



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 03:20 pm GMT

PDB ID : 3CXC
Title : The structure of an enhanced oxazolidinone inhibitor bound to the 50S ribosomal subunit of *H. marismortui*
Authors : Ippolito, J.A.; Wang, D.; Kanyo, Z.F.; Duffy, E.M.
Deposited on : 2008-04-24
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

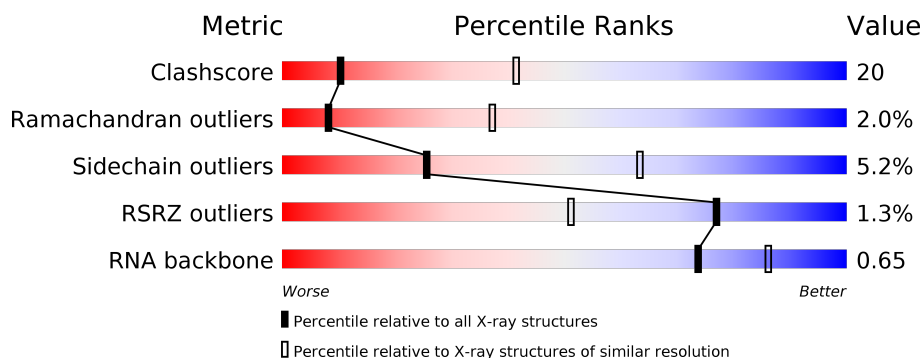
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 122126 | 2167 (3.00-3.00) |
| Ramachandran outliers | 120053 | 2101 (3.00-3.00) |
| Sidechain outliers | 120020 | 2104 (3.00-3.00) |
| RSRZ outliers | 108989 | 1751 (3.00-3.00) |
| RNA backbone | 2636 | 1017 (3.30-2.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | 0 | 2922 | <div> <div></div> <div> <div></div> <div>47%</div> <div>40%</div> <div>6%</div> <div>6%</div> </div> </div> |
| 2 | 9 | 122 | <div> <div>4%</div> <div> <div></div> <div>38%</div> <div>49%</div> <div>11%</div> </div> </div> |
| 3 | 4 | 3 | <div> <div> <div></div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div> |
| 4 | A | 239 | <div> <div></div> <div> <div></div> <div>54%</div> <div>41%</div> <div>5%</div> </div> </div> |
| 5 | B | 337 | <div> <div></div> <div> <div></div> <div>53%</div> <div>42%</div> <div>6%</div> </div> </div> |
| 6 | C | 246 | <div> <div> <div></div> <div>55%</div> <div>39%</div> <div>5%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 7 | D | 176 | |
| 8 | E | 177 | |
| 9 | F | 119 | |
| 10 | G | 348 | |
| 11 | H | 167 | |
| 12 | I | 145 | |
| 13 | J | 132 | |
| 14 | K | 164 | |
| 15 | L | 194 | |
| 16 | M | 186 | |
| 17 | N | 115 | |
| 18 | O | 148 | |
| 19 | P | 95 | |
| 20 | Q | 154 | |
| 21 | R | 84 | |
| 22 | S | 119 | |
| 23 | T | 66 | |
| 24 | U | 70 | |
| 25 | V | 154 | |
| 26 | W | 91 | |
| 27 | X | 240 | |
| 28 | Y | 73 | |
| 29 | Z | 56 | |
| 30 | 1 | 48 | |
| 31 | 2 | 92 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 33 | MG | 0 | 8024 | - | - | - | X |
| 33 | MG | 0 | 8114 | - | - | - | X |
| 35 | NA | 0 | 8329 | - | - | - | X |
| 35 | NA | 0 | 8363 | - | - | - | X |
| 35 | NA | 0 | 8371 | - | - | - | X |
| 35 | NA | 0 | 8384 | - | - | - | X |
| 35 | NA | H | 8322 | - | - | - | X |
| 35 | NA | Q | 8386 | - | - | - | X |
| 35 | NA | R | 8312 | - | - | - | X |
| 37 | CD | 2 | 8404 | - | - | X | - |

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98635 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 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | 0 | 2754 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59017 | 26346 | 10878 | 19048 | 2745 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 0 | 560 | C | U | CONFLICT | GB 3377779 |

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | 9 | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2600 | 1160 | 472 | 847 | 121 | | | |

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*A)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3 | 4 | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59 | 28 | 11 | 18 | 2 | | | |

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | A | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1754 | 1072 | 352 | 325 | 5 | | | |

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | B | 337 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2625 | 1616 | 493 | 511 | 5 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| B | 310 | ARG | PRO | CONFLICT | UNP P20279 |

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | C | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1859 | 1131 | 344 | 383 | 1 | | | |

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | D | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1094 | 685 | 195 | 210 | 4 | | | |

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | E | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1357 | 840 | 224 | 289 | 4 | | | |

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L7AE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | F | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 552 | 141 | 192 | 1 | | | |

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | G | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 240 | 149 | 39 | 51 | 1 | | | |

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | H | 156 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1216 | 766 | 233 | 213 | 4 | | | |

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | I | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1120 | 696 | 199 | 222 | 3 | | | |

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | J | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 994 | 609 | 189 | 192 | 4 | | | |

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | K | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1118 | 670 | 222 | 226 | | | | |

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | L | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1606 | 988 | 346 | 267 | 5 | | | |

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | M | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 895 | 262 | 286 | 2 | | | |

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | N | 115 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 865 | 529 | 161 | 175 | | | | |

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L19E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | O | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 680 | 230 | 223 | | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| O | 71 | LYS | TYR | CONFLICT | UNP P14119 |

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L21E.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19 | P | 95 | Total | C | N | O | 0 | 0 | 0 |
| | | | 735 | 450 | 141 | 144 | | | |

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | Q | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1149 | 713 | 209 | 223 | 4 | | | |

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | R | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 641 | 389 | 111 | 138 | 3 | | | |

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 22 | S | 119 | Total | C | N | O | 0 | 0 | 0 |
| | | | 950 | 568 | 180 | 202 | | | |

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 23 | T | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 410 | 244 | 75 | 86 | 5 | | | |

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 24 | U | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 499 | 304 | 94 | 100 | 1 | | | |

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | V | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1196 | 737 | 209 | 244 | 6 | | | |

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L31E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | W | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 654 | 402 | 129 | 122 | 1 | | | |

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L32E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | X | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1130 | 686 | 228 | 216 | | | | |

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37AE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 28 | Y | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 564 | 359 | 111 | 87 | 7 | | | |

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | Z | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 431 | 258 | 86 | 83 | 4 | | | |

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L39E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | 1 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 394 | 238 | 86 | 69 | 1 | | | |

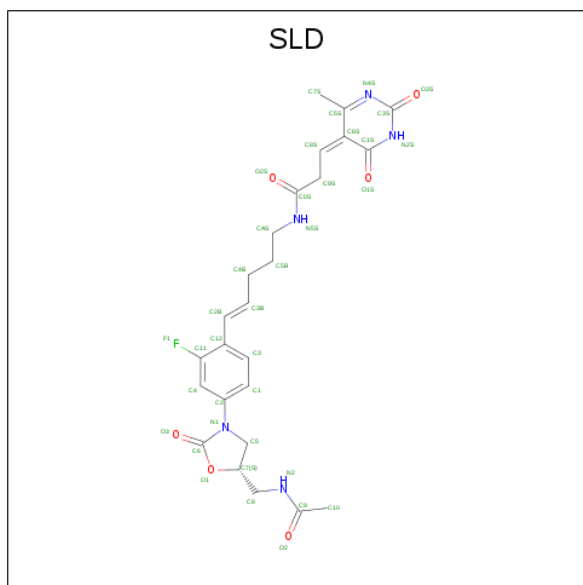
There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 1 | ? | - | ARG | DELETION | UNP P22452 |

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | 2 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 458 | 153 | 137 | 7 | | | |

- Molecule 32 is (3Z)-N-[(4E)-5-(4-{(5S)-5-[(acetylamino)methyl]-2-oxo-1,3-oxazolidin-3-yl}-2-fluorophenyl)pent-4-en-1-yl]-3-(4-methyl-2,6-dioxo-1,6-dihydropyrimidin-5(2H)-ylidene)propanamide (three-letter code: SLD) (formula: C₂₅H₂₈FN₅O₆).



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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 33 | 9 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 33 | S | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 34 | 0 | 2 | Total | K | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 35 | 0 | 73 | Total | Na | 0 | 0 |
| | | | 73 | 73 | | |
| 35 | P | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | Q | 2 | Total | Na | 0 | 0 |
| | | | 2 | 2 | | |
| 35 | K | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | H | 2 | Total | Na | 0 | 0 |
| | | | 2 | 2 | | |
| 35 | I | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | C | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | A | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | R | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | 9 | 2 | Total | Na | 0 | 0 |
| | | | 2 | 2 | | |
| 35 | L | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 36 | 0 | 8 | Total | Cl | 0 | 0 |
| | | | 8 | 8 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 36 | P | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | J | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | Q | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | K | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | B | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | I | 3 | Total 3 | Cl 3 | 0 | 0 |
| 36 | A | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | N | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | X | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | 2 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | L | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | M | 1 | Total 1 | Cl 1 | 0 | 0 |

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 37 | Z | 1 | Total 1 | Cd 1 | 0 | 0 |
| 37 | Y | 1 | Total 1 | Cd 1 | 0 | 0 |
| 37 | T | 1 | Total 1 | Cd 1 | 0 | 0 |
| 37 | 2 | 1 | Total 1 | Cd 1 | 0 | 0 |
| 37 | N | 1 | Total 1 | Cd 1 | 0 | 0 |

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 38 | 0 | 5806 | Total O 5806 5806 | 0 | 0 |
| 38 | 9 | 147 | Total O 147 147 | 0 | 0 |
| 38 | 4 | 1 | Total O 1 1 | 0 | 0 |
| 38 | A | 136 | Total O 136 136 | 0 | 0 |
| 38 | B | 160 | Total O 160 160 | 0 | 0 |
| 38 | C | 180 | Total O 180 180 | 0 | 0 |
| 38 | D | 49 | Total O 49 49 | 0 | 0 |
| 38 | E | 47 | Total O 47 47 | 0 | 0 |
| 38 | F | 26 | Total O 26 26 | 0 | 0 |
| 38 | G | 21 | Total O 21 21 | 0 | 0 |
| 38 | H | 82 | Total O 82 82 | 0 | 0 |
| 38 | I | 61 | Total O 61 61 | 0 | 0 |
| 38 | J | 63 | Total O 63 63 | 0 | 0 |
| 38 | K | 85 | Total O 85 85 | 0 | 0 |
| 38 | L | 130 | Total O 130 130 | 0 | 0 |
| 38 | M | 69 | Total O 69 69 | 0 | 0 |
| 38 | N | 45 | Total O 45 45 | 0 | 0 |
| 38 | O | 70 | Total O 70 70 | 0 | 0 |
| 38 | P | 56 | Total O 56 56 | 0 | 0 |
| 38 | Q | 92 | Total O 92 92 | 0 | 0 |
| 38 | R | 40 | Total O 40 40 | 0 | 0 |
| 38 | S | 37 | Total O 37 37 | 0 | 0 |

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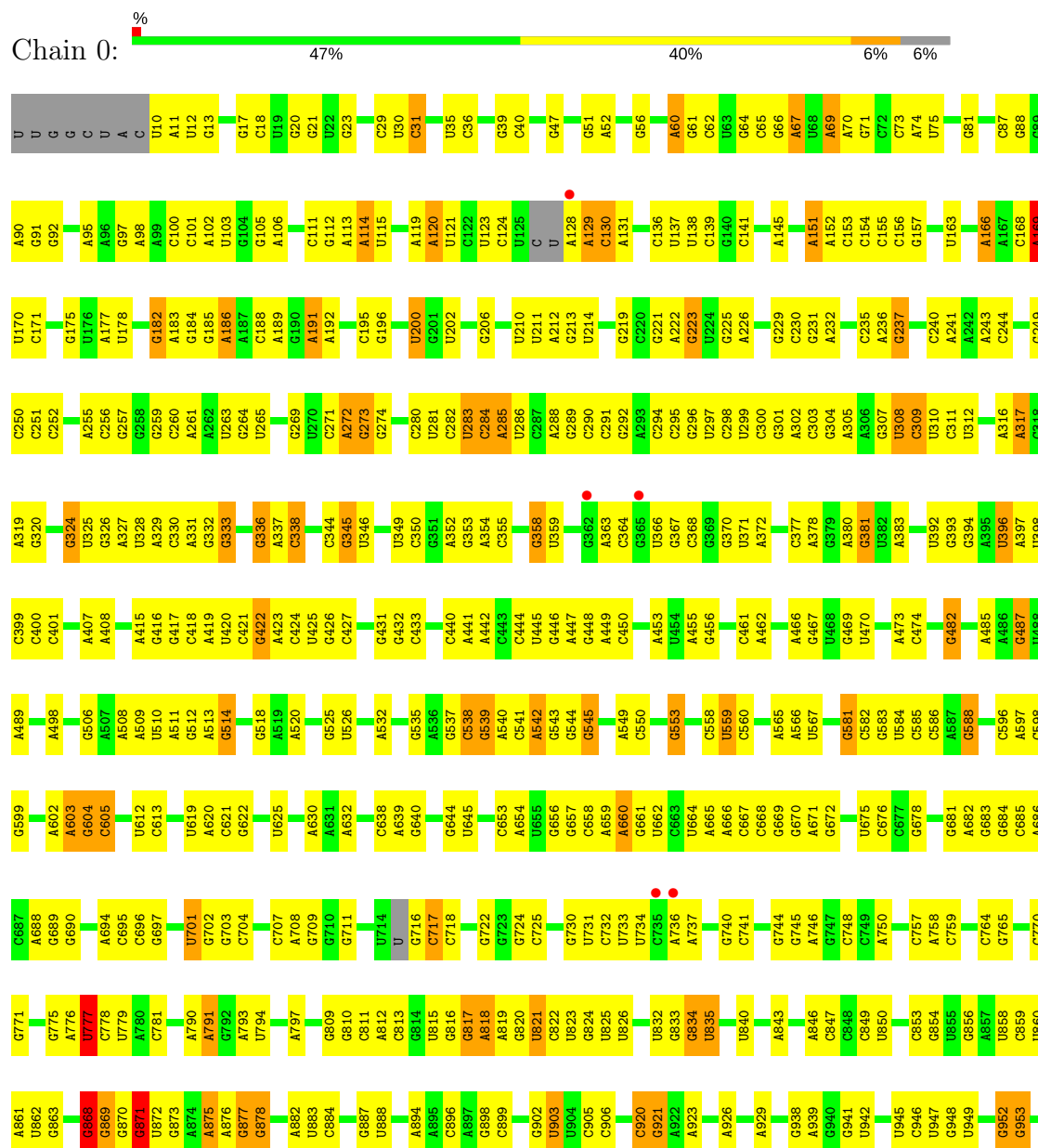
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 38 | T | 27 | Total 27 | O 27 | 0 | 0 |
| 38 | U | 13 | Total 13 | O 13 | 0 | 0 |
| 38 | V | 74 | Total 74 | O 74 | 0 | 0 |
| 38 | W | 29 | Total 29 | O 29 | 0 | 0 |
| 38 | X | 105 | Total 105 | O 105 | 0 | 0 |
| 38 | Y | 41 | Total 41 | O 41 | 0 | 0 |
| 38 | Z | 57 | Total 57 | O 57 | 0 | 0 |
| 38 | 1 | 45 | Total 45 | O 45 | 0 | 0 |
| 38 | 2 | 76 | Total 76 | O 76 | 0 | 0 |

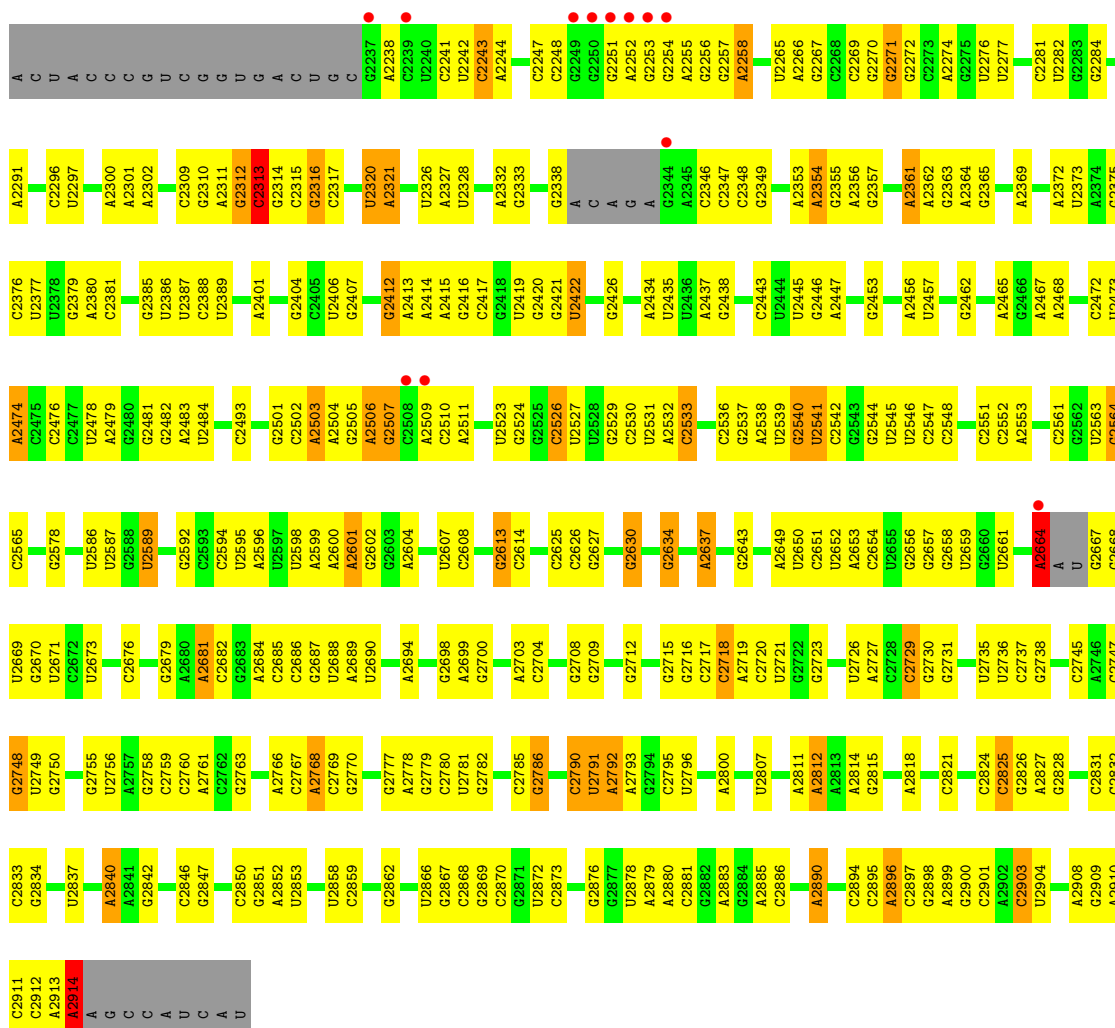
3 Residue-property plots

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.

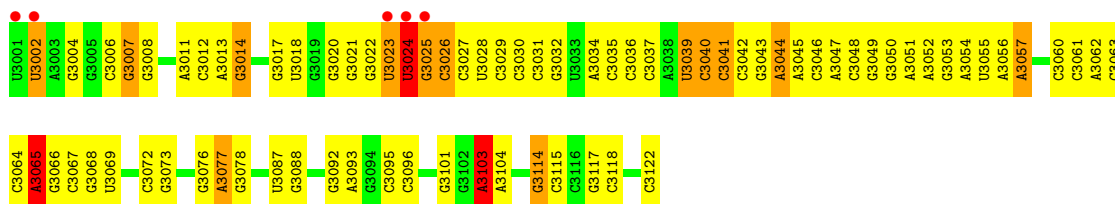
• Molecule 1: 23S RIBOSOMAL RNA



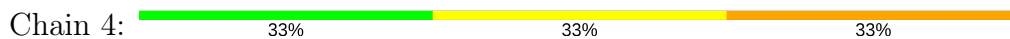
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| U | A2083 | U1992 | G1917 | A1822 | G1751 | A1657 | C1575 | U1499 | C1420 | U1314 | G1224 | G1155 | U1030 | C959 |
| G | C1993 | A1918 | U1918 | G1823 | G1752 | A1658 | A1580 | U1500 | U1421 | A1320 | C1225 | C1156 | G1031 | G960 |
| G | A2089 | C1994 | A1919 | U1825 | A1755 | C1666 | U1503 | U1503 | C1423 | A1321 | G1226 | G1158 | C1044 | A961 |
| U | G2090 | G1995 | C1920 | C1826 | A1667 | C1667 | C1584 | A1504 | U1424 | G1322 | G1229 | G1159 | G1045 | C962 |
| A | G2091 | U1996 | A1921 | G1827 | G1756 | U1668 | C1585 | U1505 | G1425 | G1323 | C1229 | G1160 | G1045 | C963 |
| G | C2094 | G2000 | A1922 | G1828 | U1757 | A1669 | C1586 | U1506 | C1426 | G1324 | C1230 | A1161 | G1052 | G964 |
| G | A2095 | C2001 | G1925 | A1829 | U1758 | G1670 | U1587 | U1511 | A1427 | G1325 | U1234 | G1162 | G1052 | G968 |
| A | A2096 | G2002 | G1926 | C1830 | A1759 | C1675 | G1592 | U1512 | G1430 | A1328 | G1235 | G1163 | G1055 | G969 |
| G | U2003 | U2003 | A1927 | C1834 | U1761 | G1576 | C1593 | C1513 | C1431 | A1329 | U1236 | U1164 | A1068 | U970 |
| C | A2101 | U2004 | C1928 | U1835 | C1762 | U1677 | C1594 | C1514 | U1432 | A1330 | U1237 | G1165 | G1059 | G |
| A | G2102 | G2005 | G1929 | C1763 | U1757 | A1678 | G1595 | U1515 | G1433 | A1331 | G1239 | A1166 | C1060 | U |
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| U | C2106 | U2008 | G1931 | A1841 | U1767 | A1682 | U1597 | U1517 | U1435 | C1333 | A1242 | U1171 | U1064 | C |
| A | U2107 | A2011 | G1932 | U1845 | C1768 | C1683 | U1598 | U1519 | U1436 | C1334 | U1244 | G1172 | G1065 | G |
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| C | G2110 | G2013 | C1935 | A1847 | C1769 | A1685 | G1603 | C1521 | U1441 | C1342 | U1246 | G1173 | A1070 | C |
| C | G2111 | G2014 | U1936 | G1848 | U1770 | A1686 | A1603 | A1522 | G1442 | C1343 | U1247 | G1174 | G1071 | U |
| A | A2112 | A2015 | C1937 | C1886 | U1771 | C1686 | G1604 | A1523 | G1443 | G1344 | A1248 | U1180 | G1072 | C |
| G | G2113 | U2016 | U1938 | U1850 | C1772 | C1687 | G1605 | U1524 | G1444 | A1345 | C1249 | A1181 | A1078 | C |
| G | C2114 | U2016 | G1938 | G1851 | G1773 | C1687 | G1605 | U1525 | G1445 | U1346 | C1250 | C1182 | A1078 | C |
| U | U2115 | A2023 | U1939 | A1852 | G1774 | C1692 | C1609 | A1526 | G1445 | U1346 | C1251 | A1079 | A1079 | A |
| A | U2116 | C2023 | C1940 | C1853 | G1774 | C1692 | C1609 | A1526 | G1445 | U1346 | C1251 | C1182 | A1079 | A |
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| C | C2119 | C2029 | A1942 | C1855 | U1779 | U1698 | G1611 | A1528 | C1451 | C1353 | U1267 | C1184 | A1081 | G |
| C | U2120 | A2030 | C1943 | C1856 | C1780 | A1698 | A1612 | G1529 | G1452 | C1354 | U1268 | U1185 | A1081 | A |
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| G | G2125 | C2035 | G1951 | G1863 | C1785 | A1711 | C1617 | C1538 | U1457 | C1365 | U1270 | G1190 | A1088 | U |
| U | U2126 | U2036 | U | C1864 | C1787 | A1712 | G1618 | U1539 | C1366 | C1366 | U1271 | A1191 | U1109 | C |
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| G | G2136 | U2042 | U | C1878 | U1791 | A1716 | A1626 | A1547 | C1463 | A1375 | U1277 | G1197 | U1116 | C |
| G | C2043 | U2043 | U | G1879 | C1792 | A1717 | G1627 | U1548 | U1464 | G1376 | U1278 | U1198 | A1117 | C |
| C | A | G2044 | G | U1879 | C1793 | C1793 | G1633 | C1549 | C1474 | C1377 | U1279 | A1199 | A1117 | A |
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| A | G | G2050 | A | C1882 | C1798 | C1723 | G1634 | G1552 | U1470 | A1372 | G1283 | C1201 | U1120 | C999 |
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| C | G | C | C | G1884 | G1800 | C1725 | G1636 | C1553 | U1472 | G1382 | C1284 | A1202 | G1002 | U1001 |
| G | C | C | C | C | A1801 | C1725 | G1636 | C1553 | U1472 | G1382 | C1284 | A1202 | G1002 | U1001 |
| G | A2054 | G2053 | C | C1894 | G1802 | C1803 | A1801 | C1557 | C1474 | C1384 | C1289 | C1204 | A1123 | U1003 |
| A | U2054 | C2054 | U | C1895 | G1802 | C1803 | A1801 | C1557 | C1474 | C1384 | C1289 | C1204 | A1123 | U1003 |
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| G | U2054 | C2055 | C | G1896 | C1803 | C1803 | A1801 | C1557 | C1474 | C1384 | C1289 | C1204 | A1123 | U1003 |
| C | C | U2055 | U | G1897 | A1804 | A1732 | C1640 | U | U1477 | A1393 | U1298 | U1206 | U1130 | A1006 |
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| A | C2061 | C2061 | G1971 | G1899 | C1804 | A1732 | C1640 | U | U1477 | A1393 | U1298 | U1206 | U1130 | A1006 |
| A | G | A | U | G1900 | G1806 | A1733 | C1641 | C1562 | C1483 | G1398 | G1299 | C1208 | G1131 | C1007 |
| C | U2063 | U2063 | A1973 | C1899 | U1807 | C1734 | C1642 | C1562 | C1483 | G1398 | G1299 | C1208 | G1131 | C1007 |
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| C | G | C | C | G1902 | C1810 | U1741 | G1649 | C1566 | C1483 | G1398 | G1299 | C1208 | G1131 | C1007 |
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| A | A2072 | C2071 | G1977 | U1903 | C1810 | U1741 | G1649 | C1566 | C1483 | G1398 | G1299 | C1208 | G1131 | C1007 |
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| A | A2072 | C2071 | G1977 | U1903 | C1810 | U1741 | G1649 | C1566 | C1483 | G1398 | G1299 | C1208 | G1131 | C1007 |
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- Molecule 2: 5S RIBOSOMAL RNA

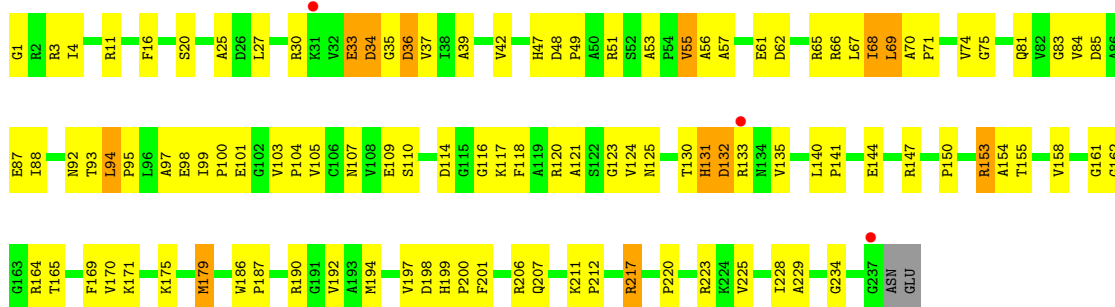


- Molecule 3: 5'-R(*CP*CP*A)-3'

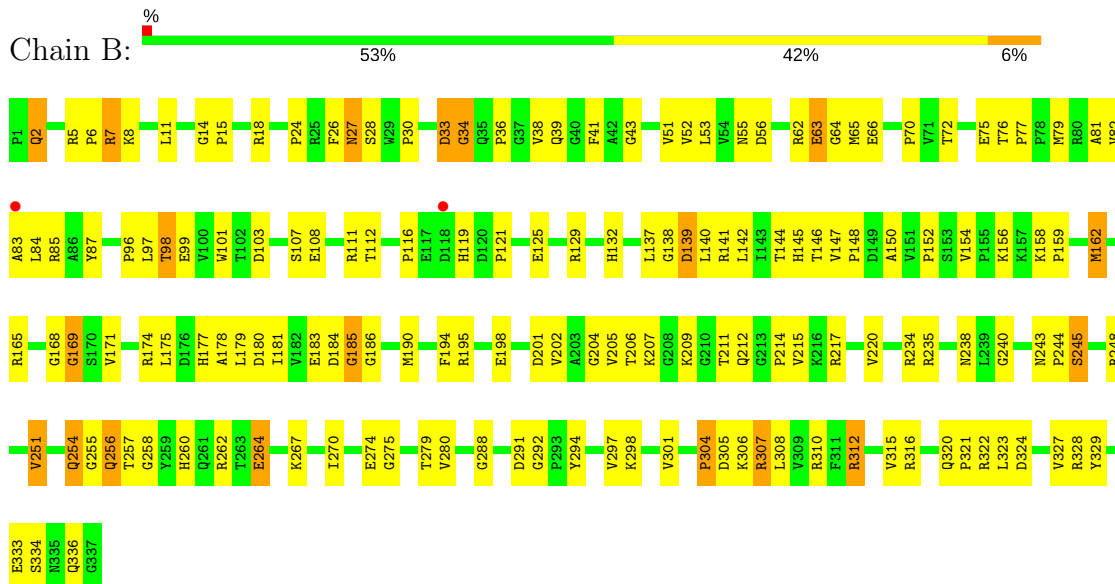


- Molecule 4: RIBOSOMAL PROTEIN L2

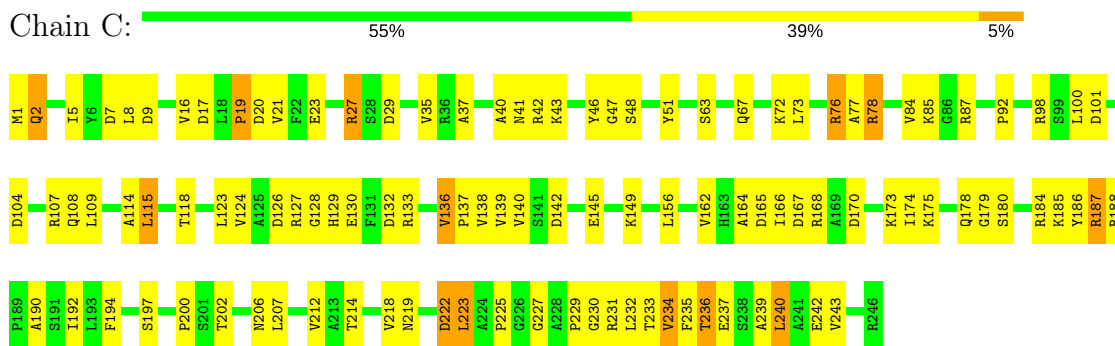




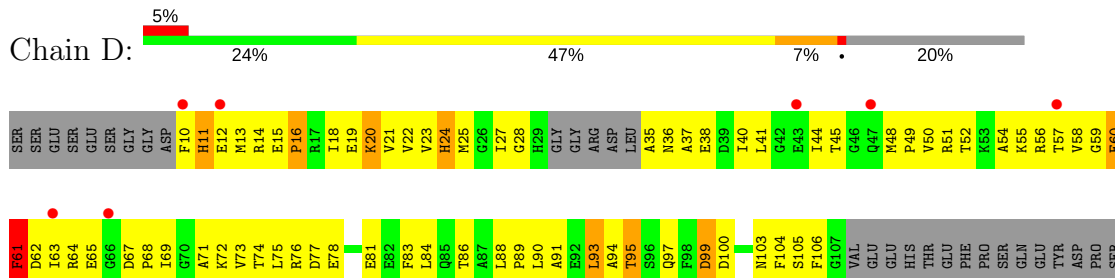
- Molecule 5: RIBOSOMAL PROTEIN L3



- Molecule 6: RIBOSOMAL PROTEIN L4



- Molecule 7: RIBOSOMAL PROTEIN L5

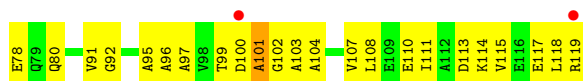
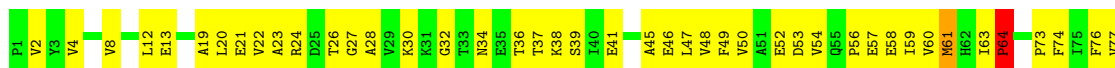
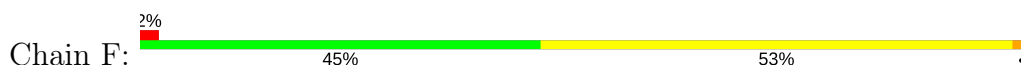




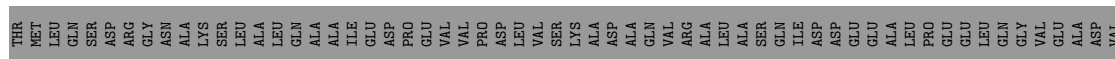
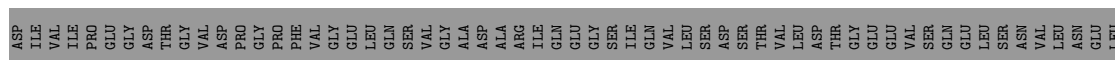
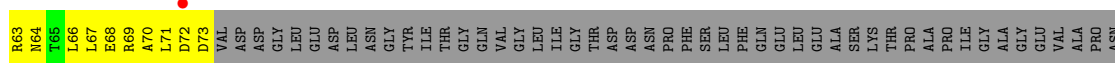
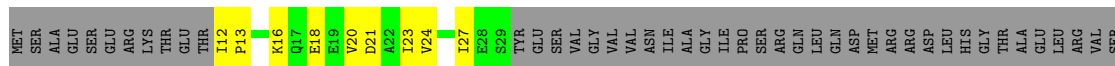
- Molecule 8: RIBOSOMAL PROTEIN L6



