AA | 1621 | 1/1 | 0.88 | 0.14 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3203 | 1/1 | 0.88 | 0.34 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3255 | 1/1 | 0.88 | 0.21 | 55,55,55,55 | 0 |
| 57 | MG | AX | 3008 | 1/1 | 0.88 | 0.15 | 76,76,76,76 | 0 |
| 57 | MG | BA | 3763 | 1/1 | 0.88 | 0.15 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3129 | 1/1 | 0.88 | 0.13 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3384 | 1/1 | 0.88 | 0.10 | 38,38,38,38 | 0 |
| 57 | MG | AA | 1605 | 1/1 | 0.88 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3638 | 1/1 | 0.88 | 0.17 | 65,65,65,65 | 0 |
| 57 | MG | AF | 3001 | 1/1 | 0.88 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3594 | 1/1 | 0.88 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3306 | 1/1 | 0.88 | 0.28 | 65,65,65,65 | 0 |
| 57 | MG | DV | 201 | 1/1 | 0.88 | 0.51 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3666 | 1/1 | 0.88 | 0.26 | 74,74,74,74 | 0 |
| 57 | MG | DA | 3522 | 1/1 | 0.88 | 0.11 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3455 | 1/1 | 0.88 | 0.09 | 64,64,64,64 | 0 |
| 57 | MG | AY | 3001 | 1/1 | 0.88 | 0.32 | 63,63,63,63 | 0 |
| 57 | MG | AA | 1704 | 1/1 | 0.88 | 0.13 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3359 | 1/1 | 0.88 | 0.06 | 60,60,60,60 | 0 |
| 57 | MG | DB | 3012 | 1/1 | 0.88 | 0.24 | 66,66,66,66 | 0 |
| 57 | MG | DU | 201 | 1/1 | 0.88 | 0.57 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3580 | 1/1 | 0.88 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3218 | 1/1 | 0.88 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3125 | 1/1 | 0.89 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | AA | 1693 | 1/1 | 0.89 | 0.20 | 76,76,76,76 | 0 |
| 57 | MG | BA | 3389 | 1/1 | 0.89 | 0.21 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3379 | 1/1 | 0.89 | 0.18 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3132 | 1/1 | 0.89 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3129 | 1/1 | 0.89 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3515 | 1/1 | 0.89 | 0.13 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3064 | 1/1 | 0.89 | 0.11 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3266 | 1/1 | 0.89 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3529 | 1/1 | 0.89 | 0.25 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3705 | 1/1 | 0.89 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1626 | 1/1 | 0.89 | 0.21 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3021 | 1/1 | 0.89 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3491 | 1/1 | 0.89 | 0.22 | 56,56,56,56 | 0 |
| 57 | MG | AA | 1739 | 1/1 | 0.89 | 0.22 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3212 | 1/1 | 0.89 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | DB | 3011 | 1/1 | 0.89 | 0.26 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3222 | 1/1 | 0.89 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3645 | 1/1 | 0.89 | 0.11 | 64,64,64,64 | 0 |
| 57 | MG | AY | 3003 | 1/1 | 0.89 | 0.15 | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3486 | 1/1 | 0.89 | 0.13 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3689 | 1/1 | 0.89 | 0.19 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1708 | 1/1 | 0.89 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3237 | 1/1 | 0.89 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3422 | 1/1 | 0.89 | 0.24 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3068 | 1/1 | 0.89 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3471 | 1/1 | 0.89 | 0.31 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3480 | 1/1 | 0.89 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | AA | 1671 | 1/1 | 0.89 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | BP | 3002 | 1/1 | 0.89 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3646 | 1/1 | 0.89 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3248 | 1/1 | 0.89 | 0.15 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3443 | 1/1 | 0.89 | 0.18 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3358 | 1/1 | 0.89 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3239 | 1/1 | 0.89 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3329 | 1/1 | 0.89 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3125 | 1/1 | 0.89 | 0.25 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3558 | 1/1 | 0.89 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3513 | 1/1 | 0.89 | 0.34 | 50,50,50,50 | 0 |
| 57 | MG | CW | 3001 | 1/1 | 0.89 | 0.19 | 66,66,66,66 | 0 |
| 57 | MG | AA | 1662 | 1/1 | 0.89 | 0.20 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3008 | 1/1 | 0.89 | 0.32 | 47,47,47,47 | 0 |
| 57 | MG | CA | 3023 | 1/1 | 0.89 | 0.10 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3299 | 1/1 | 0.89 | 0.21 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3609 | 1/1 | 0.89 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3558 | 1/1 | 0.89 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3274 | 1/1 | 0.89 | 0.27 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3554 | 1/1 | 0.89 | 0.09 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3766 | 1/1 | 0.89 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3622 | 1/1 | 0.89 | 0.21 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3291 | 1/1 | 0.89 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3232 | 1/1 | 0.89 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | AA | 1759 | 1/1 | 0.89 | 0.15 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3065 | 1/1 | 0.89 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1652 | 1/1 | 0.89 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | AA | 1712 | 1/1 | 0.89 | 0.21 | 69,69,69,69 | 0 |
| 57 | MG | AX | 3015 | 1/1 | 0.89 | 0.29 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3295 | 1/1 | 0.89 | 0.22 | 23,23,23,23 | 0 |
| 57 | MG | BA | 3536 | 1/1 | 0.89 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3194 | 1/1 | 0.89 | 0.25 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3601 | 1/1 | 0.89 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3390 | 1/1 | 0.89 | 0.10 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3735 | 1/1 | 0.89 | 0.23 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3077 | 1/1 | 0.89 | 0.21 | 60,60,60,60 | 0 |
| 57 | MG | CA | 3119 | 1/1 | 0.89 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3325 | 1/1 | 0.89 | 0.15 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3219 | 1/1 | 0.89 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3407 | 1/1 | 0.89 | 0.17 | 32,32,32,32 | 0 |
| 57 | MG | CA | 3029 | 1/1 | 0.89 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3522 | 1/1 | 0.89 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | AM | 3002 | 1/1 | 0.89 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | CA | 3137 | 1/1 | 0.89 | 0.15 | 78,78,78,78 | 0 |
| 57 | MG | DA | 3552 | 1/1 | 0.89 | 0.13 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3451 | 1/1 | 0.89 | 0.08 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3148 | 1/1 | 0.89 | 0.15 | 68,68,68,68 | 0 |
| 57 | MG | CA | 3063 | 1/1 | 0.89 | 0.23 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3367 | 1/1 | 0.89 | 0.22 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3138 | 1/1 | 0.89 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3406 | 1/1 | 0.89 | 0.10 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3079 | 1/1 | 0.89 | 0.37 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3034 | 1/1 | 0.89 | 0.23 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3574 | 1/1 | 0.89 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3501 | 1/1 | 0.89 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3393 | 1/1 | 0.89 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3095 | 1/1 | 0.89 | 0.16 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3377 | 1/1 | 0.89 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | DP | 202 | 1/1 | 0.89 | 0.09 | 49,49,49,49 | 0 |
| 57 | MG | BB | 3009 | 1/1 | 0.90 | 0.09 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3546 | 1/1 | 0.90 | 0.14 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3063 | 1/1 | 0.90 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3476 | 1/1 | 0.90 | 0.08 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3694 | 1/1 | 0.90 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3658 | 1/1 | 0.90 | 0.12 | 61,61,61,61 | 0 |
| 57 | MG | DQ | 3002 | 1/1 | 0.90 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3651 | 1/1 | 0.90 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3117 | 1/1 | 0.90 | 0.64 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3087 | 1/1 | 0.90 | 0.38 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3273 | 1/1 | 0.90 | 0.21 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3532 | 1/1 | 0.90 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3631 | 1/1 | 0.90 | 0.26 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3171 | 1/1 | 0.90 | 0.32 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3765 | 1/1 | 0.90 | 0.24 | 49,49,49,49 | 0 |
| 57 | MG | AA | 1635 | 1/1 | 0.90 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | BB | 3016 | 1/1 | 0.90 | 0.14 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3761 | 1/1 | 0.90 | 0.10 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3115 | 1/1 | 0.90 | 0.23 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3110 | 1/1 | 0.90 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3399 | 1/1 | 0.90 | 0.15 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3372 | 1/1 | 0.90 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3404 | 1/1 | 0.90 | 0.34 | 59,59,59,59 | 0 |
| 57 | MG | CA | 3135 | 1/1 | 0.90 | 0.06 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3590 | 1/1 | 0.90 | 0.22 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3505 | 1/1 | 0.90 | 0.08 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3333 | 1/1 | 0.90 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3406 | 1/1 | 0.90 | 0.17 | 70,70,70,70 | 0 |
| 57 | MG | BA | 3264 | 1/1 | 0.90 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3573 | 1/1 | 0.90 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3099 | 1/1 | 0.90 | 0.09 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3572 | 1/1 | 0.90 | 0.19 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3166 | 1/1 | 0.90 | 0.19 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3211 | 1/1 | 0.90 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3518 | 1/1 | 0.90 | 0.20 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3217 | 1/1 | 0.90 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3055 | 1/1 | 0.90 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3619 | 1/1 | 0.90 | 0.14 | 28,28,28,28 | 0 |
| 57 | MG | BV | 204 | 1/1 | 0.90 | 0.26 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3091 | 1/1 | 0.90 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3636 | 1/1 | 0.90 | 0.19 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3485 | 1/1 | 0.90 | 0.09 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3158 | 1/1 | 0.90 | 0.39 | 56,56,56,56 | 0 |
| 57 | MG | CA | 3131 | 1/1 | 0.90 | 0.24 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3439 | 1/1 | 0.90 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3063 | 1/1 | 0.90 | 0.33 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3244 | 1/1 | 0.90 | 0.27 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3413 | 1/1 | 0.90 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3459 | 1/1 | 0.90 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3704 | 1/1 | 0.90 | 0.18 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3625 | 1/1 | 0.90 | 0.14 | 33,33,33,33 | 0 |
| 57 | MG | AA | 1674 | 1/1 | 0.90 | 0.20 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3658 | 1/1 | 0.90 | 0.49 | 62,62,62,62 | 0 |
| 57 | MG | AA | 1768 | 1/1 | 0.90 | 0.11 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3336 | 1/1 | 0.90 | 0.09 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3110 | 1/1 | 0.90 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3570 | 1/1 | 0.90 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3141 | 1/1 | 0.90 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3089 | 1/1 | 0.90 | 0.23 | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3446 | 1/1 | 0.90 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3556 | 1/1 | 0.90 | 0.13 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3147 | 1/1 | 0.90 | 0.20 | 36,36,36,36 | 0 |
| 57 | MG | CA | 3126 | 1/1 | 0.90 | 0.09 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3448 | 1/1 | 0.90 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3786 | 1/1 | 0.90 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3429 | 1/1 | 0.90 | 0.26 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3296 | 1/1 | 0.90 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3410 | 1/1 | 0.90 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3523 | 1/1 | 0.90 | 0.14 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3692 | 1/1 | 0.90 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3408 | 1/1 | 0.90 | 0.17 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3243 | 1/1 | 0.90 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3803 | 1/1 | 0.90 | 0.34 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3096 | 1/1 | 0.90 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | CA | 3026 | 1/1 | 0.90 | 0.21 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3388 | 1/1 | 0.90 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3532 | 1/1 | 0.90 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3414 | 1/1 | 0.90 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | AA | 1687 | 1/1 | 0.90 | 0.21 | 46,46,46,46 | 0 |
| 57 | MG | AA | 1756 | 1/1 | 0.90 | 0.33 | 45,45,45,45 | 0 |