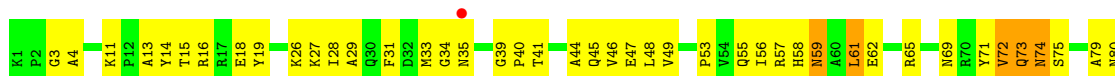
- Molecule 9: RIBOSOMAL PROTEIN L7AE

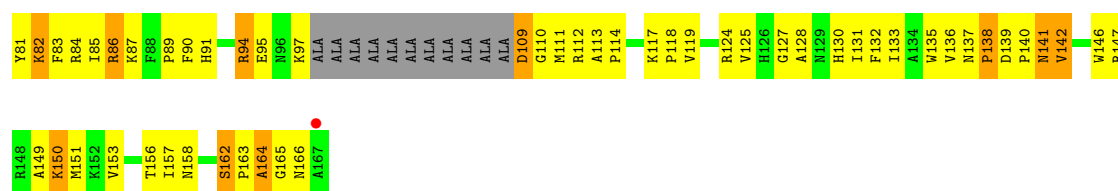


- Molecule 10: RIBOSOMAL PROTEIN L10



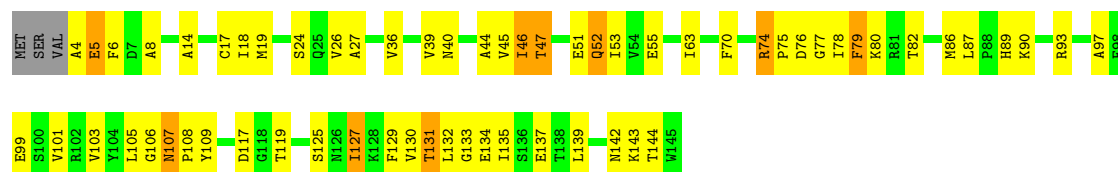
- Molecule 11: RIBOSOMAL PROTEIN L10E





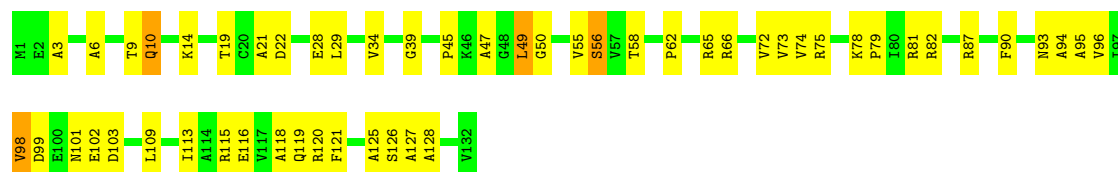
• Molecule 12: RIBOSOMAL PROTEIN L13

Chain I: 55% 37% 6%



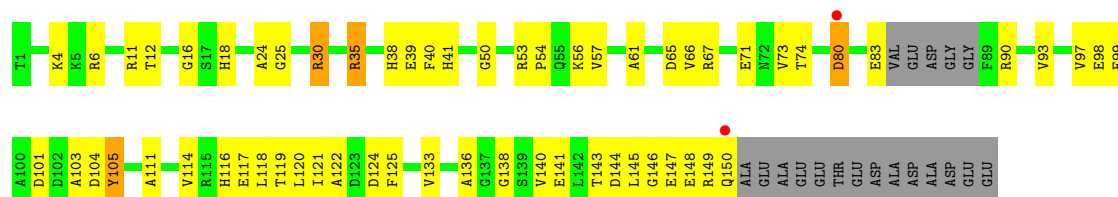
• Molecule 13: RIBOSOMAL PROTEIN L14

Chain J: 60% 37%



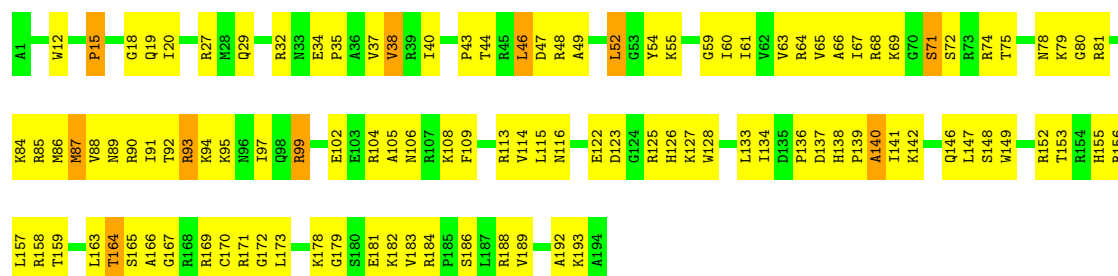
• Molecule 14: RIBOSOMAL PROTEIN L15

Chain K: 51% 35% 12%

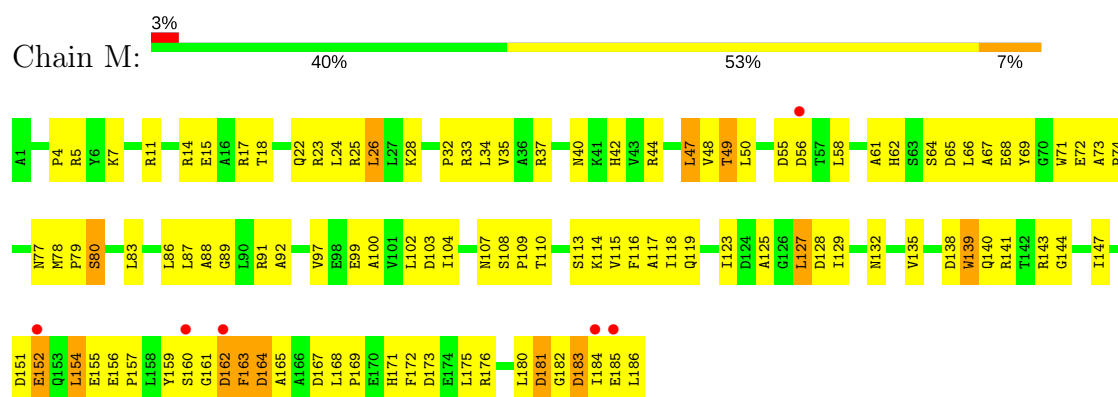


• Molecule 15: RIBOSOMAL PROTEIN L15E

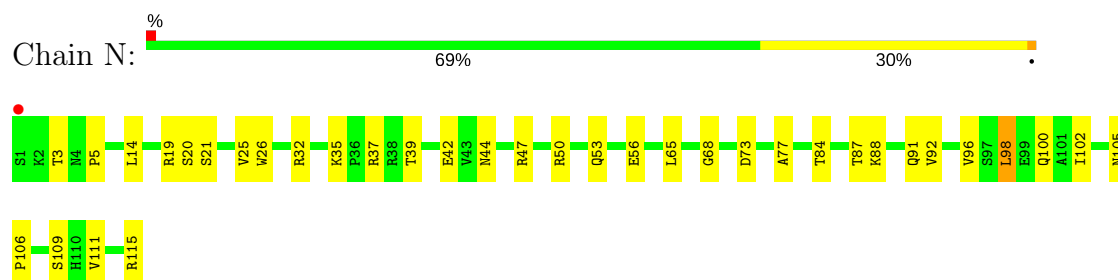
Chain L: 43% 52% 5%



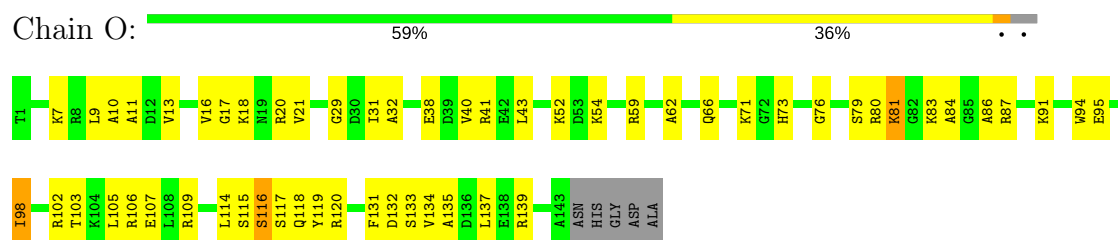
• Molecule 16: RIBOSOMAL PROTEIN L18



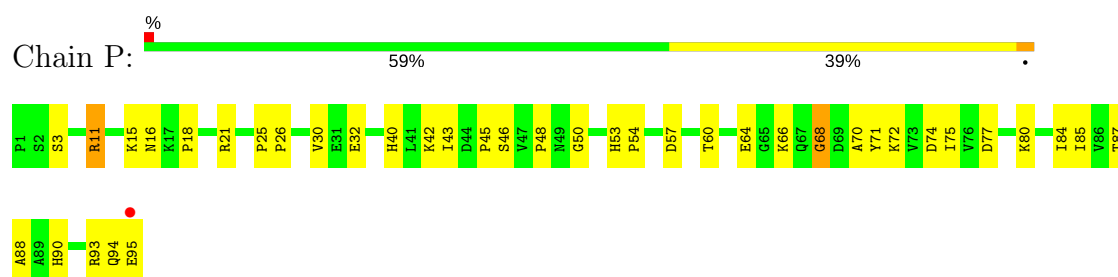
• Molecule 17: RIBOSOMAL PROTEIN L18E



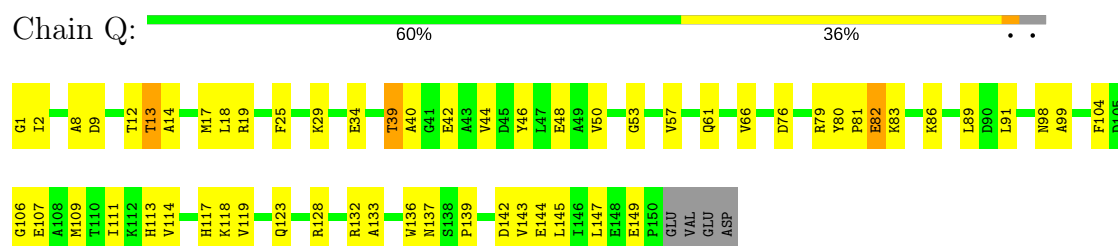
• Molecule 18: RIBOSOMAL PROTEIN L19E



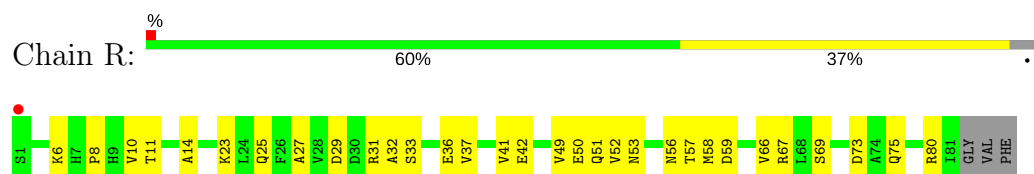
• Molecule 19: RIBOSOMAL PROTEIN L21E



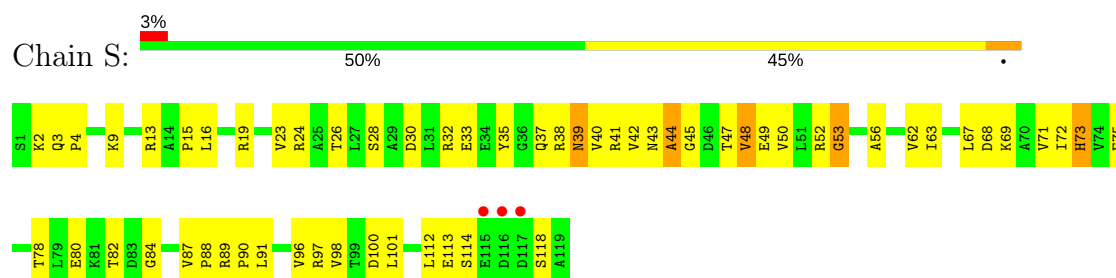
• Molecule 20: RIBOSOMAL PROTEIN L22



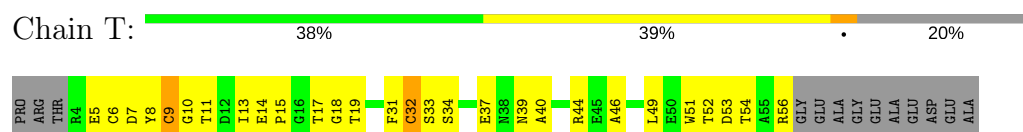
- Molecule 21: RIBOSOMAL PROTEIN L23



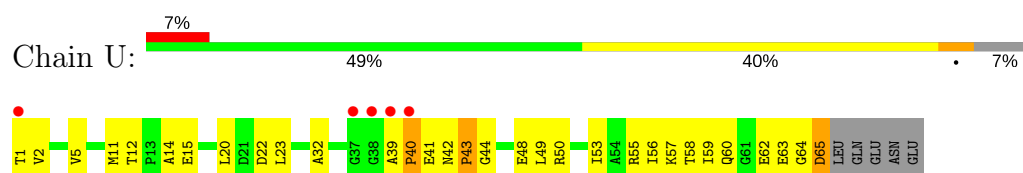
- Molecule 22: RIBOSOMAL PROTEIN L24



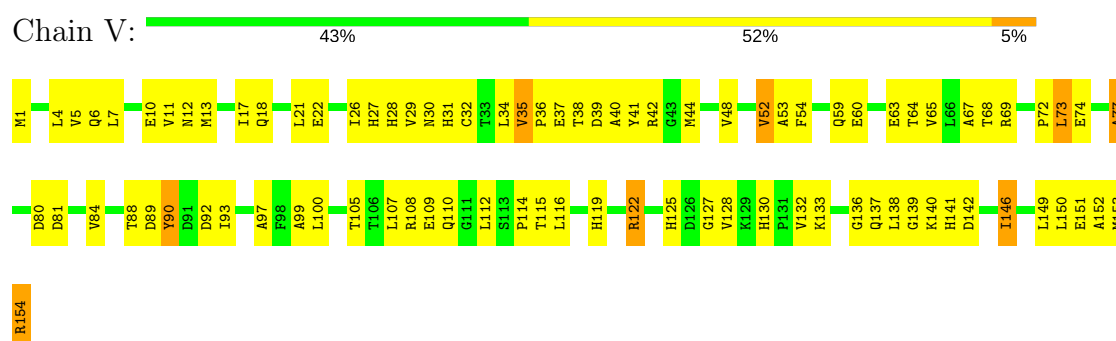
- Molecule 23: RIBOSOMAL PROTEIN L24E



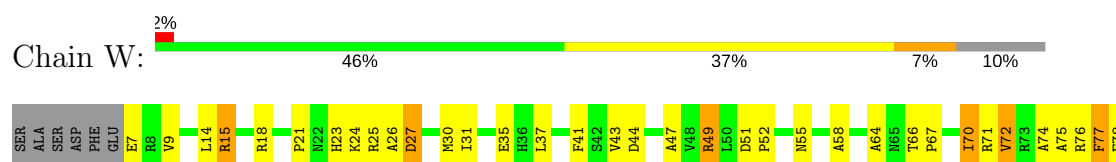
- Molecule 24: RIBOSOMAL PROTEIN L29



- Molecule 25: RIBOSOMAL PROTEIN L30



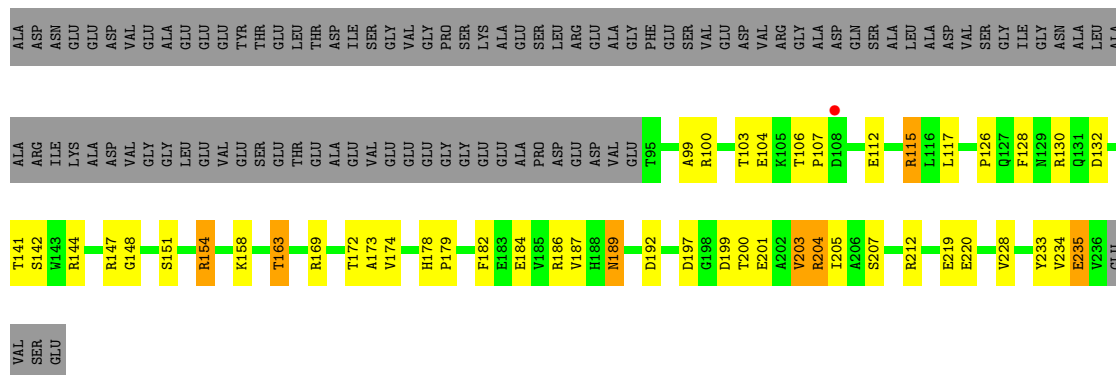
- Molecule 26: RIBOSOMAL PROTEIN L31E





• Molecule 27: RIBOSOMAL PROTEIN L32E

Chain X: 39% 18% 41%



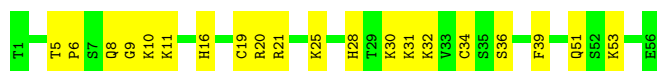
• Molecule 28: RIBOSOMAL PROTEIN L37AE

Chain Y: 38% 52% 10%



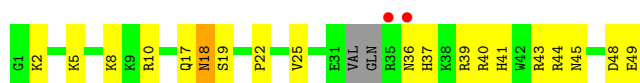
• Molecule 29: RIBOSOMAL PROTEIN L37E

Chain Z: 64% 36%



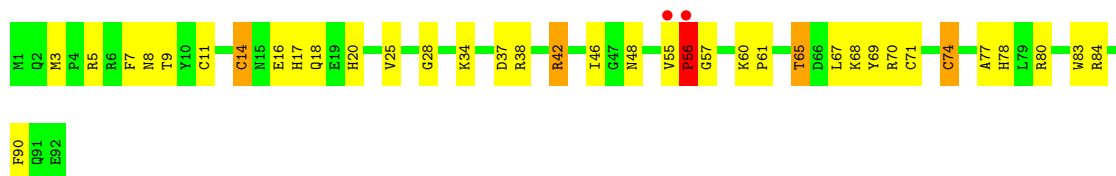
• Molecule 30: RIBOSOMAL PROTEIN L39E

Chain 1: 4% 56% 38%



• Molecule 31: RIBOSOMAL PROTEIN L44E

Chain 2: 2% 60% 35%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 213.66Å 300.71Å 575.37Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.00 20.00 – 2.99 | Depositor EDS |
| % Data completeness (in resolution range) | 91.4 (20.00-3.00) 90.8 (20.00-2.99) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.77 (at 2.98Å) | Xtriage |
| Refinement program | CNX | Depositor |
| R, R_{free} | 0.186 , 0.229 0.186 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | wwPDB-VP |
| Wilson B-factor (Å ²) | 66.9 | Xtriage |
| Anisotropy | 0.417 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 63.5 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 98635 | wwPDB-VP |
| Average B, all atoms (Å ²) | 70.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, CD, SLD

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 | 0 | 0.52 | 4/66076 (0.0%) | 0.71 | 23/103052 (0.0%) |
| 2 | 9 | 0.46 | 0/2905 | 0.76 | 3/4528 (0.1%) |
| 3 | 4 | 0.89 | 0/65 | 1.01 | 0/99 |
| 4 | A | 0.39 | 0/1787 | 0.70 | 0/2409 |
| 5 | B | 0.40 | 0/2690 | 0.68 | 0/3652 |
| 6 | C | 0.45 | 0/1884 | 0.71 | 0/2551 |
| 7 | D | 0.37 | 0/1111 | 0.62 | 0/1498 |
| 8 | E | 0.38 | 0/1382 | 0.61 | 0/1880 |
| 9 | F | 0.38 | 0/897 | 0.60 | 0/1219 |
| 10 | G | 0.38 | 0/241 | 0.58 | 0/324 |
| 11 | H | 0.44 | 0/1247 | 0.79 | 3/1686 (0.2%) |
| 12 | I | 0.43 | 0/1136 | 0.65 | 0/1530 |
| 13 | J | 0.41 | 0/1004 | 0.72 | 0/1351 |
| 14 | K | 0.41 | 0/1130 | 0.71 | 0/1509 |
| 15 | L | 0.49 | 0/1634 | 0.75 | 1/2180 (0.0%) |
| 16 | M | 0.39 | 0/1474 | 0.68 | 0/1999 |
| 17 | N | 0.41 | 0/874 | 0.67 | 0/1181 |
| 18 | O | 0.41 | 0/1143 | 0.60 | 0/1521 |
| 19 | P | 0.44 | 0/749 | 0.74 | 1/1005 (0.1%) |
| 20 | Q | 0.44 | 0/1172 | 0.69 | 0/1578 |
| 21 | R | 0.38 | 0/648 | 0.62 | 0/875 |
| 22 | S | 0.40 | 0/958 | 0.69 | 0/1289 |
| 23 | T | 0.61 | 2/417 (0.5%) | 0.68 | 0/562 |
| 24 | U | 0.36 | 0/502 | 0.60 | 0/675 |
| 25 | V | 0.43 | 0/1219 | 0.67 | 0/1655 |
| 26 | W | 0.41 | 0/664 | 0.65 | 0/895 |
| 27 | X | 0.43 | 0/1146 | 0.68 | 0/1536 |
| 28 | Y | 0.54 | 1/576 (0.2%) | 0.80 | 0/763 |
| 29 | Z | 0.54 | 0/438 | 0.78 | 2/578 (0.3%) |
| 30 | 1 | 0.43 | 0/399 | 0.58 | 0/527 |
| 31 | 2 | 0.73 | 2/771 (0.3%) | 0.72 | 0/1024 |
| All | All | 0.49 | 9/98339 (0.0%) | 0.70 | 33/147131 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 0 | 0 | 70 |
| 2 | 9 | 0 | 2 |
| 25 | V | 0 | 1 |
| All | All | 0 | 73 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 31 | 2 | 14 | CYS | CB-SG | -12.55 | 1.60 | 1.82 |
| 1 | 0 | 2102 | G | C6-O6 | -6.72 | 1.18 | 1.24 |
| 28 | Y | 60 | CYS | CB-SG | -6.10 | 1.71 | 1.82 |
| 1 | 0 | 2474 | A | N1-C2 | 5.85 | 1.39 | 1.34 |
| 23 | T | 9 | CYS | CB-SG | -5.75 | 1.72 | 1.81 |
| 31 | 2 | 74 | CYS | CB-SG | -5.65 | 1.72 | 1.81 |
| 1 | 0 | 456 | G | C6-O6 | -5.58 | 1.19 | 1.24 |
| 23 | T | 32 | CYS | CB-SG | -5.19 | 1.73 | 1.81 |
| 1 | 0 | 2474 | A | C5-C6 | 5.03 | 1.45 | 1.41 |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | 9 | 3024 | U | C2'-C3'-O3' | 8.48 | 128.16 | 109.50 |
| 1 | 0 | 1979 | G | C2'-C3'-O3' | 6.90 | 124.75 | 113.70 |
| 11 | H | 74 | ASN | N-CA-C | -6.85 | 92.50 | 111.00 |
| 2 | 9 | 3103 | A | C5'-C4'-O4' | 6.75 | 117.20 | 109.10 |
| 1 | 0 | 1563 | G | C2'-C3'-O3' | 6.72 | 124.45 | 113.70 |
| 1 | 0 | 871 | G | C5'-C4'-O4' | -6.35 | 101.48 | 109.10 |
| 1 | 0 | 1942 | A | C5'-C4'-O4' | -6.12 | 101.76 | 109.10 |
| 29 | Z | 34 | CYS | CA-CB-SG | -6.09 | 103.05 | 114.00 |
| 1 | 0 | 1559 | A | C2'-C3'-O3' | 6.08 | 123.42 | 113.70 |
| 19 | P | 68 | GLY | N-CA-C | -6.05 | 97.98 | 113.10 |
| 1 | 0 | 1120 | U | C5'-C4'-C3' | -5.95 | 106.48 | 116.00 |
| 15 | L | 52 | LEU | CB-CG-CD1 | -5.86 | 101.05 | 111.00 |
| 1 | 0 | 2338 | G | C2'-C3'-O3' | 5.85 | 123.06 | 113.70 |
| 1 | 0 | 1942 | A | C5'-C4'-C3' | 5.81 | 125.30 | 116.00 |
| 11 | H | 141 | ASN | N-CA-C | -5.75 | 95.47 | 111.00 |
| 29 | Z | 19 | CYS | CA-CB-SG | -5.71 | 103.72 | 114.00 |
| 1 | 0 | 2313 | C | C5'-C4'-O4' | 5.69 | 115.93 | 109.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 0 | 1819 | G | C5'-C4'-C3' | 5.58 | 124.92 | 116.00 |
| 1 | 0 | 2664 | A | N9-C1'-C2' | 5.56 | 121.22 | 114.00 |
| 1 | 0 | 2914 | A | C2'-C3'-O3' | 5.53 | 122.55 | 113.70 |
| 1 | 0 | 1342 | C | N1-C1'-C2' | -5.53 | 105.92 | 112.00 |
| 1 | 0 | 2316 | G | C5'-C4'-C3' | -5.44 | 107.29 | 116.00 |
| 1 | 0 | 2313 | C | O4'-C1'-N1 | 5.41 | 112.52 | 108.20 |
| 2 | 9 | 3039 | U | N1-C1'-C2' | 5.40 | 121.02 | 114.00 |
| 11 | H | 110 | GLY | N-CA-C | -5.39 | 99.61 | 113.10 |
| 1 | 0 | 206 | G | C5'-C4'-C3' | -5.39 | 107.38 | 116.00 |
| 1 | 0 | 535 | G | N9-C1'-C2' | 5.34 | 120.94 | 114.00 |
| 1 | 0 | 1592 | G | N9-C1'-C2' | 5.25 | 120.82 | 114.00 |
| 1 | 0 | 169 | A | C5'-C4'-O4' | -5.21 | 102.85 | 109.10 |
| 1 | 0 | 868 | G | O4'-C1'-N9 | 5.19 | 112.36 | 108.20 |
| 1 | 0 | 1863 | G | N9-C1'-C2' | -5.16 | 106.33 | 112.00 |
| 1 | 0 | 777 | U | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 1 | 0 | 2313 | C | C5'-C4'-C3' | 5.07 | 124.11 | 116.00 |

There are no chirality outliers.

All (73) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | 0 | 1055 | G | Sidechain |
| 1 | 0 | 1078 | A | Sidechain |
| 1 | 0 | 1226 | G | Sidechain |
| 1 | 0 | 1236 | A | Sidechain |
| 1 | 0 | 1309 | U | Sidechain |
| 1 | 0 | 1342 | C | Sidechain |
| 1 | 0 | 1417 | G | Sidechain |
| 1 | 0 | 1430 | G | Sidechain |
| 1 | 0 | 1595 | G | Sidechain |
| 1 | 0 | 1635 | U | Sidechain |
| 1 | 0 | 1744 | G | Sidechain |
| 1 | 0 | 1809 | G | Sidechain |
| 1 | 0 | 1819 | G | Sidechain |
| 1 | 0 | 182 | G | Sidechain |
| 1 | 0 | 1822 | A | Sidechain |
| 1 | 0 | 1829 | A | Sidechain |
| 1 | 0 | 1835 | U | Sidechain |
| 1 | 0 | 1845 | A | Sidechain |
| 1 | 0 | 1848 | G | Sidechain |
| 1 | 0 | 1861 | C | Sidechain |
| 1 | 0 | 1863 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | 0 | 1877 | G | Sidechain |
| 1 | 0 | 1878 | G | Sidechain |
| 1 | 0 | 1933 | G | Sidechain |
| 1 | 0 | 1978 | A | Sidechain |
| 1 | 0 | 202 | U | Sidechain |
| 1 | 0 | 2023 | G | Sidechain |
| 1 | 0 | 223 | G | Sidechain |
| 1 | 0 | 2312 | G | Sidechain |
| 1 | 0 | 2313 | C | Sidechain |
| 1 | 0 | 2316 | G | Sidechain |
| 1 | 0 | 2412 | G | Sidechain |
| 1 | 0 | 2465 | A | Sidechain |
| 1 | 0 | 2493 | C | Sidechain |
| 1 | 0 | 2503 | A | Sidechain |
| 1 | 0 | 2506 | A | Sidechain |
| 1 | 0 | 2526 | C | Sidechain |
| 1 | 0 | 2564 | G | Sidechain |
| 1 | 0 | 2607 | U | Sidechain |
| 1 | 0 | 261 | A | Sidechain |
| 1 | 0 | 2630 | G | Sidechain |
| 1 | 0 | 2637 | A | Sidechain |
| 1 | 0 | 2643 | G | Sidechain |
| 1 | 0 | 2673 | U | Sidechain |
| 1 | 0 | 2727 | A | Sidechain |
| 1 | 0 | 2729 | C | Sidechain |
| 1 | 0 | 2790 | C | Sidechain |
| 1 | 0 | 2793 | A | Sidechain |
| 1 | 0 | 2840 | A | Sidechain |
| 1 | 0 | 2853 | U | Sidechain |
| 1 | 0 | 324 | G | Sidechain |
| 1 | 0 | 333 | G | Sidechain |
| 1 | 0 | 396 | U | Sidechain |
| 1 | 0 | 422 | G | Sidechain |
| 1 | 0 | 469 | G | Sidechain |
| 1 | 0 | 482 | G | Sidechain |
| 1 | 0 | 518 | G | Sidechain |
| 1 | 0 | 532 | A | Sidechain |
| 1 | 0 | 619 | U | Sidechain |
| 1 | 0 | 664 | U | Sidechain |
| 1 | 0 | 722 | G | Sidechain |
| 1 | 0 | 781 | C | Sidechain |
| 1 | 0 | 791 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | 0 | 815 | U | Sidechain |
| 1 | 0 | 817 | G | Sidechain |
| 1 | 0 | 818 | A | Sidechain |
| 1 | 0 | 868 | G | Sidechain |
| 1 | 0 | 903 | U | Sidechain |
| 1 | 0 | 939 | A | Sidechain |
| 1 | 0 | 952 | G | Sidechain |
| 2 | 9 | 3065 | A | Sidechain |
| 2 | 9 | 3087 | U | Sidechain |
| 25 | V | 90 | TYR | Sidechain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 0 | 59017 | 0 | 29800 | 1222 | 0 |
| 2 | 9 | 2600 | 0 | 1326 | 88 | 0 |
| 3 | 4 | 59 | 0 | 35 | 2 | 0 |
| 4 | A | 1754 | 0 | 1763 | 127 | 0 |
| 5 | B | 2625 | 0 | 2533 | 170 | 0 |
| 6 | C | 1859 | 0 | 1816 | 112 | 0 |
| 7 | D | 1094 | 0 | 1085 | 125 | 0 |
| 8 | E | 1357 | 0 | 1266 | 65 | 0 |
| 9 | F | 886 | 0 | 854 | 67 | 0 |
| 10 | G | 240 | 0 | 231 | 22 | 0 |
| 11 | H | 1216 | 0 | 1215 | 155 | 0 |
| 12 | I | 1120 | 0 | 1098 | 69 | 0 |
| 13 | J | 994 | 0 | 1027 | 57 | 0 |
| 14 | K | 1118 | 0 | 1076 | 64 | 0 |
| 15 | L | 1606 | 0 | 1676 | 142 | 0 |
| 16 | M | 1445 | 0 | 1401 | 139 | 0 |
| 17 | N | 865 | 0 | 873 | 35 | 0 |
| 18 | O | 1133 | 0 | 1127 | 57 | 0 |
| 19 | P | 735 | 0 | 729 | 29 | 0 |
| 20 | Q | 1149 | 0 | 1122 | 61 | 0 |
| 21 | R | 641 | 0 | 605 | 24 | 0 |
| 22 | S | 950 | 0 | 923 | 53 | 0 |
| 23 | T | 410 | 0 | 364 | 33 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24 | U | 499 | 0 | 511 | 32 | 0 |
| 25 | V | 1196 | 0 | 1137 | 97 | 0 |
| 26 | W | 654 | 0 | 653 | 46 | 0 |
| 27 | X | 1130 | 0 | 1133 | 51 | 0 |
| 28 | Y | 564 | 0 | 598 | 54 | 0 |
| 29 | Z | 431 | 0 | 426 | 24 | 0 |
| 30 | 1 | 394 | 0 | 406 | 32 | 0 |
| 31 | 2 | 755 | 0 | 729 | 51 | 0 |
| 32 | 0 | 37 | 0 | 28 | 4 | 0 |
| 33 | 0 | 107 | 0 | 0 | 0 | 0 |
| 33 | 2 | 1 | 0 | 0 | 0 | 0 |
| 33 | 4 | 1 | 0 | 0 | 0 | 0 |
| 33 | 9 | 2 | 0 | 0 | 0 | 0 |
| 33 | A | 2 | 0 | 0 | 0 | 0 |
| 33 | B | 1 | 0 | 0 | 0 | 0 |
| 33 | J | 1 | 0 | 0 | 0 | 0 |
| 33 | S | 1 | 0 | 0 | 0 | 0 |
| 33 | X | 1 | 0 | 0 | 0 | 0 |
| 34 | 0 | 2 | 0 | 0 | 0 | 0 |
| 35 | 0 | 73 | 0 | 0 | 0 | 0 |
| 35 | 9 | 2 | 0 | 0 | 0 | 0 |
| 35 | A | 1 | 0 | 0 | 0 | 0 |
| 35 | C | 1 | 0 | 0 | 0 | 0 |
| 35 | H | 2 | 0 | 0 | 0 | 0 |
| 35 | I | 1 | 0 | 0 | 0 | 0 |
| 35 | K | 1 | 0 | 0 | 0 | 0 |
| 35 | L | 1 | 0 | 0 | 0 | 0 |
| 35 | P | 1 | 0 | 0 | 0 | 0 |
| 35 | Q | 2 | 0 | 0 | 0 | 0 |
| 35 | R | 1 | 0 | 0 | 0 | 0 |
| 36 | 0 | 8 | 0 | 0 | 1 | 0 |
| 36 | 2 | 1 | 0 | 0 | 0 | 0 |
| 36 | A | 1 | 0 | 0 | 0 | 0 |
| 36 | B | 1 | 0 | 0 | 0 | 0 |
| 36 | I | 3 | 0 | 0 | 1 | 0 |
| 36 | J | 1 | 0 | 0 | 0 | 0 |
| 36 | K | 1 | 0 | 0 | 0 | 0 |
| 36 | L | 1 | 0 | 0 | 1 | 0 |
| 36 | M | 1 | 0 | 0 | 1 | 0 |
| 36 | N | 1 | 0 | 0 | 0 | 0 |
| 36 | P | 1 | 0 | 0 | 0 | 0 |
| 36 | Q | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36 | X | 1 | 0 | 0 | 0 | 0 |
| 37 | 2 | 1 | 0 | 0 | 2 | 0 |
| 37 | N | 1 | 0 | 0 | 0 | 0 |
| 37 | T | 1 | 0 | 0 | 0 | 0 |
| 37 | Y | 1 | 0 | 0 | 0 | 0 |
| 37 | Z | 1 | 0 | 0 | 0 | 0 |
| 38 | 0 | 5806 | 0 | 0 | 72 | 0 |
| 38 | 1 | 45 | 0 | 0 | 1 | 0 |
| 38 | 2 | 76 | 0 | 0 | 4 | 0 |
| 38 | 4 | 1 | 0 | 0 | 0 | 0 |
| 38 | 9 | 147 | 0 | 0 | 5 | 0 |
| 38 | A | 136 | 0 | 0 | 11 | 0 |
| 38 | B | 160 | 0 | 0 | 17 | 0 |
| 38 | C | 180 | 0 | 0 | 10 | 0 |
| 38 | D | 49 | 0 | 0 | 8 | 0 |
| 38 | E | 47 | 0 | 0 | 1 | 0 |
| 38 | F | 26 | 0 | 0 | 6 | 0 |
| 38 | G | 21 | 0 | 0 | 2 | 0 |
| 38 | H | 82 | 0 | 0 | 9 | 0 |
| 38 | I | 61 | 0 | 0 | 3 | 0 |
| 38 | J | 63 | 0 | 0 | 4 | 0 |
| 38 | K | 85 | 0 | 0 | 9 | 0 |
| 38 | L | 130 | 0 | 0 | 5 | 0 |
| 38 | M | 69 | 0 | 0 | 8 | 0 |
| 38 | N | 45 | 0 | 0 | 5 | 0 |
| 38 | O | 70 | 0 | 0 | 0 | 0 |
| 38 | P | 56 | 0 | 0 | 1 | 0 |
| 38 | Q | 92 | 0 | 0 | 4 | 0 |
| 38 | R | 40 | 0 | 0 | 1 | 0 |
| 38 | S | 37 | 0 | 0 | 3 | 0 |
| 38 | T | 27 | 0 | 0 | 2 | 0 |
| 38 | U | 13 | 0 | 0 | 1 | 0 |
| 38 | V | 74 | 0 | 0 | 6 | 0 |
| 38 | W | 29 | 0 | 0 | 3 | 0 |
| 38 | X | 105 | 0 | 0 | 4 | 0 |
| 38 | Y | 41 | 0 | 0 | 5 | 0 |
| 38 | Z | 57 | 0 | 0 | 1 | 0 |
| All | All | 98635 | 0 | 59566 | 2990 | 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 20.