| 57 | MG | CX | 3002 | 1/1 | 0.90 | 0.14 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3049 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 57 | MG | AA | 1816 | 1/1 | 0.90 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | CA | 3121 | 1/1 | 0.90 | 0.13 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3072 | 1/1 | 0.90 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3416 | 1/1 | 0.90 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3533 | 1/1 | 0.90 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3769 | 1/1 | 0.90 | 0.20 | 47,47,47,47 | 0 |
| 57 | MG | CA | 3123 | 1/1 | 0.90 | 0.32 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3526 | 1/1 | 0.90 | 0.26 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3078 | 1/1 | 0.90 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3482 | 1/1 | 0.90 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | CJ | 5001 | 1/1 | 0.90 | 0.18 | 77,77,77,77 | 0 |
| 57 | MG | BA | 3497 | 1/1 | 0.90 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | AA | 1619 | 1/1 | 0.90 | 0.11 | 64,64,64,64 | 0 |
| 57 | MG | CA | 3027 | 1/1 | 0.90 | 0.19 | 65,65,65,65 | 0 |
| 57 | MG | CA | 3095 | 1/1 | 0.91 | 0.13 | 71,71,71,71 | 0 |
| 57 | MG | AA | 1609 | 1/1 | 0.91 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | AT | 3001 | 1/1 | 0.91 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3554 | 1/1 | 0.91 | 0.09 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3042 | 1/1 | 0.91 | 0.13 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1814 | 1/1 | 0.91 | 0.15 | 57,57,57,57 | 0 |
| 57 | MG | AA | 1781 | 1/1 | 0.91 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3645 | 1/1 | 0.91 | 0.18 | 47,47,47,47 | 0 |
| 57 | MG | CA | 3082 | 1/1 | 0.91 | 0.13 | 66,66,66,66 | 0 |
| 57 | MG | BW | 3004 | 1/1 | 0.91 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3103 | 1/1 | 0.91 | 0.15 | 73,73,73,73 | 0 |
| 57 | MG | DA | 3154 | 1/1 | 0.91 | 0.08 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3031 | 1/1 | 0.91 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | AA | 1798 | 1/1 | 0.91 | 0.11 | 62,62,62,62 | 0 |
| 57 | MG | DO | 202 | 1/1 | 0.91 | 0.12 | 60,60,60,60 | 0 |
| 57 | MG | CA | 3076 | 1/1 | 0.91 | 0.20 | 77,77,77,77 | 0 |
| 57 | MG | DA | 3260 | 1/1 | 0.91 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3261 | 1/1 | 0.91 | 0.16 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3166 | 1/1 | 0.91 | 0.15 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3081 | 1/1 | 0.91 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3126 | 1/1 | 0.91 | 0.23 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3328 | 1/1 | 0.91 | 0.21 | 42,42,42,42 | 0 |
| 57 | MG | BB | 3017 | 1/1 | 0.91 | 0.16 | 81,81,81,81 | 0 |
| 57 | MG | BA | 3358 | 1/1 | 0.91 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3446 | 1/1 | 0.91 | 0.09 | 59,59,59,59 | 0 |
| 57 | MG | BD | 3003 | 1/1 | 0.91 | 0.30 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3036 | 1/1 | 0.91 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3420 | 1/1 | 0.91 | 0.18 | 25,25,25,25 | 0 |
| 57 | MG | CA | 3152 | 1/1 | 0.91 | 0.10 | 71,71,71,71 | 0 |
| 57 | MG | BA | 3740 | 1/1 | 0.91 | 0.19 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3545 | 1/1 | 0.91 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3470 | 1/1 | 0.91 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | AA | 1753 | 1/1 | 0.91 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3034 | 1/1 | 0.91 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3323 | 1/1 | 0.91 | 0.19 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3419 | 1/1 | 0.91 | 0.20 | 25,25,25,25 | 0 |
| 57 | MG | CA | 3100 | 1/1 | 0.91 | 0.15 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3209 | 1/1 | 0.91 | 0.24 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3292 | 1/1 | 0.91 | 0.11 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3647 | 1/1 | 0.91 | 0.08 | 53,53,53,53 | 0 |
| 57 | MG | AX | 3004 | 1/1 | 0.91 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3435 | 1/1 | 0.91 | 0.22 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3615 | 1/1 | 0.91 | 0.13 | 71,71,71,71 | 0 |
| 57 | MG | BF | 306 | 1/1 | 0.91 | 0.33 | 49,49,49,49 | 0 |
| 57 | MG | CA | 3160 | 1/1 | 0.91 | 0.14 | 73,73,73,73 | 0 |
| 57 | MG | BA | 3524 | 1/1 | 0.91 | 0.21 | 33,33,33,33 | 0 |
| 57 | MG | AA | 1705 | 1/1 | 0.91 | 0.23 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3128 | 1/1 | 0.91 | 0.19 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3361 | 1/1 | 0.91 | 0.08 | 33,33,33,33 | 0 |
| 57 | MG | BB | 3013 | 1/1 | 0.91 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3388 | 1/1 | 0.91 | 0.20 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3008 | 1/1 | 0.91 | 0.14 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3796 | 1/1 | 0.91 | 0.17 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3160 | 1/1 | 0.91 | 0.34 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3197 | 1/1 | 0.91 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1717 | 1/1 | 0.91 | 0.16 | 75,75,75,75 | 0 |
| 57 | MG | DA | 3565 | 1/1 | 0.91 | 0.04 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3553 | 1/1 | 0.91 | 0.19 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3308 | 1/1 | 0.91 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3737 | 1/1 | 0.91 | 0.17 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3531 | 1/1 | 0.91 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3613 | 1/1 | 0.91 | 0.23 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3479 | 1/1 | 0.91 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3021 | 1/1 | 0.91 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3019 | 1/1 | 0.91 | 0.28 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3181 | 1/1 | 0.91 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | BY | 502 | 1/1 | 0.91 | 0.24 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3378 | 1/1 | 0.91 | 0.24 | 39,39,39,39 | 0 |
| 57 | MG | AA | 1643 | 1/1 | 0.91 | 0.21 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3122 | 1/1 | 0.91 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3069 | 1/1 | 0.91 | 0.08 | 43,43,43,43 | 0 |
| 57 | MG | AA | 1729 | 1/1 | 0.91 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3344 | 1/1 | 0.91 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3409 | 1/1 | 0.91 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3511 | 1/1 | 0.91 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3593 | 1/1 | 0.91 | 0.08 | 60,60,60,60 | 0 |
| 59 | ZN | CN | 501 | 1/1 | 0.91 | 0.06 | 100,100,100,100 | 0 |
| 57 | MG | DA | 3107 | 1/1 | 0.91 | 0.11 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3639 | 1/1 | 0.91 | 0.18 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3517 | 1/1 | 0.91 | 0.23 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3802 | 1/1 | 0.91 | 0.23 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3618 | 1/1 | 0.91 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3403 | 1/1 | 0.91 | 0.09 | 49,49,49,49 | 0 |
| 57 | MG | B7 | 103 | 1/1 | 0.91 | 0.30 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3259 | 1/1 | 0.91 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3507 | 1/1 | 0.91 | 0.26 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3081 | 1/1 | 0.91 | 0.11 | 51,51,51,51 | 0 |
| 57 | MG | AA | 1639 | 1/1 | 0.91 | 0.07 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3614 | 1/1 | 0.91 | 0.14 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3030 | 1/1 | 0.91 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3252 | 1/1 | 0.91 | 0.19 | 36,36,36,36 | 0 |
| 57 | MG | BX | 3001 | 1/1 | 0.91 | 0.35 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3557 | 1/1 | 0.91 | 0.19 | 57,57,57,57 | 0 |
| 57 | MG | AA | 1721 | 1/1 | 0.91 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3814 | 1/1 | 0.91 | 0.28 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3127 | 1/1 | 0.91 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3535 | 1/1 | 0.91 | 0.20 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3055 | 1/1 | 0.91 | 0.18 | 63,63,63,63 | 0 |
| 57 | MG | BN | 3001 | 1/1 | 0.91 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3191 | 1/1 | 0.91 | 0.19 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3163 | 1/1 | 0.91 | 0.49 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3524 | 1/1 | 0.91 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3728 | 1/1 | 0.91 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3452 | 1/1 | 0.91 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3241 | 1/1 | 0.91 | 0.13 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1801 | 1/1 | 0.91 | 0.09 | 71,71,71,71 | 0 |
| 57 | MG | DA | 3550 | 1/1 | 0.91 | 0.04 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3132 | 1/1 | 0.91 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3179 | 1/1 | 0.91 | 0.06 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3159 | 1/1 | 0.91 | 0.11 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3207 | 1/1 | 0.91 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | D0 | 101 | 1/1 | 0.91 | 0.13 | 71,71,71,71 | 0 |
| 57 | MG | BA | 3781 | 1/1 | 0.91 | 0.16 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3084 | 1/1 | 0.91 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1714 | 1/1 | 0.91 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | CA | 3151 | 1/1 | 0.91 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3516 | 1/1 | 0.91 | 0.24 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3327 | 1/1 | 0.91 | 0.15 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3685 | 1/1 | 0.91 | 0.20 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3368 | 1/1 | 0.91 | 0.09 | 67,67,67,67 | 0 |
| 57 | MG | AA | 1726 | 1/1 | 0.92 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | CT | 3001 | 1/1 | 0.92 | 0.17 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3156 | 1/1 | 0.92 | 0.23 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3768 | 1/1 | 0.92 | 0.13 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3672 | 1/1 | 0.92 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | BF | 311 | 1/1 | 0.92 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3662 | 1/1 | 0.92 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3543 | 1/1 | 0.92 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3314 | 1/1 | 0.92 | 0.18 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3542 | 1/1 | 0.92 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3682 | 1/1 | 0.92 | 0.14 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | CA | 3035 | 1/1 | 0.92 | 0.11 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3405 | 1/1 | 0.92 | 0.07 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3773 | 1/1 | 0.92 | 0.21 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3256 | 1/1 | 0.92 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3010 | 1/1 | 0.92 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3500 | 1/1 | 0.92 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | DE | 3005 | 1/1 | 0.92 | 0.14 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3512 | 1/1 | 0.92 | 0.21 | 23,23,23,23 | 0 |
| 57 | MG | BZ | 302 | 1/1 | 0.92 | 0.17 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3022 | 1/1 | 0.92 | 0.45 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3146 | 1/1 | 0.92 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3242 | 1/1 | 0.92 | 0.09 | 52,52,52,52 | 0 |
| 57 | MG | AA | 1745 | 1/1 | 0.92 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3362 | 1/1 | 0.92 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3100 | 1/1 | 0.92 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3053 | 1/1 | 0.92 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3305 | 1/1 | 0.92 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3470 | 1/1 | 0.92 | 0.08 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3366 | 1/1 | 0.92 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3806 | 1/1 | 0.92 | 0.17 | 43,43,43,43 | 0 |
| 57 | MG | DF | 301 | 1/1 | 0.92 | 0.31 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3741 | 1/1 | 0.92 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3729 | 1/1 | 0.92 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | AW | 3002 | 1/1 | 0.92 | 0.14 | 79,79,79,79 | 0 |
| 57 | MG | AA | 1688 | 1/1 | 0.92 | 0.21 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3641 | 1/1 | 0.92 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3094 | 1/1 | 0.92 | 0.06 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3151 | 1/1 | 0.92 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3460 | 1/1 | 0.92 | 0.11 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3310 | 1/1 | 0.92 | 0.13 | 35,35,35,35 | 0 |
| 57 | MG | AA | 1692 | 1/1 | 0.92 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | B4 | 502 | 1/1 | 0.92 | 0.09 | 70,70,70,70 | 0 |
| 57 | MG | BF | 307 | 1/1 | 0.92 | 0.13 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3141 | 1/1 | 0.92 | 0.32 | 38,38,38,38 | 0 |
| 57 | MG | AA | 1815 | 1/1 | 0.92 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3001 | 1/1 | 0.92 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3364 | 1/1 | 0.92 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3425 | 1/1 | 0.92 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3575 | 1/1 | 0.92 | 0.08 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3300 | 1/1 | 0.92 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3156 | 1/1 | 0.92 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3481 | 1/1 | 0.92 | 0.13 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3431 | 1/1 | 0.92 | 0.23 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3623 | 1/1 | 0.92 | 0.17 | 43,43,43,43 | 0 |
| 57 | MG | AA | 1797 | 1/1 | 0.92 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3134 | 1/1 | 0.92 | 0.19 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3124 | 1/1 | 0.92 | 0.28 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3582 | 1/1 | 0.92 | 0.05 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3086 | 1/1 | 0.92 | 0.33 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3028 | 1/1 | 0.92 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3113 | 1/1 | 0.92 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3587 | 1/1 | 0.92 | 0.11 | 46,46,46,46 | 0 |