All (2990) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:U:12:THR:HG22 | 24:U:15:GLU:HG3 | 1.24 | 1.14 |
| 13:J:10:GLN:NE2 | 13:J:10:GLN:H | 1.47 | 1.13 |
| 1:O:871:G:H8 | 1:O:871:G:H5' | 1.13 | 1.10 |
| 11:H:86:ARG:NH1 | 11:H:133:ILE:HG13 | 1.66 | 1.08 |
| 15:L:87:MET:HB3 | 31:2:46:ILE:HD13 | 1.31 | 1.07 |
| 6:C:236:THR:HG22 | 6:C:239:ALA:H | 1.17 | 1.07 |
| 15:L:164:THR:HG22 | 15:L:167:GLY:H | 1.20 | 1.06 |
| 1:O:1160:G:H5' | 1:O:1161:A:H5' | 1.33 | 1.06 |
| 1:O:871:G:C8 | 1:O:871:G:H5' | 1.90 | 1.06 |
| 13:J:10:GLN:N | 13:J:10:GLN:HE21 | 1.54 | 1.05 |
| 22:S:71:VAL:HG11 | 22:S:90:PRO:HB3 | 1.37 | 1.05 |
| 6:C:127:ARG:NH2 | 6:C:225:PRO:HG2 | 1.74 | 1.03 |
| 1:O:156:C:H5'' | 15:L:171:ARG:HD3 | 1.36 | 1.03 |
| 2:9:3023:U:H3' | 2:9:3024:U:H5'' | 1.39 | 1.03 |
| 11:H:86:ARG:HH11 | 11:H:133:ILE:HG13 | 0.87 | 1.02 |
| 2:9:3056:A:H2' | 2:9:3057:A:H5'' | 1.40 | 1.02 |
| 1:O:1119:G:H2' | 12:I:52:GLN:HE22 | 1.25 | 1.02 |
| 15:L:106:ASN:ND2 | 36:L:8518:CL:CL | 2.30 | 1.02 |
| 6:C:5:ILE:HD11 | 6:C:16:VAL:HG23 | 1.43 | 1.01 |
| 11:H:45:GLN:HB3 | 11:H:163:PRO:HD2 | 1.42 | 0.99 |
| 1:O:1751:G:H2' | 1:O:1752:G:H5'' | 1.44 | 0.99 |
| 2:9:3076:G:H3' | 2:9:3077:A:H5'' | 1.44 | 0.99 |
| 5:B:238:ASN:HD22 | 5:B:240:GLY:H | 1.08 | 0.98 |
| 13:J:62:PRO:HG3 | 13:J:65:ARG:HH21 | 1.29 | 0.96 |
| 11:H:162:SER:HB2 | 11:H:163:PRO:HD3 | 1.46 | 0.95 |
| 7:D:105:SER:HB2 | 7:D:131:THR:HG23 | 1.49 | 0.95 |
| 5:B:162:MET:HE3 | 5:B:308:LEU:HD21 | 1.46 | 0.95 |
| 6:C:115:LEU:HD13 | 6:C:223:LEU:HD21 | 1.49 | 0.95 |
| 11:H:86:ARG:HH11 | 11:H:133:ILE:CG1 | 1.80 | 0.94 |
| 1:O:1164:U:H4' | 1:O:1165:G:OP1 | 1.68 | 0.94 |
| 31:2:71:CYS:HG | 37:2:8404:CD:CD | 0.84 | 0.94 |
| 1:O:289:G:H22 | 1:O:363:A:H2 | 1.14 | 0.93 |
| 16:M:47:LEU:HD11 | 16:M:127:LEU:HD21 | 1.49 | 0.93 |
| 7:D:134:LEU:HD11 | 7:D:166:ILE:HD11 | 1.50 | 0.93 |
| 11:H:29:ALA:HB3 | 11:H:65:ARG:HH12 | 1.31 | 0.92 |
| 1:O:545:G:H8 | 1:O:545:G:H5' | 1.34 | 0.92 |
| 1:O:870:G:H2' | 1:O:871:G:H5'' | 1.51 | 0.92 |
| 1:O:1242:A:H5' | 12:I:82:THR:HG23 | 1.51 | 0.92 |
| 2:9:3006:C:H5'' | 16:M:37:ARG:NH1 | 1.85 | 0.92 |
| 11:H:26:LYS:HD2 | 11:H:28:ILE:HD12 | 1.50 | 0.91 |
| 28:Y:46:LYS:HD3 | 28:Y:59:HIS:HB2 | 1.52 | 0.91 |
| 26:W:37:LEU:HD13 | 26:W:85:VAL:HG21 | 1.50 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1134:G:H4' | 11:H:151:MET:HE1 | 1.53 | 0.90 |
| 1:0:2812:A:H2 | 1:0:2814:A:H62 | 1.14 | 0.90 |
| 31:2:71:CYS:SG | 37:2:8404:CD:CD | 1.79 | 0.90 |
| 18:O:115:SER:H | 18:O:118:GLN:HE21 | 0.96 | 0.89 |
| 1:0:182:G:H4' | 15:L:157:LEU:HD13 | 1.51 | 0.89 |
| 11:H:55:GLN:HE21 | 11:H:124:ARG:HE | 1.14 | 0.89 |
| 28:Y:38:LYS:HG2 | 28:Y:45:LYS:HG2 | 1.54 | 0.89 |
| 2:9:3024:U:O2' | 2:9:3025:G:H4' | 1.73 | 0.88 |
| 7:D:25:MET:HE2 | 7:D:41:LEU:HG | 1.54 | 0.88 |
| 1:0:1120:U:H6 | 1:0:1120:U:H5'' | 1.39 | 0.88 |
| 15:L:102:GLU:OE1 | 15:L:164:THR:HG21 | 1.72 | 0.88 |
| 27:X:187:VAL:HG23 | 27:X:192:ASP:HB2 | 1.56 | 0.88 |
| 26:W:15:ARG:HH11 | 26:W:15:ARG:HB3 | 1.37 | 0.87 |
| 5:B:264:GLU:HG2 | 5:B:267:LYS:HE2 | 1.57 | 0.87 |
| 7:D:154:LYS:HD2 | 7:D:154:LYS:H | 1.38 | 0.87 |
| 7:D:27:ILE:HG22 | 7:D:28:GLY:H | 1.37 | 0.87 |
| 11:H:139:ASP:N | 11:H:140:PRO:HD3 | 1.90 | 0.87 |
| 1:0:1116:U:O2' | 1:0:1118:A:H2 | 1.56 | 0.86 |
| 16:M:49:THR:HG22 | 16:M:56:ASP:HB2 | 1.56 | 0.86 |
| 20:Q:99:ALA:HB1 | 20:Q:109:MET:HE1 | 1.55 | 0.86 |
| 25:V:72:PRO:HG2 | 25:V:77:ALA:HB3 | 1.57 | 0.86 |
| 1:0:1835:U:H5 | 1:0:1840:A:N7 | 1.74 | 0.86 |
| 11:H:162:SER:HB2 | 11:H:163:PRO:CD | 2.06 | 0.85 |
| 25:V:4:LEU:HD22 | 25:V:52:VAL:HG21 | 1.59 | 0.85 |
| 25:V:88:THR:HG23 | 25:V:110:GLN:NE2 | 1.91 | 0.85 |
| 7:D:25:MET:HE1 | 7:D:37:ALA:HB1 | 1.58 | 0.85 |
| 11:H:26:LYS:HG2 | 11:H:28:ILE:H | 1.42 | 0.84 |
| 1:0:2717:C:C2' | 1:0:2718:C:H5'' | 2.07 | 0.84 |
| 30:1:41:HIS:H | 30:1:45:ASN:HD22 | 1.24 | 0.84 |
| 1:0:506:G:H22 | 1:0:509:A:H5' | 1.42 | 0.84 |
| 18:O:103:THR:HA | 18:O:106:ARG:NH1 | 1.91 | 0.84 |
| 25:V:6:GLN:HB2 | 25:V:26:ILE:HD12 | 1.58 | 0.84 |
| 15:L:35:PRO:CG | 15:L:38:VAL:HG23 | 2.06 | 0.83 |
| 1:0:2506:A:HO2' | 1:0:2507:G:H8 | 0.85 | 0.83 |
| 1:0:56:G:H5'' | 24:U:50:ARG:HH12 | 1.43 | 0.83 |
| 8:E:6:GLU:HA | 8:E:46:THR:HG22 | 1.58 | 0.83 |
| 28:Y:38:LYS:HE2 | 28:Y:45:LYS:HE2 | 1.60 | 0.83 |
| 12:I:131:THR:HG22 | 12:I:134:GLU:H | 1.44 | 0.83 |
| 1:0:1771:U:H4' | 28:Y:20:LEU:HD21 | 1.61 | 0.83 |
| 1:0:2717:C:H2' | 1:0:2718:C:H5'' | 1.57 | 0.83 |
| 9:F:63:ILE:HB | 9:F:64:PRO:HD3 | 1.57 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:2502:C:C2' | 1:O:2503:A:H5' | 2.09 | 0.83 |
| 5:B:212:GLN:HB2 | 5:B:257:THR:HG21 | 1.61 | 0.83 |
| 18:O:115:SER:N | 18:O:118:GLN:HE21 | 1.76 | 0.83 |
| 25:V:122:ARG:HH11 | 25:V:122:ARG:HG2 | 1.42 | 0.83 |
| 25:V:88:THR:HG22 | 25:V:89:ASP:H | 1.44 | 0.83 |
| 8:E:23:GLU:HG2 | 8:E:28:SER:HB3 | 1.62 | 0.82 |
| 11:H:27:LYS:H | 11:H:58:HIS:HD2 | 1.23 | 0.82 |
| 15:L:106:ASN:HD22 | 15:L:114:VAL:HG23 | 1.44 | 0.82 |
| 26:W:76:ARG:HG3 | 26:W:76:ARG:HH11 | 1.44 | 0.82 |
| 7:D:37:ALA:O | 7:D:40:ILE:HG12 | 1.80 | 0.82 |
| 4:A:194:MET:HE2 | 4:A:199:HIS:HB2 | 1.62 | 0.82 |
| 1:O:2502:C:H2' | 1:O:2503:A:H5' | 1.62 | 0.82 |
| 1:O:1450:C:H4' | 1:O:1451:C:OP2 | 1.78 | 0.82 |
| 2:9:3023:U:H3' | 2:9:3024:U:C5' | 2.10 | 0.82 |
| 13:J:74:VAL:HG11 | 13:J:113:ILE:HG12 | 1.62 | 0.82 |
| 1:O:21:G:H5' | 20:Q:2:ILE:HA | 1.61 | 0.82 |
| 28:Y:28:ASP:O | 28:Y:31:ILE:HG22 | 1.79 | 0.82 |
| 15:L:87:MET:HB2 | 15:L:91:ILE:HD11 | 1.61 | 0.81 |
| 5:B:27:ASN:H | 5:B:27:ASN:HD22 | 1.25 | 0.81 |
| 1:O:2506:A:O2' | 1:O:2507:G:H8 | 1.64 | 0.81 |
| 1:O:506:G:H22 | 1:O:509:A:C5' | 1.93 | 0.81 |
| 6:C:142:ASP:OD1 | 6:C:237:GLU:HB3 | 1.81 | 0.81 |
| 1:O:1603:A:H5' | 1:O:1605:G:O4' | 1.80 | 0.81 |
| 6:C:162:VAL:HG12 | 6:C:192:ILE:HD11 | 1.62 | 0.81 |
| 1:O:870:G:C2' | 1:O:871:G:H5'' | 2.11 | 0.81 |
| 22:S:9:LYS:HE3 | 22:S:13:ARG:NH1 | 1.95 | 0.81 |
| 1:O:2533:C:H5' | 1:O:2533:C:H6 | 1.46 | 0.81 |
| 13:J:39:GLY:HA2 | 38:J:4183:HOH:O | 1.78 | 0.80 |
| 24:U:1:THR:HG23 | 24:U:2:VAL:H | 1.46 | 0.80 |
| 25:V:137:GLN:HE21 | 25:V:141:HIS:HE1 | 1.26 | 0.80 |
| 12:I:74:ARG:HB3 | 12:I:74:ARG:HH11 | 1.44 | 0.80 |
| 28:Y:37:HIS:HB2 | 28:Y:47:LEU:HB2 | 1.63 | 0.80 |
| 1:O:450:C:OP1 | 6:C:184:ARG:NH2 | 2.15 | 0.80 |
| 2:9:3056:A:C2' | 2:9:3057:A:H5'' | 2.12 | 0.80 |
| 20:Q:39:THR:HG22 | 20:Q:42:GLU:H | 1.47 | 0.79 |
| 11:H:45:GLN:HE21 | 11:H:135:TRP:HE1 | 1.31 | 0.79 |
| 1:O:2586:U:H3 | 1:O:2592:G:H22 | 1.30 | 0.79 |
| 4:A:36:ASP:OD2 | 4:A:85:ASP:HB2 | 1.83 | 0.79 |
| 11:H:139:ASP:H | 11:H:140:PRO:HD3 | 1.47 | 0.79 |
| 1:O:2526:C:O2' | 1:O:2527:U:H5' | 1.82 | 0.79 |
| 4:A:194:MET:CE | 4:A:199:HIS:HB2 | 2.13 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:M:87:LEU:HD12 | 16:M:186:LEU:HD21 | 1.65 | 0.79 |
| 5:B:304:PRO:HD2 | 5:B:307:ARG:HD2 | 1.64 | 0.79 |
| 5:B:195:ARG:HG2 | 5:B:323:LEU:HD22 | 1.63 | 0.79 |
| 5:B:18:ARG:HG3 | 5:B:256:GLN:HG3 | 1.64 | 0.79 |
| 31:2:70:ARG:HG2 | 31:2:77:ALA:HB2 | 1.65 | 0.78 |
| 2:9:3025:G:H3' | 2:9:3026:C:C5' | 2.13 | 0.78 |
| 1:0:1201:C:H5'' | 38:0:7119:HOH:O | 1.83 | 0.78 |
| 8:E:20:ILE:HD11 | 8:E:40:VAL:HG11 | 1.64 | 0.78 |
| 1:0:2420:G:O2' | 1:0:2421:G:H5' | 1.82 | 0.78 |
| 4:A:69:LEU:HD21 | 4:A:120:ARG:HB3 | 1.65 | 0.78 |
| 5:B:201:ASP:HB2 | 5:B:312:ARG:HD2 | 1.64 | 0.78 |
| 8:E:107:PHE:CE2 | 8:E:108:LEU:HD13 | 2.19 | 0.78 |
| 15:L:139:PRO:O | 15:L:140:ALA:HB3 | 1.81 | 0.78 |
| 1:0:2679:G:H2' | 1:0:2681:A:OP2 | 1.82 | 0.78 |
| 24:U:12:THR:HG22 | 24:U:15:GLU:CG | 2.12 | 0.78 |
| 1:0:1474:C:H5' | 1:0:1474:C:H6 | 1.49 | 0.78 |
| 1:0:1164:U:H3 | 1:0:1192:A:H2 | 1.32 | 0.77 |
| 9:F:46:GLU:O | 9:F:73:PRO:HD2 | 1.85 | 0.77 |
| 1:0:542:A:H5' | 1:0:542:A:H8 | 1.48 | 0.77 |
| 13:J:14:LYS:HB2 | 13:J:45:PRO:HG2 | 1.65 | 0.77 |
| 21:R:33:SER:O | 21:R:37:VAL:HG23 | 1.84 | 0.77 |
| 9:F:2:VAL:HG22 | 9:F:57:GLU:OE1 | 1.85 | 0.77 |
| 1:0:1119:G:H2' | 12:I:52:GLN:NE2 | 1.98 | 0.77 |
| 6:C:236:THR:HG22 | 6:C:239:ALA:N | 1.98 | 0.77 |
| 18:O:115:SER:OG | 18:O:118:GLN:HG3 | 1.84 | 0.77 |
| 26:W:41:PHE:O | 26:W:43:VAL:HG23 | 1.83 | 0.77 |
| 20:Q:8:ALA:HB1 | 20:Q:13:THR:HG21 | 1.66 | 0.77 |
| 26:W:72:VAL:HG22 | 26:W:85:VAL:HG12 | 1.64 | 0.77 |
| 15:L:164:THR:HG23 | 15:L:165:SER:N | 2.00 | 0.77 |
| 20:Q:44:VAL:O | 20:Q:48:GLU:HG3 | 1.85 | 0.77 |
| 2:9:3025:G:H3' | 2:9:3026:C:H5' | 1.64 | 0.77 |
| 1:0:1166:A:H1' | 1:0:1192:A:C2 | 2.19 | 0.76 |
| 1:0:240:C:H4' | 15:L:146:GLN:NE2 | 2.00 | 0.76 |
| 20:Q:99:ALA:HB1 | 20:Q:109:MET:CE | 2.14 | 0.76 |
| 1:0:1116:U:H3 | 1:0:1246:A:H62 | 1.30 | 0.76 |
| 1:0:2094:G:H4' | 5:B:245:SER:HB3 | 1.66 | 0.76 |
| 13:J:29:LEU:HB3 | 13:J:55:VAL:HG11 | 1.65 | 0.76 |
| 25:V:88:THR:HB | 38:V:6679:HOH:O | 1.83 | 0.76 |
| 1:0:1119:G:N2 | 1:0:1246:A:C2 | 2.52 | 0.76 |
| 1:0:282:C:H1' | 1:0:368:C:N4 | 2.00 | 0.76 |
| 25:V:13:MET:HE3 | 25:V:17:ILE:HG22 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:V:21:LEU:HD22 | 25:V:26:ILE:HD11 | 1.67 | 0.76 |
| 5:B:238:ASN:ND2 | 5:B:240:GLY:H | 1.81 | 0.76 |
| 7:D:19:GLU:O | 7:D:20:LYS:HG2 | 1.85 | 0.76 |
| 25:V:4:LEU:HD23 | 25:V:54:PHE:HB3 | 1.67 | 0.76 |
| 4:A:211:LYS:HB3 | 4:A:212:PRO:HD2 | 1.66 | 0.76 |
| 16:M:7:LYS:HE3 | 19:P:21:ARG:O | 1.86 | 0.76 |
| 11:H:75:SER:O | 11:H:79:ALA:HB2 | 1.86 | 0.76 |
| 1:O:1751:G:C2' | 1:O:1752:G:H5'' | 2.15 | 0.76 |
| 2:9:3069:U:OP1 | 16:M:4:PRO:HG3 | 1.86 | 0.76 |
| 4:A:35:GLY:O | 4:A:36:ASP:HB3 | 1.86 | 0.76 |
| 20:Q:106:GLY:HA2 | 20:Q:109:MET:HE3 | 1.67 | 0.76 |
| 1:O:794:U:H3 | 1:O:819:A:H61 | 1.34 | 0.76 |
| 12:I:52:GLN:HG3 | 12:I:53:ILE:N | 1.99 | 0.76 |
| 1:O:2694:A:H4' | 8:E:91:PHE:HE1 | 1.50 | 0.75 |
| 14:K:136:ALA:HB3 | 38:K:8579:HOH:O | 1.86 | 0.75 |
| 1:O:656:G:OP2 | 17:N:37:ARG:HD2 | 1.87 | 0.75 |
| 1:O:871:G:H8 | 1:O:871:G:C5' | 1.95 | 0.75 |
| 11:H:55:GLN:NE2 | 11:H:124:ARG:HE | 1.85 | 0.75 |
| 1:O:1206:U:H6 | 1:O:1206:U:H5' | 1.50 | 0.75 |
| 15:L:60:ILE:C | 15:L:61:ILE:HD12 | 2.07 | 0.75 |
| 18:O:59:ARG:NH2 | 18:O:66:GLN:HE22 | 1.85 | 0.75 |
| 1:O:1116:U:HO2' | 1:O:1118:A:H2 | 0.77 | 0.75 |
| 5:B:125:GLU:O | 5:B:129:ARG:HG3 | 1.86 | 0.75 |
| 8:E:15:GLN:HG3 | 8:E:20:ILE:HG12 | 1.68 | 0.75 |
| 1:O:2502:C:H4' | 11:H:151:MET:HG2 | 1.67 | 0.75 |
| 11:H:162:SER:CB | 11:H:163:PRO:HD3 | 2.16 | 0.75 |
| 1:O:2890:A:H1' | 23:T:56:ARG:NH2 | 2.02 | 0.75 |
| 6:C:139:VAL:HG13 | 38:C:8461:HOH:O | 1.85 | 0.75 |
| 27:X:187:VAL:HG23 | 27:X:192:ASP:CB | 2.17 | 0.75 |
| 16:M:113:SER:HB2 | 38:M:8559:HOH:O | 1.86 | 0.74 |
| 31:2:25:VAL:HG22 | 31:2:68:LYS:HG3 | 1.68 | 0.74 |
| 1:O:21:G:C5' | 20:Q:2:ILE:HA | 2.17 | 0.74 |
| 10:G:12:ILE:N | 10:G:13:PRO:HD3 | 2.01 | 0.74 |
| 1:O:1120:U:H5'' | 1:O:1120:U:C6 | 2.22 | 0.74 |
| 1:O:962:C:H1' | 16:M:5:ARG:NH1 | 2.03 | 0.74 |
| 16:M:11:ARG:HG3 | 16:M:14:ARG:NH1 | 2.03 | 0.74 |
| 6:C:162:VAL:HG13 | 6:C:232:LEU:HD21 | 1.70 | 0.74 |
| 21:R:51:GLN:HE21 | 21:R:53:ASN:HD21 | 1.34 | 0.74 |
| 1:O:1160:G:H5' | 1:O:1161:A:C5' | 2.16 | 0.74 |
| 7:D:146:LYS:NZ | 16:M:107:ASN:HD21 | 1.86 | 0.74 |
| 17:N:32:ARG:O | 17:N:32:ARG:HD3 | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:C:78:ARG:HG3 | 6:C:78:ARG:HH11 | 1.52 | 0.73 |
| 1:O:284:C:H4' | 1:O:285:A:O5' | 1.87 | 0.73 |
| 16:M:86:LEU:HD12 | 16:M:125:ALA:HB2 | 1.71 | 0.73 |
| 7:D:22:VAL:HG22 | 7:D:74:THR:HG22 | 1.70 | 0.73 |
| 9:F:91:VAL:HG12 | 9:F:92:GLY:N | 2.03 | 0.73 |
| 11:H:47:GLU:HB3 | 11:H:133:ILE:HD13 | 1.70 | 0.73 |
| 13:J:62:PRO:HG3 | 13:J:65:ARG:NH2 | 2.03 | 0.73 |
| 5:B:119:HIS:O | 5:B:121:PRO:HD3 | 1.89 | 0.73 |
| 1:O:56:G:H5'' | 24:U:50:ARG:NH1 | 2.02 | 0.73 |
| 5:B:297:VAL:HB | 38:B:8619:HOH:O | 1.88 | 0.73 |
| 1:O:1834:C:H2' | 1:O:1840:A:N6 | 2.03 | 0.73 |
| 1:O:2507:G:H2' | 1:O:2510:C:H42 | 1.52 | 0.73 |
| 11:H:53:PRO:HG3 | 11:H:127:GLY:H | 1.52 | 0.73 |
| 15:L:104:ARG:O | 15:L:108:LYS:HE2 | 1.88 | 0.73 |
| 25:V:13:MET:HE1 | 25:V:18:GLN:HA | 1.69 | 0.73 |
| 1:O:2851:G:O2' | 1:O:2852:A:H5' | 1.87 | 0.73 |
| 7:D:57:THR:HG23 | 7:D:63:ILE:HG22 | 1.71 | 0.73 |
| 1:O:1080:C:H4' | 1:O:1081:A:OP1 | 1.87 | 0.73 |
| 7:D:135:VAL:HG21 | 7:D:139:TYR:CD1 | 2.24 | 0.72 |
| 11:H:59:ASN:HD22 | 11:H:59:ASN:N | 1.87 | 0.72 |
| 2:9:3092:G:H2' | 2:9:3093:A:C8 | 2.24 | 0.72 |
| 11:H:130:HIS:CD2 | 11:H:133:ILE:HD11 | 2.24 | 0.72 |
| 11:H:56:ILE:HG22 | 11:H:61:LEU:HD22 | 1.70 | 0.72 |
| 1:O:541:C:C2' | 1:O:542:A:H5'' | 2.20 | 0.72 |
| 1:O:545:G:C8 | 1:O:545:G:H5' | 2.23 | 0.72 |
| 7:D:41:LEU:HA | 7:D:44:ILE:HG22 | 1.72 | 0.72 |
| 7:D:88:LEU:HB2 | 7:D:89:PRO:HD3 | 1.71 | 0.72 |
| 16:M:184:ILE:HG22 | 16:M:185:GLU:HG3 | 1.70 | 0.72 |
| 1:O:603:A:H5'' | 1:O:604:G:OP1 | 1.88 | 0.72 |
| 10:G:16:LYS:O | 10:G:20:VAL:HG23 | 1.89 | 0.72 |
| 1:O:447:A:OP1 | 22:S:2:LYS:HG2 | 1.90 | 0.72 |
| 14:K:143:THR:HG22 | 14:K:145:LEU:H | 1.54 | 0.72 |
| 16:M:159:TYR:HB3 | 16:M:162:ASP:HB2 | 1.72 | 0.72 |
| 16:M:89:GLY:O | 16:M:92:ALA:HB3 | 1.89 | 0.72 |
| 20:Q:9:ASP:O | 20:Q:13:THR:HB | 1.90 | 0.72 |
| 8:E:23:GLU:HG2 | 8:E:28:SER:CB | 2.20 | 0.72 |
| 1:O:121:U:OP2 | 30:1:10:ARG:NH2 | 2.23 | 0.71 |
| 8:E:11:VAL:HG12 | 8:E:12:ASP:N | 2.04 | 0.71 |
| 1:O:289:G:N2 | 1:O:363:A:H2 | 1.86 | 0.71 |
| 1:O:1118:A:H3' | 1:O:1118:A:C8 | 2.25 | 0.71 |
| 7:D:99:ASP:HB3 | 7:D:103:ASN:H | 1.56 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:J:109:LEU:HD13 | 13:J:113:ILE:HD11 | 1.72 | 0.71 |
| 25:V:21:LEU:HD22 | 25:V:26:ILE:CD1 | 2.21 | 0.71 |
| 1:0:541:C:H2' | 1:0:542:A:H5'' | 1.71 | 0.71 |
| 7:D:105:SER:CB | 7:D:131:THR:HG23 | 2.19 | 0.71 |
| 1:0:1160:G:C5' | 1:0:1161:A:H5' | 2.14 | 0.71 |
| 1:0:2827:A:H2' | 1:0:2828:G:O4' | 1.89 | 0.71 |
| 4:A:217:ARG:HG2 | 4:A:229:ALA:HB2 | 1.71 | 0.71 |
| 11:H:28:ILE:HA | 11:H:62:GLU:OE1 | 1.90 | 0.71 |
| 2:9:3048:C:H4' | 16:M:141:ARG:HH21 | 1.55 | 0.71 |
| 20:Q:14:ALA:HB3 | 20:Q:147:LEU:HB2 | 1.72 | 0.71 |
| 25:V:88:THR:HG22 | 25:V:89:ASP:N | 2.05 | 0.71 |
| 25:V:4:LEU:HD22 | 25:V:52:VAL:CG2 | 2.20 | 0.71 |
| 24:U:39:ALA:N | 24:U:40:PRO:HD2 | 2.06 | 0.71 |
| 16:M:144:GLY:O | 16:M:147:ILE:HG22 | 1.90 | 0.71 |
| 6:C:127:ARG:HG2 | 6:C:127:ARG:HH11 | 1.56 | 0.71 |
| 12:I:93:ARG:HB3 | 12:I:93:ARG:HH11 | 1.56 | 0.71 |
| 23:T:9:CYS:HA | 23:T:52:THR:HG23 | 1.72 | 0.71 |
| 31:2:17:HIS:O | 31:2:18:GLN:HG3 | 1.90 | 0.71 |
| 5:B:24:PRO:CG | 5:B:204:GLY:HA2 | 2.21 | 0.71 |
| 11:H:137:ASN:O | 11:H:139:ASP:N | 2.23 | 0.71 |
| 1:0:1328:A:OP1 | 27:X:169:ARG:HD2 | 1.90 | 0.70 |
| 7:D:64:ARG:HG2 | 7:D:67:ASP:HB3 | 1.73 | 0.70 |
| 11:H:55:GLN:HE21 | 11:H:124:ARG:NE | 1.89 | 0.70 |
| 26:W:78:GLU:HG2 | 26:W:79:GLU:H | 1.56 | 0.70 |
| 1:0:1185:U:H2' | 1:0:1186:C:C6 | 2.27 | 0.70 |
| 1:0:2256:G:O2' | 1:0:2257:G:H5' | 1.89 | 0.70 |
| 25:V:88:THR:HG23 | 25:V:110:GLN:HE21 | 1.54 | 0.70 |
| 1:0:31:C:H4' | 38:S:7242:HOH:O | 1.90 | 0.70 |
| 15:L:34:GLU:HB3 | 15:L:35:PRO:HD2 | 1.74 | 0.70 |
| 1:0:1805:G:H2' | 1:0:1806:G:H8 | 1.56 | 0.70 |
| 1:0:2716:G:H5'' | 5:B:206:THR:HG21 | 1.72 | 0.70 |
| 4:A:88:ILE:HD13 | 4:A:100:PRO:HD3 | 1.74 | 0.70 |
| 11:H:35:ASN:ND2 | 11:H:80:ASN:HA | 2.07 | 0.70 |
| 28:Y:40:PRO:HD3 | 28:Y:47:LEU:HD11 | 1.73 | 0.70 |
| 1:0:1535:G:H2' | 1:0:1536:C:C6 | 2.27 | 0.70 |
| 20:Q:18:LEU:HB2 | 20:Q:143:VAL:HG12 | 1.72 | 0.70 |
| 27:X:189:ASN:C | 27:X:189:ASN:HD22 | 1.95 | 0.70 |
| 1:0:1684:A:H1' | 30:1:43:ARG:HH22 | 1.55 | 0.70 |
| 29:Z:25:LYS:HD2 | 30:1:49:GLU:H | 1.55 | 0.70 |
| 16:M:138:ASP:O | 16:M:140:GLN:N | 2.23 | 0.70 |
| 1:0:371:U:H2' | 1:0:372:A:H8 | 1.57 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:D:27:ILE:HG22 | 7:D:28:GLY:N | 2.07 | 0.70 |
| 9:F:58:GLU:HA | 9:F:61:MET:HG3 | 1.72 | 0.70 |
| 23:T:52:THR:HG22 | 23:T:54:THR:H | 1.57 | 0.70 |
| 4:A:190:ARG:NH2 | 4:A:207:GLN:OE1 | 2.24 | 0.70 |
| 23:T:39:ASN:ND2 | 23:T:44:ARG:HH11 | 1.89 | 0.70 |
| 4:A:94:LEU:HG | 4:A:99:ILE:HD11 | 1.73 | 0.69 |
| 26:W:71:ARG:HB3 | 26:W:88:GLU:OE1 | 1.92 | 0.69 |
| 6:C:115:LEU:O | 6:C:118:THR:HB | 1.92 | 0.69 |
| 1:O:2694:A:H4' | 8:E:91:PHE:CE1 | 2.26 | 0.69 |
| 1:O:1165:G:H4' | 1:O:1174:A:O2' | 1.91 | 0.69 |
| 4:A:51:ARG:HB2 | 38:A:8617:HOH:O | 1.91 | 0.69 |
| 15:L:139:PRO:O | 15:L:140:ALA:CB | 2.39 | 0.69 |
| 5:B:177:HIS:O | 5:B:181:ILE:HG13 | 1.93 | 0.69 |
| 16:M:132:ASN:O | 16:M:135:VAL:HG12 | 1.92 | 0.69 |
| 16:M:48:VAL:CG1 | 16:M:55:ASP:HB3 | 2.22 | 0.69 |
| 6:C:107:ARG:NH1 | 6:C:107:ARG:HB3 | 2.07 | 0.69 |
| 16:M:119:GLN:O | 16:M:123:ILE:HG13 | 1.93 | 0.69 |
| 6:C:236:THR:CG2 | 6:C:239:ALA:H | 2.01 | 0.69 |
| 14:K:133:VAL:HA | 38:K:8579:HOH:O | 1.91 | 0.69 |
| 11:H:45:GLN:HG3 | 11:H:135:TRP:NE1 | 2.08 | 0.69 |
| 1:O:236:A:H4' | 1:O:237:G:H5' | 1.75 | 0.69 |
| 5:B:55:ASN:HB3 | 5:B:63:GLU:HA | 1.73 | 0.69 |
| 1:O:1130:U:H2' | 1:O:1131:G:O4' | 1.93 | 0.69 |
| 1:O:1926:G:H2' | 1:O:1927:A:H8 | 1.58 | 0.69 |
| 26:W:15:ARG:NH1 | 26:W:15:ARG:HB3 | 2.06 | 0.69 |
| 1:O:1942:A:H3' | 38:O:8223:HOH:O | 1.92 | 0.69 |
| 8:E:20:ILE:CD1 | 8:E:40:VAL:HG11 | 2.22 | 0.69 |
| 20:Q:39:THR:HG23 | 20:Q:107:GLU:O | 1.93 | 0.69 |
| 1:O:560:C:H42 | 1:O:597:A:H61 | 1.41 | 0.68 |
| 5:B:321:PRO:HA | 38:B:8672:HOH:O | 1.92 | 0.68 |
| 15:L:35:PRO:HG2 | 15:L:38:VAL:HG23 | 1.75 | 0.68 |
| 22:S:32:ARG:NH1 | 22:S:38:ARG:HH12 | 1.90 | 0.68 |
| 1:O:1118:A:H3' | 1:O:1118:A:H8 | 1.57 | 0.68 |
| 1:O:2908:A:H2' | 1:O:2909:G:O4' | 1.94 | 0.68 |
| 1:O:285:A:H2' | 1:O:286:U:O4' | 1.94 | 0.68 |
| 4:A:153:ARG:HH11 | 4:A:153:ARG:HB2 | 1.57 | 0.68 |
| 17:N:47:ARG:HA | 17:N:50:ARG:NH1 | 2.08 | 0.68 |
| 24:U:12:THR:CG2 | 24:U:15:GLU:HG3 | 2.14 | 0.68 |
| 1:O:1790:C:H2' | 1:O:1791:U:H6 | 1.59 | 0.68 |
| 4:A:131:HIS:O | 4:A:132:ASP:HB2 | 1.92 | 0.68 |
| 1:O:188:C:H5'' | 15:L:163:LEU:HD21 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:2414:A:H2' | 1:O:2415:A:C8 | 2.29 | 0.68 |
| 22:S:71:VAL:HG11 | 22:S:90:PRO:CB | 2.20 | 0.68 |
| 27:X:187:VAL:CG2 | 27:X:192:ASP:HB2 | 2.23 | 0.68 |
| 1:O:2346:C:O2' | 7:D:52:THR:HG21 | 1.93 | 0.68 |
| 6:C:219:ASN:O | 6:C:222:ASP:OD1 | 2.12 | 0.68 |
| 15:L:164:THR:CG2 | 15:L:165:SER:N | 2.56 | 0.68 |
| 16:M:164:ASP:CG | 16:M:167:ASP:HA | 2.14 | 0.68 |
| 16:M:169:PRO:O | 16:M:172:PHE:HB3 | 1.93 | 0.68 |
| 22:S:47:THR:HB | 22:S:100:ASP:HB3 | 1.75 | 0.68 |
| 26:W:72:VAL:HG22 | 26:W:85:VAL:CG1 | 2.24 | 0.68 |
| 7:D:20:LYS:HA | 7:D:75:LEU:O | 1.93 | 0.68 |
| 8:E:37:ASP:OD1 | 12:I:125:SER:HB3 | 1.94 | 0.68 |
| 1:O:1450:C:O2' | 1:O:1494:A:H5' | 1.93 | 0.68 |
| 5:B:258:GLY:H | 5:B:260:HIS:CE1 | 2.11 | 0.68 |
| 15:L:12:TRP:CE2 | 15:L:20:ILE:HD11 | 2.28 | 0.68 |
| 15:L:164:THR:HG22 | 15:L:167:GLY:N | 2.02 | 0.68 |
| 1:O:1209:C:H2' | 1:O:1210:G:H8 | 1.56 | 0.67 |
| 13:J:74:VAL:HG13 | 13:J:113:ILE:HG23 | 1.76 | 0.67 |
| 15:L:37:VAL:HG21 | 15:L:108:LYS:HG3 | 1.75 | 0.67 |
| 5:B:41:PHE:HA | 5:B:79:MET:HE2 | 1.76 | 0.67 |
| 6:C:1:MET:HG2 | 6:C:2:GLN:H | 1.58 | 0.67 |
| 17:N:47:ARG:HA | 17:N:50:ARG:HH12 | 1.59 | 0.67 |
| 5:B:168:GLY:H | 5:B:174:ARG:HD3 | 1.57 | 0.67 |
| 1:O:1191:A:H3' | 1:O:1192:A:H5'' | 1.76 | 0.67 |
| 1:O:2768:A:H2' | 1:O:2769:C:O4' | 1.93 | 0.67 |
| 7:D:50:VAL:O | 7:D:71:ALA:HA | 1.95 | 0.67 |
| 12:I:133:GLY:O | 12:I:137:GLU:HG3 | 1.95 | 0.67 |
| 1:O:1244:U:OP1 | 12:I:18:ILE:HD13 | 1.94 | 0.67 |
| 14:K:67:ARG:O | 14:K:71:GLU:HG3 | 1.94 | 0.67 |
| 15:L:55:LYS:O | 15:L:60:ILE:HD12 | 1.95 | 0.67 |
| 1:O:2274:A:H1' | 15:L:86:MET:SD | 2.34 | 0.67 |
| 17:N:44:ASN:OD1 | 17:N:65:LEU:HB2 | 1.95 | 0.67 |
| 1:O:1666:C:H2' | 1:O:1667:A:H5' | 1.77 | 0.67 |
| 1:O:288:A:H61 | 1:O:364:C:H42 | 1.42 | 0.67 |
| 1:O:2897:C:H2' | 1:O:2898:G:H8 | 1.59 | 0.67 |
| 4:A:192:VAL:HB | 38:A:8604:HOH:O | 1.94 | 0.67 |
| 4:A:36:ASP:HA | 4:A:83:GLY:HA3 | 1.77 | 0.67 |
| 15:L:65:VAL:HG21 | 15:L:105:ALA:HB2 | 1.75 | 0.67 |
| 22:S:50:VAL:HG12 | 22:S:56:ALA:HA | 1.76 | 0.67 |
| 1:O:2769:C:O2' | 1:O:2770:G:H5' | 1.94 | 0.67 |
| 5:B:254:GLN:HG2 | 5:B:255:GLY:N | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:K:73:VAL:HG23 | 14:K:74:THR:H | 1.60 | 0.67 |
| 24:U:64:GLY:O | 24:U:65:ASP:HB2 | 1.93 | 0.67 |
| 1:0:2780:C:H1' | 8:E:143:GLN:HE21 | 1.59 | 0.67 |
| 1:0:1930:A:H2' | 1:0:1931:A:C8 | 2.30 | 0.67 |
| 1:0:2265:U:H2' | 1:0:2266:A:C8 | 2.30 | 0.67 |
| 5:B:24:PRO:HG2 | 5:B:204:GLY:HA2 | 1.76 | 0.67 |
| 1:0:1008:C:H5'' | 11:H:16:ARG:HH12 | 1.59 | 0.67 |
| 28:Y:53:GLY:HA2 | 28:Y:67:GLY:O | 1.94 | 0.67 |
| 9:F:107:VAL:O | 9:F:111:ILE:HG13 | 1.95 | 0.67 |
| 1:0:1299:G:O6 | 14:K:6:ARG:HD3 | 1.95 | 0.67 |
| 1:0:820:G:OP2 | 4:A:171:LYS:NZ | 2.27 | 0.67 |
| 1:0:559:U:H5' | 1:0:559:U:H6 | 1.59 | 0.66 |
| 2:9:3023:U:C3' | 2:9:3024:U:H5'' | 2.20 | 0.66 |
| 25:V:6:GLN:HB2 | 25:V:26:ILE:CD1 | 2.25 | 0.66 |
| 17:N:73:ASP:HA | 17:N:92:VAL:O | 1.95 | 0.66 |
| 1:0:1926:G:H2' | 1:0:1927:A:C8 | 2.29 | 0.66 |
| 1:0:2256:G:C2' | 1:0:2257:G:H5' | 2.25 | 0.66 |
| 6:C:233:THR:HG22 | 6:C:234:VAL:H | 1.60 | 0.66 |
| 12:I:117:ASP:O | 12:I:119:THR:HG23 | 1.96 | 0.66 |
| 12:I:19:MET:CE | 12:I:132:LEU:HD11 | 2.25 | 0.66 |
| 25:V:122:ARG:NH2 | 25:V:154:ARG:OXT | 2.26 | 0.66 |
| 1:0:2769:C:H2' | 1:0:2770:G:O4' | 1.95 | 0.66 |
| 2:9:3039:U:H1' | 2:9:3044:A:H61 | 1.61 | 0.66 |
| 7:D:64:ARG:CG | 7:D:67:ASP:HB3 | 2.26 | 0.66 |
| 11:H:26:LYS:HD2 | 11:H:28:ILE:CD1 | 2.25 | 0.66 |
| 20:Q:18:LEU:HB2 | 20:Q:143:VAL:CG1 | 2.26 | 0.66 |
| 27:X:203:VAL:HG12 | 27:X:228:VAL:HG22 | 1.78 | 0.66 |
| 1:0:2421:G:H3' | 1:0:2422:U:H5'' | 1.76 | 0.66 |
| 5:B:41:PHE:HB3 | 5:B:190:MET:HE1 | 1.78 | 0.66 |
| 5:B:7:ARG:HG2 | 5:B:7:ARG:HH11 | 1.61 | 0.66 |
| 11:H:47:GLU:HB3 | 11:H:133:ILE:CD1 | 2.26 | 0.66 |
| 23:T:14:GLU:O | 23:T:17:THR:HB | 1.95 | 0.66 |
| 28:Y:30:GLU:O | 28:Y:33:HIS:HB3 | 1.95 | 0.66 |
| 1:0:2506:A:O2' | 1:0:2507:G:O5' | 2.14 | 0.66 |
| 1:0:2594:C:O2' | 1:0:2595:U:H5' | 1.95 | 0.66 |
| 7:D:135:VAL:HG22 | 7:D:136:ARG:H | 1.61 | 0.66 |
| 11:H:150:LYS:HB2 | 11:H:157:ILE:HD12 | 1.78 | 0.66 |
| 5:B:162:MET:CE | 5:B:308:LEU:HD21 | 2.22 | 0.66 |
| 11:H:33:MET:HB2 | 11:H:83:PHE:HB3 | 1.77 | 0.66 |
| 13:J:81:ARG:HB2 | 13:J:87:ARG:NH1 | 2.11 | 0.66 |
| 28:Y:11:THR:OG1 | 28:Y:23:ARG:HB2 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:B:195:ARG:HD2 | 5:B:324:ASP:OD1 | 1.96 | 0.65 |
| 5:B:238:ASN:HD22 | 5:B:240:GLY:N | 1.87 | 0.65 |
| 5:B:280:VAL:CG1 | 5:B:334:SER:HA | 2.27 | 0.65 |
| 15:L:72:SER:HB2 | 15:L:93:ARG:HG2 | 1.77 | 0.65 |
| 1:O:2269:C:C2' | 1:O:2270:G:H5' | 2.26 | 0.65 |
| 1:O:1641:A:H2' | 1:O:1642:A:H5' | 1.78 | 0.65 |
| 1:O:2578:G:H5' | 1:O:2578:G:H8 | 1.61 | 0.65 |
| 5:B:175:LEU:C | 5:B:175:LEU:HD23 | 2.17 | 0.65 |
| 8:E:11:VAL:HG12 | 8:E:12:ASP:H | 1.61 | 0.65 |
| 1:O:1771:U:C4' | 28:Y:20:LEU:HD21 | 2.26 | 0.65 |
| 1:O:2271:G:H5' | 38:A:8579:HOH:O | 1.95 | 0.65 |
| 31:2:55:VAL:O | 31:2:56:PRO:O | 2.15 | 0.65 |
| 11:H:13:ALA:HA | 11:H:91:HIS:HE1 | 1.62 | 0.65 |
| 28:Y:38:LYS:HE2 | 28:Y:45:LYS:CE | 2.27 | 0.65 |
| 1:O:111:C:O2' | 29:Z:20:ARG:HG2 | 1.96 | 0.65 |
| 1:O:1505:U:H6 | 1:O:1505:U:H5' | 1.60 | 0.65 |
| 1:O:1835:U:C5 | 1:O:1840:A:N7 | 2.61 | 0.65 |
| 1:O:877:G:H5' | 1:O:878:G:OP1 | 1.96 | 0.65 |
| 5:B:168:GLY:N | 5:B:174:ARG:HD3 | 2.11 | 0.65 |
| 5:B:312:ARG:HD3 | 5:B:315:VAL:HG13 | 1.78 | 0.65 |
| 16:M:154:LEU:O | 16:M:155:GLU:HB3 | 1.96 | 0.65 |
| 21:R:37:VAL:O | 21:R:41:VAL:HG23 | 1.96 | 0.65 |
| 16:M:163:PHE:HE1 | 16:M:171:HIS:HD1 | 1.44 | 0.65 |
| 20:Q:29:LYS:HD3 | 38:Q:8542:HOH:O | 1.96 | 0.65 |
| 1:O:1234:U:N3 | 5:B:244:PRO:HB3 | 2.12 | 0.65 |
| 1:O:544:G:H2' | 1:O:545:G:H5'' | 1.79 | 0.65 |
| 2:9:3054:A:O2' | 2:9:3055:U:H5' | 1.97 | 0.65 |
| 11:H:140:PRO:HA | 11:H:142:VAL:HG12 | 1.78 | 0.65 |
| 15:L:37:VAL:HG21 | 15:L:108:LYS:CG | 2.27 | 0.65 |
| 1:O:2717:C:O2' | 1:O:2718:C:H5'' | 1.97 | 0.64 |
| 1:O:2878:U:H2' | 1:O:2879:A:O4' | 1.97 | 0.64 |
| 9:F:50:VAL:HG13 | 9:F:60:VAL:HG11 | 1.77 | 0.64 |
| 12:I:19:MET:HE3 | 12:I:132:LEU:HD11 | 1.78 | 0.64 |
| 29:Z:28:HIS:CE1 | 29:Z:31:LYS:HE2 | 2.32 | 0.64 |
| 2:9:3006:C:OP1 | 16:M:37:ARG:NH1 | 2.29 | 0.64 |
| 14:K:54:PRO:HG2 | 14:K:57:VAL:HG21 | 1.78 | 0.64 |
| 23:T:52:THR:HG22 | 23:T:54:THR:N | 2.13 | 0.64 |
| 28:Y:29:VAL:O | 28:Y:33:HIS:HB2 | 1.97 | 0.64 |
| 5:B:275:GLY:O | 5:B:291:ASP:HA | 1.97 | 0.64 |
| 6:C:235:PHE:HE2 | 6:C:243:VAL:HG21 | 1.62 | 0.64 |
| 5:B:307:ARG:HB2 | 5:B:307:ARG:HH11 | 1.63 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:36:PRO:HA | 5:B:168:GLY:CA | 2.27 | 0.64 |
| 1:0:184:G:H5'' | 15:L:153:THR:HG22 | 1.78 | 0.64 |
| 2:9:3028:U:H5'' | 16:M:40:ASN:HD21 | 1.63 | 0.64 |
| 26:W:25:ARG:HD3 | 26:W:64:ALA:O | 1.97 | 0.64 |
| 2:9:3049:G:O2' | 2:9:3050:G:H5' | 1.96 | 0.64 |
| 1:0:2094:G:C4' | 5:B:245:SER:HB3 | 2.27 | 0.64 |
| 9:F:53:ASP:OD1 | 9:F:80:GLN:HB2 | 1.96 | 0.64 |
| 24:U:49:LEU:O | 24:U:53:ILE:HG13 | 1.97 | 0.64 |
| 28:Y:33:HIS:CE1 | 28:Y:49:ARG:HD2 | 2.33 | 0.64 |
| 1:0:1803:C:H2' | 1:0:1804:A:C8 | 2.33 | 0.64 |
| 1:0:407:A:H2' | 1:0:408:A:C8 | 2.33 | 0.64 |
| 1:0:541:C:H2' | 1:0:542:A:C5' | 2.26 | 0.64 |
| 4:A:140:LEU:HB3 | 4:A:141:PRO:HD2 | 1.77 | 0.64 |
| 12:I:74:ARG:CB | 12:I:74:ARG:HH11 | 2.10 | 0.64 |
| 13:J:74:VAL:CG1 | 13:J:113:ILE:HG12 | 2.26 | 0.64 |
| 20:Q:25:PHE:CE2 | 20:Q:29:LYS:HE2 | 2.32 | 0.64 |
| 21:R:57:THR:HG22 | 21:R:59:ASP:N | 2.12 | 0.64 |
| 17:N:32:ARG:HE | 17:N:35:LYS:HD2 | 1.63 | 0.64 |
| 20:Q:18:LEU:HD12 | 20:Q:143:VAL:HG11 | 1.80 | 0.64 |
| 11:H:44:ALA:HA | 11:H:163:PRO:O | 1.98 | 0.64 |
| 14:K:104:ASP:O | 14:K:105:TYR:HB3 | 1.96 | 0.64 |
| 22:S:101:LEU:HD13 | 22:S:112:LEU:HD11 | 1.79 | 0.64 |
| 1:0:2613:G:O2' | 1:0:2614:C:H5' | 1.98 | 0.64 |
| 23:T:52:THR:CG2 | 23:T:54:THR:HB | 2.28 | 0.64 |
| 7:D:64:ARG:CD | 7:D:67:ASP:HB3 | 2.28 | 0.64 |
| 11:H:27:LYS:N | 11:H:58:HIS:HD2 | 1.94 | 0.64 |
| 12:I:27:ALA:HB1 | 12:I:87:LEU:HD21 | 1.80 | 0.64 |
| 1:0:1972:U:H2' | 1:0:1973:A:H5' | 1.80 | 0.63 |
| 14:K:143:THR:HG22 | 14:K:144:ASP:N | 2.13 | 0.63 |
| 7:D:25:MET:CE | 7:D:41:LEU:HG | 2.27 | 0.63 |
| 1:0:157:G:H4' | 15:L:95:LYS:HE3 | 1.80 | 0.63 |
| 4:A:48:ASP:HB3 | 38:A:8617:HOH:O | 1.97 | 0.63 |
| 11:H:14:TYR:H | 11:H:91:HIS:CE1 | 2.15 | 0.63 |
| 12:I:107:ASN:ND2 | 12:I:109:TYR:H | 1.96 | 0.63 |
| 13:J:55:VAL:HG12 | 13:J:56:SER:H | 1.62 | 0.63 |
| 1:0:1595:G:O2' | 1:0:1596:U:H5' | 1.99 | 0.63 |
| 1:0:871:G:C8 | 1:0:871:G:C5' | 2.74 | 0.63 |
| 4:A:88:ILE:HD13 | 4:A:100:PRO:CD | 2.28 | 0.63 |
| 15:L:87:MET:HB3 | 31:2:46:ILE:HG21 | 1.80 | 0.63 |
| 23:T:14:GLU:OE1 | 23:T:15:PRO:HD2 | 1.98 | 0.63 |
| 7:D:23:VAL:HG22 | 7:D:73:VAL:HB | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:M:183:ASP:OD2 | 16:M:186:LEU:HD12 | 1.99 | 0.63 |
| 22:S:49:GLU:OE2 | 22:S:97:ARG:HD2 | 1.98 | 0.63 |
| 1:O:2690:U:O2' | 8:E:111:LYS:HE3 | 1.98 | 0.63 |
| 10:G:64:ASN:N | 10:G:64:ASN:HD22 | 1.94 | 0.63 |
| 11:H:147:ARG:HA | 11:H:150:LYS:NZ | 2.14 | 0.63 |
| 11:H:84:ARG:NH2 | 11:H:135:TRP:HH2 | 1.96 | 0.63 |
| 14:K:24:ALA:HB2 | 14:K:30:ARG:HD2 | 1.81 | 0.63 |
| 26:W:30:MET:HE1 | 26:W:55:ASN:HA | 1.79 | 0.63 |
| 1:O:136:C:H2' | 1:O:137:U:O4' | 1.98 | 0.63 |
| 1:O:1596:U:H2' | 1:O:1598:A:OP2 | 1.99 | 0.63 |
| 1:O:960:G:H2' | 1:O:960:G:N3 | 2.14 | 0.63 |
| 5:B:202:VAL:HG11 | 5:B:301:VAL:HG13 | 1.81 | 0.63 |
| 10:G:64:ASN:O | 10:G:68:GLU:HG3 | 1.98 | 0.63 |
| 12:I:45:VAL:HG21 | 12:I:129:PHE:CD1 | 2.34 | 0.63 |
| 15:L:52:LEU:HD13 | 15:L:116:ASN:HB3 | 1.80 | 0.63 |
| 26:W:15:ARG:HH11 | 26:W:15:ARG:CB | 2.10 | 0.63 |
| 1:O:1474:C:H5' | 1:O:1474:C:C6 | 2.33 | 0.63 |
| 11:H:26:LYS:HD3 | 11:H:89:PRO:HG3 | 1.80 | 0.63 |
| 1:O:2270:G:H4' | 4:A:223:ARG:HH12 | 1.64 | 0.63 |
| 6:C:104:ASP:HA | 6:C:107:ARG:HH12 | 1.63 | 0.63 |
| 6:C:46:TYR:CE2 | 6:C:98:ARG:NH1 | 2.67 | 0.63 |
| 1:O:1741:U:H5' | 1:O:1742:A:OP1 | 1.99 | 0.62 |
| 32:O:9500:SLD:C6S | 3:4:76:A:H5'' | 2.29 | 0.62 |
| 4:A:94:LEU:N | 4:A:94:LEU:HD23 | 2.14 | 0.62 |
| 11:H:13:ALA:HA | 11:H:91:HIS:CE1 | 2.33 | 0.62 |
| 13:J:10:GLN:H | 13:J:10:GLN:HE21 | 0.75 | 0.62 |
| 14:K:114:VAL:HG11 | 38:K:8579:HOH:O | 1.99 | 0.62 |
| 1:O:553:G:P | 27:X:204:ARG:HH22 | 2.22 | 0.62 |
| 4:A:164:ARG:HB2 | 28:Y:68:CYS:SG | 2.39 | 0.62 |
| 1:O:2070:G:H2' | 1:O:2072:G:OP1 | 2.00 | 0.62 |
| 1:O:2265:U:H2' | 1:O:2266:A:H8 | 1.64 | 0.62 |
| 2:9:3020:G:O2' | 2:9:3021:G:H5' | 1.99 | 0.62 |
| 2:9:3040:C:N4 | 7:D:51:ARG:HB2 | 2.13 | 0.62 |
| 21:R:57:THR:HG22 | 21:R:59:ASP:H | 1.65 | 0.62 |
| 27:X:186:ARG:HG2 | 27:X:186:ARG:HH11 | 1.64 | 0.62 |
| 1:O:1667:A:H8 | 1:O:1667:A:H5' | 1.64 | 0.62 |
| 2:9:3051:A:H5' | 16:M:160:SER:HB3 | 1.81 | 0.62 |
| 5:B:56:ASP:HB3 | 5:B:322:ARG:HH21 | 1.65 | 0.62 |
| 1:O:1636:G:O2' | 1:O:1637:A:H5' | 1.98 | 0.62 |
| 1:O:2780:C:H2' | 1:O:2781:U:C6 | 2.34 | 0.62 |
| 1:O:731:U:H2' | 1:O:732:C:C6 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:2:65:THR:HG23 | 31:2:67:LEU:HG | 1.80 | 0.62 |
| 28:Y:62:TYR:CE2 | 28:Y:64:ILE:HG23 | 2.34 | 0.62 |
| 1:0:2256:G:H2' | 1:0:2257:G:H5' | 1.82 | 0.62 |
| 1:0:2456:A:H2' | 1:0:2457:U:C6 | 2.34 | 0.62 |
| 9:F:21:GLU:O | 9:F:24:ARG:HG3 | 1.99 | 0.62 |
| 22:S:32:ARG:NH1 | 22:S:38:ARG:NH1 | 2.47 | 0.62 |
| 25:V:68:THR:HG23 | 25:V:69:ARG:HG2 | 1.79 | 0.62 |
| 1:0:2269:C:O2' | 1:0:2270:G:H5' | 2.00 | 0.62 |
| 14:K:138:GLY:HA3 | 38:K:8558:HOH:O | 2.00 | 0.62 |
| 2:9:3006:C:H5'' | 16:M:37:ARG:HH12 | 1.63 | 0.62 |
| 1:0:2054:A:N3 | 20:Q:128:ARG:NH2 | 2.47 | 0.62 |
| 25:V:137:GLN:HE21 | 25:V:141:HIS:CE1 | 2.13 | 0.62 |
| 1:0:2421:G:H3' | 1:0:2422:U:C5' | 2.27 | 0.62 |
| 4:A:81:GLN:HB2 | 4:A:92:ASN:ND2 | 2.14 | 0.62 |
| 11:H:48:LEU:HG | 11:H:157:ILE:HG21 | 1.82 | 0.62 |
| 18:O:76:GLY:O | 18:O:79:SER:N | 2.32 | 0.62 |
| 1:0:638:C:H2' | 1:0:639:A:C8 | 2.35 | 0.62 |
| 1:0:702:G:O2' | 1:0:703:G:H5' | 2.00 | 0.62 |
| 29:Z:21:ARG:HD2 | 29:Z:39:PHE:HB2 | 1.82 | 0.62 |
| 1:0:2505:G:O2' | 1:0:2506:A:H5' | 2.00 | 0.61 |
| 1:0:558:C:O2' | 1:0:559:U:H5'' | 1.99 | 0.61 |
| 2:9:3030:C:OP1 | 7:D:137:PRO:O | 2.18 | 0.61 |
| 4:A:101:GLU:OE2 | 4:A:131:HIS:HB2 | 2.00 | 0.61 |
| 13:J:98:VAL:HG13 | 13:J:102:GLU:HA | 1.82 | 0.61 |
| 18:O:7:LYS:HD3 | 18:O:21:VAL:CG2 | 2.30 | 0.61 |
| 4:A:121:ALA:O | 4:A:124:VAL:HG22 | 1.99 | 0.61 |
| 11:H:29:ALA:HB3 | 11:H:65:ARG:NH1 | 2.09 | 0.61 |
| 22:S:9:LYS:CE | 22:S:13:ARG:NH1 | 2.62 | 0.61 |
| 27:X:112:GLU:OE1 | 27:X:112:GLU:HA | 2.00 | 0.61 |
| 28:Y:30:GLU:HA | 28:Y:33:HIS:HB3 | 1.81 | 0.61 |
| 1:0:2375:G:H2' | 1:0:2376:C:C6 | 2.35 | 0.61 |
| 2:9:3044:A:O4' | 7:D:76:ARG:NE | 2.33 | 0.61 |
| 9:F:96:ALA:HA | 38:F:3111:HOH:O | 2.00 | 0.61 |
| 20:Q:40:ALA:O | 20:Q:44:VAL:HG23 | 2.01 | 0.61 |
| 1:0:470:U:O2' | 29:Z:16:HIS:HD2 | 1.82 | 0.61 |
| 1:0:1850:U:H2' | 1:0:1851:G:H8 | 1.65 | 0.61 |
| 1:0:1909:A:H2' | 1:0:1910:A:C8 | 2.35 | 0.61 |
| 1:0:2533:C:C6 | 1:0:2533:C:H5' | 2.33 | 0.61 |
| 1:0:2795:C:O2' | 1:0:2796:U:H5' | 2.00 | 0.61 |
| 6:C:5:ILE:HD11 | 6:C:16:VAL:CG2 | 2.24 | 0.61 |
| 15:L:48:ARG:HH11 | 15:L:52:LEU:HD21 | 1.64 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:M:48:VAL:HG11 | 16:M:55:ASP:HB3 | 1.82 | 0.61 |
| 16:M:91:ARG:HG3 | 16:M:186:LEU:HD23 | 1.81 | 0.61 |
| 23:T:11:THR:HG22 | 23:T:53:ASP:OD2 | 2.01 | 0.61 |
| 1:0:1250:C:O2' | 1:0:1251:C:H5' | 2.01 | 0.61 |
| 1:0:281:U:H2' | 1:0:282:C:O4' | 2.01 | 0.61 |
| 1:0:696:C:O2' | 1:0:697:G:H5' | 2.00 | 0.61 |
| 1:0:1422:U:H2' | 1:0:1423:C:C6 | 2.35 | 0.61 |
| 1:0:669:G:O2' | 1:0:670:G:H5' | 2.00 | 0.61 |
| 12:I:74:ARG:O | 12:I:78:ILE:HG12 | 2.00 | 0.61 |
| 1:0:1882:C:H2' | 1:0:1883:U:H6 | 1.64 | 0.61 |
| 2:9:3013:A:O2' | 2:9:3014:G:H5'' | 2.00 | 0.61 |
| 8:E:31:ARG:HH12 | 8:E:68:HIS:CG | 2.19 | 0.61 |
| 10:G:23:ILE:HD13 | 10:G:67:LEU:HD23 | 1.83 | 0.61 |
| 1:0:2502:C:C4' | 11:H:151:MET:HG2 | 2.30 | 0.61 |
| 16:M:152:GLU:C | 16:M:154:LEU:H | 2.03 | 0.61 |
| 27:X:200:THR:HG22 | 27:X:201:GLU:HG3 | 1.83 | 0.61 |
| 1:0:1170:U:O2' | 1:0:1172:G:N7 | 2.32 | 0.61 |
| 1:0:2840:A:OP1 | 5:B:211:THR:HG23 | 2.01 | 0.61 |
| 1:0:657:G:OP1 | 6:C:27:ARG:NH2 | 2.28 | 0.61 |
| 5:B:145:HIS:HD2 | 5:B:146:THR:O | 1.84 | 0.61 |
| 9:F:56:PRO:HG2 | 15:L:44:THR:HA | 1.82 | 0.61 |
| 6:C:47:GLY:HA2 | 6:C:92:PRO:HB2 | 1.81 | 0.61 |
| 10:G:71:LEU:C | 10:G:73:ASP:H | 2.04 | 0.61 |
| 25:V:84:VAL:HG12 | 38:V:6679:HOH:O | 1.99 | 0.61 |
| 4:A:199:HIS:HD2 | 4:A:201:PHE:HB2 | 1.66 | 0.61 |
| 24:U:39:ALA:C | 24:U:41:GLU:H | 2.04 | 0.61 |
| 25:V:122:ARG:NH1 | 25:V:152:ALA:O | 2.34 | 0.61 |
| 1:0:1666:C:O2' | 1:0:1667:A:H5'' | 2.00 | 0.60 |
| 26:W:9:VAL:HG22 | 26:W:88:GLU:OE2 | 2.01 | 0.60 |
| 1:0:1003:U:HO2' | 11:H:90:PHE:HE1 | 1.49 | 0.60 |
| 1:0:1393:A:H2' | 1:0:1394:C:C6 | 2.36 | 0.60 |
| 1:0:1666:C:C2' | 1:0:1667:A:H5' | 2.31 | 0.60 |
| 2:9:3025:G:C3' | 2:9:3026:C:H5' | 2.31 | 0.60 |
| 4:A:27:LEU:HD21 | 4:A:55:VAL:HG21 | 1.83 | 0.60 |
| 9:F:56:PRO:CG | 15:L:44:THR:HA | 2.32 | 0.60 |
| 6:C:27:ARG:HD2 | 17:N:5:PRO:HD2 | 1.81 | 0.60 |
| 1:0:1119:G:H22 | 1:0:1246:A:H2 | 1.48 | 0.60 |
| 1:0:777:U:O2' | 29:Z:11:LYS:HG2 | 2.01 | 0.60 |
| 31:2:42:ARG:HH11 | 31:2:42:ARG:HG3 | 1.65 | 0.60 |
| 12:I:75:PRO:HG2 | 12:I:105:LEU:HD21 | 1.82 | 0.60 |
| 11:H:95:GLU:HB3 | 11:H:119:VAL:HG11 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:Q:106:GLY:HA2 | 20:Q:109:MET:CE | 2.32 | 0.60 |
| 1:0:2001:G:O2' | 1:0:2002:C:H5' | 2.01 | 0.60 |
| 1:0:241:A:C2 | 1:0:378:A:H4' | 2.36 | 0.60 |
| 1:0:645:U:OP2 | 14:K:4:LYS:HE2 | 2.00 | 0.60 |
| 12:I:52:GLN:HG3 | 12:I:53:ILE:H | 1.64 | 0.60 |
| 23:T:49:LEU:HG | 38:T:3805:HOH:O | 2.00 | 0.60 |
| 1:0:1158:G:O2' | 1:0:1159:G:H5' | 2.01 | 0.60 |
| 1:0:2291:A:C8 | 1:0:2309:C:H5' | 2.37 | 0.60 |
| 31:2:60:LYS:HG3 | 31:2:61:PRO:HD2 | 1.84 | 0.60 |
| 28:Y:30:GLU:HA | 28:Y:33:HIS:CB | 2.32 | 0.60 |
| 1:0:2028:U:H2' | 1:0:2029:C:C6 | 2.36 | 0.60 |
| 1:0:2266:A:H2' | 1:0:2267:G:C8 | 2.36 | 0.60 |
| 12:I:45:VAL:HG23 | 12:I:130:VAL:O | 2.01 | 0.60 |
| 13:J:28:GLU:HG2 | 13:J:58:THR:HB | 1.84 | 0.60 |
| 1:0:2415:A:N3 | 16:M:26:LEU:HD13 | 2.17 | 0.60 |
| 1:0:2598:U:O2 | 1:0:2600:A:H8 | 1.83 | 0.60 |
| 4:A:164:ARG:HA | 28:Y:69:TYR:CE1 | 2.36 | 0.60 |
| 6:C:118:THR:O | 6:C:136:VAL:HG13 | 2.01 | 0.60 |
| 6:C:78:ARG:HG3 | 6:C:78:ARG:NH1 | 2.13 | 0.60 |
| 11:H:27:LYS:H | 11:H:58:HIS:CD2 | 2.13 | 0.60 |
| 1:0:2241:C:H2' | 1:0:2242:U:C6 | 2.37 | 0.60 |
| 1:0:256:C:H2' | 1:0:257:G:O4' | 2.02 | 0.60 |
| 16:M:165:ALA:HB1 | 38:M:8526:HOH:O | 2.02 | 0.60 |
| 20:Q:18:LEU:HG | 20:Q:91:LEU:HD13 | 1.84 | 0.60 |
| 1:0:2720:C:O2 | 13:J:87:ARG:NH2 | 2.35 | 0.60 |
| 1:0:2779:G:H21 | 8:E:143:GLN:NE2 | 2.00 | 0.60 |
| 1:0:29:C:O2' | 1:0:30:U:H5' | 2.02 | 0.60 |
| 5:B:5:ARG:HD2 | 5:B:8:LYS:NZ | 2.17 | 0.60 |
| 7:D:135:VAL:HG22 | 7:D:136:ARG:N | 2.17 | 0.60 |
| 7:D:44:ILE:HG23 | 7:D:45:THR:HG23 | 1.83 | 0.60 |
| 11:H:139:ASP:N | 11:H:140:PRO:CD | 2.65 | 0.60 |
| 18:O:59:ARG:HH22 | 18:O:66:GLN:HE22 | 1.48 | 0.60 |
| 1:0:2320:U:H4' | 1:0:2321:A:O4' | 2.02 | 0.59 |
| 1:0:2361:A:H2' | 1:0:2362:A:C8 | 2.37 | 0.59 |
| 8:E:86:VAL:CG1 | 8:E:129:GLU:HA | 2.31 | 0.59 |
| 11:H:31:PHE:CD2 | 11:H:85:ILE:HG23 | 2.37 | 0.59 |
| 15:L:74:ARG:HG3 | 15:L:74:ARG:HH11 | 1.66 | 0.59 |
| 25:V:64:THR:O | 25:V:68:THR:HG22 | 2.02 | 0.59 |
| 1:0:2256:G:H2' | 1:0:2257:G:C5' | 2.31 | 0.59 |
| 1:0:902:G:N7 | 14:K:18:HIS:HD2 | 1.99 | 0.59 |
| 5:B:51:VAL:HG13 | 5:B:53:LEU:HD13 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:D:95:THR:O | 7:D:97:GLN:N | 2.31 | 0.59 |
| 15:L:48:ARG:NH1 | 15:L:52:LEU:HD21 | 2.17 | 0.59 |
| 20:Q:61:GLN:NE2 | 38:Q:8542:HOH:O | 2.35 | 0.59 |
| 25:V:149:LEU:HG | 25:V:153:MET:CE | 2.32 | 0.59 |
| 1:O:1790:C:H2' | 1:O:1791:U:C6 | 2.37 | 0.59 |
| 2:9:3014:G:H8 | 2:9:3014:G:H5' | 1.67 | 0.59 |
| 14:K:35:ARG:O | 14:K:40:PHE:HA | 2.02 | 0.59 |
| 9:F:58:GLU:OE1 | 15:L:27:ARG:NH2 | 2.34 | 0.59 |
| 31:2:84:ARG:HD3 | 38:2:8554:HOH:O | 2.02 | 0.59 |
| 8:E:11:VAL:HG13 | 8:E:23:GLU:O | 2.03 | 0.59 |
| 10:G:12:ILE:N | 10:G:13:PRO:CD | 2.64 | 0.59 |
| 26:W:76:ARG:O | 26:W:77:PHE:HB3 | 2.01 | 0.59 |
| 1:O:2507:G:H2' | 1:O:2510:C:N4 | 2.17 | 0.59 |
| 30:1:40:ARG:HG2 | 30:1:40:ARG:HH11 | 1.67 | 0.59 |
| 6:C:1:MET:HG2 | 6:C:2:GLN:NE2 | 2.16 | 0.59 |
| 11:H:127:GLY:O | 11:H:128:ALA:HB3 | 2.03 | 0.59 |
| 13:J:115:ARG:HG3 | 13:J:116:GLU:N | 2.18 | 0.59 |
| 1:O:1461:U:H2' | 1:O:1462:C:C6 | 2.37 | 0.59 |
| 1:O:947:U:H2' | 1:O:948:G:C8 | 2.37 | 0.59 |
| 16:M:155:GLU:O | 16:M:156:GLU:HG3 | 2.02 | 0.59 |
| 1:O:2356:A:H2' | 1:O:2357:G:O4' | 2.03 | 0.59 |
| 1:O:303:C:O2' | 1:O:304:G:H5' | 2.03 | 0.59 |
| 7:D:86:THR:O | 7:D:90:LEU:HG | 2.02 | 0.59 |
| 15:L:138:HIS:ND1 | 15:L:139:PRO:O | 2.31 | 0.59 |
| 1:O:2413:A:N7 | 16:M:109:PRO:HB3 | 2.17 | 0.59 |
| 20:Q:12:THR:HG22 | 20:Q:149:GLU:OE1 | 2.03 | 0.59 |
| 26:W:43:VAL:HG12 | 26:W:44:ASP:N | 2.17 | 0.59 |
| 27:X:235:GLU:CD | 27:X:235:GLU:H | 2.03 | 0.59 |
| 1:O:449:A:N7 | 6:C:43:LYS:HG2 | 2.18 | 0.59 |
| 4:A:194:MET:HE2 | 4:A:199:HIS:CB | 2.32 | 0.59 |
| 11:H:46:VAL:HG12 | 11:H:146:TRP:HZ3 | 1.68 | 0.59 |
| 14:K:54:PRO:HG2 | 14:K:57:VAL:CG2 | 2.32 | 0.59 |
| 16:M:33:ARG:NH1 | 16:M:103:ASP:OD2 | 2.26 | 0.59 |
| 16:M:151:ASP:O | 16:M:154:LEU:HB2 | 2.01 | 0.59 |
| 2:9:3039:U:H1' | 2:9:3044:A:N6 | 2.17 | 0.59 |
| 1:O:1855:G:H8 | 4:A:144:GLU:OE2 | 1.85 | 0.59 |
| 16:M:164:ASP:OD2 | 16:M:167:ASP:HA | 2.02 | 0.59 |
| 1:O:1552:G:H2' | 1:O:1553:C:C6 | 2.38 | 0.59 |
| 7:D:25:MET:CE | 7:D:37:ALA:HB1 | 2.31 | 0.59 |
| 23:T:52:THR:HG22 | 23:T:54:THR:HB | 1.85 | 0.59 |
| 25:V:110:GLN:NE2 | 25:V:110:GLN:HA | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:W:76:ARG:HG3 | 26:W:76:ARG:NH1 | 2.16 | 0.59 |
| 1:0:282:C:O2' | 1:0:283:U:H5' | 2.03 | 0.58 |
| 1:0:95:A:H5'' | 1:0:97:G:O4' | 2.03 | 0.58 |
| 30:1:41:HIS:HD2 | 30:1:44:ARG:H | 1.51 | 0.58 |
| 6:C:233:THR:HG22 | 6:C:234:VAL:N | 2.17 | 0.58 |
| 1:0:2363:G:O2' | 19:P:11:ARG:HG3 | 2.03 | 0.58 |
| 1:0:1187:U:O2' | 1:0:1189:A:H2 | 1.86 | 0.58 |
| 1:0:338:C:H4' | 6:C:174:ILE:CD1 | 2.32 | 0.58 |
| 9:F:91:VAL:HG12 | 9:F:92:GLY:H | 1.64 | 0.58 |
| 14:K:149:ARG:O | 14:K:150:GLN:HB2 | 2.03 | 0.58 |
| 1:0:694:A:H2' | 1:0:695:C:H5' | 1.84 | 0.58 |
| 4:A:110:SER:HA | 4:A:118:PHE:HE1 | 1.68 | 0.58 |
| 16:M:143:ARG:HA | 16:M:172:PHE:CD2 | 2.38 | 0.58 |
| 17:N:14:LEU:HG | 17:N:102:ILE:HD11 | 1.85 | 0.58 |
| 1:0:625:U:H5'' | 1:0:1044:C:N4 | 2.18 | 0.58 |
| 2:9:3055:U:H4' | 2:9:3056:A:C8 | 2.37 | 0.58 |
| 7:D:94:ALA:HB3 | 7:D:174:VAL:CA | 2.33 | 0.58 |
| 16:M:25:ARG:HA | 16:M:28:LYS:HG3 | 1.84 | 0.58 |
| 27:X:200:THR:HG22 | 27:X:201:GLU:CG | 2.32 | 0.58 |
| 1:0:292:G:H2' | 1:0:358:G:N2 | 2.17 | 0.58 |
| 5:B:36:PRO:HA | 5:B:168:GLY:HA3 | 1.85 | 0.58 |