| 57 | MG | BB | 3022 | 1/1 | 0.92 | 0.20 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3566 | 1/1 | 0.92 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3189 | 1/1 | 0.92 | 0.23 | 47,47,47,47 | 0 |
| 57 | MG | AA | 1694 | 1/1 | 0.92 | 0.08 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3025 | 1/1 | 0.92 | 0.18 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3640 | 1/1 | 0.92 | 0.17 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3561 | 1/1 | 0.92 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3036 | 1/1 | 0.92 | 0.16 | 73,73,73,73 | 0 |
| 57 | MG | DA | 3077 | 1/1 | 0.92 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | AL | 202 | 1/1 | 0.92 | 0.26 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3186 | 1/1 | 0.92 | 0.15 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3431 | 1/1 | 0.92 | 0.28 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3576 | 1/1 | 0.92 | 0.16 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3096 | 1/1 | 0.92 | 0.19 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3236 | 1/1 | 0.92 | 0.13 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3478 | 1/1 | 0.92 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | DR | 3001 | 1/1 | 0.92 | 0.13 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3090 | 1/1 | 0.92 | 0.31 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3454 | 1/1 | 0.92 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3348 | 1/1 | 0.92 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3296 | 1/1 | 0.92 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3064 | 1/1 | 0.92 | 0.21 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3426 | 1/1 | 0.92 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3137 | 1/1 | 0.92 | 0.25 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3268 | 1/1 | 0.92 | 0.22 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3626 | 1/1 | 0.92 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3643 | 1/1 | 0.92 | 0.07 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3119 | 1/1 | 0.92 | 0.26 | 50,50,50,50 | 0 |
| 57 | MG | DQ | 3001 | 1/1 | 0.92 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3051 | 1/1 | 0.92 | 0.23 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3155 | 1/1 | 0.92 | 0.24 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3483 | 1/1 | 0.92 | 0.17 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3541 | 1/1 | 0.92 | 0.20 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3219 | 1/1 | 0.92 | 0.50 | 58,58,58,58 | 0 |
| 57 | MG | AA | 1754 | 1/1 | 0.92 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3553 | 1/1 | 0.92 | 0.07 | 72,72,72,72 | 0 |
| 57 | MG | AA | 1799 | 1/1 | 0.92 | 0.11 | 78,78,78,78 | 0 |
| 57 | MG | BA | 3790 | 1/1 | 0.92 | 0.54 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3349 | 1/1 | 0.92 | 0.18 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3528 | 1/1 | 0.92 | 0.20 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3563 | 1/1 | 0.92 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3352 | 1/1 | 0.92 | 0.09 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3458 | 1/1 | 0.92 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3170 | 1/1 | 0.92 | 0.17 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3080 | 1/1 | 0.92 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3407 | 1/1 | 0.92 | 0.08 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3569 | 1/1 | 0.92 | 0.24 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3506 | 1/1 | 0.92 | 0.08 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3375 | 1/1 | 0.92 | 0.22 | 39,39,39,39 | 0 |
| 57 | MG | AA | 1691 | 1/1 | 0.92 | 0.27 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3559 | 1/1 | 0.92 | 0.15 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3001 | 1/1 | 0.92 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3663 | 1/1 | 0.92 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3290 | 1/1 | 0.92 | 0.21 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3662 | 1/1 | 0.92 | 0.22 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3436 | 1/1 | 0.92 | 0.15 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3528 | 1/1 | 0.92 | 0.14 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3091 | 1/1 | 0.92 | 0.40 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3309 | 1/1 | 0.92 | 0.17 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3357 | 1/1 | 0.92 | 0.13 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3075 | 1/1 | 0.92 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1778 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 57 | MG | AA | 1648 | 1/1 | 0.92 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3339 | 1/1 | 0.92 | 0.20 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3789 | 1/1 | 0.92 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3374 | 1/1 | 0.92 | 0.22 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3630 | 1/1 | 0.92 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3363 | 1/1 | 0.92 | 0.09 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3062 | 1/1 | 0.92 | 0.11 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3400 | 1/1 | 0.92 | 0.24 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3298 | 1/1 | 0.92 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3464 | 1/1 | 0.93 | 0.30 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3101 | 1/1 | 0.93 | 0.24 | 37,37,37,37 | 0 |
| 57 | MG | CA | 3015 | 1/1 | 0.93 | 0.19 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3414 | 1/1 | 0.93 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | B6 | 103 | 1/1 | 0.93 | 0.15 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3337 | 1/1 | 0.93 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3622 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3322 | 1/1 | 0.93 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | CA | 3073 | 1/1 | 0.93 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1800 | 1/1 | 0.93 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3624 | 1/1 | 0.93 | 0.13 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3391 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3428 | 1/1 | 0.93 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | CA | 3165 | 1/1 | 0.93 | 0.09 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3499 | 1/1 | 0.93 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3150 | 1/1 | 0.93 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3047 | 1/1 | 0.93 | 0.22 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3657 | 1/1 | 0.93 | 0.11 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3282 | 1/1 | 0.93 | 0.24 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3006 | 1/1 | 0.93 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3127 | 1/1 | 0.93 | 0.08 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3303 | 1/1 | 0.93 | 0.23 | 26,26,26,26 | 0 |
| 57 | MG | BN | 3003 | 1/1 | 0.93 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | AA | 1607 | 1/1 | 0.93 | 0.13 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3071 | 1/1 | 0.93 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3366 | 1/1 | 0.93 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3247 | 1/1 | 0.93 | 0.17 | 29,29,29,29 | 0 |
| 57 | MG | CA | 3124 | 1/1 | 0.93 | 0.22 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3207 | 1/1 | 0.93 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3335 | 1/1 | 0.93 | 0.25 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3321 | 1/1 | 0.93 | 0.13 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3754 | 1/1 | 0.93 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3120 | 1/1 | 0.93 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3599 | 1/1 | 0.93 | 0.16 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3543 | 1/1 | 0.93 | 0.23 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3150 | 1/1 | 0.93 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3342 | 1/1 | 0.93 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | BE | 304 | 1/1 | 0.93 | 0.23 | 23,23,23,23 | 0 |
| 57 | MG | CA | 3054 | 1/1 | 0.93 | 0.33 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3222 | 1/1 | 0.93 | 0.23 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3504 | 1/1 | 0.93 | 0.09 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3161 | 1/1 | 0.93 | 0.29 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1690 | 1/1 | 0.93 | 0.42 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3330 | 1/1 | 0.93 | 0.15 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3301 | 1/1 | 0.93 | 0.18 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1654 | 1/1 | 0.93 | 0.23 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3649 | 1/1 | 0.93 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1791 | 1/1 | 0.93 | 0.08 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3083 | 1/1 | 0.93 | 0.26 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3210 | 1/1 | 0.93 | 0.08 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3449 | 1/1 | 0.93 | 0.13 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3195 | 1/1 | 0.93 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3179 | 1/1 | 0.93 | 0.23 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3371 | 1/1 | 0.93 | 0.17 | 34,34,34,34 | 0 |
| 57 | MG | AA | 1641 | 1/1 | 0.93 | 0.17 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3466 | 1/1 | 0.93 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3302 | 1/1 | 0.93 | 0.15 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3305 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | AA | 1751 | 1/1 | 0.93 | 0.23 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3249 | 1/1 | 0.93 | 0.08 | 65,65,65,65 | 0 |
| 57 | MG | CA | 3078 | 1/1 | 0.93 | 0.16 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3785 | 1/1 | 0.93 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3659 | 1/1 | 0.93 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3651 | 1/1 | 0.93 | 0.14 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3644 | 1/1 | 0.93 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | AK | 3101 | 1/1 | 0.93 | 0.17 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3403 | 1/1 | 0.93 | 0.29 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3579 | 1/1 | 0.93 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3048 | 1/1 | 0.93 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | DY | 502 | 1/1 | 0.93 | 0.17 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1657 | 1/1 | 0.93 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3177 | 1/1 | 0.93 | 0.23 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3775 | 1/1 | 0.93 | 0.33 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3595 | 1/1 | 0.93 | 0.13 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3055 | 1/1 | 0.93 | 0.23 | 37,37,37,37 | 0 |
| 57 | MG | BR | 5001 | 1/1 | 0.93 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3462 | 1/1 | 0.93 | 0.11 | 53,53,53,53 | 0 |
| 57 | MG | AA | 1782 | 1/1 | 0.93 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3746 | 1/1 | 0.93 | 0.14 | 78,78,78,78 | 0 |
| 57 | MG | B0 | 3001 | 1/1 | 0.93 | 0.19 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3315 | 1/1 | 0.93 | 0.13 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3686 | 1/1 | 0.93 | 0.19 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3757 | 1/1 | 0.93 | 0.18 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3066 | 1/1 | 0.93 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3104 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3396 | 1/1 | 0.93 | 0.17 | 46,46,46,46 | 0 |
| 57 | MG | AA | 1752 | 1/1 | 0.93 | 0.14 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3269 | 1/1 | 0.93 | 0.25 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3540 | 1/1 | 0.93 | 0.16 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3552 | 1/1 | 0.93 | 0.15 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3798 | 1/1 | 0.93 | 0.24 | 22,22,22,22 | 0 |
| 57 | MG | DA | 3433 | 1/1 | 0.93 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3661 | 1/1 | 0.93 | 0.24 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3092 | 1/1 | 0.93 | 0.29 | 40,40,40,40 | 0 |
| 57 | MG | CA | 3025 | 1/1 | 0.93 | 0.24 | 53,53,53,53 | 0 |
| 57 | MG | B5 | 102 | 1/1 | 0.93 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | AY | 3002 | 1/1 | 0.93 | 0.31 | 52,52,52,52 | 0 |
| 57 | MG | DF | 305 | 1/1 | 0.93 | 0.59 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3220 | 1/1 | 0.93 | 0.16 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3421 | 1/1 | 0.93 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3105 | 1/1 | 0.93 | 0.22 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3697 | 1/1 | 0.93 | 0.18 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3123 | 1/1 | 0.93 | 0.09 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3159 | 1/1 | 0.93 | 0.13 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3536 | 1/1 | 0.93 | 0.08 | 52,52,52,52 | 0 |
| 57 | MG | AA | 1737 | 1/1 | 0.93 | 0.09 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3684 | 1/1 | 0.93 | 0.22 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3699 | 1/1 | 0.93 | 0.20 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3177 | 1/1 | 0.93 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3539 | 1/1 | 0.93 | 0.08 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3117 | 1/1 | 0.93 | 0.09 | 63,63,63,63 | 0 |
| 57 | MG | AA | 1656 | 1/1 | 0.93 | 0.16 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3081 | 1/1 | 0.93 | 0.30 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3289 | 1/1 | 0.93 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3449 | 1/1 | 0.93 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3218 | 1/1 | 0.93 | 0.15 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3432 | 1/1 | 0.93 | 0.22 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3571 | 1/1 | 0.93 | 0.28 | 45,45,45,45 | 0 |
| 57 | MG | AA | 1638 | 1/1 | 0.93 | 0.23 | 60,60,60,60 | 0 |
| 57 | MG | AA | 1802 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3181 | 1/1 | 0.93 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3282 | 1/1 | 0.93 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3304 | 1/1 | 0.93 | 0.18 | 39,39,39,39 | 0 |
| 57 | MG | AX | 3011 | 1/1 | 0.93 | 0.13 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3237 | 1/1 | 0.93 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3563 | 1/1 | 0.93 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | AA | 1790 | 1/1 | 0.93 | 0.08 | 81,81,81,81 | 0 |
| 57 | MG | DA | 3133 | 1/1 | 0.93 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3026 | 1/1 | 0.93 | 0.72 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BB | 3005 | 1/1 | 0.93 | 0.28 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3441 | 1/1 | 0.93 | 0.20 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3461 | 1/1 | 0.93 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3131 | 1/1 | 0.93 | 0.25 | 49,49,49,49 | 0 |
| 57 | MG | DD | 303 | 1/1 | 0.93 | 0.34 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3587 | 1/1 | 0.93 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | B6 | 101 | 1/1 | 0.93 | 0.32 | 60,60,60,60 | 0 |
| 57 | MG | CA | 3101 | 1/1 | 0.93 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3646 | 1/1 | 0.93 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3148 | 1/1 | 0.93 | 0.28 | 38,38,38,38 | 0 |
| 57 | MG | AA | 1675 | 1/1 | 0.93 | 0.24 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3415 | 1/1 | 0.93 | 0.23 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3673 | 1/1 | 0.93 | 0.28 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3613 | 1/1 | 0.93 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3690 | 1/1 | 0.93 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3279 | 1/1 | 0.93 | 0.32 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3098 | 1/1 | 0.93 | 0.11 | 54,54,54,54 | 0 |
| 57 | MG | AA | 1645 | 1/1 | 0.93 | 0.15 | 61,61,61,61 | 0 |
| 57 | MG | AA | 1765 | 1/1 | 0.93 | 0.13 | 65,65,65,65 | 0 |
| 57 | MG | AX | 3014 | 1/1 | 0.93 | 0.24 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3527 | 1/1 | 0.93 | 0.19 | 24,24,24,24 | 0 |
| 57 | MG | DA | 3273 | 1/1 | 0.93 | 0.12 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3367 | 1/1 | 0.93 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3139 | 1/1 | 0.94 | 0.11 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3294 | 1/1 | 0.94 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | AA | 1728 | 1/1 | 0.94 | 0.25 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3526 | 1/1 | 0.94 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3804 | 1/1 | 0.94 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | BB | 3012 | 1/1 | 0.94 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3475 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3012 | 1/1 | 0.94 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3012 | 1/1 | 0.94 | 0.17 | 25,25,25,25 | 0 |
| 57 | MG | AA | 1806 | 1/1 | 0.94 | 0.18 | 74,74,74,74 | 0 |
| 57 | MG | BA | 3620 | 1/1 | 0.94 | 0.14 | 29,29,29,29 | 0 |
| 57 | MG | BF | 302 | 1/1 | 0.94 | 0.31 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3126 | 1/1 | 0.94 | 0.15 | 59,59,59,59 | 0 |
| 57 | MG | BF | 301 | 1/1 | 0.94 | 0.25 | 40,40,40,40 | 0 |
| 57 | MG | AA | 1659 | 1/1 | 0.94 | 0.19 | 65,65,65,65 | 0 |
| 57 | MG | AA | 1733 | 1/1 | 0.94 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3018 | 1/1 | 0.94 | 0.10 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3551 | 1/1 | 0.94 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3242 | 1/1 | 0.94 | 0.69 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3703 | 1/1 | 0.94 | 0.33 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3564 | 1/1 | 0.94 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3176 | 1/1 | 0.94 | 0.24 | 38,38,38,38 | 0 |
| 57 | MG | BW | 3002 | 1/1 | 0.94 | 0.27 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3187 | 1/1 | 0.94 | 0.22 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3220 | 1/1 | 0.94 | 0.32 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3144 | 1/1 | 0.94 | 0.13 | 82,82,82,82 | 0 |
| 57 | MG | BA | 3165 | 1/1 | 0.94 | 0.31 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3138 | 1/1 | 0.94 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | AA | 1649 | 1/1 | 0.94 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3142 | 1/1 | 0.94 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3419 | 1/1 | 0.94 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | AM | 3001 | 1/1 | 0.94 | 0.09 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3285 | 1/1 | 0.94 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3334 | 1/1 | 0.94 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | BB | 3003 | 1/1 | 0.94 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | AA | 1805 | 1/1 | 0.94 | 0.07 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3298 | 1/1 | 0.94 | 0.15 | 27,27,27,27 | 0 |
| 57 | MG | CA | 3072 | 1/1 | 0.94 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3244 | 1/1 | 0.94 | 0.26 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3241 | 1/1 | 0.94 | 0.16 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3226 | 1/1 | 0.94 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3236 | 1/1 | 0.94 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3048 | 1/1 | 0.94 | 0.22 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3437 | 1/1 | 0.94 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3084 | 1/1 | 0.94 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | D3 | 3001 | 1/1 | 0.94 | 0.27 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3540 | 1/1 | 0.94 | 0.06 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3074 | 1/1 | 0.94 | 0.08 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3373 | 1/1 | 0.94 | 0.22 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3223 | 1/1 | 0.94 | 0.19 | 39,39,39,39 | 0 |
| 57 | MG | BU | 201 | 1/1 | 0.94 | 0.36 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3722 | 1/1 | 0.94 | 0.19 | 64,64,64,64 | 0 |
| 57 | MG | AA | 1808 | 1/1 | 0.94 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | DB | 3004 | 1/1 | 0.94 | 0.21 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3193 | 1/1 | 0.94 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3548 | 1/1 | 0.94 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | AA | 1646 | 1/1 | 0.94 | 0.23 | 58,58,58,58 | 0 |
| 57 | MG | BE | 303 | 1/1 | 0.94 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3585 | 1/1 | 0.94 | 0.25 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3288 | 1/1 | 0.94 | 0.16 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3292 | 1/1 | 0.94 | 0.24 | 26,26,26,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3517 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3240 | 1/1 | 0.94 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3105 | 1/1 | 0.94 | 0.12 | 46,46,46,46 | 0 |
| 57 | MG | CA | 3106 | 1/1 | 0.94 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3771 | 1/1 | 0.94 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3097 | 1/1 | 0.94 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3004 | 1/1 | 0.94 | 0.20 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3206 | 1/1 | 0.94 | 0.16 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3534 | 1/1 | 0.94 | 0.10 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3268 | 1/1 | 0.94 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3100 | 1/1 | 0.94 | 0.25 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3635 | 1/1 | 0.94 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3210 | 1/1 | 0.94 | 0.25 | 41,41,41,41 | 0 |
| 57 | MG | AX | 3002 | 1/1 | 0.94 | 0.30 | 71,71,71,71 | 0 |
| 57 | MG | DA | 3283 | 1/1 | 0.94 | 0.07 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3332 | 1/1 | 0.94 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3474 | 1/1 | 0.94 | 0.27 | 33,33,33,33 | 0 |
| 57 | MG | AB | 3001 | 1/1 | 0.94 | 0.13 | 77,77,77,77 | 0 |
| 57 | MG | CA | 3046 | 1/1 | 0.94 | 0.18 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3609 | 1/1 | 0.94 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3733 | 1/1 | 0.94 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3567 | 1/1 | 0.94 | 0.26 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3164 | 1/1 | 0.94 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3134 | 1/1 | 0.94 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3399 | 1/1 | 0.94 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3098 | 1/1 | 0.94 | 0.22 | 23,23,23,23 | 0 |
| 57 | MG | BA | 3192 | 1/1 | 0.94 | 0.20 | 19,19,19,19 | 0 |
| 57 | MG | DA | 3401 | 1/1 | 0.94 | 0.06 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3038 | 1/1 | 0.94 | 0.23 | 20,20,20,20 | 0 |
| 57 | MG | BA | 3009 | 1/1 | 0.94 | 0.17 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3384 | 1/1 | 0.94 | 0.11 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3706 | 1/1 | 0.94 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3631 | 1/1 | 0.94 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3799 | 1/1 | 0.94 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3743 | 1/1 | 0.94 | 0.59 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3040 | 1/1 | 0.94 | 0.27 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3758 | 1/1 | 0.94 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3148 | 1/1 | 0.94 | 0.21 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3069 | 1/1 | 0.94 | 0.34 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3095 | 1/1 | 0.94 | 0.23 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3113 | 1/1 | 0.94 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3047 | 1/1 | 0.94 | 0.16 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3679 | 1/1 | 0.94 | 0.22 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3602 | 1/1 | 0.94 | 0.26 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3202 | 1/1 | 0.94 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3483 | 1/1 | 0.94 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3714 | 1/1 | 0.94 | 0.12 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3211 | 1/1 | 0.94 | 0.18 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3605 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3114 | 1/1 | 0.94 | 0.14 | 71,71,71,71 | 0 |
| 57 | MG | DA | 3659 | 1/1 | 0.94 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3450 | 1/1 | 0.94 | 0.25 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3616 | 1/1 | 0.94 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3596 | 1/1 | 0.94 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3784 | 1/1 | 0.94 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | DB | 3006 | 1/1 | 0.94 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3660 | 1/1 | 0.94 | 0.52 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3372 | 1/1 | 0.94 | 0.13 | 53,53,53,53 | 0 |
| 59 | ZN | B4 | 501 | 1/1 | 0.94 | 0.10 | 118,118,118,118 | 0 |
| 57 | MG | DA | 3206 | 1/1 | 0.94 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3584 | 1/1 | 0.94 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3280 | 1/1 | 0.94 | 0.21 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3317 | 1/1 | 0.94 | 0.21 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3535 | 1/1 | 0.94 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3169 | 1/1 | 0.94 | 0.18 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3489 | 1/1 | 0.94 | 0.25 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3608 | 1/1 | 0.94 | 0.09 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3198 | 1/1 | 0.94 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3695 | 1/1 | 0.94 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | AA | 1731 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3255 | 1/1 | 0.94 | 0.24 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3251 | 1/1 | 0.94 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | CA | 3069 | 1/1 | 0.94 | 0.22 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3467 | 1/1 | 0.94 | 0.24 | 52,52,52,52 | 0 |
| 57 | MG | DE | 3003 | 1/1 | 0.94 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3185 | 1/1 | 0.94 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3394 | 1/1 | 0.94 | 0.28 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3064 | 1/1 | 0.94 | 0.23 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3112 | 1/1 | 0.94 | 0.26 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3059 | 1/1 | 0.94 | 0.14 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3246 | 1/1 | 0.94 | 0.31 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3027 | 1/1 | 0.94 | 0.41 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3128 | 1/1 | 0.94 | 0.28 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3744 | 1/1 | 0.94 | 0.18 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BO | 5001 | 1/1 | 0.94 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3601 | 1/1 | 0.94 | 0.32 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3044 | 1/1 | 0.94 | 0.35 | 43,43,43,43 | 0 |
| 57 | MG | DB | 3002 | 1/1 | 0.94 | 0.26 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3438 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3247 | 1/1 | 0.94 | 0.16 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3788 | 1/1 | 0.94 | 0.24 | 44,44,44,44 | 0 |
| 57 | MG | BE | 306 | 1/1 | 0.94 | 0.10 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3113 | 1/1 | 0.94 | 0.13 | 35,35,35,35 | 0 |