| 7:D:99:ASP:HA | 38:D:5675:HOH:O | 2.04 | 0.58 |
| 9:F:110:GLU:HA | 9:F:113:ASP:OD2 | 2.03 | 0.58 |
| 15:L:74:ARG:NH1 | 15:L:74:ARG:HG3 | 2.17 | 0.58 |
| 15:L:80:GLY:O | 15:L:81:ARG:HD2 | 2.04 | 0.58 |
| 5:B:144:THR:HG22 | 5:B:145:HIS:N | 2.18 | 0.58 |
| 7:D:44:ILE:HG12 | 7:D:83:PHE:HE1 | 1.68 | 0.58 |
| 11:H:166:ASN:N | 11:H:166:ASN:HD22 | 1.99 | 0.58 |
| 17:N:87:THR:O | 17:N:91:GLN:HG3 | 2.04 | 0.58 |
| 18:O:9:LEU:O | 18:O:13:VAL:HG12 | 2.03 | 0.58 |
| 24:U:56:ILE:O | 24:U:60:GLN:HG3 | 2.03 | 0.58 |
| 1:0:1643:C:O2' | 1:0:1644:C:H5' | 2.04 | 0.58 |
| 7:D:49:PRO:HA | 7:D:73:VAL:HG22 | 1.86 | 0.58 |
| 14:K:145:LEU:O | 14:K:148:GLU:HG3 | 2.03 | 0.58 |
| 18:O:115:SER:H | 18:O:118:GLN:NE2 | 1.82 | 0.58 |
| 1:0:21:G:H4' | 20:Q:2:ILE:HG22 | 1.84 | 0.58 |
| 1:0:2300:A:H4' | 1:0:2301:A:O5' | 2.03 | 0.58 |
| 5:B:96:PRO:HG2 | 38:B:8648:HOH:O | 2.03 | 0.58 |
| 15:L:37:VAL:HG13 | 15:L:63:VAL:HG11 | 1.86 | 0.58 |
| 25:V:122:ARG:HH11 | 25:V:122:ARG:CG | 2.14 | 0.58 |
| 25:V:65:VAL:HG12 | 25:V:116:LEU:HD13 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1164:U:C4' | 1:0:1165:G:OP1 | 2.48 | 0.58 |
| 1:0:812:A:H2' | 1:0:813:C:C6 | 2.39 | 0.58 |
| 14:K:93:VAL:HG12 | 14:K:97:VAL:HG23 | 1.85 | 0.58 |
| 1:0:1864:C:OP1 | 15:L:75:THR:HG23 | 2.03 | 0.58 |
| 1:0:1444:G:O2' | 1:0:1445:G:H5' | 2.02 | 0.58 |
| 1:0:2668:G:H2' | 1:0:2669:U:C6 | 2.38 | 0.58 |
| 1:0:2894:C:O2' | 1:0:2895:C:H5' | 2.04 | 0.58 |
| 1:0:862:U:H2' | 1:0:863:G:H8 | 1.68 | 0.58 |
| 31:2:11:CYS:HB2 | 31:2:20:HIS:CE1 | 2.38 | 0.58 |
| 5:B:141:ARG:HG2 | 5:B:165:ARG:HA | 1.85 | 0.58 |
| 23:T:17:THR:HG22 | 23:T:18:GLY:N | 2.18 | 0.58 |
| 1:0:10:U:HO2' | 1:0:11:A:H8 | 1.50 | 0.57 |
| 1:0:544:G:C2' | 1:0:545:G:H5'' | 2.34 | 0.57 |
| 7:D:19:GLU:O | 7:D:133:ASN:HB3 | 2.03 | 0.57 |
| 8:E:132:THR:O | 8:E:132:THR:HG23 | 2.03 | 0.57 |
| 11:H:46:VAL:O | 11:H:146:TRP:HH2 | 1.87 | 0.57 |
| 12:I:39:VAL:HG12 | 12:I:40:ASN:ND2 | 2.18 | 0.57 |
| 22:S:73:HIS:CD2 | 22:S:88:PRO:HG3 | 2.38 | 0.57 |
| 1:0:1804:A:H2' | 1:0:1805:G:C8 | 2.39 | 0.57 |
| 1:0:566:A:H2' | 1:0:567:U:O4' | 2.04 | 0.57 |
| 4:A:66:ARG:HH11 | 4:A:66:ARG:HB2 | 1.67 | 0.57 |
| 13:J:72:VAL:HG11 | 13:J:121:PHE:CD1 | 2.39 | 0.57 |
| 16:M:97:VAL:HG12 | 16:M:127:LEU:HD11 | 1.86 | 0.57 |
| 2:9:3048:C:H4' | 16:M:141:ARG:NH2 | 2.17 | 0.57 |
| 21:R:6:LYS:HB2 | 21:R:27:ALA:O | 2.04 | 0.57 |
| 1:0:1441:G:O2' | 1:0:1442:A:H5' | 2.03 | 0.57 |
| 1:0:820:G:C6 | 4:A:171:LYS:HB2 | 2.39 | 0.57 |
| 4:A:33:GLU:O | 4:A:34:ASP:HB2 | 2.03 | 0.57 |
| 11:H:47:GLU:CB | 11:H:133:ILE:HD13 | 2.35 | 0.57 |
| 11:H:26:LYS:HE3 | 11:H:28:ILE:HB | 1.86 | 0.57 |
| 17:N:77:ALA:HB1 | 17:N:98:LEU:HD12 | 1.86 | 0.57 |
| 23:T:13:ILE:HG12 | 23:T:32:CYS:HB3 | 1.85 | 0.57 |
| 1:0:1496:G:H5' | 1:0:1572:A:H1' | 1.86 | 0.57 |
| 1:0:2756:U:H3 | 1:0:2896:A:H2 | 1.53 | 0.57 |
| 13:J:55:VAL:HG12 | 13:J:56:SER:N | 2.19 | 0.57 |
| 18:O:13:VAL:HG11 | 18:O:40:VAL:HG11 | 1.86 | 0.57 |
| 1:0:1783:A:O2' | 1:0:1784:U:H5' | 2.04 | 0.57 |
| 1:0:297:U:H2' | 1:0:298:C:H6 | 1.69 | 0.57 |
| 5:B:190:MET:HE2 | 5:B:194:PHE:CD1 | 2.39 | 0.57 |
| 7:D:64:ARG:HB3 | 7:D:67:ASP:OD2 | 2.04 | 0.57 |
| 9:F:117:GLU:C | 9:F:119:ARG:H | 2.08 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:H:71:TYR:C | 11:H:73:GLN:H | 2.08 | 0.57 |
| 12:I:39:VAL:HG13 | 12:I:106:GLY:O | 2.03 | 0.57 |
| 16:M:78:MET:HB2 | 16:M:79:PRO:HD3 | 1.87 | 0.57 |
| 24:U:44:GLY:O | 24:U:48:GLU:HG2 | 2.04 | 0.57 |
| 1:0:832:U:H2' | 1:0:833:G:C8 | 2.39 | 0.57 |
| 2:9:3028:U:H2' | 2:9:3029:C:C6 | 2.40 | 0.57 |
| 11:H:53:PRO:HA | 11:H:125:VAL:O | 2.05 | 0.57 |
| 27:X:99:ALA:HB2 | 27:X:233:TYR:CZ | 2.40 | 0.57 |
| 1:0:1827:G:H2' | 1:0:1828:G:C8 | 2.39 | 0.57 |
| 13:J:99:ASP:OD1 | 13:J:101:ASN:N | 2.36 | 0.57 |
| 15:L:186:SER:O | 15:L:189:VAL:HG12 | 2.04 | 0.57 |
| 25:V:38:THR:HG22 | 25:V:39:ASP:N | 2.20 | 0.57 |
| 28:Y:19:GLY:O | 28:Y:23:ARG:HG2 | 2.05 | 0.57 |
| 1:0:1333:U:H2' | 1:0:1334:C:C6 | 2.40 | 0.57 |
| 1:0:1667:A:H2' | 1:0:1668:U:C6 | 2.40 | 0.57 |
| 4:A:199:HIS:CD2 | 4:A:201:PHE:H | 2.23 | 0.57 |
| 11:H:83:PHE:HZ | 11:H:146:TRP:HE1 | 1.47 | 0.57 |
| 12:I:107:ASN:HD21 | 12:I:109:TYR:HB2 | 1.70 | 0.57 |
| 1:0:962:C:H1' | 16:M:5:ARG:HH12 | 1.69 | 0.57 |
| 24:U:11:MET:HB3 | 24:U:15:GLU:HB2 | 1.87 | 0.57 |
| 25:V:151:GLU:O | 25:V:154:ARG:HB3 | 2.04 | 0.57 |
| 1:0:797:A:H4' | 28:Y:10:ARG:N | 2.19 | 0.57 |
| 28:Y:50:ALA:HB3 | 28:Y:54:ILE:HG22 | 1.85 | 0.57 |
| 1:0:1189:A:H3' | 38:0:8560:HOH:O | 2.05 | 0.57 |
| 1:0:1205:U:C2' | 1:0:1206:U:H5'' | 2.35 | 0.57 |
| 1:0:170:U:H2' | 1:0:171:C:H5' | 1.87 | 0.57 |
| 1:0:1803:C:H2' | 1:0:1804:A:H8 | 1.68 | 0.57 |
| 1:0:2717:C:H2' | 1:0:2718:C:C5' | 2.30 | 0.57 |
| 4:A:87:GLU:HB3 | 38:A:8635:HOH:O | 2.04 | 0.57 |
| 5:B:140:LEU:HA | 38:B:8592:HOH:O | 2.04 | 0.57 |
| 6:C:162:VAL:CG1 | 6:C:192:ILE:HD11 | 2.34 | 0.57 |
| 11:H:49:VAL:O | 11:H:157:ILE:HG23 | 2.05 | 0.57 |
| 38:0:6828:HOH:O | 11:H:4:ALA:HB3 | 2.05 | 0.57 |
| 28:Y:57:CYS:SG | 28:Y:59:HIS:HB3 | 2.45 | 0.57 |
| 1:0:1234:U:C4 | 5:B:244:PRO:HB3 | 2.40 | 0.57 |
| 1:0:2456:A:H2' | 1:0:2457:U:H6 | 1.69 | 0.57 |
| 1:0:371:U:H2' | 1:0:372:A:C8 | 2.40 | 0.57 |
| 4:A:39:ALA:HB3 | 4:A:61:GLU:OE2 | 2.04 | 0.57 |
| 8:E:31:ARG:HH12 | 8:E:68:HIS:CD2 | 2.23 | 0.57 |
| 28:Y:10:ARG:HA | 38:Y:8416:HOH:O | 2.03 | 0.57 |
| 1:0:12:U:H2' | 1:0:13:G:H5' | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2729:C:O2' | 1:0:2730:G:H5' | 2.05 | 0.56 |
| 1:0:2780:C:H2' | 1:0:2781:U:H6 | 1.68 | 0.56 |
| 9:F:19:ALA:O | 9:F:22:VAL:HG22 | 2.04 | 0.56 |
| 18:O:80:ARG:HG2 | 18:O:87:ARG:CZ | 2.35 | 0.56 |
| 1:0:1398:G:H2' | 1:0:1399:A:C8 | 2.41 | 0.56 |
| 1:0:290:C:O2' | 1:0:291:C:H5' | 2.05 | 0.56 |
| 4:A:1:GLY:HA2 | 4:A:197:VAL:HG23 | 1.87 | 0.56 |
| 10:G:23:ILE:O | 10:G:27:ILE:HG13 | 2.04 | 0.56 |
| 29:Z:25:LYS:HD2 | 30:1:49:GLU:N | 2.19 | 0.56 |
| 1:0:1352:A:N1 | 6:C:48:SER:HB3 | 2.20 | 0.56 |
| 1:0:1766:U:O2 | 1:0:1778:A:H5' | 2.06 | 0.56 |
| 1:0:1829:A:H2' | 1:0:1830:C:H5' | 1.88 | 0.56 |
| 1:0:392:U:O2' | 15:L:182:LYS:HE2 | 2.05 | 0.56 |
| 1:0:431:G:P | 15:L:48:ARG:HH12 | 2.28 | 0.56 |
| 2:9:3023:U:H6 | 2:9:3023:U:H5'' | 1.69 | 0.56 |
| 7:D:41:LEU:HA | 7:D:44:ILE:CG2 | 2.35 | 0.56 |
| 11:H:35:ASN:HD21 | 11:H:80:ASN:HA | 1.69 | 0.56 |
| 14:K:90:ARG:NH2 | 14:K:121:ILE:HD11 | 2.21 | 0.56 |
| 15:L:172:GLY:O | 15:L:183:VAL:HG11 | 2.04 | 0.56 |
| 1:0:2404:G:O5' | 19:P:68:GLY:HA3 | 2.04 | 0.56 |
| 20:Q:82:GLU:HG3 | 20:Q:83:LYS:N | 2.20 | 0.56 |
| 22:S:28:SER:O | 22:S:32:ARG:HG3 | 2.05 | 0.56 |
| 24:U:39:ALA:N | 24:U:40:PRO:CD | 2.67 | 0.56 |
| 26:W:78:GLU:HG2 | 26:W:79:GLU:N | 2.18 | 0.56 |
| 1:0:1209:C:H2' | 1:0:1210:G:C8 | 2.39 | 0.56 |
| 6:C:104:ASP:HA | 6:C:107:ARG:NH1 | 2.19 | 0.56 |
| 12:I:26:VAL:HG13 | 12:I:36:VAL:HG11 | 1.88 | 0.56 |
| 16:M:143:ARG:NH1 | 16:M:173:ASP:OD2 | 2.36 | 0.56 |
| 17:N:47:ARG:HH11 | 17:N:47:ARG:HG3 | 1.70 | 0.56 |
| 21:R:52:VAL:HG22 | 21:R:66:VAL:HG22 | 1.88 | 0.56 |
| 1:0:2269:C:H2' | 1:0:2270:G:H5' | 1.86 | 0.56 |
| 1:0:64:G:H2' | 1:0:65:C:C6 | 2.40 | 0.56 |
| 2:9:3055:U:H4' | 2:9:3056:A:H8 | 1.71 | 0.56 |
| 5:B:24:PRO:HG3 | 5:B:204:GLY:HA2 | 1.87 | 0.56 |
| 7:D:146:LYS:HZ1 | 16:M:107:ASN:HD21 | 1.51 | 0.56 |
| 9:F:47:LEU:HB2 | 9:F:108:LEU:HD11 | 1.88 | 0.56 |
| 15:L:155:HIS:CE1 | 15:L:158:ARG:HE | 2.23 | 0.56 |
| 16:M:71:TRP:HE3 | 16:M:175:LEU:HD22 | 1.71 | 0.56 |
| 24:U:58:THR:O | 24:U:62:GLU:HG3 | 2.05 | 0.56 |
| 25:V:21:LEU:HD21 | 25:V:48:VAL:HG11 | 1.88 | 0.56 |
| 1:0:1139:U:H2' | 1:0:1140:C:C6 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:2011:A:H4' | 1:0:2012:U:O5' | 2.06 | 0.56 |
| 1:0:445:U:H2' | 1:0:446:G:H8 | 1.69 | 0.56 |
| 1:0:558:C:H2' | 1:0:559:U:H5' | 1.86 | 0.56 |
| 1:0:960:G:H4' | 38:0:8921:HOH:O | 2.05 | 0.56 |
| 2:9:3028:U:H5'' | 16:M:40:ASN:ND2 | 2.20 | 0.56 |
| 19:P:64:GLU:HG3 | 19:P:74:ASP:OD2 | 2.05 | 0.56 |
| 1:0:1669:A:H2' | 1:0:1670:G:C8 | 2.41 | 0.56 |
| 1:0:732:C:H2' | 1:0:733:U:C6 | 2.40 | 0.56 |
| 2:9:3025:G:H5'' | 2:9:3026:C:C6 | 2.40 | 0.56 |
| 5:B:175:LEU:O | 5:B:175:LEU:HD23 | 2.05 | 0.56 |
| 6:C:27:ARG:HG3 | 6:C:29:ASP:OD1 | 2.06 | 0.56 |
| 11:H:97:LYS:HD3 | 11:H:117:LYS:HD3 | 1.86 | 0.56 |
| 12:I:74:ARG:NH1 | 12:I:76:ASP:HB2 | 2.20 | 0.56 |
| 18:O:16:VAL:HG12 | 18:O:17:GLY:N | 2.20 | 0.56 |
| 1:0:2364:A:H5'' | 19:P:15:LYS:HD3 | 1.87 | 0.56 |
| 26:W:37:LEU:CD1 | 26:W:85:VAL:HG21 | 2.32 | 0.56 |
| 1:0:1586:G:O2' | 1:0:1587:U:H5' | 2.06 | 0.56 |
| 1:0:2054:A:C2 | 20:Q:128:ARG:NH2 | 2.74 | 0.56 |
| 1:0:2768:A:O2' | 1:0:2769:C:H5' | 2.05 | 0.56 |
| 1:0:862:U:H2' | 1:0:863:G:C8 | 2.39 | 0.56 |
| 2:9:3029:C:H2' | 2:9:3030:C:H5' | 1.87 | 0.56 |
| 4:A:51:ARG:NH1 | 4:A:120:ARG:O | 2.38 | 0.56 |
| 38:0:6414:HOH:O | 5:B:298:LYS:HD3 | 2.06 | 0.56 |
| 1:0:2310:G:OP2 | 11:H:114:PRO:HD2 | 2.05 | 0.56 |
| 7:D:25:MET:SD | 7:D:40:ILE:HD11 | 2.46 | 0.56 |
| 7:D:69:ILE:O | 7:D:69:ILE:HG22 | 2.05 | 0.56 |
| 8:E:31:ARG:NH1 | 8:E:68:HIS:CG | 2.73 | 0.56 |
| 15:L:134:ILE:O | 15:L:136:PRO:HD3 | 2.05 | 0.56 |
| 1:0:1154:A:H2' | 1:0:1155:G:C8 | 2.40 | 0.56 |
| 1:0:1453:G:H2' | 1:0:1454:U:O4' | 2.06 | 0.56 |
| 1:0:2119:C:O2' | 1:0:2120:U:H5' | 2.06 | 0.56 |
| 1:0:2426:G:H1' | 38:0:6980:HOH:O | 2.05 | 0.56 |
| 1:0:2909:G:O2' | 1:0:2910:A:H5' | 2.06 | 0.56 |
| 1:0:2435:U:OP1 | 31:2:28:GLY:HA3 | 2.06 | 0.56 |
| 5:B:82:VAL:HG12 | 5:B:82:VAL:O | 2.06 | 0.56 |
| 6:C:20:ASP:O | 6:C:23:GLU:HB2 | 2.06 | 0.56 |
| 7:D:10:PHE:CG | 7:D:11:HIS:N | 2.73 | 0.56 |
| 12:I:27:ALA:HB1 | 12:I:87:LEU:CD2 | 2.36 | 0.56 |
| 1:0:1733:A:H4' | 5:B:212:GLN:HA | 1.88 | 0.56 |
| 1:0:485:A:N3 | 1:0:487:G:H5'' | 2.21 | 0.56 |
| 4:A:100:PRO:HG2 | 4:A:103:VAL:HG21 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:B:56:ASP:OD1 | 5:B:322:ARG:HB3 | 2.05 | 0.56 |
| 6:C:72:LYS:HG2 | 6:C:77:ALA:HA | 1.86 | 0.56 |
| 11:H:157:ILE:HG22 | 11:H:158:ASN:N | 2.21 | 0.56 |
| 12:I:99:GLU:HA | 38:I:7377:HOH:O | 2.06 | 0.56 |
| 13:J:81:ARG:HB2 | 13:J:87:ARG:HH11 | 1.70 | 0.56 |
| 26:W:66:THR:HG23 | 26:W:67:PRO:HD2 | 1.88 | 0.56 |
| 1:O:1882:C:H2' | 1:O:1883:U:C6 | 2.42 | 0.55 |
| 4:A:192:VAL:HG12 | 4:A:192:VAL:O | 2.05 | 0.55 |
| 16:M:77:ASN:OD1 | 16:M:79:PRO:HD2 | 2.05 | 0.55 |
| 20:Q:104:PHE:HB2 | 20:Q:109:MET:HE1 | 1.88 | 0.55 |
| 23:T:44:ARG:HB3 | 38:T:3805:HOH:O | 2.06 | 0.55 |
| 1:O:1657:A:H2' | 1:O:1658:A:C8 | 2.41 | 0.55 |
| 30:I:18:ASN:ND2 | 30:I:40:ARG:H | 2.04 | 0.55 |
| 2:9:3023:U:H4' | 2:9:3024:U:OP2 | 2.05 | 0.55 |
| 17:N:53:GLN:HG2 | 17:N:56:GLU:OE1 | 2.07 | 0.55 |
| 1:O:596:C:H2' | 1:O:597:A:C8 | 2.41 | 0.55 |
| 4:A:125:ASN:CB | 4:A:158:VAL:HG12 | 2.36 | 0.55 |
| 5:B:280:VAL:HG13 | 5:B:334:SER:HA | 1.88 | 0.55 |
| 11:H:46:VAL:HG21 | 38:H:8387:HOH:O | 2.05 | 0.55 |
| 38:O:7746:HOH:O | 15:L:178:LYS:HB2 | 2.06 | 0.55 |
| 18:O:7:LYS:HD3 | 18:O:21:VAL:HG21 | 1.87 | 0.55 |
| 25:V:21:LEU:HD21 | 25:V:48:VAL:CG1 | 2.36 | 0.55 |
| 1:O:1223:G:O2' | 1:O:1224:G:H5' | 2.06 | 0.55 |
| 1:O:671:A:O2' | 1:O:672:G:H2' | 2.07 | 0.55 |
| 31:2:3:MET:O | 31:2:90:PHE:HA | 2.05 | 0.55 |
| 6:C:168:ARG:NH2 | 6:C:190:ALA:O | 2.39 | 0.55 |
| 14:K:66:VAL:HG23 | 14:K:67:ARG:N | 2.21 | 0.55 |
| 9:F:61:MET:HB3 | 15:L:19:GLN:OE1 | 2.05 | 0.55 |
| 25:V:149:LEU:HG | 25:V:153:MET:HE2 | 1.87 | 0.55 |
| 27:X:103:THR:HG22 | 27:X:104:GLU:OE2 | 2.07 | 0.55 |
| 1:O:319:A:H4' | 1:O:338:C:C4 | 2.41 | 0.55 |
| 1:O:542:A:H2' | 1:O:543:G:O4' | 2.07 | 0.55 |
| 4:A:105:VAL:CG1 | 4:A:154:ALA:HB1 | 2.36 | 0.55 |
| 7:D:99:ASP:HB2 | 7:D:103:ASN:HB2 | 1.88 | 0.55 |
| 8:E:81:GLU:HG2 | 8:E:134:SER:HB3 | 1.88 | 0.55 |
| 9:F:56:PRO:HG2 | 15:L:43:PRO:O | 2.06 | 0.55 |
| 1:O:1789:G:O6 | 18:O:73:HIS:HE1 | 1.89 | 0.55 |
| 1:O:793:A:H5'' | 18:O:83:LYS:HG2 | 1.89 | 0.55 |
| 21:R:32:ALA:HA | 21:R:36:GLU:OE1 | 2.06 | 0.55 |
| 26:W:31:ILE:O | 26:W:35:GLU:HG3 | 2.06 | 0.55 |
| 28:Y:42:CYS:SG | 28:Y:44:PHE:HB2 | 2.47 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:Y:56:MET:HA | 28:Y:62:TYR:O | 2.06 | 0.55 |
| 1:O:1249:U:H2' | 1:O:1250:C:C6 | 2.41 | 0.55 |
| 1:O:420:U:H2' | 1:O:421:C:C6 | 2.42 | 0.55 |
| 1:O:67:A:H5'' | 1:O:69:A:C8 | 2.41 | 0.55 |
| 1:O:2715:G:O2' | 5:B:262:ARG:HD2 | 2.06 | 0.55 |
| 6:C:124:VAL:HA | 6:C:230:GLY:O | 2.07 | 0.55 |
| 9:F:37:THR:O | 9:F:41:GLU:HG3 | 2.07 | 0.55 |
| 6:C:139:VAL:CG2 | 6:C:240:LEU:HD12 | 2.37 | 0.55 |
| 15:L:12:TRP:O | 15:L:15:PRO:HD3 | 2.07 | 0.55 |
| 15:L:47:ASP:CG | 15:L:48:ARG:H | 2.09 | 0.55 |
| 1:O:432:G:O2' | 1:O:433:C:H5' | 2.07 | 0.55 |
| 4:A:36:ASP:HB2 | 4:A:84:VAL:N | 2.22 | 0.55 |
| 7:D:23:VAL:HG21 | 7:D:45:THR:HG21 | 1.87 | 0.55 |
| 10:G:71:LEU:O | 10:G:73:ASP:N | 2.40 | 0.55 |
| 15:L:134:ILE:HG23 | 15:L:141:ILE:HD13 | 1.89 | 0.55 |
| 22:S:71:VAL:HG13 | 22:S:91:LEU:O | 2.07 | 0.55 |
| 4:A:179:MET:HG2 | 4:A:186:TRP:CG | 2.42 | 0.55 |
| 8:E:7:ILE:HG22 | 8:E:45:ASP:O | 2.07 | 0.55 |
| 11:H:31:PHE:HA | 11:H:85:ILE:CG2 | 2.37 | 0.55 |
| 2:9:3114:G:O6 | 16:M:11:ARG:HD3 | 2.06 | 0.55 |
| 4:A:125:ASN:HB3 | 4:A:158:VAL:HG12 | 1.88 | 0.55 |
| 6:C:218:VAL:N | 38:C:8434:HOH:O | 2.40 | 0.55 |
| 7:D:54:ALA:HB2 | 7:D:69:ILE:HD12 | 1.88 | 0.55 |
| 9:F:91:VAL:CG1 | 9:F:92:GLY:N | 2.70 | 0.55 |
| 13:J:74:VAL:HG12 | 13:J:75:ARG:HG3 | 1.89 | 0.55 |
| 15:L:149:TRP:O | 15:L:152:ARG:HG2 | 2.07 | 0.55 |
| 28:Y:27:ALA:HA | 38:Y:8416:HOH:O | 2.07 | 0.55 |
| 1:O:1165:G:H1' | 1:O:1174:A:H1' | 1.89 | 0.54 |
| 1:O:1942:A:H2' | 1:O:1943:C:H6 | 1.72 | 0.54 |
| 1:O:2600:A:H2' | 1:O:2601:A:O4' | 2.07 | 0.54 |
| 1:O:596:C:H2' | 1:O:597:A:H8 | 1.72 | 0.54 |
| 1:O:832:U:H2' | 1:O:833:G:H8 | 1.72 | 0.54 |
| 21:R:11:THR:H | 21:R:14:ALA:HB3 | 1.71 | 0.54 |
| 4:A:170:VAL:HG13 | 28:Y:22:ILE:HG21 | 1.89 | 0.54 |
| 1:O:1943:C:O4' | 4:A:212:PRO:HA | 2.08 | 0.54 |
| 1:O:2777:G:O2' | 1:O:2778:A:H5' | 2.07 | 0.54 |
| 1:O:398:U:H2' | 1:O:399:C:C6 | 2.43 | 0.54 |
| 9:F:50:VAL:HG21 | 9:F:63:ILE:HG21 | 1.89 | 0.54 |
| 13:J:75:ARG:HG2 | 13:J:90:PHE:CD2 | 2.42 | 0.54 |
| 25:V:125:HIS:CD2 | 25:V:127:GLY:H | 2.25 | 0.54 |
| 1:O:1377:C:H6 | 1:O:1377:C:H5' | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:2072:G:C6 | 1:0:2533:C:H1' | 2.42 | 0.54 |
| 1:0:2502:C:H2' | 1:0:2503:A:C5' | 2.36 | 0.54 |
| 1:0:2718:C:H6 | 1:0:2718:C:H5' | 1.71 | 0.54 |
| 1:0:2769:C:C2' | 1:0:2770:G:H5' | 2.37 | 0.54 |
| 1:0:2885:A:H2' | 1:0:2886:C:H6 | 1.71 | 0.54 |
| 1:0:506:G:N2 | 1:0:509:A:H5' | 2.19 | 0.54 |
| 1:0:825:U:H5'' | 1:0:826:U:OP1 | 2.07 | 0.54 |
| 8:E:5:LEU:HD21 | 8:E:66:GLN:HG3 | 1.89 | 0.54 |
| 11:H:3:GLY:HA2 | 11:H:57:ARG:NH1 | 2.23 | 0.54 |
| 24:U:57:LYS:HA | 24:U:60:GLN:HE21 | 1.71 | 0.54 |
| 25:V:90:TYR:CE2 | 25:V:99:ALA:HB2 | 2.41 | 0.54 |
| 1:0:2419:U:H5'' | 1:0:2420:G:H5' | 1.89 | 0.54 |
| 1:0:263:U:O4' | 9:F:59:ILE:HD13 | 2.07 | 0.54 |
| 2:9:3064:C:C2' | 2:9:3065:A:H5' | 2.37 | 0.54 |
| 6:C:40:ALA:CB | 6:C:100:LEU:HD12 | 2.37 | 0.54 |
| 14:K:65:ASP:CG | 14:K:111:ALA:HB3 | 2.28 | 0.54 |
| 21:R:57:THR:C | 21:R:59:ASP:H | 2.11 | 0.54 |
| 1:0:1119:G:N2 | 1:0:1246:A:H2 | 2.05 | 0.54 |
| 1:0:2050:G:H5'' | 20:Q:80:TYR:O | 2.07 | 0.54 |
| 1:0:2766:A:O2' | 1:0:2767:C:H5' | 2.07 | 0.54 |
| 9:F:28:ALA:HB3 | 9:F:99:THR:O | 2.07 | 0.54 |
| 14:K:73:VAL:HG23 | 14:K:74:THR:N | 2.22 | 0.54 |
| 25:V:125:HIS:HD2 | 25:V:127:GLY:H | 1.55 | 0.54 |
| 26:W:21:PRO:HG2 | 26:W:24:LYS:HD3 | 1.90 | 0.54 |
| 1:0:1666:C:O2' | 1:0:1667:A:C5' | 2.55 | 0.54 |
| 1:0:2897:C:H2' | 1:0:2898:G:C8 | 2.41 | 0.54 |
| 31:2:69:TYR:HB2 | 31:2:78:HIS:CE1 | 2.43 | 0.54 |
| 2:9:3076:G:C3' | 2:9:3077:A:H5'' | 2.28 | 0.54 |
| 4:A:42:VAL:HG21 | 4:A:74:VAL:CG1 | 2.38 | 0.54 |
| 1:0:2676:C:H4' | 12:I:70:PHE:CE1 | 2.42 | 0.54 |
| 1:0:100:C:H4' | 22:S:16:LEU:HB2 | 1.90 | 0.54 |
| 1:0:1331:A:OP2 | 27:X:142:SER:OG | 2.23 | 0.54 |
| 1:0:2112:A:H2' | 1:0:2113:G:C8 | 2.41 | 0.54 |
| 1:0:263:U:C4 | 9:F:54:VAL:HG13 | 2.42 | 0.54 |
| 1:0:282:C:H1' | 1:0:368:C:H42 | 1.70 | 0.54 |
| 1:0:660:A:H4' | 1:0:661:G:O5' | 2.08 | 0.54 |
| 5:B:248:ARG:O | 5:B:251:VAL:HG13 | 2.08 | 0.54 |
| 5:B:305:ASP:O | 5:B:306:LYS:HB2 | 2.08 | 0.54 |
| 6:C:16:VAL:HG12 | 6:C:17:ASP:N | 2.22 | 0.54 |
| 2:9:3056:A:H1' | 7:D:14:ARG:HG2 | 1.90 | 0.54 |
| 8:E:24:GLY:HA3 | 8:E:76:VAL:HB | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:H:31:PHE:HD2 | 11:H:85:ILE:O | 1.90 | 0.54 |
| 18:O:29:GLY:O | 18:O:32:ALA:HB3 | 2.07 | 0.54 |
| 28:Y:48:LYS:HG2 | 38:Y:8435:HOH:O | 2.08 | 0.54 |
| 1:O:2379:G:H4' | 1:O:2380:A:H5'' | 1.90 | 0.54 |
| 30:1:39:ARG:HG2 | 38:1:3143:HOH:O | 2.06 | 0.54 |
| 7:D:140:ARG:O | 7:D:144:ARG:HG2 | 2.07 | 0.54 |
| 9:F:28:ALA:CB | 9:F:99:THR:HG23 | 2.37 | 0.54 |
| 2:9:3006:C:C5' | 16:M:37:ARG:NH1 | 2.67 | 0.54 |
| 1:O:947:U:H2' | 1:O:948:G:H8 | 1.70 | 0.54 |
| 16:M:34:LEU:HD22 | 16:M:129:ILE:HD13 | 1.88 | 0.54 |
| 20:Q:98:ASN:HD22 | 20:Q:98:ASN:N | 2.04 | 0.54 |
| 1:O:1641:A:C2' | 1:O:1642:A:H5' | 2.38 | 0.54 |
| 1:O:2437:A:H2' | 1:O:2438:G:C8 | 2.42 | 0.54 |
| 1:O:512:G:O3' | 1:O:513:A:H8 | 1.91 | 0.54 |
| 1:O:60:A:O2' | 1:O:61:G:H5' | 2.08 | 0.54 |
| 4:A:53:ALA:HB3 | 38:A:8617:HOH:O | 2.08 | 0.54 |
| 16:M:154:LEU:HD11 | 38:M:8526:HOH:O | 2.08 | 0.54 |
| 1:O:1123:A:C2 | 1:O:1129:C:H4' | 2.43 | 0.53 |
| 1:O:168:C:O2' | 1:O:169:A:H5' | 2.08 | 0.53 |
| 1:O:249:G:O2' | 1:O:250:C:H5' | 2.08 | 0.53 |
| 1:O:415:A:O2' | 1:O:416:G:H5' | 2.09 | 0.53 |
| 5:B:52:VAL:O | 5:B:53:LEU:HD12 | 2.06 | 0.53 |
| 8:E:84:MET:HB2 | 8:E:131:LEU:HB2 | 1.89 | 0.53 |
| 13:J:28:GLU:OE2 | 13:J:58:THR:HG21 | 2.08 | 0.53 |
| 16:M:139:TRP:HA | 16:M:139:TRP:CE3 | 2.42 | 0.53 |
| 16:M:34:LEU:HA | 16:M:47:LEU:HD23 | 1.89 | 0.53 |
| 29:Z:28:HIS:HD2 | 29:Z:30:LYS:H | 1.56 | 0.53 |
| 1:O:316:A:N3 | 1:O:336:G:O2' | 2.39 | 0.53 |
| 1:O:352:A:H2' | 1:O:353:G:C8 | 2.43 | 0.53 |
| 1:O:639:A:H2' | 1:O:640:G:C8 | 2.43 | 0.53 |
| 31:2:56:PRO:HA | 38:2:8553:HOH:O | 2.07 | 0.53 |
| 7:D:94:ALA:HB3 | 7:D:174:VAL:HA | 1.89 | 0.53 |
| 9:F:52:GLU:HG3 | 9:F:77:VAL:O | 2.09 | 0.53 |
| 15:L:87:MET:HB2 | 15:L:91:ILE:CD1 | 2.36 | 0.53 |
| 38:9:8461:HOH:O | 19:P:25:PRO:HB2 | 2.08 | 0.53 |
| 1:O:1528:A:H2' | 1:O:1529:G:O4' | 2.08 | 0.53 |
| 1:O:1666:C:H2' | 1:O:1667:A:H8 | 1.73 | 0.53 |
| 1:O:2276:U:H2' | 1:O:2277:U:C6 | 2.43 | 0.53 |
| 1:O:2791:U:H1' | 1:O:2792:A:H5'' | 1.91 | 0.53 |
| 1:O:381:G:H5'' | 38:0:5237:HOH:O | 2.06 | 0.53 |
| 1:O:447:A:O2' | 1:O:448:G:H5' | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:1884:G:O6 | 4:A:190:ARG:HD2 | 2.07 | 0.53 |
| 7:D:54:ALA:CB | 7:D:69:ILE:HD12 | 2.38 | 0.53 |
| 14:K:61:ALA:HA | 38:K:8569:HOH:O | 2.08 | 0.53 |
| 22:S:19:ARG:NH1 | 22:S:68:ASP:O | 2.41 | 0.53 |
| 28:Y:30:GLU:HB2 | 38:Y:8416:HOH:O | 2.07 | 0.53 |
| 1:O:1182:C:H1' | 1:O:1192:A:H8 | 1.73 | 0.53 |
| 1:O:1471:A:H2' | 1:O:1472:C:C6 | 2.43 | 0.53 |
| 1:O:1805:G:H2' | 1:O:1806:G:C8 | 2.40 | 0.53 |
| 1:O:1825:U:O2' | 1:O:1826:C:H5' | 2.08 | 0.53 |
| 1:O:2243:C:HO2' | 1:O:2244:A:H8 | 1.56 | 0.53 |
| 1:O:810:G:H2' | 1:O:811:C:C6 | 2.43 | 0.53 |
| 7:D:59:GLY:O | 7:D:61:PHE:N | 2.35 | 0.53 |
| 9:F:63:ILE:HB | 9:F:64:PRO:CD | 2.33 | 0.53 |
| 13:J:34:VAL:HG22 | 13:J:47:ALA:HB2 | 1.90 | 0.53 |
| 13:J:98:VAL:CG1 | 13:J:102:GLU:HA | 2.38 | 0.53 |
| 16:M:11:ARG:HG3 | 16:M:14:ARG:HH12 | 1.72 | 0.53 |