| 57 | MG | AA | 1673 | 1/1 | 0.94 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3555 | 1/1 | 0.94 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | BV | 201 | 1/1 | 0.94 | 0.36 | 31,31,31,31 | 0 |
| 57 | MG | AA | 1683 | 1/1 | 0.94 | 0.13 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3037 | 1/1 | 0.94 | 0.21 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3519 | 1/1 | 0.94 | 0.19 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3056 | 1/1 | 0.94 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | AA | 1715 | 1/1 | 0.94 | 0.23 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3009 | 1/1 | 0.94 | 0.17 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3060 | 1/1 | 0.94 | 0.28 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3070 | 1/1 | 0.94 | 0.24 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3030 | 1/1 | 0.94 | 0.24 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3135 | 1/1 | 0.94 | 0.45 | 56,56,56,56 | 0 |
| 57 | MG | BB | 3010 | 1/1 | 0.94 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3445 | 1/1 | 0.94 | 0.23 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3320 | 1/1 | 0.94 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3621 | 1/1 | 0.94 | 0.49 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3147 | 1/1 | 0.94 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | BA | 3422 | 1/1 | 0.94 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3230 | 1/1 | 0.94 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3402 | 1/1 | 0.94 | 0.09 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3028 | 1/1 | 0.94 | 0.20 | 37,37,37,37 | 0 |
| 57 | MG | DB | 3009 | 1/1 | 0.94 | 0.14 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3277 | 1/1 | 0.94 | 0.13 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3581 | 1/1 | 0.94 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3675 | 1/1 | 0.94 | 0.26 | 56,56,56,56 | 0 |
| 57 | MG | AA | 1676 | 1/1 | 0.94 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3480 | 1/1 | 0.94 | 0.18 | 47,47,47,47 | 0 |
| 57 | MG | B8 | 5001 | 1/1 | 0.94 | 0.20 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3509 | 1/1 | 0.94 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | AA | 1749 | 1/1 | 0.94 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | AA | 1698 | 1/1 | 0.94 | 0.23 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3529 | 1/1 | 0.94 | 0.07 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3351 | 1/1 | 0.94 | 0.19 | 45,45,45,45 | 0 |
| 57 | MG | AA | 1785 | 1/1 | 0.94 | 0.11 | 72,72,72,72 | 0 |
| 57 | MG | CA | 3060 | 1/1 | 0.94 | 0.08 | 71,71,71,71 | 0 |
| 57 | MG | BA | 3202 | 1/1 | 0.94 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3075 | 1/1 | 0.94 | 0.24 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3386 | 1/1 | 0.94 | 0.14 | 28,28,28,28 | 0 |
| 57 | MG | CA | 3136 | 1/1 | 0.94 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | AA | 1617 | 1/1 | 0.94 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3427 | 1/1 | 0.94 | 0.17 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3616 | 1/1 | 0.94 | 0.20 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3018 | 1/1 | 0.94 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3531 | 1/1 | 0.94 | 0.07 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3395 | 1/1 | 0.94 | 0.20 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3589 | 1/1 | 0.94 | 0.23 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1780 | 1/1 | 0.94 | 0.11 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3460 | 1/1 | 0.94 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3677 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3642 | 1/1 | 0.94 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3019 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3465 | 1/1 | 0.94 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3166 | 1/1 | 0.94 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1636 | 1/1 | 0.94 | 0.31 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3556 | 1/1 | 0.94 | 0.07 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3562 | 1/1 | 0.94 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3272 | 1/1 | 0.94 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | CA | 3024 | 1/1 | 0.94 | 0.16 | 67,67,67,67 | 0 |
| 57 | MG | BR | 5002 | 1/1 | 0.94 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3167 | 1/1 | 0.94 | 0.21 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3353 | 1/1 | 0.94 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3496 | 1/1 | 0.95 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3269 | 1/1 | 0.95 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | AA | 1786 | 1/1 | 0.95 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | DE | 3002 | 1/1 | 0.95 | 0.16 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3716 | 1/1 | 0.95 | 0.25 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3610 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3354 | 1/1 | 0.95 | 0.12 | 47,47,47,47 | 0 |
| 57 | MG | BW | 3003 | 1/1 | 0.95 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3118 | 1/1 | 0.95 | 0.21 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3385 | 1/1 | 0.95 | 0.07 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3421 | 1/1 | 0.95 | 0.26 | 62,62,62,62 | 0 |
| 59 | ZN | BY | 501 | 1/1 | 0.95 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3228 | 1/1 | 0.95 | 0.10 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DB | 3008 | 1/1 | 0.95 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3208 | 1/1 | 0.95 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3057 | 1/1 | 0.95 | 0.14 | 84,84,84,84 | 0 |
| 57 | MG | BA | 3708 | 1/1 | 0.95 | 0.21 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3003 | 1/1 | 0.95 | 0.23 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3752 | 1/1 | 0.95 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3277 | 1/1 | 0.95 | 0.43 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3607 | 1/1 | 0.95 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3801 | 1/1 | 0.95 | 0.16 | 71,71,71,71 | 0 |
| 57 | MG | BA | 3061 | 1/1 | 0.95 | 0.30 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3199 | 1/1 | 0.95 | 0.30 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3284 | 1/1 | 0.95 | 0.10 | 57,57,57,57 | 0 |
| 57 | MG | AA | 1709 | 1/1 | 0.95 | 0.26 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3037 | 1/1 | 0.95 | 0.28 | 42,42,42,42 | 0 |
| 57 | MG | AA | 1769 | 1/1 | 0.95 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | AX | 3006 | 1/1 | 0.95 | 0.15 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3116 | 1/1 | 0.95 | 0.35 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3102 | 1/1 | 0.95 | 0.32 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3583 | 1/1 | 0.95 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3238 | 1/1 | 0.95 | 0.48 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3617 | 1/1 | 0.95 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3043 | 1/1 | 0.95 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3252 | 1/1 | 0.95 | 0.07 | 50,50,50,50 | 0 |
| 57 | MG | AA | 1807 | 1/1 | 0.95 | 0.07 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3153 | 1/1 | 0.95 | 0.15 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3145 | 1/1 | 0.95 | 0.32 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3401 | 1/1 | 0.95 | 0.25 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3478 | 1/1 | 0.95 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3184 | 1/1 | 0.95 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3363 | 1/1 | 0.95 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3580 | 1/1 | 0.95 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3287 | 1/1 | 0.95 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3076 | 1/1 | 0.95 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3511 | 1/1 | 0.95 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3093 | 1/1 | 0.95 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1757 | 1/1 | 0.95 | 0.25 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3178 | 1/1 | 0.95 | 0.17 | 32,32,32,32 | 0 |
| 57 | MG | AA | 1700 | 1/1 | 0.95 | 0.08 | 71,71,71,71 | 0 |
| 57 | MG | DA | 3641 | 1/1 | 0.95 | 0.07 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3017 | 1/1 | 0.95 | 0.28 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3346 | 1/1 | 0.95 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3158 | 1/1 | 0.95 | 0.17 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3278 | 1/1 | 0.95 | 0.10 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3389 | 1/1 | 0.95 | 0.19 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3404 | 1/1 | 0.95 | 0.08 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3459 | 1/1 | 0.95 | 0.15 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3193 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3093 | 1/1 | 0.95 | 0.24 | 41,41,41,41 | 0 |
| 57 | MG | BB | 3018 | 1/1 | 0.95 | 0.06 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3656 | 1/1 | 0.95 | 0.25 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3033 | 1/1 | 0.95 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | BB | 3014 | 1/1 | 0.95 | 0.12 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3169 | 1/1 | 0.95 | 0.24 | 50,50,50,50 | 0 |
| 57 | MG | AA | 1750 | 1/1 | 0.95 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3709 | 1/1 | 0.95 | 0.34 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3812 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3753 | 1/1 | 0.95 | 0.19 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3251 | 1/1 | 0.95 | 0.25 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3423 | 1/1 | 0.95 | 0.20 | 37,37,37,37 | 0 |
| 57 | MG | AA | 1804 | 1/1 | 0.95 | 0.12 | 70,70,70,70 | 0 |
| 57 | MG | DA | 3149 | 1/1 | 0.95 | 0.08 | 46,46,46,46 | 0 |
| 57 | MG | CA | 3097 | 1/1 | 0.95 | 0.27 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3664 | 1/1 | 0.95 | 0.21 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3575 | 1/1 | 0.95 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3038 | 1/1 | 0.95 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3115 | 1/1 | 0.95 | 0.29 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3142 | 1/1 | 0.95 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3071 | 1/1 | 0.95 | 0.31 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3537 | 1/1 | 0.95 | 0.08 | 43,43,43,43 | 0 |
| 57 | MG | CX | 3001 | 1/1 | 0.95 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3322 | 1/1 | 0.95 | 0.16 | 42,42,42,42 | 0 |
| 57 | MG | B7 | 101 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3774 | 1/1 | 0.95 | 0.32 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3042 | 1/1 | 0.95 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3359 | 1/1 | 0.95 | 0.16 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3328 | 1/1 | 0.95 | 0.19 | 27,27,27,27 | 0 |
| 57 | MG | AA | 1794 | 1/1 | 0.95 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3080 | 1/1 | 0.95 | 0.14 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3444 | 1/1 | 0.95 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3337 | 1/1 | 0.95 | 0.06 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3261 | 1/1 | 0.95 | 0.21 | 18,18,18,18 | 0 |
| 57 | MG | DA | 3225 | 1/1 | 0.95 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3335 | 1/1 | 0.95 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3578 | 1/1 | 0.95 | 0.35 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3188 | 1/1 | 0.95 | 0.19 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3152 | 1/1 | 0.95 | 0.26 | 23,23,23,23 | 0 |
| 57 | MG | BA | 3629 | 1/1 | 0.95 | 0.25 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3481 | 1/1 | 0.95 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | BU | 202 | 1/1 | 0.95 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3032 | 1/1 | 0.95 | 0.21 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3465 | 1/1 | 0.95 | 0.09 | 48,48,48,48 | 0 |
| 57 | MG | BB | 3008 | 1/1 | 0.95 | 0.36 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3295 | 1/1 | 0.95 | 0.19 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3378 | 1/1 | 0.95 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3509 | 1/1 | 0.95 | 0.06 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3213 | 1/1 | 0.95 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3224 | 1/1 | 0.95 | 0.08 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3589 | 1/1 | 0.95 | 0.08 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3567 | 1/1 | 0.95 | 0.25 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3293 | 1/1 | 0.95 | 0.11 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3324 | 1/1 | 0.95 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3165 | 1/1 | 0.95 | 0.21 | 55,55,55,55 | 0 |
| 57 | MG | BV | 202 | 1/1 | 0.95 | 0.26 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3410 | 1/1 | 0.95 | 0.22 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3691 | 1/1 | 0.95 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3074 | 1/1 | 0.95 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | DN | 5001 | 1/1 | 0.95 | 0.11 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3748 | 1/1 | 0.95 | 0.17 | 61,61,61,61 | 0 |
| 57 | MG | CA | 3040 | 1/1 | 0.95 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3223 | 1/1 | 0.95 | 0.18 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3168 | 1/1 | 0.95 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3171 | 1/1 | 0.95 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | AA | 1742 | 1/1 | 0.95 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3474 | 1/1 | 0.95 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | AA | 1746 | 1/1 | 0.95 | 0.10 | 56,56,56,56 | 0 |
| 57 | MG | CD | 502 | 1/1 | 0.95 | 0.27 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3433 | 1/1 | 0.95 | 0.20 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3350 | 1/1 | 0.95 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3325 | 1/1 | 0.95 | 0.23 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3175 | 1/1 | 0.95 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3586 | 1/1 | 0.95 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3469 | 1/1 | 0.95 | 0.16 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3594 | 1/1 | 0.95 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | DD | 301 | 1/1 | 0.95 | 0.22 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3451 | 1/1 | 0.95 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1774 | 1/1 | 0.95 | 0.17 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | CA | 3134 | 1/1 | 0.95 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3495 | 1/1 | 0.95 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3429 | 1/1 | 0.95 | 0.15 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3527 | 1/1 | 0.95 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3082 | 1/1 | 0.95 | 0.22 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3510 | 1/1 | 0.95 | 0.26 | 64,64,64,64 | 0 |
| 57 | MG | AA | 1776 | 1/1 | 0.95 | 0.16 | 73,73,73,73 | 0 |
| 57 | MG | AA | 1783 | 1/1 | 0.95 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3520 | 1/1 | 0.95 | 0.25 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3043 | 1/1 | 0.95 | 0.17 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3471 | 1/1 | 0.95 | 0.19 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3572 | 1/1 | 0.95 | 0.26 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3266 | 1/1 | 0.95 | 0.12 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3124 | 1/1 | 0.95 | 0.17 | 43,43,43,43 | 0 |
| 57 | MG | BE | 305 | 1/1 | 0.95 | 0.07 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3299 | 1/1 | 0.95 | 0.09 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3364 | 1/1 | 0.95 | 0.10 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3331 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3780 | 1/1 | 0.95 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3088 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3355 | 1/1 | 0.95 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | BD | 3007 | 1/1 | 0.95 | 0.30 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3297 | 1/1 | 0.95 | 0.22 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3276 | 1/1 | 0.95 | 0.40 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1615 | 1/1 | 0.95 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3258 | 1/1 | 0.95 | 0.35 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3550 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3490 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 57 | MG | CA | 3053 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3329 | 1/1 | 0.95 | 0.10 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3455 | 1/1 | 0.95 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3116 | 1/1 | 0.95 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3023 | 1/1 | 0.95 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3555 | 1/1 | 0.95 | 0.21 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3479 | 1/1 | 0.95 | 0.06 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3498 | 1/1 | 0.95 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | AX | 3009 | 1/1 | 0.95 | 0.37 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3671 | 1/1 | 0.95 | 0.19 | 24,24,24,24 | 0 |
| 57 | MG | BQ | 3002 | 1/1 | 0.95 | 0.28 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3143 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3168 | 1/1 | 0.95 | 0.24 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3434 | 1/1 | 0.95 | 0.07 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3147 | 1/1 | 0.95 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1670 | 1/1 | 0.95 | 0.17 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3120 | 1/1 | 0.95 | 0.18 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3443 | 1/1 | 0.95 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3588 | 1/1 | 0.95 | 0.15 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1775 | 1/1 | 0.95 | 0.11 | 73,73,73,73 | 0 |
| 57 | MG | DA | 3382 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3312 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3262 | 1/1 | 0.96 | 0.27 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3724 | 1/1 | 0.96 | 0.18 | 20,20,20,20 | 0 |
| 57 | MG | DA | 3573 | 1/1 | 0.96 | 0.05 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3590 | 1/1 | 0.96 | 0.15 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3031 | 1/1 | 0.96 | 0.27 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3502 | 1/1 | 0.96 | 0.19 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3602 | 1/1 | 0.96 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3082 | 1/1 | 0.96 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | DW | 3001 | 1/1 | 0.96 | 0.21 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3648 | 1/1 | 0.96 | 0.22 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3464 | 1/1 | 0.96 | 0.13 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3215 | 1/1 | 0.96 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | AA | 1647 | 1/1 | 0.96 | 0.22 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3293 | 1/1 | 0.96 | 0.15 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3787 | 1/1 | 0.96 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | BB | 3015 | 1/1 | 0.96 | 0.26 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3011 | 1/1 | 0.96 | 0.07 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3336 | 1/1 | 0.96 | 0.17 | 20,20,20,20 | 0 |
| 57 | MG | AA | 1725 | 1/1 | 0.96 | 0.22 | 51,51,51,51 | 0 |
| 57 | MG | BG | 201 | 1/1 | 0.96 | 0.14 | 39,39,39,39 | 0 |
| 57 | MG | B7 | 105 | 1/1 | 0.96 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3307 | 1/1 | 0.96 | 0.19 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3119 | 1/1 | 0.96 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | BF | 303 | 1/1 | 0.96 | 0.26 | 33,33,33,33 | 0 |
| 57 | MG | AA | 1767 | 1/1 | 0.96 | 0.11 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3638 | 1/1 | 0.96 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3201 | 1/1 | 0.96 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3432 | 1/1 | 0.96 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3397 | 1/1 | 0.96 | 0.15 | 28,28,28,28 | 0 |
| 57 | MG | CA | 3066 | 1/1 | 0.96 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3151 | 1/1 | 0.96 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3157 | 1/1 | 0.96 | 0.13 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3044 | 1/1 | 0.96 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3263 | 1/1 | 0.96 | 0.13 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3308 | 1/1 | 0.96 | 0.23 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3117 | 1/1 | 0.96 | 0.09 | 56,56,56,56 | 0 |
| 57 | MG | BF | 304 | 1/1 | 0.96 | 0.39 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3791 | 1/1 | 0.96 | 0.38 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3396 | 1/1 | 0.96 | 0.23 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3172 | 1/1 | 0.96 | 0.26 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3402 | 1/1 | 0.96 | 0.18 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3144 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 57 | MG | AA | 1706 | 1/1 | 0.96 | 0.22 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3430 | 1/1 | 0.96 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3380 | 1/1 | 0.96 | 0.04 | 66,66,66,66 | 0 |
| 57 | MG | CF | 3001 | 1/1 | 0.96 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3457 | 1/1 | 0.96 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3503 | 1/1 | 0.96 | 0.22 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3409 | 1/1 | 0.96 | 0.23 | 22,22,22,22 | 0 |
| 57 | MG | BA | 3392 | 1/1 | 0.96 | 0.18 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3046 | 1/1 | 0.96 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3482 | 1/1 | 0.96 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3610 | 1/1 | 0.96 | 0.09 | 61,61,61,61 | 0 |
| 57 | MG | AA | 1773 | 1/1 | 0.96 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3059 | 1/1 | 0.96 | 0.10 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3473 | 1/1 | 0.96 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3643 | 1/1 | 0.96 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3155 | 1/1 | 0.96 | 0.15 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3258 | 1/1 | 0.96 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3137 | 1/1 | 0.96 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3450 | 1/1 | 0.96 | 0.06 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3196 | 1/1 | 0.96 | 0.23 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3034 | 1/1 | 0.96 | 0.23 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3525 | 1/1 | 0.96 | 0.15 | 28,28,28,28 | 0 |
| 57 | MG | AA | 1716 | 1/1 | 0.96 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3098 | 1/1 | 0.96 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3215 | 1/1 | 0.96 | 0.42 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3050 | 1/1 | 0.96 | 0.15 | 32,32,32,32 | 0 |
| 57 | MG | BF | 308 | 1/1 | 0.96 | 0.08 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3265 | 1/1 | 0.96 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | BP | 3001 | 1/1 | 0.96 | 0.14 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3090 | 1/1 | 0.96 | 0.26 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3360 | 1/1 | 0.96 | 0.09 | 31,31,31,31 | 0 |
| 57 | MG | CA | 3138 | 1/1 | 0.96 | 0.10 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3762 | 1/1 | 0.96 | 0.18 | 20,20,20,20 | 0 |
| 57 | MG | BA | 3521 | 1/1 | 0.96 | 0.22 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3152 | 1/1 | 0.96 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3405 | 1/1 | 0.96 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | AA | 1779 | 1/1 | 0.96 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | AA | 1685 | 1/1 | 0.96 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3568 | 1/1 | 0.96 | 0.23 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3249 | 1/1 | 0.96 | 0.23 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3438 | 1/1 | 0.96 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3398 | 1/1 | 0.96 | 0.22 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3503 | 1/1 | 0.96 | 0.10 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3276 | 1/1 | 0.96 | 0.16 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3162 | 1/1 | 0.96 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3228 | 1/1 | 0.96 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3130 | 1/1 | 0.96 | 0.46 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3454 | 1/1 | 0.96 | 0.17 | 46,46,46,46 | 0 |
| 57 | MG | AA | 1608 | 1/1 | 0.96 | 0.22 | 43,43,43,43 | 0 |
| 57 | MG | DE | 3004 | 1/1 | 0.96 | 0.17 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3246 | 1/1 | 0.96 | 0.06 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3795 | 1/1 | 0.96 | 0.25 | 19,19,19,19 | 0 |
| 57 | MG | B9 | 502 | 1/1 | 0.96 | 0.34 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3035 | 1/1 | 0.96 | 0.27 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3808 | 1/1 | 0.96 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | AA | 1736 | 1/1 | 0.96 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3565 | 1/1 | 0.96 | 0.14 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3013 | 1/1 | 0.96 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | AA | 1813 | 1/1 | 0.96 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3270 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3028 | 1/1 | 0.96 | 0.27 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3493 | 1/1 | 0.96 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3167 | 1/1 | 0.96 | 0.18 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3183 | 1/1 | 0.96 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | AA | 1793 | 1/1 | 0.96 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3149 | 1/1 | 0.96 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3664 | 1/1 | 0.96 | 0.09 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3595 | 1/1 | 0.96 | 0.09 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3797 | 1/1 | 0.96 | 0.32 | 51,51,51,51 | 0 |
| 57 | MG | AA | 1811 | 1/1 | 0.96 | 0.21 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3468 | 1/1 | 0.96 | 0.19 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3756 | 1/1 | 0.96 | 0.19 | 18,18,18,18 | 0 |
| 57 | MG | BA | 3142 | 1/1 | 0.96 | 0.31 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3440 | 1/1 | 0.96 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3343 | 1/1 | 0.96 | 0.15 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3783 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1744 | 1/1 | 0.96 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3038 | 1/1 | 0.96 | 0.09 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3430 | 1/1 | 0.96 | 0.24 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3720 | 1/1 | 0.96 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | AA | 1748 | 1/1 | 0.96 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3121 | 1/1 | 0.96 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3507 | 1/1 | 0.96 | 0.07 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3319 | 1/1 | 0.96 | 0.22 | 23,23,23,23 | 0 |
| 57 | MG | BA | 3514 | 1/1 | 0.96 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3306 | 1/1 | 0.96 | 0.17 | 15,15,15,15 | 0 |
| 57 | MG | BA | 3204 | 1/1 | 0.96 | 0.27 | 67,67,67,67 | 0 |
| 57 | MG | BE | 302 | 1/1 | 0.96 | 0.16 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3291 | 1/1 | 0.96 | 0.26 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3350 | 1/1 | 0.96 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3447 | 1/1 | 0.96 | 0.32 | 52,52,52,52 | 0 |