| 18:O:131:PHE:CD1 | 18:O:137:LEU:HD13 | 2.43 | 0.53 |
| 22:S:37:GLN:OE1 | 22:S:118:SER:HA | 2.09 | 0.53 |
| 1:O:797:A:C4' | 28:Y:10:ARG:N | 2.72 | 0.53 |
| 1:O:1516:C:H2' | 1:O:1517:U:C6 | 2.44 | 0.53 |
| 1:O:2247:C:O2' | 1:O:2248:C:H5' | 2.07 | 0.53 |
| 1:O:2781:U:O2' | 1:O:2782:G:H5' | 2.08 | 0.53 |
| 31:2:65:THR:HB | 31:2:83:TRP:H | 1.73 | 0.53 |
| 6:C:127:ARG:HG2 | 6:C:127:ARG:NH1 | 2.20 | 0.53 |
| 1:O:1058:A:H2' | 1:O:1060:C:H5'' | 1.91 | 0.53 |
| 1:O:111:C:O2' | 1:O:112:G:H5' | 2.07 | 0.53 |
| 1:O:1934:A:C8 | 1:O:1935:C:C5 | 2.96 | 0.53 |
| 1:O:2353:A:O2' | 16:M:7:LYS:HB3 | 2.08 | 0.53 |
| 1:O:861:A:H2' | 1:O:862:U:C6 | 2.43 | 0.53 |
| 1:O:462:A:C2 | 30:1:37:HIS:HB3 | 2.43 | 0.53 |
| 7:D:57:THR:HG23 | 7:D:63:ILE:CG2 | 2.38 | 0.53 |
| 14:K:133:VAL:HG13 | 38:K:8558:HOH:O | 2.09 | 0.53 |
| 15:L:32:ARG:HH21 | 15:L:123:ASP:HB3 | 1.74 | 0.53 |
| 20:Q:18:LEU:HD12 | 20:Q:143:VAL:CG1 | 2.38 | 0.53 |
| 25:V:52:VAL:HG22 | 25:V:53:ALA:H | 1.74 | 0.53 |
| 25:V:81:ASP:OD1 | 25:V:92:ASP:HB2 | 2.09 | 0.53 |
| 1:O:120:A:N3 | 1:O:120:A:H2' | 2.23 | 0.53 |
| 1:O:1132:A:N6 | 1:O:1229:C:H2' | 2.24 | 0.53 |
| 1:O:1701:A:H4' | 1:O:1702:U:H5'' | 1.89 | 0.53 |
| 1:O:2721:U:H4' | 13:J:87:ARG:HG3 | 1.91 | 0.53 |
| 1:O:280:C:H2' | 1:O:281:U:O4' | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:D:41:LEU:CA | 7:D:44:ILE:HG22 | 2.37 | 0.53 |
| 16:M:167:ASP:O | 16:M:168:LEU:HD23 | 2.08 | 0.53 |
| 1:O:2712:G:H5' | 38:J:4183:HOH:O | 2.09 | 0.53 |
| 1:O:703:G:O2' | 1:O:704:C:H5' | 2.09 | 0.53 |
| 4:A:220:PRO:HD2 | 4:A:223:ARG:HD3 | 1.90 | 0.53 |
| 7:D:23:VAL:HG23 | 7:D:41:LEU:HD22 | 1.89 | 0.53 |
| 38:O:4718:HOH:O | 15:L:189:VAL:HG21 | 2.08 | 0.53 |
| 16:M:71:TRP:CE3 | 16:M:175:LEU:HD22 | 2.43 | 0.53 |
| 20:Q:118:LYS:HE3 | 20:Q:139:PRO:HB3 | 1.91 | 0.53 |
| 25:V:108:ARG:HE | 25:V:114:PRO:HG3 | 1.74 | 0.53 |
| 1:O:1304:U:H2' | 1:O:1305:C:C6 | 2.44 | 0.53 |
| 1:O:394:G:H1 | 15:L:181:GLU:CD | 2.12 | 0.53 |
| 1:O:661:G:C5 | 1:O:686:A:C2 | 2.96 | 0.53 |
| 2:9:3060:C:O2' | 2:9:3061:C:H5' | 2.08 | 0.53 |
| 12:I:46:ILE:HG12 | 12:I:53:ILE:HD13 | 1.91 | 0.53 |
| 20:Q:29:LYS:HB3 | 38:Q:8533:HOH:O | 2.08 | 0.53 |
| 24:U:39:ALA:O | 24:U:41:GLU:N | 2.42 | 0.53 |
| 25:V:10:GLU:HG3 | 25:V:11:VAL:N | 2.24 | 0.53 |
| 1:O:1515:A:H2' | 1:O:1516:C:C6 | 2.43 | 0.53 |
| 1:O:1714:C:O2' | 1:O:1715:C:H5' | 2.08 | 0.53 |
| 1:O:1878:G:O2' | 1:O:1879:U:P | 2.67 | 0.53 |
| 1:O:324:G:O2' | 1:O:325:U:H5' | 2.09 | 0.53 |
| 2:9:3041:C:O4' | 7:D:50:VAL:HG23 | 2.08 | 0.53 |
| 5:B:87:TYR:HD1 | 38:B:8592:HOH:O | 1.91 | 0.53 |
| 7:D:95:THR:C | 7:D:97:GLN:H | 2.13 | 0.53 |
| 11:H:147:ARG:HA | 11:H:150:LYS:HZ3 | 1.73 | 0.53 |
| 22:S:35:TYR:CG | 22:S:112:LEU:HD22 | 2.43 | 0.53 |
| 1:O:1829:A:H5'' | 38:O:4035:HOH:O | 2.09 | 0.52 |
| 1:O:1850:U:H2' | 1:O:1851:G:C8 | 2.44 | 0.52 |
| 6:C:130:GLU:HG2 | 6:C:168:ARG:HD3 | 1.91 | 0.52 |
| 6:C:175:LYS:HD3 | 6:C:184:ARG:O | 2.09 | 0.52 |
| 15:L:87:MET:CB | 31:2:46:ILE:HG21 | 2.38 | 0.52 |
| 25:V:1:MET:N | 25:V:37:GLU:HG3 | 2.24 | 0.52 |
| 1:O:1899:C:O2' | 1:O:1900:A:H5' | 2.09 | 0.52 |
| 1:O:2115:U:H2' | 1:O:2116:U:C6 | 2.44 | 0.52 |
| 1:O:2812:A:C2 | 1:O:2814:A:N6 | 2.72 | 0.52 |
| 1:O:695:C:O2' | 1:O:696:C:H5' | 2.08 | 0.52 |
| 1:O:858:U:H2' | 1:O:859:C:H6 | 1.74 | 0.52 |
| 1:O:949:U:O2' | 19:P:40:HIS:HE1 | 1.92 | 0.52 |
| 1:O:470:U:O2' | 29:Z:16:HIS:CD2 | 2.61 | 0.52 |
| 1:O:1821:A:O2' | 1:O:1822:A:H5' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:88:ILE:HG22 | 4:A:88:ILE:O | 2.09 | 0.52 |
| 9:F:13:GLU:OE2 | 9:F:78:GLU:HG2 | 2.09 | 0.52 |
| 11:H:26:LYS:CD | 11:H:28:ILE:HB | 2.39 | 0.52 |
| 28:Y:31:ILE:HG23 | 28:Y:32:LYS:N | 2.25 | 0.52 |
| 1:0:1206:U:C6 | 1:0:1206:U:H5' | 2.37 | 0.52 |
| 1:0:1568:G:O2' | 1:0:1569:U:H5' | 2.08 | 0.52 |
| 1:0:1634:G:H2' | 1:0:1635:U:C6 | 2.44 | 0.52 |
| 1:0:1638:U:O2' | 1:0:1639:U:H5' | 2.09 | 0.52 |
| 1:0:332:G:O2' | 1:0:333:G:H5' | 2.10 | 0.52 |
| 1:0:2468:A:H61 | 31:2:48:ASN:HD21 | 1.58 | 0.52 |
| 4:A:94:LEU:HG | 4:A:99:ILE:CD1 | 2.38 | 0.52 |
| 7:D:154:LYS:H | 7:D:154:LYS:CD | 2.17 | 0.52 |
| 1:0:1055:G:OP2 | 11:H:94:ARG:NH1 | 2.43 | 0.52 |
| 16:M:151:ASP:OD1 | 16:M:154:LEU:HD13 | 2.10 | 0.52 |
| 1:0:1268:C:H2' | 1:0:1269:G:H8 | 1.75 | 0.52 |
| 1:0:2346:C:O5' | 1:0:2346:C:H6 | 1.92 | 0.52 |
| 1:0:858:U:H2' | 1:0:859:C:C6 | 2.43 | 0.52 |
| 2:9:3064:C:H2' | 2:9:3065:A:H5' | 1.91 | 0.52 |
| 7:D:23:VAL:O | 7:D:23:VAL:HG23 | 2.09 | 0.52 |
| 9:F:49:PHE:O | 9:F:95:ALA:HA | 2.09 | 0.52 |
| 25:V:65:VAL:CG1 | 25:V:116:LEU:HD13 | 2.38 | 0.52 |
| 1:0:621:C:H5' | 27:X:132:ASP:OD2 | 2.10 | 0.52 |
| 1:0:1191:A:C3' | 1:0:1192:A:H5'' | 2.38 | 0.52 |
| 1:0:221:G:H2' | 1:0:222:A:C8 | 2.44 | 0.52 |
| 1:0:2326:U:H4' | 1:0:2412:G:H4' | 1.90 | 0.52 |
| 1:0:2781:U:C2' | 1:0:2782:G:H5' | 2.40 | 0.52 |
| 1:0:1787:C:H4' | 1:0:2883:A:O4' | 2.10 | 0.52 |
| 4:A:192:VAL:O | 4:A:207:GLN:HG2 | 2.10 | 0.52 |
| 5:B:162:MET:HE3 | 5:B:308:LEU:CD2 | 2.31 | 0.52 |
| 1:0:330:C:H5 | 6:C:170:ASP:OD2 | 1.92 | 0.52 |
| 1:0:1456:C:H2' | 1:0:1457:U:C6 | 2.44 | 0.52 |
| 1:0:1513:C:O2' | 1:0:1514:C:H5' | 2.10 | 0.52 |
| 1:0:2266:A:OP2 | 15:L:90:ARG:NH2 | 2.42 | 0.52 |
| 1:0:240:C:O2 | 1:0:240:C:H2' | 2.10 | 0.52 |
| 5:B:101:TRP:HB2 | 5:B:119:HIS:CD2 | 2.45 | 0.52 |
| 1:0:1134:G:OP2 | 11:H:156:THR:HG23 | 2.09 | 0.52 |
| 1:0:1730:G:H5' | 1:0:1731:C:C5 | 2.45 | 0.52 |
| 1:0:269:G:O3' | 1:0:274:G:H4' | 2.09 | 0.52 |
| 1:0:2909:G:H2' | 1:0:2910:A:H8 | 1.75 | 0.52 |
| 6:C:236:THR:O | 6:C:239:ALA:N | 2.43 | 0.52 |
| 8:E:15:GLN:HG2 | 8:E:19:ASP:O | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:L:52:LEU:HD13 | 15:L:116:ASN:CG | 2.30 | 0.52 |
| 16:M:62:HIS:HB3 | 16:M:65:ASP:OD1 | 2.09 | 0.52 |
| 22:S:71:VAL:HG12 | 22:S:72:ILE:N | 2.23 | 0.52 |
| 22:S:9:LYS:HE3 | 22:S:13:ARG:HH11 | 1.70 | 0.52 |
| 25:V:38:THR:HG22 | 25:V:39:ASP:H | 1.74 | 0.52 |
| 1:0:105:G:O2' | 1:0:106:A:H5' | 2.10 | 0.52 |
| 1:0:1497:G:H4' | 1:0:1627:G:O2' | 2.10 | 0.52 |
| 1:0:1878:G:O2' | 1:0:1879:U:C6 | 2.60 | 0.52 |
| 1:0:2269:C:H2' | 1:0:2270:G:C5' | 2.40 | 0.52 |
| 1:0:2903:C:O2' | 1:0:2904:U:H5' | 2.10 | 0.52 |
| 1:0:289:G:O2' | 1:0:290:C:H5' | 2.10 | 0.52 |
| 1:0:226:A:H1' | 1:0:393:G:C5 | 2.45 | 0.52 |
| 5:B:36:PRO:HA | 5:B:168:GLY:HA2 | 1.92 | 0.52 |
| 8:E:15:GLN:HB2 | 8:E:20:ILE:HG23 | 1.92 | 0.52 |
| 1:0:1345:A:H2' | 1:0:1346:U:C6 | 2.45 | 0.52 |
| 1:0:1527:A:H1' | 1:0:1528:A:C8 | 2.45 | 0.52 |
| 1:0:155:C:O2' | 1:0:156:C:H5' | 2.10 | 0.52 |
| 1:0:175:G:H2' | 15:L:192:ALA:HB3 | 1.91 | 0.52 |
| 1:0:542:A:C8 | 1:0:542:A:H5' | 2.37 | 0.52 |
| 7:D:38:GLU:OE2 | 7:D:51:ARG:CZ | 2.57 | 0.52 |
| 9:F:30:LYS:HB2 | 9:F:97:ALA:HB3 | 1.91 | 0.52 |
| 11:H:47:GLU:HG2 | 11:H:133:ILE:HD12 | 1.91 | 0.52 |
| 11:H:59:ASN:ND2 | 11:H:59:ASN:N | 2.56 | 0.52 |
| 15:L:47:ASP:CG | 15:L:48:ARG:N | 2.64 | 0.52 |
| 16:M:180:LEU:O | 16:M:181:ASP:HB3 | 2.08 | 0.52 |
| 17:N:84:THR:CG2 | 17:N:88:LYS:HE3 | 2.40 | 0.52 |
| 22:S:63:ILE:HD11 | 22:S:75:GLU:HB2 | 1.91 | 0.52 |
| 1:0:1634:G:H2' | 1:0:1635:U:H6 | 1.74 | 0.51 |
| 1:0:255:A:H2' | 1:0:256:C:C6 | 2.45 | 0.51 |
| 13:J:98:VAL:HG13 | 13:J:99:ASP:N | 2.24 | 0.51 |
| 1:0:189:A:OP1 | 15:L:171:ARG:NH2 | 2.43 | 0.51 |
| 19:P:26:PRO:O | 19:P:30:VAL:HG23 | 2.10 | 0.51 |
| 1:0:1820:G:C6 | 1:0:2030:A:C2 | 2.98 | 0.51 |
| 1:0:1909:A:N1 | 1:0:2128:G:H1' | 2.25 | 0.51 |
| 1:0:2531:U:O2' | 1:0:2532:A:H5' | 2.10 | 0.51 |
| 1:0:2781:U:H1' | 8:E:139:GLU:OE2 | 2.10 | 0.51 |
| 1:0:820:G:C5 | 4:A:171:LYS:HB2 | 2.46 | 0.51 |
| 5:B:62:ARG:HA | 5:B:65:MET:HE2 | 1.92 | 0.51 |
| 5:B:63:GLU:HG3 | 5:B:63:GLU:O | 2.10 | 0.51 |
| 5:B:62:ARG:HA | 5:B:65:MET:CE | 2.38 | 0.51 |
| 9:F:48:VAL:CG2 | 9:F:74:PHE:HB3 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:L:52:LEU:HD13 | 15:L:116:ASN:CB | 2.40 | 0.51 |
| 15:L:147:LEU:O | 15:L:149:TRP:N | 2.43 | 0.51 |
| 1:O:2296:C:H5 | 19:P:3:SER:HG | 1.58 | 0.51 |
| 19:P:42:LYS:NZ | 19:P:43:ILE:O | 2.42 | 0.51 |
| 22:S:9:LYS:HB2 | 38:S:7242:HOH:O | 2.10 | 0.51 |
| 25:V:13:MET:CE | 25:V:17:ILE:HG22 | 2.39 | 0.51 |
| 25:V:26:ILE:HG13 | 25:V:26:ILE:O | 2.10 | 0.51 |
| 25:V:73:LEU:O | 25:V:74:GLU:HG3 | 2.11 | 0.51 |
| 27:X:178:HIS:CG | 27:X:179:PRO:HD2 | 2.46 | 0.51 |
| 1:O:1218:U:H2' | 1:O:1219:U:C6 | 2.44 | 0.51 |
| 1:O:419:A:H1' | 1:O:1921:A:C2 | 2.45 | 0.51 |
| 1:O:2121:G:H1' | 38:O:5481:HOH:O | 2.10 | 0.51 |
| 1:O:816:G:H5' | 1:O:1598:A:H4' | 1.93 | 0.51 |
| 2:9:3007:G:H5' | 38:9:8479:HOH:O | 2.09 | 0.51 |
| 5:B:304:PRO:CG | 5:B:307:ARG:NH1 | 2.73 | 0.51 |
| 7:D:170:TYR:O | 7:D:171:ASP:HB3 | 2.09 | 0.51 |
| 17:N:96:VAL:HG13 | 17:N:100:GLN:HB2 | 1.93 | 0.51 |
| 1:O:958:G:H2' | 1:O:959:C:C6 | 2.45 | 0.51 |
| 5:B:280:VAL:HG13 | 5:B:333:GLU:O | 2.10 | 0.51 |
| 5:B:72:THR:HB | 38:B:8619:HOH:O | 2.09 | 0.51 |
| 8:E:11:VAL:CG1 | 8:E:12:ASP:N | 2.72 | 0.51 |
| 16:M:115:VAL:HG23 | 38:M:8559:HOH:O | 2.10 | 0.51 |
| 1:O:1159:G:H21 | 1:O:1189:A:H8 | 1.58 | 0.51 |
| 5:B:212:GLN:HB2 | 5:B:257:THR:CG2 | 2.38 | 0.51 |
| 6:C:173:LYS:HB3 | 6:C:187:ARG:HG3 | 1.90 | 0.51 |
| 16:M:154:LEU:O | 16:M:155:GLU:CB | 2.58 | 0.51 |
| 19:P:32:GLU:HA | 19:P:71:TYR:OH | 2.11 | 0.51 |
| 22:S:78:THR:HB | 22:S:87:VAL:O | 2.11 | 0.51 |
| 24:U:64:GLY:O | 24:U:65:ASP:CB | 2.58 | 0.51 |
| 1:O:2241:C:O2' | 1:O:2242:U:H5' | 2.11 | 0.51 |
| 1:O:2346:C:O2' | 1:O:2347:C:H5' | 2.11 | 0.51 |
| 1:O:39:G:H2' | 1:O:40:C:O4' | 2.11 | 0.51 |
| 8:E:31:ARG:HH12 | 8:E:68:HIS:CE1 | 2.29 | 0.51 |
| 11:H:151:MET:CE | 11:H:151:MET:HA | 2.41 | 0.51 |
| 12:I:90:LYS:HB2 | 36:I:8502:CL:CL | 2.47 | 0.51 |
| 15:L:38:VAL:O | 15:L:38:VAL:HG12 | 2.11 | 0.51 |
| 17:N:96:VAL:CG1 | 17:N:100:GLN:HB2 | 2.41 | 0.51 |
| 1:O:1385:G:O3' | 26:W:49:ARG:NH1 | 2.43 | 0.51 |
| 1:O:1332:C:O2' | 1:O:1333:U:H5' | 2.11 | 0.51 |
| 1:O:1810:C:OP1 | 23:T:44:ARG:NE | 2.32 | 0.51 |
| 1:O:184:G:H5'' | 15:L:153:THR:CG2 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2547:C:OP2 | 5:B:5:ARG:NH1 | 2.44 | 0.51 |
| 1:0:2598:U:O2 | 1:0:2600:A:C8 | 2.63 | 0.51 |
| 1:0:2785:C:H4' | 1:0:2786:G:OP2 | 2.11 | 0.51 |
| 1:0:506:G:H22 | 1:0:509:A:H5'' | 1.73 | 0.51 |
| 30:1:36:ASN:HB3 | 30:1:39:ARG:NE | 2.25 | 0.51 |
| 31:2:55:VAL:HG23 | 31:2:55:VAL:O | 2.10 | 0.51 |
| 5:B:294:TYR:HE2 | 38:B:8665:HOH:O | 1.94 | 0.51 |
| 6:C:109:LEU:O | 6:C:109:LEU:HD12 | 2.10 | 0.51 |
| 16:M:87:LEU:CD1 | 16:M:186:LEU:HD21 | 2.39 | 0.51 |
| 16:M:64:SER:C | 16:M:66:LEU:H | 2.12 | 0.51 |
| 25:V:4:LEU:CD2 | 25:V:54:PHE:HB3 | 2.38 | 0.51 |
| 26:W:9:VAL:HG13 | 26:W:88:GLU:OE2 | 2.11 | 0.51 |
| 1:0:1333:U:H2' | 1:0:1334:C:H6 | 1.76 | 0.51 |
| 1:0:222:A:H2' | 1:0:223:G:O4' | 2.10 | 0.51 |
| 1:0:920:C:H5'' | 1:0:921:G:O5' | 2.11 | 0.51 |
| 31:2:14:CYS:HB3 | 31:2:16:GLU:HG2 | 1.93 | 0.51 |
| 15:L:27:ARG:NH2 | 15:L:44:THR:HG23 | 2.26 | 0.51 |
| 27:X:99:ALA:HB2 | 27:X:233:TYR:CE2 | 2.45 | 0.51 |
| 1:0:1189:A:H1' | 1:0:1209:C:O4' | 2.11 | 0.51 |
| 1:0:1855:G:H4' | 1:0:1856:C:O5' | 2.09 | 0.51 |
| 1:0:1920:C:O2' | 1:0:1921:A:H5' | 2.11 | 0.51 |
| 31:2:69:TYR:O | 31:2:77:ALA:HA | 2.10 | 0.51 |
| 2:9:3045:A:H2' | 2:9:3046:C:H6 | 1.75 | 0.51 |
| 1:0:1654:U:H2' | 4:A:47:HIS:CD2 | 2.46 | 0.51 |
| 15:L:155:HIS:ND1 | 15:L:158:ARG:NE | 2.54 | 0.51 |
| 28:Y:22:ILE:O | 28:Y:26:VAL:HG23 | 2.11 | 0.51 |
| 1:0:1819:G:H2' | 1:0:1820:G:H4' | 1.93 | 0.51 |
| 1:0:1849:G:H1' | 1:0:2011:A:N1 | 2.26 | 0.51 |
| 1:0:2676:C:H4' | 12:I:70:PHE:HE1 | 1.76 | 0.51 |
| 1:0:1855:G:O6 | 4:A:141:PRO:HG2 | 2.11 | 0.51 |
| 5:B:75:GLU:C | 5:B:77:PRO:HD3 | 2.32 | 0.51 |
| 8:E:11:VAL:CG1 | 8:E:12:ASP:H | 2.24 | 0.51 |
| 11:H:26:LYS:HD3 | 11:H:89:PRO:CG | 2.40 | 0.51 |
| 1:0:195:C:H2' | 1:0:196:G:H5' | 1.93 | 0.50 |
| 1:0:2314:G:C2' | 1:0:2315:C:H5' | 2.41 | 0.50 |
| 1:0:243:A:H61 | 1:0:269:G:H1' | 1.75 | 0.50 |
| 1:0:2667:G:H1' | 1:0:2914:A:N3 | 2.25 | 0.50 |
| 31:2:70:ARG:HH11 | 31:2:70:ARG:HG2 | 1.76 | 0.50 |
| 4:A:200:PRO:HG2 | 4:A:225:VAL:HG21 | 1.94 | 0.50 |
| 11:H:165:GLY:C | 11:H:166:ASN:HD22 | 2.14 | 0.50 |
| 11:H:85:ILE:HG23 | 11:H:85:ILE:O | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:R:33:SER:OG | 21:R:36:GLU:HG3 | 2.12 | 0.50 |
| 25:V:13:MET:HE3 | 25:V:17:ILE:CG2 | 2.38 | 0.50 |
| 28:Y:26:VAL:O | 28:Y:30:GLU:HG3 | 2.11 | 0.50 |
| 1:0:426:G:H2' | 1:0:427:C:O4' | 2.12 | 0.50 |
| 6:C:165:ASP:O | 6:C:168:ARG:HB3 | 2.12 | 0.50 |
| 14:K:90:ARG:NH1 | 14:K:119:THR:HG21 | 2.26 | 0.50 |
| 19:P:75:ILE:HD13 | 19:P:84:ILE:HD11 | 1.94 | 0.50 |
| 24:U:20:LEU:HD22 | 24:U:60:GLN:HE22 | 1.75 | 0.50 |
| 26:W:85:VAL:HG12 | 26:W:86:GLU:N | 2.26 | 0.50 |
| 1:0:1192:A:O2' | 1:0:1193:A:OP1 | 2.29 | 0.50 |
| 1:0:1197:G:N2 | 38:0:7119:HOH:O | 2.39 | 0.50 |
| 1:0:213:G:N2 | 1:0:225:G:H2' | 2.26 | 0.50 |
| 1:0:2758:G:H2' | 1:0:2759:C:C6 | 2.47 | 0.50 |
| 1:0:283:U:H5 | 1:0:284:C:N4 | 2.09 | 0.50 |
| 1:0:288:A:H2' | 1:0:289:G:C8 | 2.45 | 0.50 |
| 1:0:1654:U:H2' | 4:A:47:HIS:HD2 | 1.75 | 0.50 |
| 14:K:125:PHE:CE1 | 14:K:140:VAL:HG13 | 2.47 | 0.50 |
| 16:M:24:LEU:HD13 | 19:P:26:PRO:HB3 | 1.93 | 0.50 |
| 19:P:46:SER:O | 19:P:48:PRO:HD3 | 2.12 | 0.50 |
| 20:Q:119:VAL:HG12 | 20:Q:119:VAL:O | 2.11 | 0.50 |
| 1:0:1398:G:O2' | 1:0:1399:A:H5' | 2.11 | 0.50 |
| 1:0:1804:A:H2' | 1:0:1805:G:H8 | 1.74 | 0.50 |
| 1:0:182:G:O2' | 1:0:183:A:H5' | 2.12 | 0.50 |
| 1:0:2540:G:O2' | 1:0:2541:U:H5'' | 2.11 | 0.50 |
| 1:0:2862:G:H4' | 5:B:336:GLN:O | 2.12 | 0.50 |
| 2:9:3041:C:C6 | 7:D:50:VAL:HG21 | 2.47 | 0.50 |
| 5:B:217:ARG:CD | 5:B:257:THR:HG22 | 2.41 | 0.50 |
| 7:D:86:THR:C | 7:D:89:PRO:HD2 | 2.31 | 0.50 |
| 11:H:165:GLY:HA3 | 38:H:8403:HOH:O | 2.11 | 0.50 |
| 11:H:166:ASN:N | 11:H:166:ASN:ND2 | 2.60 | 0.50 |
| 13:J:82:ARG:NH2 | 13:J:115:ARG:HG2 | 2.26 | 0.50 |
| 18:O:134:VAL:O | 18:O:137:LEU:HB3 | 2.11 | 0.50 |
| 20:Q:119:VAL:CG2 | 20:Q:142:ASP:HB2 | 2.42 | 0.50 |
| 21:R:51:GLN:HB3 | 21:R:67:ARG:NH1 | 2.26 | 0.50 |
| 25:V:22:GLU:HG2 | 25:V:27:HIS:CD2 | 2.46 | 0.50 |
| 1:0:1822:A:O2' | 1:0:1823:G:H5' | 2.11 | 0.50 |
| 1:0:559:U:H2' | 1:0:560:C:O4' | 2.11 | 0.50 |
| 31:2:8:ASN:O | 31:2:9:THR:HB | 2.10 | 0.50 |
| 2:9:3002:U:OP2 | 2:9:3002:U:H4' | 2.11 | 0.50 |
| 4:A:100:PRO:O | 4:A:103:VAL:HG23 | 2.11 | 0.50 |
| 7:D:99:ASP:CB | 7:D:103:ASN:HB2 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:E:107:PHE:CD2 | 8:E:108:LEU:HD13 | 2.47 | 0.50 |
| 8:E:137:ASP:OD1 | 8:E:139:GLU:HB2 | 2.11 | 0.50 |
| 8:E:16:ASP:O | 8:E:17:HIS:HB2 | 2.11 | 0.50 |
| 23:T:33:SER:O | 23:T:37:GLU:HG3 | 2.12 | 0.50 |
| 25:V:38:THR:O | 25:V:42:ARG:HB2 | 2.11 | 0.50 |
| 1:O:1008:C:OP1 | 11:H:16:ARG:NH2 | 2.44 | 0.50 |
| 1:O:1762:C:O2' | 1:O:1763:C:H5' | 2.11 | 0.50 |
| 1:O:667:C:H2' | 1:O:668:C:H6 | 1.76 | 0.50 |
| 5:B:207:LYS:HG2 | 5:B:304:PRO:HB3 | 1.93 | 0.50 |
| 7:D:97:GLN:HG2 | 7:D:97:GLN:O | 2.11 | 0.50 |
| 11:H:86:ARG:HD3 | 11:H:130:HIS:HD2 | 1.77 | 0.50 |
| 1:O:20:G:H21 | 20:Q:117:HIS:HD2 | 1.60 | 0.50 |
| 20:Q:132:ARG:HG2 | 20:Q:133:ALA:N | 2.26 | 0.50 |
| 26:W:9:VAL:HG13 | 26:W:88:GLU:OE1 | 2.12 | 0.50 |
| 1:O:1538:C:O2' | 1:O:1539:U:H5' | 2.12 | 0.50 |
| 1:O:241:A:N1 | 1:O:378:A:H4' | 2.27 | 0.50 |
| 1:O:2626:C:H2' | 1:O:2627:G:C8 | 2.47 | 0.50 |
| 11:H:59:ASN:HD22 | 11:H:59:ASN:H | 1.59 | 0.50 |
| 12:I:19:MET:HE1 | 12:I:132:LEU:HD21 | 1.93 | 0.50 |
| 38:O:5742:HOH:O | 12:I:47:THR:HB | 2.11 | 0.50 |
| 14:K:104:ASP:HB3 | 38:K:8569:HOH:O | 2.11 | 0.50 |
| 14:K:148:GLU:HA | 38:K:8578:HOH:O | 2.10 | 0.50 |
| 15:L:166:ALA:HA | 15:L:169:ARG:NH1 | 2.27 | 0.50 |
| 22:S:71:VAL:CG1 | 22:S:90:PRO:HB3 | 2.25 | 0.50 |
| 25:V:122:ARG:CG | 25:V:122:ARG:NH1 | 2.74 | 0.50 |
| 1:O:2251:G:H2' | 1:O:2252:A:C8 | 2.46 | 0.50 |
| 1:O:2699:A:H2' | 1:O:2700:G:O4' | 2.11 | 0.50 |
| 1:O:151:A:C2 | 1:O:442:A:C8 | 3.00 | 0.50 |
| 6:C:237:GLU:HB2 | 38:C:8441:HOH:O | 2.11 | 0.50 |
| 1:O:2101:A:H2' | 6:C:63:SER:OG | 2.11 | 0.50 |
| 7:D:57:THR:HG23 | 7:D:63:ILE:CB | 2.42 | 0.50 |
| 9:F:91:VAL:CG1 | 9:F:92:GLY:H | 2.25 | 0.50 |
| 11:H:130:HIS:CG | 11:H:133:ILE:HD11 | 2.47 | 0.50 |
| 38:O:5524:HOH:O | 17:N:35:LYS:HD3 | 2.12 | 0.50 |
| 18:O:38:GLU:HA | 18:O:41:ARG:NH1 | 2.27 | 0.50 |
| 20:Q:111:ILE:HG23 | 20:Q:145:LEU:HD11 | 1.92 | 0.50 |
| 22:S:48:VAL:HG22 | 22:S:98:VAL:HA | 1.92 | 0.50 |
| 25:V:60:GLU:O | 25:V:63:GLU:HB2 | 2.12 | 0.50 |
| 25:V:63:GLU:HG2 | 25:V:93:ILE:HG22 | 1.92 | 0.50 |
| 28:Y:38:LYS:CE | 28:Y:45:LYS:HE2 | 2.38 | 0.50 |
| 1:O:1171:A:H2' | 1:O:1172:G:H5' | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1463:A:H2' | 1:0:1464:U:C6 | 2.47 | 0.50 |
| 1:0:2541:U:H2' | 1:0:2542:C:C6 | 2.47 | 0.50 |
| 1:0:352:A:H2' | 1:0:353:G:H8 | 1.75 | 0.50 |
| 1:0:353:G:H2' | 1:0:354:A:C8 | 2.46 | 0.50 |
| 1:0:90:A:H2' | 1:0:91:G:O4' | 2.12 | 0.50 |
| 4:A:199:HIS:CD2 | 4:A:201:PHE:HB2 | 2.47 | 0.50 |
| 5:B:304:PRO:HD2 | 5:B:307:ARG:NH1 | 2.27 | 0.50 |
| 11:H:142:VAL:HG13 | 38:H:8387:HOH:O | 2.12 | 0.50 |
| 13:J:49:LEU:HD21 | 13:J:74:VAL:O | 2.12 | 0.50 |
| 38:0:4491:HOH:O | 15:L:152:ARG:HG3 | 2.12 | 0.50 |
| 1:0:154:C:P | 15:L:188:ARG:HH12 | 2.34 | 0.50 |
| 15:L:38:VAL:C | 15:L:63:VAL:HG13 | 2.33 | 0.50 |
| 22:S:19:ARG:HD3 | 22:S:67:LEU:O | 2.12 | 0.50 |
| 1:0:1266:U:H4' | 27:X:115:ARG:HH21 | 1.76 | 0.49 |
| 1:0:2416:G:H2' | 1:0:2417:C:C6 | 2.47 | 0.49 |
| 1:0:2818:A:H2 | 38:B:8648:HOH:O | 1.93 | 0.49 |
| 1:0:281:U:O2' | 1:0:282:C:H5' | 2.11 | 0.49 |
| 1:0:354:A:H2' | 1:0:355:C:C6 | 2.47 | 0.49 |
| 1:0:694:A:C2' | 1:0:695:C:H5' | 2.42 | 0.49 |
| 1:0:962:C:H2' | 1:0:963:C:H5' | 1.94 | 0.49 |
| 6:C:166:ILE:HD13 | 6:C:207:LEU:HD22 | 1.93 | 0.49 |
| 12:I:93:ARG:CB | 12:I:93:ARG:HH11 | 2.25 | 0.49 |
| 18:O:98:ILE:HD12 | 18:O:102:ARG:NE | 2.27 | 0.49 |
| 18:O:71:LYS:O | 18:O:71:LYS:HG3 | 2.12 | 0.49 |
| 26:W:14:LEU:HD12 | 26:W:67:PRO:O | 2.12 | 0.49 |
| 1:0:1174:A:C5 | 1:0:1201:C:H4' | 2.46 | 0.49 |
| 1:0:2547:C:H2' | 1:0:2548:C:H6 | 1.77 | 0.49 |
| 1:0:2911:C:H2' | 1:0:2912:C:C6 | 2.48 | 0.49 |
| 1:0:396:U:OP2 | 31:2:38:ARG:NH1 | 2.37 | 0.49 |
| 5:B:53:LEU:HD21 | 5:B:270:ILE:HD12 | 1.94 | 0.49 |
| 7:D:40:ILE:HG23 | 38:D:5583:HOH:O | 2.11 | 0.49 |
| 12:I:39:VAL:HG11 | 12:I:107:ASN:HB2 | 1.92 | 0.49 |
| 14:K:143:THR:CG2 | 14:K:144:ASP:N | 2.76 | 0.49 |
| 1:0:1425:G:O2' | 1:0:1426:C:H5' | 2.12 | 0.49 |
| 1:0:1925:G:O2' | 1:0:1926:G:H5' | 2.12 | 0.49 |
| 1:0:2028:U:H2' | 1:0:2029:C:H6 | 1.78 | 0.49 |
| 1:0:2587:U:H2' | 1:0:2589:U:H5'' | 1.94 | 0.49 |
| 1:0:297:U:H2' | 1:0:298:C:C6 | 2.47 | 0.49 |
| 30:1:41:HIS:N | 30:1:45:ASN:HD22 | 2.02 | 0.49 |
| 2:9:3017:G:O2' | 2:9:3018:U:H5' | 2.12 | 0.49 |
| 6:C:164:ALA:O | 6:C:167:ASP:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:F:27:GLY:HA3 | 9:F:101:ALA:O | 2.12 | 0.49 |
| 8:E:34:TRP:O | 12:I:127:ILE:HD11 | 2.12 | 0.49 |
| 29:Z:8:GLN:HE22 | 29:Z:11:LYS:NZ | 2.11 | 0.49 |
| 1:0:119:A:H2' | 1:0:120:A:H5'' | 1.95 | 0.49 |
| 1:0:1483:C:O2' | 1:0:1484:G:H5' | 2.12 | 0.49 |
| 1:0:1935:C:H2' | 1:0:1936:C:H6 | 1.76 | 0.49 |
| 1:0:214:U:H5' | 38:0:7028:HOH:O | 2.11 | 0.49 |
| 1:0:657:G:H2' | 1:0:658:C:C6 | 2.48 | 0.49 |
| 1:0:962:C:C2' | 1:0:963:C:H5' | 2.42 | 0.49 |
| 2:9:3023:U:C3' | 2:9:3024:U:C5' | 2.87 | 0.49 |
| 15:L:137:ASP:C | 15:L:142:LYS:HE3 | 2.33 | 0.49 |