| 57 | MG | AA | 1760 | 1/1 | 0.96 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | CA | 3156 | 1/1 | 0.96 | 0.08 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3029 | 1/1 | 0.96 | 0.57 | 45,45,45,45 | 0 |
| 57 | MG | CK | 5001 | 1/1 | 0.96 | 0.05 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3214 | 1/1 | 0.96 | 0.50 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3349 | 1/1 | 0.96 | 0.16 | 34,34,34,34 | 0 |
| 57 | MG | BF | 309 | 1/1 | 0.96 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3058 | 1/1 | 0.96 | 0.08 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3216 | 1/1 | 0.96 | 0.28 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3652 | 1/1 | 0.96 | 0.16 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3374 | 1/1 | 0.96 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3214 | 1/1 | 0.96 | 0.08 | 51,51,51,51 | 0 |
| 57 | MG | DE | 3007 | 1/1 | 0.96 | 0.11 | 58,58,58,58 | 0 |
| 57 | MG | AA | 1637 | 1/1 | 0.96 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3205 | 1/1 | 0.96 | 0.43 | 57,57,57,57 | 0 |
| 57 | MG | AA | 1719 | 1/1 | 0.96 | 0.16 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3159 | 1/1 | 0.96 | 0.18 | 27,27,27,27 | 0 |
| 57 | MG | DA | 3109 | 1/1 | 0.96 | 0.13 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3352 | 1/1 | 0.96 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3221 | 1/1 | 0.96 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3076 | 1/1 | 0.96 | 0.38 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3226 | 1/1 | 0.96 | 0.22 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3361 | 1/1 | 0.96 | 0.08 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3585 | 1/1 | 0.96 | 0.16 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3486 | 1/1 | 0.96 | 0.13 | 41,41,41,41 | 0 |
| 57 | MG | AE | 3001 | 1/1 | 0.96 | 0.07 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3654 | 1/1 | 0.96 | 0.11 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3022 | 1/1 | 0.96 | 0.11 | 25,25,25,25 | 0 |
| 57 | MG | DA | 3598 | 1/1 | 0.96 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3285 | 1/1 | 0.96 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3764 | 1/1 | 0.96 | 0.20 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3231 | 1/1 | 0.96 | 0.18 | 61,61,61,61 | 0 |
| 57 | MG | AA | 1734 | 1/1 | 0.96 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3278 | 1/1 | 0.96 | 0.78 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3380 | 1/1 | 0.96 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3108 | 1/1 | 0.96 | 0.21 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3711 | 1/1 | 0.96 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3376 | 1/1 | 0.96 | 0.19 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3437 | 1/1 | 0.96 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3484 | 1/1 | 0.96 | 0.07 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3365 | 1/1 | 0.96 | 0.14 | 19,19,19,19 | 0 |
| 57 | MG | CA | 3083 | 1/1 | 0.96 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3466 | 1/1 | 0.96 | 0.17 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3234 | 1/1 | 0.96 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3387 | 1/1 | 0.96 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3354 | 1/1 | 0.96 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3216 | 1/1 | 0.96 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3492 | 1/1 | 0.96 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3309 | 1/1 | 0.96 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3647 | 1/1 | 0.96 | 0.11 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3140 | 1/1 | 0.96 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3213 | 1/1 | 0.97 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3341 | 1/1 | 0.97 | 0.20 | 18,18,18,18 | 0 |
| 57 | MG | BQ | 3001 | 1/1 | 0.97 | 0.26 | 37,37,37,37 | 0 |
| 57 | MG | DF | 304 | 1/1 | 0.97 | 0.07 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3120 | 1/1 | 0.97 | 0.33 | 56,56,56,56 | 0 |
| 57 | MG | CA | 3105 | 1/1 | 0.97 | 0.11 | 75,75,75,75 | 0 |
| 57 | MG | CA | 3048 | 1/1 | 0.97 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | BD | 3005 | 1/1 | 0.97 | 0.24 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3190 | 1/1 | 0.97 | 0.28 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3180 | 1/1 | 0.97 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3331 | 1/1 | 0.97 | 0.20 | 53,53,53,53 | 0 |
| 57 | MG | CA | 3128 | 1/1 | 0.97 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3448 | 1/1 | 0.97 | 0.18 | 17,17,17,17 | 0 |
| 57 | MG | BA | 3136 | 1/1 | 0.97 | 0.36 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3548 | 1/1 | 0.97 | 0.13 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3492 | 1/1 | 0.97 | 0.07 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3669 | 1/1 | 0.97 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3039 | 1/1 | 0.97 | 0.16 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3077 | 1/1 | 0.97 | 0.20 | 15,15,15,15 | 0 |
| 57 | MG | AA | 1653 | 1/1 | 0.97 | 0.23 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3004 | 1/1 | 0.97 | 0.22 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3810 | 1/1 | 0.97 | 0.21 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3040 | 1/1 | 0.97 | 0.14 | 28,28,28,28 | 0 |
| 57 | MG | BB | 3021 | 1/1 | 0.97 | 0.18 | 41,41,41,41 | 0 |
| 57 | MG | AA | 1661 | 1/1 | 0.97 | 0.37 | 54,54,54,54 | 0 |
| 57 | MG | AN | 502 | 1/1 | 0.97 | 0.29 | 62,62,62,62 | 0 |
| 57 | MG | DD | 304 | 1/1 | 0.97 | 0.09 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3302 | 1/1 | 0.97 | 0.23 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3634 | 1/1 | 0.97 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3043 | 1/1 | 0.97 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1727 | 1/1 | 0.97 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3736 | 1/1 | 0.97 | 0.16 | 22,22,22,22 | 0 |
| 57 | MG | DA | 3386 | 1/1 | 0.97 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3053 | 1/1 | 0.97 | 0.27 | 23,23,23,23 | 0 |
| 57 | MG | BB | 3007 | 1/1 | 0.97 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | B7 | 102 | 1/1 | 0.97 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3036 | 1/1 | 0.97 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3303 | 1/1 | 0.97 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3083 | 1/1 | 0.97 | 0.34 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3157 | 1/1 | 0.97 | 0.20 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3144 | 1/1 | 0.97 | 0.23 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3011 | 1/1 | 0.97 | 0.15 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3725 | 1/1 | 0.97 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | AA | 1703 | 1/1 | 0.97 | 0.29 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3621 | 1/1 | 0.97 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3045 | 1/1 | 0.97 | 0.22 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3501 | 1/1 | 0.97 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | CA | 3084 | 1/1 | 0.97 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3629 | 1/1 | 0.97 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3385 | 1/1 | 0.97 | 0.23 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3256 | 1/1 | 0.97 | 0.34 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3290 | 1/1 | 0.97 | 0.14 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3628 | 1/1 | 0.97 | 0.28 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3473 | 1/1 | 0.97 | 0.19 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3203 | 1/1 | 0.97 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3661 | 1/1 | 0.97 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | BB | 3011 | 1/1 | 0.97 | 0.20 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3062 | 1/1 | 0.97 | 0.11 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3760 | 1/1 | 0.97 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3174 | 1/1 | 0.97 | 0.53 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3496 | 1/1 | 0.97 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | AA | 1611 | 1/1 | 0.97 | 0.19 | 20,20,20,20 | 0 |
| 57 | MG | DA | 3307 | 1/1 | 0.97 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3287 | 1/1 | 0.97 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3315 | 1/1 | 0.97 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3304 | 1/1 | 0.97 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3490 | 1/1 | 0.97 | 0.17 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3348 | 1/1 | 0.97 | 0.21 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3606 | 1/1 | 0.97 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3495 | 1/1 | 0.97 | 0.05 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3045 | 1/1 | 0.97 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3047 | 1/1 | 0.97 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | DE | 3006 | 1/1 | 0.97 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | CA | 3096 | 1/1 | 0.97 | 0.18 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3264 | 1/1 | 0.97 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3370 | 1/1 | 0.97 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3362 | 1/1 | 0.97 | 0.22 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3356 | 1/1 | 0.97 | 0.24 | 31,31,31,31 | 0 |
| 57 | MG | BH | 201 | 1/1 | 0.97 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3461 | 1/1 | 0.97 | 0.11 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3387 | 1/1 | 0.97 | 0.20 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3749 | 1/1 | 0.97 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3612 | 1/1 | 0.97 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3260 | 1/1 | 0.97 | 0.20 | 19,19,19,19 | 0 |
| 57 | MG | BA | 3544 | 1/1 | 0.97 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3267 | 1/1 | 0.97 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3323 | 1/1 | 0.97 | 0.21 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3560 | 1/1 | 0.97 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3776 | 1/1 | 0.97 | 0.22 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3180 | 1/1 | 0.97 | 0.27 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3316 | 1/1 | 0.97 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3248 | 1/1 | 0.97 | 0.11 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3566 | 1/1 | 0.97 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3186 | 1/1 | 0.97 | 0.27 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3770 | 1/1 | 0.97 | 0.44 | 49,49,49,49 | 0 |
| 57 | MG | AA | 1624 | 1/1 | 0.97 | 0.25 | 66,66,66,66 | 0 |
| 57 | MG | BB | 3023 | 1/1 | 0.97 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | B5 | 104 | 1/1 | 0.97 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3037 | 1/1 | 0.97 | 0.12 | 26,26,26,26 | 0 |
| 57 | MG | CA | 3158 | 1/1 | 0.97 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3221 | 1/1 | 0.97 | 0.21 | 29,29,29,29 | 0 |
| 57 | MG | AA | 1627 | 1/1 | 0.97 | 0.14 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3357 | 1/1 | 0.97 | 0.07 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3073 | 1/1 | 0.97 | 0.08 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3683 | 1/1 | 0.97 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3412 | 1/1 | 0.97 | 0.17 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3434 | 1/1 | 0.97 | 0.12 | 19,19,19,19 | 0 |
| 57 | MG | BA | 3185 | 1/1 | 0.97 | 0.15 | 33,33,33,33 | 0 |
| 57 | MG | AA | 1803 | 1/1 | 0.97 | 0.12 | 46,46,46,46 | 0 |
| 57 | MG | BD | 3001 | 1/1 | 0.97 | 0.14 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3294 | 1/1 | 0.97 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3316 | 1/1 | 0.97 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3326 | 1/1 | 0.97 | 0.10 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3640 | 1/1 | 0.97 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3132 | 1/1 | 0.97 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | AA | 1642 | 1/1 | 0.97 | 0.23 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3184 | 1/1 | 0.97 | 0.21 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3544 | 1/1 | 0.97 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3198 | 1/1 | 0.97 | 0.16 | 52,52,52,52 | 0 |
| 59 | ZN | DY | 501 | 1/1 | 0.97 | 0.11 | 90,90,90,90 | 0 |
| 57 | MG | BA | 3627 | 1/1 | 0.97 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | AA | 1668 | 1/1 | 0.97 | 0.10 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3133 | 1/1 | 0.97 | 0.17 | 82,82,82,82 | 0 |
| 57 | MG | BA | 3635 | 1/1 | 0.97 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | BV | 203 | 1/1 | 0.97 | 0.21 | 23,23,23,23 | 0 |
| 57 | MG | BU | 203 | 1/1 | 0.97 | 0.31 | 34,34,34,34 | 0 |
| 57 | MG | CA | 3118 | 1/1 | 0.97 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3334 | 1/1 | 0.97 | 0.22 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3311 | 1/1 | 0.97 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3436 | 1/1 | 0.97 | 0.11 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3229 | 1/1 | 0.97 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | AA | 1809 | 1/1 | 0.97 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3654 | 1/1 | 0.97 | 0.19 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3413 | 1/1 | 0.97 | 0.17 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3072 | 1/1 | 0.97 | 0.24 | 49,49,49,49 | 0 |
| 57 | MG | AA | 1665 | 1/1 | 0.97 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3494 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3424 | 1/1 | 0.97 | 0.29 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3777 | 1/1 | 0.97 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3007 | 1/1 | 0.97 | 0.13 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3005 | 1/1 | 0.97 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3537 | 1/1 | 0.97 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3586 | 1/1 | 0.97 | 0.11 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3391 | 1/1 | 0.97 | 0.15 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59 | ZN | D9 | 501 | 1/1 | 0.97 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3370 | 1/1 | 0.97 | 0.24 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3169 | 1/1 | 0.97 | 0.28 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3603 | 1/1 | 0.97 | 0.28 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3393 | 1/1 | 0.97 | 0.20 | 23,23,23,23 | 0 |
| 57 | MG | BA | 3227 | 1/1 | 0.97 | 0.17 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3321 | 1/1 | 0.97 | 0.15 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3547 | 1/1 | 0.97 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3639 | 1/1 | 0.97 | 0.18 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3162 | 1/1 | 0.97 | 0.29 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3655 | 1/1 | 0.97 | 0.08 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3089 | 1/1 | 0.97 | 0.19 | 36,36,36,36 | 0 |
| 57 | MG | BD | 3004 | 1/1 | 0.97 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | AA | 1735 | 1/1 | 0.97 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3518 | 1/1 | 0.97 | 0.10 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3576 | 1/1 | 0.97 | 0.24 | 30,30,30,30 | 0 |
| 57 | MG | AU | 101 | 1/1 | 0.97 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3630 | 1/1 | 0.97 | 0.25 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3319 | 1/1 | 0.97 | 0.14 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3463 | 1/1 | 0.97 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3182 | 1/1 | 0.97 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3133 | 1/1 | 0.97 | 0.27 | 37,37,37,37 | 0 |
| 59 | ZN | D6 | 501 | 1/1 | 0.97 | 0.18 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3007 | 1/1 | 0.97 | 0.23 | 21,21,21,21 | 0 |
| 57 | MG | BA | 3054 | 1/1 | 0.97 | 0.22 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3440 | 1/1 | 0.97 | 0.13 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3698 | 1/1 | 0.97 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3353 | 1/1 | 0.97 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3342 | 1/1 | 0.97 | 0.29 | 67,67,67,67 | 0 |
| 57 | MG | CA | 3167 | 1/1 | 0.97 | 0.30 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3027 | 1/1 | 0.97 | 0.53 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3674 | 1/1 | 0.97 | 0.34 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3033 | 1/1 | 0.97 | 0.40 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3340 | 1/1 | 0.97 | 0.14 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3559 | 1/1 | 0.97 | 0.22 | 26,26,26,26 | 0 |
| 57 | MG | DA | 3489 | 1/1 | 0.97 | 0.09 | 48,48,48,48 | 0 |
| 59 | ZN | AN | 501 | 1/1 | 0.97 | 0.16 | 77,77,77,77 | 0 |
| 57 | MG | DA | 3428 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3605 | 1/1 | 0.97 | 0.18 | 47,47,47,47 | 0 |
| 57 | MG | BD | 3010 | 1/1 | 0.97 | 0.20 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3344 | 1/1 | 0.97 | 0.10 | 71,71,71,71 | 0 |
| 57 | MG | DA | 3262 | 1/1 | 0.97 | 0.13 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3014 | 1/1 | 0.97 | 0.22 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3297 | 1/1 | 0.98 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3368 | 1/1 | 0.98 | 0.24 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3521 | 1/1 | 0.98 | 0.09 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3533 | 1/1 | 0.98 | 0.18 | 23,23,23,23 | 0 |
| 57 | MG | BA | 3772 | 1/1 | 0.98 | 0.15 | 36,36,36,36 | 0 |
| 58 | SF4 | AD | 501 | 8/8 | 0.98 | 0.15 | 59,68,73,79 | 0 |
| 57 | MG | BA | 3813 | 1/1 | 0.98 | 0.13 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3178 | 1/1 | 0.98 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3146 | 1/1 | 0.98 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3584 | 1/1 | 0.98 | 0.09 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3547 | 1/1 | 0.98 | 0.08 | 48,48,48,48 | 0 |
| 57 | MG | DE | 3001 | 1/1 | 0.98 | 0.44 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3300 | 1/1 | 0.98 | 0.10 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3182 | 1/1 | 0.98 | 0.67 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3425 | 1/1 | 0.98 | 0.25 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3013 | 1/1 | 0.98 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | BB | 3002 | 1/1 | 0.98 | 0.28 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3467 | 1/1 | 0.98 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3779 | 1/1 | 0.98 | 0.19 | 17,17,17,17 | 0 |
| 57 | MG | DA | 3581 | 1/1 | 0.98 | 0.07 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1732 | 1/1 | 0.98 | 0.20 | 63,63,63,63 | 0 |
| 57 | MG | AA | 1792 | 1/1 | 0.98 | 0.12 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3312 | 1/1 | 0.98 | 0.19 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3382 | 1/1 | 0.98 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3477 | 1/1 | 0.98 | 0.11 | 53,53,53,53 | 0 |
| 57 | MG | AA | 1730 | 1/1 | 0.98 | 0.25 | 27,27,27,27 | 0 |
| 57 | MG | DA | 3093 | 1/1 | 0.98 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3453 | 1/1 | 0.98 | 0.17 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3615 | 1/1 | 0.98 | 0.09 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3701 | 1/1 | 0.98 | 0.23 | 39,39,39,39 | 0 |
| 58 | SF4 | CD | 501 | 8/8 | 0.98 | 0.14 | 64,67,74,91 | 0 |
| 57 | MG | DA | 3085 | 1/1 | 0.98 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | BD | 3002 | 1/1 | 0.98 | 0.21 | 28,28,28,28 | 0 |
| 57 | MG | CA | 3163 | 1/1 | 0.98 | 0.19 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3054 | 1/1 | 0.98 | 0.10 | 27,27,27,27 | 0 |
| 57 | MG | AA | 1702 | 1/1 | 0.98 | 0.27 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3163 | 1/1 | 0.98 | 0.21 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3472 | 1/1 | 0.98 | 0.20 | 24,24,24,24 | 0 |
| 57 | MG | DA | 3217 | 1/1 | 0.98 | 0.24 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3050 | 1/1 | 0.98 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1677 | 1/1 | 0.98 | 0.21 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3408 | 1/1 | 0.98 | 0.23 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3168 | 1/1 | 0.98 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | AA | 1796 | 1/1 | 0.98 | 0.07 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3025 | 1/1 | 0.98 | 0.45 | 47,47,47,47 | 0 |
| 57 | MG | AA | 1795 | 1/1 | 0.98 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3326 | 1/1 | 0.98 | 0.15 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3750 | 1/1 | 0.98 | 0.22 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3195 | 1/1 | 0.98 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3447 | 1/1 | 0.98 | 0.16 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3597 | 1/1 | 0.98 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3188 | 1/1 | 0.98 | 0.24 | 35,35,35,35 | 0 |
| 57 | MG | AA | 1740 | 1/1 | 0.98 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3782 | 1/1 | 0.98 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3075 | 1/1 | 0.98 | 0.20 | 24,24,24,24 | 0 |
| 57 | MG | AA | 1722 | 1/1 | 0.98 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3371 | 1/1 | 0.98 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3373 | 1/1 | 0.98 | 0.09 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3751 | 1/1 | 0.98 | 0.23 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3020 | 1/1 | 0.98 | 0.21 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3259 | 1/1 | 0.98 | 0.18 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3267 | 1/1 | 0.98 | 0.30 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3173 | 1/1 | 0.98 | 0.28 | 32,32,32,32 | 0 |
| 57 | MG | BD | 3009 | 1/1 | 0.98 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | DO | 201 | 1/1 | 0.98 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3381 | 1/1 | 0.98 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3534 | 1/1 | 0.98 | 0.23 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3742 | 1/1 | 0.98 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3539 | 1/1 | 0.98 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3245 | 1/1 | 0.98 | 0.08 | 58,58,58,58 | 0 |
| 57 | MG | BD | 3008 | 1/1 | 0.98 | 0.30 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3546 | 1/1 | 0.98 | 0.04 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3599 | 1/1 | 0.98 | 0.09 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3793 | 1/1 | 0.98 | 0.22 | 11,11,11,11 | 0 |
| 57 | MG | CA | 3104 | 1/1 | 0.98 | 0.23 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3719 | 1/1 | 0.98 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | BU | 204 | 1/1 | 0.98 | 0.31 | 47,47,47,47 | 0 |
| 57 | MG | AA | 1720 | 1/1 | 0.98 | 0.19 | 55,55,55,55 | 0 |
| 57 | MG | AA | 1718 | 1/1 | 0.98 | 0.11 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3039 | 1/1 | 0.98 | 0.19 | 36,36,36,36 | 0 |
| 57 | MG | CA | 3145 | 1/1 | 0.98 | 0.12 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3457 | 1/1 | 0.98 | 0.19 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3562 | 1/1 | 0.98 | 0.12 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3103 | 1/1 | 0.98 | 0.22 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3591 | 1/1 | 0.98 | 0.39 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3067 | 1/1 | 0.98 | 0.24 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3274 | 1/1 | 0.98 | 0.22 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3189 | 1/1 | 0.98 | 0.22 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3632 | 1/1 | 0.98 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | AA | 1724 | 1/1 | 0.98 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3739 | 1/1 | 0.98 | 0.11 | 21,21,21,21 | 0 |
| 57 | MG | BA | 3650 | 1/1 | 0.98 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3488 | 1/1 | 0.98 | 0.13 | 20,20,20,20 | 0 |
| 57 | MG | DA | 3345 | 1/1 | 0.98 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | AA | 1762 | 1/1 | 0.98 | 0.21 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3020 | 1/1 | 0.98 | 0.12 | 26,26,26,26 | 0 |
| 57 | MG | DA | 3469 | 1/1 | 0.98 | 0.07 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3339 | 1/1 | 0.98 | 0.21 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3114 | 1/1 | 0.98 | 0.20 | 39,39,39,39 | 0 |
| 57 | MG | AA | 1761 | 1/1 | 0.98 | 0.20 | 70,70,70,70 | 0 |
| 57 | MG | BA | 3345 | 1/1 | 0.98 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3665 | 1/1 | 0.98 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | BF | 305 | 1/1 | 0.98 | 0.14 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3067 | 1/1 | 0.98 | 0.21 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3021 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3079 | 1/1 | 0.98 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3811 | 1/1 | 0.98 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3080 | 1/1 | 0.98 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | DB | 3013 | 1/1 | 0.99 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | CA | 3092 | 1/1 | 0.99 | 0.24 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3104 | 1/1 | 0.99 | 0.19 | 24,24,24,24 | 0 |
| 59 | ZN | D5 | 501 | 1/1 | 0.99 | 0.19 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3355 | 1/1 | 0.99 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3551 | 1/1 | 0.99 | 0.15 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3718 | 1/1 | 0.99 | 0.17 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3085 | 1/1 | 0.99 | 0.29 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3583 | 1/1 | 0.99 | 0.15 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3398 | 1/1 | 0.99 | 0.08 | 40,40,40,40 | 0 |
| 57 | MG | CA | 3085 | 1/1 | 0.99 | 0.15 | 41,41,41,41 | 0 |
| 57 | MG | AA | 1772 | 1/1 | 0.99 | 0.20 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3476 | 1/1 | 0.99 | 0.16 | 48,48,48,48 | 0 |
| 57 | MG | BV | 205 | 1/1 | 0.99 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | AA | 1770 | 1/1 | 0.99 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3392 | 1/1 | 0.99 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3731 | 1/1 | 0.99 | 0.14 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59 | ZN | B6 | 102 | 1/1 | 0.99 | 0.26 | 50,50,50,50 | 0 |
| 57 | MG | AA | 1758 | 1/1 | 0.99 | 0.09 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3800 | 1/1 | 0.99 | 0.19 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3472 | 1/1 | 0.99 | 0.14 | 25,25,25,25 | 0 |
| 57 | MG | AA | 1678 | 1/1 | 0.99 | 0.25 | 47,47,47,47 | 0 |
| 57 | MG | CA | 3010 | 1/1 | 0.99 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | CA | 3044 | 1/1 | 0.99 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3310 | 1/1 | 0.99 | 0.23 | 26,26,26,26 | 0 |
| 57 | MG | B5 | 101 | 1/1 | 0.99 | 0.27 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3209 | 1/1 | 0.99 | 0.09 | 49,49,49,49 | 0 |
| 59 | ZN | B5 | 103 | 1/1 | 0.99 | 0.21 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3383 | 1/1 | 0.99 | 0.13 | 28,28,28,28 | 0 |
| 57 | MG | AA | 1681 | 1/1 | 0.99 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | BD | 3006 | 1/1 | 0.99 | 0.09 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3417 | 1/1 | 0.99 | 0.21 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3707 | 1/1 | 0.99 | 0.19 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3499 | 1/1 | 0.99 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | AA | 1672 | 1/1 | 0.99 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3582 | 1/1 | 0.99 | 0.12 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3412 | 1/1 | 0.99 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3003 | 1/1 | 0.99 | 0.17 | 33,33,33,33 | 0 |
| 59 | ZN | B9 | 501 | 1/1 | 1.00 | 0.23 | 49,49,49,49 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.