| 16:M:159:TYR:HE2 | 16:M:163:PHE:HE2 | 1.60 | 0.49 |
| 19:P:72:LYS:HG2 | 19:P:85:ILE:HD13 | 1.93 | 0.49 |
| 25:V:107:LEU:O | 25:V:112:LEU:HB2 | 2.11 | 0.49 |
| 25:V:90:TYR:N | 25:V:90:TYR:CD1 | 2.80 | 0.49 |
| 1:0:1213:C:O2' | 1:0:1214:G:H5' | 2.12 | 0.49 |
| 1:0:1834:C:H2' | 1:0:1840:A:H62 | 1.75 | 0.49 |
| 1:0:1902:G:O2' | 1:0:1903:U:H5' | 2.12 | 0.49 |
| 1:0:2478:U:H2' | 1:0:2479:A:C8 | 2.47 | 0.49 |
| 30:1:40:ARG:NH1 | 30:1:40:ARG:HG2 | 2.28 | 0.49 |
| 30:1:41:HIS:O | 30:1:45:ASN:HB2 | 2.11 | 0.49 |
| 15:L:87:MET:HG2 | 31:2:46:ILE:HG21 | 1.94 | 0.49 |
| 16:M:110:THR:HB | 16:M:113:SER:OG | 2.12 | 0.49 |
| 18:O:13:VAL:HG21 | 18:O:41:ARG:HG2 | 1.94 | 0.49 |
| 20:Q:111:ILE:HG23 | 20:Q:145:LEU:CD1 | 2.42 | 0.49 |
| 1:0:21:G:H5'' | 20:Q:1:GLY:O | 2.12 | 0.49 |
| 5:B:329:TYR:CE2 | 23:T:15:PRO:HG2 | 2.48 | 0.49 |
| 1:0:1687:C:O2 | 29:Z:9:GLY:HA2 | 2.13 | 0.49 |
| 1:0:1205:U:H2' | 1:0:1206:U:H5'' | 1.94 | 0.49 |
| 1:0:2446:G:H2' | 1:0:2447:A:H8 | 1.78 | 0.49 |
| 1:0:2563:U:H2' | 1:0:2565:C:O5' | 2.12 | 0.49 |
| 1:0:74:A:H2' | 1:0:75:U:C6 | 2.47 | 0.49 |
| 1:0:853:C:H2' | 1:0:854:G:O4' | 2.12 | 0.49 |
| 5:B:304:PRO:CD | 5:B:307:ARG:NH1 | 2.76 | 0.49 |
| 6:C:107:ARG:HH11 | 6:C:107:ARG:HB3 | 1.74 | 0.49 |
| 9:F:26:THR:HG21 | 9:F:103:ALA:CB | 2.43 | 0.49 |
| 12:I:6:PHE:HB3 | 12:I:109:TYR:OH | 2.12 | 0.49 |
| 13:J:6:ALA:HB3 | 13:J:116:GLU:HG2 | 1.93 | 0.49 |
| 16:M:22:GLN:HG2 | 16:M:26:LEU:HD22 | 1.95 | 0.49 |
| 25:V:4:LEU:O | 25:V:32:CYS:HA | 2.12 | 0.49 |
| 1:0:1563:G:O2' | 1:0:1564:C:OP2 | 2.23 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1735:C:O2' | 1:0:1736:A:H5' | 2.13 | 0.49 |
| 2:9:3014:G:C8 | 2:9:3014:G:H5' | 2.47 | 0.49 |
| 2:9:3035:C:H5'' | 38:9:8457:HOH:O | 2.12 | 0.49 |
| 1:0:894:A:C2 | 6:C:87:ARG:NH2 | 2.81 | 0.49 |
| 11:H:62:GLU:HA | 38:H:8390:HOH:O | 2.12 | 0.49 |
| 38:0:4656:HOH:O | 15:L:157:LEU:HD11 | 2.12 | 0.49 |
| 20:Q:119:VAL:HG21 | 20:Q:142:ASP:CG | 2.33 | 0.49 |
| 20:Q:82:GLU:O | 20:Q:86:LYS:HG3 | 2.13 | 0.49 |
| 22:S:71:VAL:CG1 | 22:S:72:ILE:N | 2.75 | 0.49 |
| 25:V:115:THR:HG23 | 38:V:5420:HOH:O | 2.12 | 0.49 |
| 1:0:1134:G:H4' | 11:H:151:MET:CE | 2.32 | 0.49 |
| 1:0:182:G:H5' | 38:0:6059:HOH:O | 2.13 | 0.49 |
| 2:9:3041:C:H4' | 7:D:48:MET:HB2 | 1.94 | 0.49 |
| 4:A:99:ILE:O | 4:A:131:HIS:HE1 | 1.96 | 0.49 |
| 6:C:21:VAL:C | 6:C:23:GLU:H | 2.16 | 0.49 |
| 7:D:58:VAL:HG12 | 7:D:59:GLY:N | 2.27 | 0.49 |
| 8:E:137:ASP:O | 8:E:141:VAL:HG23 | 2.13 | 0.49 |
| 11:H:131:ILE:HG23 | 11:H:132:PHE:CD1 | 2.48 | 0.49 |
| 11:H:139:ASP:HA | 38:H:8375:HOH:O | 2.13 | 0.49 |
| 1:0:1994:A:P | 13:J:66:ARG:HH22 | 2.36 | 0.49 |
| 15:L:164:THR:HB | 38:L:8519:HOH:O | 2.12 | 0.49 |
| 25:V:67:ALA:HB2 | 25:V:93:ILE:HD13 | 1.93 | 0.49 |
| 29:Z:28:HIS:O | 29:Z:32:LYS:N | 2.40 | 0.49 |
| 1:0:1181:A:O2' | 1:0:1182:C:H5' | 2.12 | 0.49 |
| 1:0:1768:C:H2' | 1:0:1769:C:O4' | 2.13 | 0.49 |
| 1:0:2252:A:C5 | 1:0:2253:G:H1' | 2.47 | 0.49 |
| 1:0:2377:U:O5' | 1:0:2377:U:H6 | 1.95 | 0.49 |
| 1:0:612:U:H2' | 1:0:613:C:C6 | 2.48 | 0.49 |
| 1:0:684:G:H2' | 1:0:685:C:C6 | 2.48 | 0.49 |
| 1:0:849:C:O2' | 1:0:850:U:H5' | 2.12 | 0.49 |
| 6:C:174:ILE:HD13 | 6:C:185:LYS:HE2 | 1.94 | 0.49 |
| 6:C:84:VAL:O | 6:C:85:LYS:HB2 | 2.13 | 0.49 |
| 9:F:46:GLU:OE1 | 9:F:100:ASP:HA | 2.13 | 0.49 |
| 12:I:93:ARG:HB3 | 12:I:93:ARG:NH1 | 2.24 | 0.49 |
| 1:0:1086:A:C6 | 25:V:11:VAL:HG11 | 2.47 | 0.49 |
| 1:0:1162:G:H2' | 1:0:1162:G:N3 | 2.27 | 0.49 |
| 1:0:1450:C:C4' | 1:0:1451:C:OP2 | 2.55 | 0.49 |
| 1:0:1942:A:O2' | 1:0:1943:C:H5' | 2.13 | 0.49 |
| 1:0:682:A:H2' | 1:0:683:G:O4' | 2.11 | 0.49 |
| 5:B:274:GLU:HA | 5:B:292:GLY:O | 2.12 | 0.49 |
| 6:C:84:VAL:HG12 | 6:C:85:LYS:HG2 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:D:99:ASP:CB | 7:D:103:ASN:H | 2.25 | 0.49 |
| 7:D:167:GLU:C | 7:D:169:THR:H | 2.16 | 0.49 |
| 10:G:64:ASN:N | 10:G:64:ASN:ND2 | 2.60 | 0.49 |
| 11:H:149:ALA:C | 11:H:151:MET:H | 2.15 | 0.49 |
| 18:O:13:VAL:HG11 | 18:O:40:VAL:CG1 | 2.42 | 0.49 |
| 24:U:1:THR:HG23 | 24:U:2:VAL:N | 2.23 | 0.49 |
| 1:O:1203:G:O2' | 1:O:1204:C:H5' | 2.13 | 0.48 |
| 1:O:1808:C:O2' | 1:O:1809:G:H5' | 2.13 | 0.48 |
| 1:O:2406:U:O2' | 1:O:2407:G:H5' | 2.13 | 0.48 |
| 1:O:2504:A:H2' | 1:O:2505:G:O4' | 2.13 | 0.48 |
| 1:O:2668:G:H2' | 1:O:2669:U:H6 | 1.78 | 0.48 |
| 1:O:887:G:H2' | 1:O:888:U:C6 | 2.48 | 0.48 |
| 30:1:18:ASN:HD21 | 30:1:40:ARG:H | 1.61 | 0.48 |
| 4:A:200:PRO:HD3 | 38:A:8522:HOH:O | 2.12 | 0.48 |
| 6:C:235:PHE:CE2 | 6:C:243:VAL:HG21 | 2.44 | 0.48 |
| 8:E:54:ASP:OD1 | 8:E:54:ASP:N | 2.46 | 0.48 |
| 13:J:34:VAL:HB | 38:J:7169:HOH:O | 2.12 | 0.48 |
| 15:L:37:VAL:CG1 | 15:L:63:VAL:HG11 | 2.43 | 0.48 |
| 18:O:59:ARG:HH22 | 18:O:66:GLN:NE2 | 2.11 | 0.48 |
| 1:O:776:A:OP1 | 29:Z:28:HIS:HE1 | 1.95 | 0.48 |
| 1:O:1007:A:H2' | 11:H:19:TYR:CZ | 2.48 | 0.48 |
| 1:O:1375:A:O2' | 1:O:1376:G:H5' | 2.12 | 0.48 |
| 1:O:1778:A:H2' | 1:O:1779:A:H5' | 1.94 | 0.48 |
| 1:O:2296:C:H2' | 1:O:2297:U:H6 | 1.78 | 0.48 |
| 2:9:3042:C:O2 | 7:D:76:ARG:NH1 | 2.46 | 0.48 |
| 7:D:93:LEU:HB3 | 7:D:97:GLN:OE1 | 2.13 | 0.48 |
| 15:L:164:THR:HG23 | 15:L:165:SER:H | 1.75 | 0.48 |
| 15:L:172:GLY:C | 15:L:183:VAL:HG11 | 2.34 | 0.48 |
| 16:M:72:GLU:HB3 | 16:M:171:HIS:HE1 | 1.78 | 0.48 |
| 1:O:1210:G:O2' | 1:O:1211:G:H5' | 2.14 | 0.48 |
| 1:O:1535:G:H2' | 1:O:1536:C:H6 | 1.78 | 0.48 |
| 1:O:2791:U:C1' | 1:O:2792:A:H5'' | 2.43 | 0.48 |
| 7:D:146:LYS:HE2 | 16:M:107:ASN:ND2 | 2.28 | 0.48 |
| 2:9:3004:G:O2' | 16:M:44:ARG:NH2 | 2.46 | 0.48 |
| 19:P:32:GLU:O | 19:P:93:ARG:NH2 | 2.45 | 0.48 |
| 25:V:88:THR:CG2 | 25:V:89:ASP:H | 2.21 | 0.48 |
| 27:X:126:PRO:HG2 | 27:X:128:PHE:CE1 | 2.47 | 0.48 |
| 1:O:1015:C:H2' | 1:O:1016:U:C6 | 2.48 | 0.48 |
| 1:O:1189:A:O2' | 1:O:1208:C:H2' | 2.12 | 0.48 |
| 1:O:120:A:H5' | 29:Z:20:ARG:HH21 | 1.78 | 0.48 |
| 1:O:1829:A:C2' | 1:O:1830:C:H5' | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:2089:A:O2' | 1:0:2090:G:H5' | 2.13 | 0.48 |
| 1:0:821:U:H2' | 1:0:822:C:H6 | 1.78 | 0.48 |
| 9:F:32:GLY:N | 38:F:3111:HOH:O | 2.45 | 0.48 |
| 13:J:49:LEU:HA | 13:J:73:VAL:HG12 | 1.95 | 0.48 |
| 25:V:11:VAL:O | 25:V:12:ASN:HB2 | 2.14 | 0.48 |
| 1:0:2387:U:H2' | 1:0:2388:C:C6 | 2.48 | 0.48 |
| 1:0:344:C:H2' | 1:0:345:G:O4' | 2.13 | 0.48 |
| 1:0:638:C:H2' | 1:0:639:A:H8 | 1.77 | 0.48 |
| 31:2:70:ARG:NH1 | 31:2:70:ARG:HG2 | 2.28 | 0.48 |
| 4:A:179:MET:HA | 4:A:179:MET:CE | 2.43 | 0.48 |
| 1:0:678:G:OP2 | 6:C:107:ARG:NH2 | 2.46 | 0.48 |
| 9:F:117:GLU:C | 9:F:119:ARG:N | 2.67 | 0.48 |
| 9:F:50:VAL:CG2 | 9:F:63:ILE:HG21 | 2.43 | 0.48 |
| 14:K:40:PHE:CD1 | 14:K:41:HIS:N | 2.82 | 0.48 |
| 20:Q:114:VAL:HA | 20:Q:144:GLU:O | 2.13 | 0.48 |
| 23:T:52:THR:HG21 | 23:T:54:THR:HB | 1.95 | 0.48 |
| 24:U:55:ARG:O | 24:U:59:ILE:HG12 | 2.14 | 0.48 |
| 26:W:30:MET:CE | 26:W:58:ALA:HB3 | 2.44 | 0.48 |
| 1:0:1166:A:N3 | 1:0:1166:A:H2' | 2.28 | 0.48 |
| 1:0:1422:U:H2' | 1:0:1423:C:H6 | 1.77 | 0.48 |
| 1:0:1882:C:O2' | 1:0:2012:U:OP2 | 2.32 | 0.48 |
| 1:0:229:G:O2' | 1:0:230:C:H5' | 2.13 | 0.48 |
| 1:0:2502:C:O2' | 1:0:2503:A:H5' | 2.13 | 0.48 |
| 1:0:2858:U:H2' | 1:0:2859:C:C6 | 2.48 | 0.48 |
| 1:0:707:C:C2 | 1:0:708:A:C8 | 3.02 | 0.48 |
| 2:9:3023:U:C6 | 2:9:3023:U:H5'' | 2.49 | 0.48 |
| 2:9:3026:C:O2' | 2:9:3027:C:H5' | 2.14 | 0.48 |
| 2:9:3063:C:O2' | 2:9:3064:C:H5' | 2.14 | 0.48 |
| 5:B:215:VAL:HA | 5:B:220:VAL:HG22 | 1.94 | 0.48 |
| 7:D:56:ARG:N | 38:D:6752:HOH:O | 2.46 | 0.48 |
| 7:D:95:THR:CG2 | 7:D:174:VAL:HG22 | 2.43 | 0.48 |
| 11:H:157:ILE:CG2 | 11:H:158:ASN:N | 2.77 | 0.48 |
| 15:L:108:LYS:N | 15:L:108:LYS:HD3 | 2.28 | 0.48 |
| 1:0:182:G:O3' | 15:L:157:LEU:CD1 | 2.62 | 0.48 |
| 18:O:94:TRP:CZ2 | 18:O:98:ILE:HG13 | 2.48 | 0.48 |
| 19:P:30:VAL:O | 19:P:30:VAL:HG12 | 2.13 | 0.48 |
| 21:R:50:GLU:OE2 | 21:R:69:SER:HB3 | 2.14 | 0.48 |
| 22:S:40:VAL:HG22 | 22:S:41:ARG:N | 2.28 | 0.48 |
| 25:V:122:ARG:HG2 | 25:V:152:ALA:O | 2.14 | 0.48 |
| 26:W:43:VAL:CG1 | 26:W:44:ASP:N | 2.75 | 0.48 |
| 26:W:51:ASP:OD2 | 26:W:52:PRO:HD2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:X:117:LEU:HD12 | 27:X:174:VAL:HG11 | 1.95 | 0.48 |
| 1:O:1321:A:H2' | 1:O:1322:G:C8 | 2.49 | 0.48 |
| 1:O:2270:G:H4' | 4:A:223:ARG:NH1 | 2.29 | 0.48 |
| 1:O:2348:C:H2' | 1:O:2349:G:H8 | 1.78 | 0.48 |
| 1:O:272:A:H5' | 1:O:273:G:OP2 | 2.13 | 0.48 |
| 1:O:2821:C:H4' | 5:B:116:PRO:HB3 | 1.95 | 0.48 |
| 5:B:146:THR:O | 5:B:148:PRO:HD3 | 2.14 | 0.48 |
| 5:B:179:LEU:O | 5:B:183:GLU:HG2 | 2.13 | 0.48 |
| 6:C:129:HIS:CE1 | 6:C:231:ARG:HA | 2.49 | 0.48 |
| 10:G:71:LEU:C | 10:G:73:ASP:N | 2.66 | 0.48 |
| 11:H:163:PRO:O | 11:H:164:ALA:HB2 | 2.14 | 0.48 |
| 21:R:73:ASP:OD1 | 21:R:75:GLN:HB2 | 2.14 | 0.48 |
| 6:C:51:TYR:CE2 | 29:Z:53:LYS:HB3 | 2.48 | 0.48 |
| 1:O:1900:A:H2' | 1:O:1901:G:H8 | 1.78 | 0.48 |
| 1:O:1905:U:H2' | 1:O:1906:C:H6 | 1.79 | 0.48 |
| 1:O:1972:U:C2' | 1:O:1973:A:H5' | 2.43 | 0.48 |
| 1:O:549:A:O2' | 1:O:550:C:H5' | 2.14 | 0.48 |
| 4:A:135:VAL:HG11 | 4:A:147:ARG:NH2 | 2.29 | 0.48 |
| 5:B:279:THR:HG22 | 5:B:280:VAL:N | 2.29 | 0.48 |
| 5:B:87:TYR:O | 5:B:138:GLY:N | 2.39 | 0.48 |
| 11:H:75:SER:C | 11:H:79:ALA:HB2 | 2.34 | 0.48 |
| 38:O:3375:HOH:O | 15:L:94:LYS:HE2 | 2.13 | 0.48 |
| 18:O:115:SER:O | 18:O:117:SER:N | 2.46 | 0.48 |
| 23:T:5:GLU:CG | 23:T:10:GLY:O | 2.61 | 0.48 |
| 24:U:12:THR:HG23 | 24:U:14:ALA:H | 1.78 | 0.48 |
| 1:O:906:C:OP2 | 27:X:147:ARG:NH2 | 2.46 | 0.48 |
| 1:O:1114:A:O2' | 1:O:1115:U:H5' | 2.12 | 0.48 |
| 1:O:1154:A:H2' | 1:O:1155:G:H8 | 1.77 | 0.48 |
| 1:O:1218:U:H2' | 1:O:1219:U:H6 | 1.79 | 0.48 |
| 1:O:1308:A:H2' | 1:O:1309:U:H6 | 1.78 | 0.48 |
| 1:O:1903:U:O2' | 1:O:1904:A:N7 | 2.46 | 0.48 |
| 1:O:466:A:H2' | 1:O:467:G:O4' | 2.13 | 0.48 |
| 31:2:69:TYR:CB | 31:2:78:HIS:CE1 | 2.97 | 0.48 |
| 5:B:147:VAL:HG12 | 5:B:150:ALA:H | 1.78 | 0.48 |
| 8:E:80:TRP:O | 8:E:134:SER:HA | 2.13 | 0.48 |
| 27:X:187:VAL:HG12 | 27:X:205:ILE:HA | 1.96 | 0.48 |
| 1:O:1268:C:H2' | 1:O:1269:G:C8 | 2.49 | 0.48 |
| 1:O:1462:C:H2' | 1:O:1463:A:C8 | 2.49 | 0.48 |
| 1:O:1573:A:H2' | 1:O:1574:C:O4' | 2.14 | 0.48 |
| 1:O:2015:A:H2' | 1:O:2016:U:O4' | 2.13 | 0.48 |
| 1:O:598:C:H2' | 1:O:599:G:H8 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:O:1652:C:O4' | 4:A:164:ARG:HG3 | 2.14 | 0.48 |
| 5:B:14:GLY:HA2 | 5:B:15:PRO:C | 2.35 | 0.48 |
| 5:B:168:GLY:H | 5:B:174:ARG:HH11 | 1.62 | 0.48 |
| 5:B:81:ALA:O | 5:B:186:GLY:HA3 | 2.13 | 0.48 |
| 14:K:144:ASP:O | 14:K:147:GLU:HB2 | 2.13 | 0.48 |
| 26:W:85:VAL:HG12 | 26:W:86:GLU:H | 1.78 | 0.48 |
| 29:Z:5:THR:HB | 29:Z:6:PRO:CD | 2.44 | 0.48 |
| 1:O:1289:C:H3' | 38:O:7289:HOH:O | 2.14 | 0.47 |
| 1:O:1298:U:H2' | 1:O:1299:G:C8 | 2.49 | 0.47 |
| 1:O:2523:U:O2' | 1:O:2524:G:H5' | 2.13 | 0.47 |
| 1:O:2735:U:H2' | 1:O:2736:U:C6 | 2.49 | 0.47 |
| 1:O:396:U:O2' | 1:O:418:C:H4' | 2.13 | 0.47 |
| 1:O:764:C:H2' | 1:O:765:G:O4' | 2.14 | 0.47 |
| 31:2:16:GLU:HG3 | 31:2:18:GLN:HE21 | 1.79 | 0.47 |
| 5:B:43:GLY:O | 5:B:308:LEU:HD12 | 2.13 | 0.47 |
| 5:B:76:THR:N | 5:B:77:PRO:HD3 | 2.28 | 0.47 |
| 6:C:132:ASP:HB3 | 38:C:8371:HOH:O | 2.14 | 0.47 |
| 6:C:118:THR:CG2 | 6:C:137:PRO:HB3 | 2.44 | 0.47 |
| 6:C:236:THR:O | 6:C:237:GLU:C | 2.52 | 0.47 |
| 8:E:7:ILE:HD11 | 8:E:11:VAL:C | 2.34 | 0.47 |
| 11:H:26:LYS:HG2 | 11:H:28:ILE:N | 2.19 | 0.47 |
| 11:H:72:VAL:HG11 | 11:H:81:TYR:CZ | 2.49 | 0.47 |
| 12:I:103:VAL:HG12 | 38:I:5907:HOH:O | 2.13 | 0.47 |
| 13:J:101:ASN:HB2 | 13:J:103:ASP:OD2 | 2.14 | 0.47 |
| 14:K:24:ALA:CB | 14:K:30:ARG:HD2 | 2.44 | 0.47 |
| 38:9:8479:HOH:O | 16:M:18:THR:HG21 | 2.14 | 0.47 |
| 22:S:41:ARG:NH1 | 22:S:42:VAL:O | 2.47 | 0.47 |
| 1:O:2044:G:OP1 | 26:W:23:HIS:HE1 | 1.97 | 0.47 |
| 1:O:1717:A:H5'' | 18:O:54:LYS:HB2 | 1.96 | 0.47 |
| 1:O:1847:A:OP1 | 4:A:175:LYS:HG3 | 2.14 | 0.47 |
| 1:O:2503:A:OP1 | 11:H:147:ARG:NH2 | 2.44 | 0.47 |
| 1:O:2539:U:C4 | 32:O:9500:SLD:H7 | 2.49 | 0.47 |
| 6:C:236:THR:H | 6:C:239:ALA:HB3 | 1.78 | 0.47 |
| 8:E:7:ILE:CG2 | 8:E:45:ASP:O | 2.62 | 0.47 |
| 9:F:28:ALA:HB3 | 9:F:99:THR:HG23 | 1.95 | 0.47 |
| 11:H:39:GLY:O | 11:H:41:THR:N | 2.47 | 0.47 |
| 11:H:69:ASN:O | 11:H:72:VAL:HG12 | 2.14 | 0.47 |
| 14:K:38:HIS:CD2 | 14:K:39:GLU:HG3 | 2.49 | 0.47 |
| 14:K:53:ARG:NH2 | 14:K:57:VAL:HG12 | 2.29 | 0.47 |
| 1:O:1266:U:O2' | 1:O:1267:C:H5' | 2.14 | 0.47 |
| 1:O:1701:A:H5' | 38:O:7166:HOH:O | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:711:G:H1' | 38:0:7966:HOH:O | 2.13 | 0.47 |
| 4:A:114:ASP:HB2 | 4:A:117:LYS:HE2 | 1.96 | 0.47 |
| 4:A:164:ARG:HA | 28:Y:69:TYR:HE1 | 1.78 | 0.47 |
| 4:A:65:ARG:C | 4:A:66:ARG:HG3 | 2.35 | 0.47 |
| 5:B:211:THR:HA | 5:B:255:GLY:O | 2.14 | 0.47 |
| 6:C:240:LEU:O | 6:C:240:LEU:HD23 | 2.13 | 0.47 |
| 1:0:157:G:H4' | 15:L:95:LYS:CE | 2.43 | 0.47 |
| 1:0:1761:U:H5' | 18:O:81:LYS:O | 2.14 | 0.47 |
| 25:V:88:THR:CG2 | 25:V:110:GLN:NE2 | 2.72 | 0.47 |
| 25:V:119:HIS:CB | 38:V:4276:HOH:O | 2.62 | 0.47 |
| 1:0:1851:G:O2' | 1:0:1852:A:H5' | 2.14 | 0.47 |
| 1:0:310:U:H2' | 1:0:311:C:C6 | 2.49 | 0.47 |
| 2:9:3114:G:H2' | 2:9:3115:C:C6 | 2.49 | 0.47 |
| 11:H:26:LYS:HD2 | 11:H:28:ILE:CG1 | 2.45 | 0.47 |
| 15:L:64:ARG:HD2 | 38:L:8587:HOH:O | 2.13 | 0.47 |
| 25:V:41:TYR:CD2 | 25:V:44:MET:HE3 | 2.49 | 0.47 |
| 1:0:1603:A:H5' | 1:0:1605:G:C4' | 2.45 | 0.47 |
| 1:0:1782:G:O2' | 1:0:1783:A:H5' | 2.15 | 0.47 |
| 1:0:2255:A:O2' | 1:0:2256:G:H5' | 2.14 | 0.47 |
| 1:0:2266:A:H2' | 1:0:2267:G:H8 | 1.77 | 0.47 |
| 1:0:2362:A:H2' | 1:0:2363:G:C8 | 2.50 | 0.47 |
| 1:0:2437:A:H2' | 1:0:2438:G:H8 | 1.79 | 0.47 |
| 1:0:2473:U:O3' | 1:0:2474:A:H3' | 2.13 | 0.47 |
| 1:0:431:G:O2' | 1:0:432:G:H5' | 2.13 | 0.47 |
| 2:9:3047:A:C2 | 2:9:3048:C:C2 | 3.02 | 0.47 |
| 4:A:99:ILE:O | 4:A:131:HIS:CE1 | 2.68 | 0.47 |
| 7:D:153:THR:O | 7:D:156:ARG:HB2 | 2.14 | 0.47 |
| 11:H:140:PRO:HB3 | 38:H:8387:HOH:O | 2.14 | 0.47 |
| 11:H:81:TYR:C | 11:H:81:TYR:CD1 | 2.86 | 0.47 |
| 14:K:124:ASP:OD1 | 14:K:125:PHE:N | 2.47 | 0.47 |
| 1:0:1594:C:OP2 | 18:O:120:ARG:HD2 | 2.15 | 0.47 |
| 22:S:24:ARG:HH21 | 22:S:39:ASN:ND2 | 2.12 | 0.47 |
| 1:0:1592:G:O2' | 1:0:1593:C:O5' | 2.32 | 0.47 |
| 1:0:1927:A:O2' | 1:0:1928:C:H5' | 2.14 | 0.47 |
| 1:0:288:A:H2' | 1:0:289:G:H8 | 1.80 | 0.47 |
| 4:A:153:ARG:CB | 4:A:153:ARG:HH11 | 2.27 | 0.47 |
| 4:A:36:ASP:CB | 4:A:85:ASP:H | 2.27 | 0.47 |
| 5:B:82:VAL:HG12 | 5:B:101:TRP:CE3 | 2.48 | 0.47 |
| 5:B:320:GLN:HG3 | 5:B:321:PRO:HD2 | 1.96 | 0.47 |
| 7:D:11:HIS:C | 7:D:13:MET:H | 2.17 | 0.47 |
| 15:L:182:LYS:HD2 | 15:L:193:LYS:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:N:39:THR:O | 17:N:115:ARG:NH2 | 2.47 | 0.47 |
| 22:S:24:ARG:HH21 | 22:S:39:ASN:HD22 | 1.60 | 0.47 |
| 1:0:1872:C:H5 | 4:A:20:SER:HB3 | 1.80 | 0.47 |
| 1:0:326:G:O2' | 1:0:327:A:H5' | 2.14 | 0.47 |
| 1:0:941:G:C5 | 1:0:942:U:C4 | 3.03 | 0.47 |
| 1:0:945:U:H2' | 1:0:946:C:C6 | 2.50 | 0.47 |
| 2:9:3029:C:C2' | 2:9:3030:C:H5' | 2.43 | 0.47 |
| 5:B:175:LEU:O | 5:B:178:ALA:HB3 | 2.14 | 0.47 |
| 1:0:1593:C:H5' | 18:O:116:SER:O | 2.14 | 0.47 |
| 27:X:234:VAL:HG12 | 27:X:235:GLU:N | 2.29 | 0.47 |
| 1:0:1151:G:OP1 | 10:G:63:ARG:NH1 | 2.47 | 0.47 |
| 1:0:1624:A:H5' | 1:0:1626:A:O4' | 2.15 | 0.47 |
| 1:0:1741:U:O2' | 1:0:2723:G:H4' | 2.15 | 0.47 |
| 1:0:1792:C:H2' | 1:0:1793:C:H6 | 1.78 | 0.47 |
| 1:0:2388:C:O2' | 1:0:2389:U:H5' | 2.15 | 0.47 |
| 1:0:319:A:H4' | 1:0:338:C:C5 | 2.50 | 0.47 |
| 31:2:7:PHE:HD1 | 31:2:8:ASN:O | 1.97 | 0.47 |
| 4:A:95:PRO:HA | 4:A:153:ARG:HA | 1.97 | 0.47 |
| 5:B:51:VAL:CG2 | 5:B:327:VAL:HG13 | 2.45 | 0.47 |
| 11:H:35:ASN:ND2 | 11:H:79:ALA:O | 2.46 | 0.47 |
| 16:M:154:LEU:HD11 | 16:M:157:PRO:HA | 1.97 | 0.47 |
| 26:W:27:ASP:N | 26:W:27:ASP:OD2 | 2.41 | 0.47 |
| 1:0:1307:A:H2' | 1:0:1308:A:C8 | 2.50 | 0.47 |
| 1:0:183:A:H5' | 15:L:157:LEU:HD12 | 1.97 | 0.47 |
| 1:0:1921:A:C6 | 1:0:1922:A:C2 | 3.03 | 0.47 |
| 1:0:2112:A:H2' | 1:0:2113:G:H8 | 1.79 | 0.47 |
| 1:0:2435:U:H1' | 38:O:6323:HOH:O | 2.13 | 0.47 |
| 1:0:2897:C:O2' | 1:0:2898:G:H5' | 2.15 | 0.47 |
| 1:0:2898:G:O2' | 1:0:2899:A:H5' | 2.15 | 0.47 |
| 1:0:474:C:O3' | 6:C:73:LEU:CD2 | 2.62 | 0.47 |
| 1:0:820:G:H5' | 1:0:821:U:H5' | 1.97 | 0.47 |
| 1:0:946:C:H2' | 1:0:947:U:C6 | 2.49 | 0.47 |
| 6:C:242:GLU:HG3 | 38:C:8390:HOH:O | 2.14 | 0.47 |
| 9:F:100:ASP:O | 9:F:101:ALA:O | 2.33 | 0.47 |
| 14:K:90:ARG:HH11 | 14:K:119:THR:HG21 | 1.80 | 0.47 |
| 1:0:1299:G:N7 | 14:K:6:ARG:NH1 | 2.62 | 0.47 |
| 16:M:61:ALA:HB3 | 16:M:88:ALA:HB2 | 1.97 | 0.47 |
| 22:S:48:VAL:CG2 | 22:S:98:VAL:HA | 2.45 | 0.47 |
| 1:0:553:G:O4' | 1:0:1325:G:H5' | 2.15 | 0.47 |
| 1:0:2687:G:O2' | 1:0:2688:U:H5' | 2.15 | 0.47 |
| 1:0:65:C:O2' | 1:0:66:G:H5' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 38:0:5858:HOH:O | 2:9:3103:A:H4' | 2.14 | 0.47 |
| 5:B:177:HIS:NE2 | 5:B:181:ILE:HD11 | 2.29 | 0.47 |
| 6:C:139:VAL:HG21 | 6:C:240:LEU:HD12 | 1.97 | 0.47 |
| 11:H:72:VAL:CG1 | 11:H:81:TYR:CZ | 2.98 | 0.47 |
| 12:I:39:VAL:CG1 | 12:I:107:ASN:HB2 | 2.44 | 0.47 |
| 13:J:49:LEU:HA | 13:J:73:VAL:CG1 | 2.45 | 0.47 |
| 14:K:57:VAL:O | 14:K:57:VAL:HG12 | 2.15 | 0.47 |
| 1:0:1217:G:H2' | 1:0:1218:U:C6 | 2.50 | 0.47 |
| 1:0:1701:A:H4' | 1:0:1702:U:C5' | 2.44 | 0.47 |
| 1:0:1800:G:O2' | 1:0:1801:A:H5' | 2.14 | 0.47 |
| 1:0:2326:U:H4' | 1:0:2412:G:C4' | 2.45 | 0.47 |
| 1:0:2729:C:H2' | 1:0:2730:G:H8 | 1.79 | 0.47 |
| 1:0:2858:U:H2' | 1:0:2859:C:H6 | 1.80 | 0.47 |
| 31:2:70:ARG:CG | 31:2:77:ALA:HB2 | 2.40 | 0.47 |
| 5:B:175:LEU:C | 5:B:175:LEU:CD2 | 2.83 | 0.47 |
| 7:D:166:ILE:HB | 38:D:6326:HOH:O | 2.15 | 0.47 |
| 7:D:91:ALA:HB1 | 38:D:5198:HOH:O | 2.13 | 0.47 |
| 9:F:39:SER:HB3 | 9:F:45:ALA:HB2 | 1.97 | 0.47 |
| 9:F:99:THR:HG23 | 9:F:99:THR:O | 2.14 | 0.47 |
| 10:G:67:LEU:O | 10:G:71:LEU:HG | 2.14 | 0.47 |
| 16:M:42:HIS:CG | 16:M:62:HIS:HE1 | 2.33 | 0.47 |
| 23:T:6:CYS:C | 23:T:8:TYR:H | 2.18 | 0.47 |
| 1:0:1181:A:H2' | 1:0:1182:C:O4' | 2.14 | 0.46 |
| 1:0:1584:C:O2' | 1:0:1585:C:H5' | 2.15 | 0.46 |
| 1:0:289:G:N1 | 1:0:363:A:C2 | 2.78 | 0.46 |
| 1:0:383:A:H4' | 38:0:6225:HOH:O | 2.15 | 0.46 |
| 1:0:581:G:O2' | 1:0:582:C:H5' | 2.15 | 0.46 |
| 30:1:19:SER:O | 30:1:36:ASN:ND2 | 2.47 | 0.46 |
| 31:2:42:ARG:HH11 | 31:2:42:ARG:CG | 2.27 | 0.46 |
| 5:B:315:VAL:HG23 | 5:B:316:ARG:HG2 | 1.97 | 0.46 |
| 13:J:75:ARG:O | 13:J:93:ASN:HA | 2.15 | 0.46 |
| 16:M:139:TRP:CH2 | 16:M:176:ARG:NH1 | 2.83 | 0.46 |
| 1:0:317:A:OP1 | 22:S:52:ARG:O | 2.32 | 0.46 |
| 28:Y:81:LYS:O | 28:Y:82:ALA:C | 2.53 | 0.46 |
| 1:0:1252:A:H2' | 1:0:1253:C:O4' | 2.15 | 0.46 |
| 1:0:1269:G:H2' | 1:0:1270:U:C6 | 2.50 | 0.46 |
| 1:0:1787:C:O2' | 1:0:1788:U:H5' | 2.15 | 0.46 |
| 1:0:1942:A:H1' | 38:A:8564:HOH:O | 2.15 | 0.46 |
| 1:0:2004:U:H4' | 38:0:6205:HOH:O | 2.16 | 0.46 |
| 1:0:2090:G:H2' | 1:0:2091:G:C8 | 2.49 | 0.46 |
| 1:0:665:A:H2' | 1:0:666:A:C8 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:B:85:ARG:NH1 | 38:B:8648:HOH:O | 2.47 | 0.46 |
| 7:D:21:VAL:HG13 | 7:D:131:THR:O | 2.14 | 0.46 |
| 9:F:110:GLU:HG2 | 38:F:6926:HOH:O | 2.14 | 0.46 |
| 11:H:109:ASP:HB2 | 38:H:8349:HOH:O | 2.15 | 0.46 |
| 11:H:162:SER:CB | 11:H:163:PRO:CD | 2.78 | 0.46 |
| 16:M:100:ALA:O | 16:M:129:ILE:HG23 | 2.15 | 0.46 |
| 20:Q:98:ASN:ND2 | 20:Q:98:ASN:N | 2.64 | 0.46 |
| 21:R:51:GLN:NE2 | 21:R:53:ASN:HD21 | 2.06 | 0.46 |
| 22:S:30:ASP:O | 22:S:33:GLU:HB3 | 2.15 | 0.46 |
| 1:O:1246:A:O2' | 1:O:1247:A:H3' | 2.15 | 0.46 |
| 1:O:1600:G:H8 | 1:O:1600:G:OP2 | 1.98 | 0.46 |
| 1:O:482:G:H4' | 1:O:508:A:N1 | 2.30 | 0.46 |
| 1:O:958:G:O2' | 1:O:959:C:H5' | 2.16 | 0.46 |
| 2:9:3095:C:O2' | 2:9:3096:C:H5' | 2.16 | 0.46 |
| 4:A:55:VAL:HG22 | 4:A:68:ILE:O | 2.15 | 0.46 |
| 5:B:274:GLU:HG3 | 5:B:275:GLY:N | 2.30 | 0.46 |
| 5:B:55:ASN:HB3 | 5:B:64:GLY:H | 1.80 | 0.46 |
| 6:C:127:ARG:HH21 | 6:C:225:PRO:HG2 | 1.70 | 0.46 |
| 8:E:126:ILE:HB | 8:E:131:LEU:CD2 | 2.45 | 0.46 |
| 9:F:113:ASP:O | 9:F:117:GLU:HG3 | 2.16 | 0.46 |
| 10:G:63:ARG:HB2 | 10:G:66:LEU:HG | 1.96 | 0.46 |
| 17:N:26:TRP:HB2 | 38:N:3062:HOH:O | 2.15 | 0.46 |
| 21:R:14:ALA:HA | 21:R:25:GLN:NE2 | 2.29 | 0.46 |
| 1:O:138:U:H5'' | 1:O:139:C:OP2 | 2.16 | 0.46 |
| 1:O:1677:U:OP2 | 30:1:8:LYS:NZ | 2.44 | 0.46 |
| 1:O:1773:G:C2' | 1:O:1774:G:H5' | 2.46 | 0.46 |
| 1:O:2311:A:O2' | 1:O:2312:G:H5' | 2.15 | 0.46 |
| 1:O:259:G:O2' | 1:O:260:C:H5' | 2.15 | 0.46 |
| 1:O:366:U:H2' | 1:O:367:G:O4' | 2.15 | 0.46 |
| 5:B:7:ARG:HB2 | 5:B:7:ARG:CZ | 2.46 | 0.46 |
| 6:C:107:ARG:CB | 6:C:107:ARG:HH11 | 2.27 | 0.46 |
| 7:D:67:ASP:O | 7:D:69:ILE:HG13 | 2.16 | 0.46 |
| 11:H:137:ASN:O | 11:H:138:PRO:C | 2.53 | 0.46 |
| 13:J:50:GLY:O | 13:J:120:ARG:NH1 | 2.43 | 0.46 |
| 16:M:74:PRO:HG2 | 16:M:159:TYR:CZ | 2.51 | 0.46 |
| 21:R:29:ASP:OD1 | 21:R:31:ARG:HG3 | 2.16 | 0.46 |
| 23:T:14:GLU:OE1 | 23:T:15:PRO:CD | 2.63 | 0.46 |
| 27:X:107:PRO:HB3 | 27:X:182:PHE:CD2 | 2.51 | 0.46 |
| 1:O:170:U:H2' | 1:O:171:C:C5' | 2.45 | 0.46 |
| 1:O:212:A:O4' | 1:O:214:U:C6 | 2.68 | 0.46 |
| 1:O:2332:A:H5' | 1:O:2333:G:OP2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:2748:G:H1' | 38:O:8782:HOH:O | 2.15 | 0.46 |
| 31:2:69:TYR:HE1 | 31:2:80:ARG:HB2 | 1.79 | 0.46 |
| 5:B:79:MET:HE1 | 38:B:8639:HOH:O | 2.14 | 0.46 |
| 7:D:11:HIS:O | 7:D:12:GLU:HB3 | 2.15 | 0.46 |
| 7:D:18:ILE:HG12 | 7:D:134:LEU:CD2 | 2.45 | 0.46 |
| 10:G:12:ILE:HG13 | 38:G:6833:HOH:O | 2.15 | 0.46 |
| 12:I:77:GLY:O | 12:I:78:ILE:C | 2.54 | 0.46 |
| 16:M:139:TRP:HA | 16:M:139:TRP:HE3 | 1.81 | 0.46 |
| 16:M:73:ALA:HB1 | 16:M:74:PRO:CD | 2.45 | 0.46 |
| 29:Z:28:HIS:ND1 | 29:Z:31:LYS:HE2 | 2.29 | 0.46 |
| 1:O:1064:U:H2' | 1:O:1065:G:C8 | 2.51 | 0.46 |
| 1:O:1503:U:H2' | 1:O:1504:A:O4' | 2.14 | 0.46 |
| 1:O:200:U:H2' | 38:O:4388:HOH:O | 2.15 | 0.46 |
| 1:O:2761:A:C4 | 1:O:2763:G:C8 | 3.04 | 0.46 |
| 1:O:2825:C:H4' | 1:O:2826:G:O5' | 2.15 | 0.46 |
| 1:O:724:G:O2' | 1:O:725:C:H5' | 2.15 | 0.46 |
| 1:O:745:G:O6 | 17:N:68:GLY:HA3 | 2.15 | 0.46 |
| 1:O:960:G:C2' | 1:O:960:G:N3 | 2.77 | 0.46 |
| 5:B:147:VAL:O | 5:B:150:ALA:HB3 | 2.15 | 0.46 |
| 7:D:104:PHE:CE2 | 7:D:132:VAL:HB | 2.51 | 0.46 |
| 15:L:67:ILE:CD1 | 15:L:104:ARG:HD2 | 2.46 | 0.46 |
| 15:L:87:MET:HB3 | 31:2:46:ILE:CD1 | 2.24 | 0.46 |
| 17:N:14:LEU:CG | 17:N:102:ILE:HD11 | 2.45 | 0.46 |
| 1:O:1118:A:H62 | 1:O:1244:U:H3 | 1.63 | 0.46 |
| 1:O:2034:U:H2' | 1:O:2035:C:H6 | 1.80 | 0.46 |
| 1:O:2064:U:H4' | 1:O:2653:A:OP1 | 2.16 | 0.46 |
| 1:O:2786:G:H2' | 38:O:8861:HOH:O | 2.15 | 0.46 |
| 4:A:199:HIS:HD2 | 4:A:201:PHE:H | 1.61 | 0.46 |
| 7:D:91:ALA:HB2 | 7:D:106:PHE:CD2 | 2.51 | 0.46 |
| 7:D:49:PRO:HG3 | 38:D:5828:HOH:O | 2.15 | 0.46 |
| 8:E:107:PHE:CE1 | 8:E:152:THR:HB | 2.51 | 0.46 |
| 8:E:68:HIS:O | 8:E:72:MET:HG3 | 2.16 | 0.46 |
| 14:K:120:LEU:HD12 | 14:K:133:VAL:HG21 | 1.97 | 0.46 |
| 16:M:83:LEU:HD13 | 16:M:175:LEU:HD23 | 1.98 | 0.46 |
| 18:O:105:LEU:CD2 | 18:O:137:LEU:HD21 | 2.45 | 0.46 |
| 22:S:73:HIS:CD2 | 22:S:88:PRO:CG | 2.99 | 0.46 |
| 25:V:59:GLN:NE2 | 25:V:97:ALA:HB3 | 2.30 | 0.46 |
| 1:O:1300:G:H1' | 38:O:5591:HOH:O | 2.15 | 0.46 |
| 1:O:1735:C:H2' | 1:O:1736:A:H8 | 1.80 | 0.46 |
| 1:O:1878:G:O2' | 1:O:1879:U:OP2 | 2.34 | 0.46 |
| 1:O:2035:C:O2' | 1:O:2036:C:H5' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2578:G:C8 | 1:0:2578:G:H5' | 2.48 | 0.46 |
| 1:0:445:U:H2' | 1:0:446:G:C8 | 2.51 | 0.46 |
| 11:H:15:THR:HG22 | 11:H:91:HIS:HA | 1.98 | 0.46 |
| 12:I:19:MET:HE1 | 12:I:132:LEU:HD11 | 1.97 | 0.46 |
| 12:I:135:ILE:O | 12:I:139:LEU:HG | 2.15 | 0.46 |
| 1:0:399:C:H5' | 15:L:179:GLY:O | 2.16 | 0.46 |
| 1:0:2365:G:H4' | 19:P:45:PRO:O | 2.15 | 0.46 |
| 27:X:184:GLU:OE1 | 27:X:204:ARG:NH1 | 2.49 | 0.46 |
| 1:0:1003:U:O2 | 11:H:90:PHE:CZ | 2.69 | 0.46 |
| 1:0:47:G:N3 | 1:0:114:A:C2 | 2.84 | 0.46 |
| 1:0:1773:G:H2' | 1:0:1774:G:H5' | 1.98 | 0.46 |
| 1:0:2453:G:H3' | 38:0:6807:HOH:O | 2.15 | 0.46 |
| 1:0:2851:G:C2' | 1:0:2852:A:H5' | 2.46 | 0.46 |
| 1:0:2899:A:O2' | 1:0:2900:G:H5' | 2.16 | 0.46 |
| 1:0:299:U:O2' | 1:0:300:C:H5' | 2.16 | 0.46 |
| 1:0:453:A:H4' | 1:0:455:A:N7 | 2.31 | 0.46 |
| 1:0:903:U:OP2 | 14:K:11:ARG:NH1 | 2.44 | 0.46 |
| 4:A:105:VAL:HG11 | 4:A:154:ALA:HB1 | 1.98 | 0.46 |
| 4:A:4:ILE:HG22 | 4:A:198:ASP:O | 2.16 | 0.46 |
| 5:B:279:THR:CG2 | 5:B:280:VAL:N | 2.79 | 0.46 |
| 13:J:62:PRO:CG | 13:J:65:ARG:HH21 | 2.14 | 0.46 |
| 1:0:926:A:O2' | 14:K:41:HIS:CD2 | 2.69 | 0.46 |
| 15:L:104:ARG:O | 15:L:108:LYS:HG2 | 2.15 | 0.46 |
| 9:F:58:GLU:CD | 15:L:27:ARG:HH22 | 2.18 | 0.46 |
| 16:M:62:HIS:O | 16:M:65:ASP:OD1 | 2.34 | 0.46 |
| 16:M:67:ALA:C | 16:M:69:TYR:H | 2.20 | 0.46 |
| 16:M:71:TRP:N | 38:M:8539:HOH:O | 2.49 | 0.46 |
| 26:W:18:ARG:HA | 38:W:5356:HOH:O | 2.16 | 0.46 |
| 1:0:101:C:H2' | 1:0:102:A:H8 | 1.81 | 0.46 |
| 1:0:1557:G:O2' | 1:0:1558:C:H5' | 2.16 | 0.46 |
| 1:0:1641:A:H2' | 1:0:1642:A:C5' | 2.45 | 0.46 |
| 1:0:232:A:H4' | 38:0:6972:HOH:O | 2.16 | 0.46 |
| 1:0:2372:A:H2' | 1:0:2373:U:C6 | 2.51 | 0.46 |
| 1:0:2698:G:H2' | 1:0:2699:A:C8 | 2.51 | 0.46 |
| 1:0:2781:U:H2' | 1:0:2782:G:H5' | 1.97 | 0.46 |
| 30:1:41:HIS:H | 30:1:45:ASN:ND2 | 2.04 | 0.46 |
| 7:D:60:GLU:O | 7:D:62:ASP:N | 2.49 | 0.46 |
| 9:F:26:THR:HB | 9:F:102:GLY:HA3 | 1.98 | 0.46 |
| 15:L:84:LYS:O | 15:L:87:MET:HG2 | 2.16 | 0.46 |
| 16:M:67:ALA:C | 16:M:69:TYR:N | 2.69 | 0.46 |
| 16:M:91:ARG:HG3 | 16:M:186:LEU:CD2 | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 25:V:34:LEU:CD1 | 25:V:100:LEU:HD13 | 2.46 | 0.46 |
| 1:0:128:A:O2' | 1:0:129:A:H5' | 2.16 | 0.45 |
| 1:0:1305:C:O2' | 1:0:1306:U:H5' | 2.15 | 0.45 |
| 1:0:1335:C:OP2 | 27:X:207:SER:CB | 2.64 | 0.45 |
| 1:0:1512:G:O2' | 1:0:1513:C:H5' | 2.16 | 0.45 |
| 1:0:156:C:H5'' | 15:L:171:ARG:CD | 2.25 | 0.45 |
| 1:0:1626:A:H2' | 1:0:1627:G:O4' | 2.16 | 0.45 |
| 31:2:69:TYR:CE1 | 31:2:80:ARG:HB2 | 2.50 | 0.45 |
| 6:C:123:LEU:HA | 6:C:123:LEU:HD23 | 1.84 | 0.45 |
| 6:C:197:SER:OG | 6:C:242:GLU:OE2 | 2.32 | 0.45 |
| 7:D:10:PHE:CD1 | 7:D:11:HIS:N | 2.84 | 0.45 |
| 9:F:110:GLU:O | 9:F:114:LYS:HG3 | 2.15 | 0.45 |
| 11:H:150:LYS:CB | 11:H:157:ILE:HD12 | 2.46 | 0.45 |
| 11:H:58:HIS:HA | 11:H:61:LEU:HD23 | 1.98 | 0.45 |
| 1:0:1593:C:OP1 | 18:O:117:SER:HB3 | 2.16 | 0.45 |
| 22:S:15:PRO:O | 22:S:19:ARG:HG3 | 2.16 | 0.45 |
| 23:T:34:SER:HA | 23:T:37:GLU:OE1 | 2.16 | 0.45 |
| 27:X:186:ARG:NH1 | 27:X:186:ARG:HG2 | 2.30 | 0.45 |
| 1:0:1058:A:H2' | 1:0:1060:C:C5' | 2.47 | 0.45 |
| 1:0:1116:U:C2' | 1:0:1118:A:H2 | 2.27 | 0.45 |
| 1:0:1171:A:C2' | 1:0:1172:G:H5' | 2.46 | 0.45 |
| 1:0:1206:U:H2' | 1:0:1207:A:O4' | 2.16 | 0.45 |
| 1:0:1421:C:O2' | 1:0:1422:U:H5' | 2.16 | 0.45 |
| 1:0:1917:G:H2' | 1:0:1918:U:C6 | 2.51 | 0.45 |
| 1:0:2256:G:C2' | 1:0:2257:G:C5' | 2.93 | 0.45 |
| 1:0:2314:G:O2' | 1:0:2315:C:H5' | 2.16 | 0.45 |
| 1:0:2546:U:H5 | 5:B:2:GLN:HE22 | 1.63 | 0.45 |
| 1:0:2885:A:H2' | 1:0:2886:C:C6 | 2.51 | 0.45 |
| 1:0:553:G:H5' | 38:O:4440:HOH:O | 2.16 | 0.45 |
| 1:0:689:G:O2' | 1:0:690:G:H5' | 2.17 | 0.45 |
| 1:0:963:C:H2' | 1:0:964:G:C8 | 2.50 | 0.45 |
| 2:9:3061:C:H2' | 2:9:3062:A:H8 | 1.82 | 0.45 |
| 4:A:192:VAL:CG1 | 4:A:192:VAL:O | 2.64 | 0.45 |
| 4:A:65:ARG:HH11 | 4:A:65:ARG:HG2 | 1.81 | 0.45 |
| 5:B:132:HIS:CE1 | 5:B:171:VAL:HG21 | 2.51 | 0.45 |
| 5:B:146:THR:O | 5:B:159:PRO:HB3 | 2.16 | 0.45 |
| 8:E:77:THR:OG1 | 8:E:78:GLU:N | 2.48 | 0.45 |
| 11:H:34:GLY:HA3 | 11:H:81:TYR:O | 2.16 | 0.45 |
| 12:I:19:MET:HE2 | 12:I:78:ILE:HG22 | 1.97 | 0.45 |
| 12:I:51:GLU:O | 12:I:55:GLU:HG3 | 2.16 | 0.45 |
| 16:M:139:TRP:HH2 | 16:M:176:ARG:HH11 | 1.62 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 18:O:31:ILE:HG12 | 18:O:43:LEU:HD13 | 1.98 | 0.45 |
| 25:V:122:ARG:HG2 | 25:V:122:ARG:NH1 | 2.20 | 0.45 |
| 25:V:4:LEU:HA | 25:V:4:LEU:HD23 | 1.74 | 0.45 |
| 1:O:1545:C:H2' | 1:O:1546:G:O4' | 2.16 | 0.45 |
| 1:O:170:U:C2' | 1:O:171:C:H5' | 2.47 | 0.45 |
| 1:O:1940:C:H5'' | 4:A:234:GLY:HA3 | 1.97 | 0.45 |
| 1:O:2355:G:H5'' | 1:O:2356:A:OP2 | 2.16 | 0.45 |
| 1:O:2453:G:H4' | 14:K:50:GLY:C | 2.37 | 0.45 |
| 1:O:251:C:O2' | 1:O:252:C:H5' | 2.16 | 0.45 |
| 1:O:2547:C:H2' | 1:O:2548:C:C6 | 2.51 | 0.45 |
| 1:O:2630:G:O6 | 4:A:206:ARG:NH2 | 2.49 | 0.45 |
| 1:O:697:G:H4' | 1:O:730:G:O3' | 2.17 | 0.45 |
| 1:O:869:G:OP1 | 15:L:79:LYS:HE2 | 2.16 | 0.45 |
| 4:A:30:ARG:HB3 | 4:A:30:ARG:HE | 1.65 | 0.45 |
| 4:A:66:ARG:HH11 | 4:A:66:ARG:CB | 2.29 | 0.45 |
| 1:O:2846:C:H4' | 5:B:156:LYS:HB3 | 1.97 | 0.45 |
| 1:O:2846:C:OP1 | 5:B:158:LYS:HD3 | 2.16 | 0.45 |
| 7:D:23:VAL:CG2 | 7:D:73:VAL:HB | 2.46 | 0.45 |
| 9:F:101:ALA:HB2 | 9:F:108:LEU:HD22 | 1.97 | 0.45 |
| 9:F:99:THR:O | 9:F:100:ASP:HB2 | 2.15 | 0.45 |
| 11:H:59:ASN:H | 11:H:59:ASN:ND2 | 2.14 | 0.45 |
| 16:M:184:ILE:HG22 | 16:M:185:GLU:N | 2.30 | 0.45 |
| 16:M:73:ALA:HB1 | 16:M:74:PRO:HD2 | 1.98 | 0.45 |
| 17:N:21:SER:OG | 17:N:106:PRO:HB2 | 2.17 | 0.45 |
| 1:O:709:G:O2' | 17:N:25:VAL:HG12 | 2.16 | 0.45 |
| 20:Q:39:THR:CG2 | 20:Q:42:GLU:HG3 | 2.46 | 0.45 |
| 1:O:489:A:C8 | 22:S:82:THR:HG22 | 2.51 | 0.45 |
| 29:Z:25:LYS:O | 29:Z:25:LYS:HG2 | 2.17 | 0.45 |
| 1:O:1381:A:N3 | 1:O:1382:G:H1' | 2.32 | 0.45 |
| 1:O:249:G:H1' | 1:O:265:U:O2 | 2.17 | 0.45 |
| 1:O:283:U:H5'' | 1:O:284:C:P | 2.56 | 0.45 |
| 1:O:295:C:H2' | 1:O:296:G:O4' | 2.16 | 0.45 |
| 1:O:541:C:C2' | 1:O:542:A:C5' | 2.91 | 0.45 |
| 1:O:711:G:C2 | 1:O:718:C:C2 | 3.05 | 0.45 |
| 2:9:3026:C:H2' | 2:9:3027:C:H6 | 1.81 | 0.45 |
| 4:A:70:ALA:HA | 4:A:71:PRO:HD3 | 1.79 | 0.45 |
| 5:B:304:PRO:HD2 | 5:B:307:ARG:CD | 2.40 | 0.45 |
| 7:D:57:THR:HG23 | 7:D:63:ILE:HA | 1.99 | 0.45 |
| 11:H:151:MET:HE3 | 11:H:151:MET:HA | 1.97 | 0.45 |
| 14:K:97:VAL:HG12 | 14:K:98:GLU:O | 2.16 | 0.45 |
| 16:M:115:VAL:HG23 | 16:M:116:PHE:H | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 16:M:182:GLY:O | 16:M:183:ASP:O | 2.34 | 0.45 |
| 21:R:51:GLN:HB3 | 21:R:67:ARG:HH12 | 1.82 | 0.45 |
| 26:W:70:ILE:O | 26:W:70:ILE:HG23 | 2.16 | 0.45 |
| 27:X:107:PRO:HB3 | 27:X:182:PHE:CE2 | 2.51 | 0.45 |
| 1:O:1517:U:C2 | 1:O:1670:G:N2 | 2.84 | 0.45 |
| 1:O:2000:G:O2' | 1:O:2001:G:H5' | 2.17 | 0.45 |
| 1:O:31:C:H2' | 38:O:8568:HOH:O | 2.15 | 0.45 |
| 1:O:539:G:H2' | 1:O:540:A:C8 | 2.52 | 0.45 |
| 1:O:583:G:H2' | 1:O:584:U:C6 | 2.51 | 0.45 |
| 2:9:3117:G:H2' | 2:9:3118:C:C6 | 2.51 | 0.45 |
| 4:A:161:GLY:O | 28:Y:68:CYS:SG | 2.75 | 0.45 |
| 4:A:57:ALA:HA | 4:A:67:LEU:HD23 | 1.98 | 0.45 |
| 7:D:35:ALA:HB2 | 38:D:5858:HOH:O | 2.16 | 0.45 |
| 7:D:73:VAL:HG21 | 38:D:5828:HOH:O | 2.15 | 0.45 |
| 7:D:95:THR:HG21 | 7:D:174:VAL:HG22 | 1.99 | 0.45 |
| 16:M:115:VAL:O | 16:M:118:ILE:HB | 2.17 | 0.45 |
| 19:P:75:ILE:CD1 | 19:P:84:ILE:HD11 | 2.46 | 0.45 |
| 25:V:130:HIS:O | 25:V:136:GLY:HA3 | 2.17 | 0.45 |
| 1:O:1184:C:H1' | 38:O:8953:HOH:O | 2.16 | 0.45 |
| 1:O:1500:U:P | 18:O:41:ARG:HH22 | 2.39 | 0.45 |
| 1:O:1735:C:H2' | 1:O:1736:A:C8 | 2.51 | 0.45 |
| 5:B:140:LEU:HD13 | 5:B:175:LEU:HA | 1.97 | 0.45 |
| 5:B:137:LEU:HD11 | 5:B:140:LEU:HD21 | 1.99 | 0.45 |
| 1:O:2716:G:C5' | 5:B:206:THR:HG21 | 2.45 | 0.45 |
| 5:B:243:ASN:HA | 5:B:244:PRO:C | 2.36 | 0.45 |
| 5:B:248:ARG:O | 5:B:251:VAL:CG1 | 2.65 | 0.45 |
| 1:O:2346:C:H4' | 7:D:52:THR:HG22 | 1.99 | 0.45 |
| 8:E:145:ALA:HB1 | 8:E:168:ILE:CD1 | 2.46 | 0.45 |
| 9:F:99:THR:HA | 38:F:3461:HOH:O | 2.17 | 0.45 |
| 11:H:112:ARG:O | 11:H:113:ALA:C | 2.55 | 0.45 |
| 13:J:118:ALA:HA | 13:J:125:ALA:HB2 | 1.99 | 0.45 |
| 16:M:77:ASN:OD1 | 16:M:80:SER:HB2 | 2.17 | 0.45 |
| 18:O:16:VAL:CG1 | 18:O:20:ARG:HB2 | 2.47 | 0.45 |
| 18:O:59:ARG:HG2 | 18:O:59:ARG:HH11 | 1.82 | 0.45 |
| 27:X:172:THR:HG22 | 27:X:173:ALA:N | 2.32 | 0.45 |
| 27:X:189:ASN:C | 27:X:189:ASN:ND2 | 2.67 | 0.45 |
| 1:O:1416:G:C2' | 1:O:1417:G:H5' | 2.46 | 0.45 |
| 1:O:1565:C:O4' | 1:O:2738:G:H1' | 2.16 | 0.45 |
| 1:O:243:A:H61 | 1:O:269:G:C1' | 2.29 | 0.45 |
| 1:O:338:C:H4' | 6:C:174:ILE:HD11 | 1.97 | 0.45 |
| 1:O:338:C:H4' | 6:C:174:ILE:HD12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:514:G:OP1 | 1:0:514:G:H2' | 2.16 | 0.45 |
| 1:0:668:C:H2' | 1:0:669:G:H8 | 1.80 | 0.45 |
| 1:0:820:G:O2' | 1:0:856:G:H4' | 2.17 | 0.45 |
| 1:0:958:G:H2' | 1:0:959:C:H6 | 1.80 | 0.45 |
| 30:1:40:ARG:HG3 | 30:1:45:ASN:CB | 2.46 | 0.45 |
| 5:B:87:TYR:CE2 | 5:B:96:PRO:HG3 | 2.51 | 0.45 |
| 10:G:27:ILE:HD12 | 10:G:70:ALA:HB1 | 1.98 | 0.45 |
| 13:J:22:ASP:OD1 | 13:J:22:ASP:C | 2.55 | 0.45 |
| 15:L:37:VAL:CG2 | 15:L:108:LYS:HG3 | 2.45 | 0.45 |
| 16:M:161:GLY:O | 16:M:162:ASP:C | 2.54 | 0.45 |
| 1:0:1813:U:O2' | 18:O:81:LYS:HE3 | 2.17 | 0.45 |
| 22:S:96:VAL:HG13 | 22:S:97:ARG:N | 2.32 | 0.45 |
| 25:V:54:PHE:CZ | 25:V:140:LYS:HB2 | 2.52 | 0.45 |
| 27:X:106:THR:HG23 | 27:X:107:PRO:HD2 | 1.99 | 0.45 |
| 27:X:141:THR:HG23 | 38:X:8599:HOH:O | 2.16 | 0.45 |
| 29:Z:8:GLN:HE22 | 29:Z:11:LYS:HZ2 | 1.63 | 0.45 |
| 1:0:1156:C:O2' | 1:0:1157:C:H5' | 2.17 | 0.45 |
| 1:0:1600:G:H4' | 38:0:6539:HOH:O | 2.17 | 0.45 |
| 1:0:2625:C:O2' | 1:0:2626:C:H5' | 2.16 | 0.45 |
| 1:0:64:G:H2' | 1:0:65:C:H6 | 1.80 | 0.45 |
| 2:9:3047:A:H2' | 2:9:3048:C:C6 | 2.51 | 0.45 |
| 4:A:69:LEU:CD2 | 4:A:120:ARG:HB3 | 2.41 | 0.45 |
| 5:B:144:THR:CG2 | 5:B:145:HIS:N | 2.79 | 0.45 |
| 6:C:126:ASP:C | 6:C:128:GLY:N | 2.70 | 0.45 |
| 9:F:20:LEU:O | 9:F:23:ALA:HB3 | 2.16 | 0.45 |
| 20:Q:113:HIS:O | 20:Q:145:LEU:HD12 | 2.17 | 0.45 |
| 1:0:1118:A:C8 | 1:0:1118:A:C3' | 2.87 | 0.45 |
| 1:0:1029:U:O2' | 1:0:1273:C:OP1 | 2.31 | 0.45 |
| 1:0:1613:C:H2' | 1:0:1614:G:O4' | 2.17 | 0.45 |
| 1:0:790:A:H1' | 1:0:1710:A:H2' | 1.99 | 0.45 |
| 1:0:1973:A:H2' | 1:0:1974:G:O4' | 2.17 | 0.45 |
| 1:0:2421:G:H4' | 38:0:5686:HOH:O | 2.17 | 0.45 |
| 1:0:740:G:O2' | 1:0:741:C:H5' | 2.17 | 0.45 |
| 1:0:953:G:H5' | 38:0:8786:HOH:O | 2.17 | 0.45 |
| 21:R:58:MET:SD | 30:1:8:LYS:HE3 | 2.57 | 0.45 |
| 31:2:11:CYS:HB2 | 31:2:20:HIS:NE2 | 2.32 | 0.45 |
| 5:B:38:VAL:HG22 | 5:B:142:LEU:HD12 | 1.99 | 0.45 |
| 5:B:7:ARG:CG | 5:B:7:ARG:HH11 | 2.23 | 0.45 |
| 8:E:162:PHE:CD1 | 8:E:162:PHE:N | 2.84 | 0.45 |
| 11:H:136:VAL:HG22 | 11:H:137:ASN:O | 2.16 | 0.45 |
| 12:I:17:CYS:HA | 12:I:119:THR:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:L:59:GLY:HA3 | 15:L:141:ILE:HD12 | 1.99 | 0.45 |
| 15:L:99:ARG:HD2 | 15:L:167:GLY:HA2 | 1.98 | 0.45 |
| 20:Q:39:THR:HG22 | 20:Q:42:GLU:HG3 | 1.98 | 0.45 |
| 20:Q:66:VAL:HG22 | 20:Q:79:ARG:CZ | 2.47 | 0.45 |
| 22:S:44:ALA:HA | 22:S:62:VAL:HG12 | 1.99 | 0.45 |
| 25:V:40:ALA:O | 25:V:44:MET:HG3 | 2.16 | 0.45 |
| 1:O:1278:A:H4' | 1:O:1279:U:C4 | 2.52 | 0.45 |
| 1:O:1514:C:H2' | 1:O:1515:A:H8 | 1.81 | 0.45 |
| 1:O:1523:G:H2' | 1:O:1524:U:C6 | 2.52 | 0.45 |
| 1:O:1758:U:H2' | 1:O:1759:A:O4' | 2.17 | 0.45 |
| 1:O:538:C:H5'' | 1:O:539:G:C8 | 2.52 | 0.45 |
| 5:B:195:ARG:N | 5:B:198:GLU:OE1 | 2.45 | 0.45 |
| 6:C:104:ASP:O | 6:C:108:GLN:HG3 | 2.17 | 0.45 |
| 6:C:140:VAL:HB | 38:C:8463:HOH:O | 2.16 | 0.45 |
| 6:C:76:ARG:HD2 | 38:C:8444:HOH:O | 2.17 | 0.45 |
| 8:E:126:ILE:HB | 8:E:131:LEU:HD23 | 1.99 | 0.45 |
| 1:O:1134:G:C4' | 11:H:151:MET:HE1 | 2.35 | 0.45 |
| 15:L:113:ARG:NH2 | 15:L:156:ARG:HG2 | 2.31 | 0.45 |
| 1:O:1470:A:OP1 | 15:L:93:ARG:HD2 | 2.17 | 0.45 |
| 17:N:14:LEU:CD2 | 17:N:102:ILE:HD11 | 2.47 | 0.45 |
| 27:X:219:GLU:HG3 | 27:X:220:GLU:N | 2.31 | 0.45 |
| 1:O:169:A:H1' | 31:2:48:ASN:ND2 | 2.31 | 0.44 |
| 1:O:653:C:H2' | 1:O:654:A:C8 | 2.51 | 0.44 |
| 2:9:3031:C:O2' | 2:9:3032:G:H5' | 2.17 | 0.44 |
| 5:B:7:ARG:CG | 5:B:7:ARG:NH1 | 2.80 | 0.44 |
| 1:O:2561:C:OP1 | 8:E:153:ARG:NH2 | 2.50 | 0.44 |
| 12:I:19:MET:HE2 | 12:I:79:PHE:HA | 1.98 | 0.44 |
| 16:M:34:LEU:HD13 | 16:M:47:LEU:HD21 | 1.99 | 0.44 |
| 17:N:47:ARG:NH1 | 17:N:47:ARG:HG3 | 2.32 | 0.44 |
| 17:N:77:ALA:HA | 17:N:96:VAL:O | 2.17 | 0.44 |
| 22:S:24:ARG:NH2 | 22:S:39:ASN:HD22 | 2.15 | 0.44 |
| 23:T:46:ALA:HB1 | 23:T:52:THR:HG21 | 2.00 | 0.44 |
| 26:W:30:MET:HE2 | 26:W:58:ALA:HB3 | 1.98 | 0.44 |
| 1:O:1384:C:H5' | 26:W:30:MET:HG2 | 1.99 | 0.44 |
| 1:O:1548:U:O2' | 1:O:1549:C:H5' | 2.17 | 0.44 |
| 1:O:1611:G:O2' | 1:O:1612:A:H5' | 2.18 | 0.44 |
| 1:O:1937:U:O2' | 1:O:1938:G:H5' | 2.17 | 0.44 |
| 1:O:2106:C:H2' | 1:O:2107:U:C6 | 2.53 | 0.44 |
| 1:O:658:C:O2' | 1:O:662:U:OP1 | 2.28 | 0.44 |
| 1:O:812:A:H2' | 1:O:813:C:H6 | 1.80 | 0.44 |
| 4:A:101:GLU:HG2 | 38:A:8580:HOH:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:132:ASP:OD1 | 4:A:133:ARG:N | 2.50 | 0.44 |
| 5:B:154:VAL:HG12 | 5:B:156:LYS:HG2 | 1.99 | 0.44 |
| 5:B:98:THR:HG22 | 5:B:99:GLU:H | 1.83 | 0.44 |
| 1:O:2709:G:H4' | 13:J:3:ALA:CB | 2.47 | 0.44 |
| 16:M:47:LEU:HD13 | 16:M:97:VAL:HG11 | 1.98 | 0.44 |
| 16:M:72:GLU:H | 16:M:171:HIS:CE1 | 2.35 | 0.44 |
| 17:N:96:VAL:HA | 38:N:4258:HOH:O | 2.17 | 0.44 |
| 18:O:7:LYS:CD | 18:O:21:VAL:CG2 | 2.95 | 0.44 |
| 19:P:77:ASP:N | 19:P:80:LYS:O | 2.49 | 0.44 |
| 25:V:149:LEU:HG | 25:V:153:MET:HE1 | 2.00 | 0.44 |
| 28:Y:31:ILE:CG2 | 28:Y:32:LYS:N | 2.80 | 0.44 |
| 1:O:1857:A:N6 | 1:O:2247:C:H1' | 2.32 | 0.44 |
| 1:O:1894:C:C2 | 1:O:1939:U:C4 | 3.05 | 0.44 |
| 1:O:2481:G:C3' | 1:O:2482:G:H5'' | 2.46 | 0.44 |
| 1:O:349:U:O2' | 1:O:350:C:H5' | 2.18 | 0.44 |
| 6:C:223:LEU:HA | 6:C:223:LEU:HD12 | 1.87 | 0.44 |
| 7:D:64:ARG:O | 7:D:67:ASP:OD2 | 2.36 | 0.44 |
| 13:J:21:ALA:O | 13:J:96:VAL:HG22 | 2.17 | 0.44 |
| 14:K:125:PHE:CZ | 14:K:140:VAL:HG13 | 2.52 | 0.44 |
| 14:K:144:ASP:HA | 14:K:147:GLU:HG3 | 1.99 | 0.44 |
| 15:L:88:VAL:HG12 | 15:L:89:ASN:N | 2.32 | 0.44 |
| 16:M:58:LEU:HD12 | 16:M:58:LEU:N | 2.32 | 0.44 |
| 23:T:17:THR:CG2 | 23:T:18:GLY:N | 2.81 | 0.44 |
| 26:W:23:HIS:HB2 | 38:W:7830:HOH:O | 2.16 | 0.44 |
| 1:O:1184:C:O2' | 1:O:1185:U:P | 2.76 | 0.44 |
| 1:O:1372:A:H3' | 38:O:8863:HOH:O | 2.18 | 0.44 |
| 1:O:1872:C:O2 | 4:A:25:ALA:HA | 2.18 | 0.44 |
| 1:O:2755:G:H1' | 38:O:5590:HOH:O | 2.18 | 0.44 |
| 1:O:328:U:O4' | 6:C:202:THR:HG22 | 2.17 | 0.44 |
| 1:O:653:C:H5'' | 38:N:7674:HOH:O | 2.16 | 0.44 |
| 1:O:731:U:H2' | 1:O:732:C:H6 | 1.80 | 0.44 |
| 1:O:81:G:N3 | 1:O:98:A:C2 | 2.85 | 0.44 |
| 8:E:69:ILE:O | 8:E:72:MET:HB2 | 2.16 | 0.44 |
| 9:F:34:ASN:O | 9:F:38:LYS:HG3 | 2.16 | 0.44 |
| 11:H:117:LYS:O | 11:H:119:VAL:HG13 | 2.18 | 0.44 |
| 11:H:139:ASP:O | 11:H:139:ASP:CG | 2.56 | 0.44 |
| 1:O:2415:A:C2 | 16:M:25:ARG:HB3 | 2.52 | 0.44 |
| 16:M:37:ARG:NE | 38:M:8534:HOH:O | 2.50 | 0.44 |
| 16:M:32:PRO:HD2 | 16:M:99:GLU:O | 2.17 | 0.44 |
| 18:O:115:SER:C | 18:O:117:SER:H | 2.20 | 0.44 |
| 18:O:10:ALA:HA | 18:O:13:VAL:CG1 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:W:78:GLU:CG | 26:W:79:GLU:H | 2.26 | 0.44 |
| 1:0:113:A:OP2 | 1:0:114:A:H2' | 2.18 | 0.44 |
| 1:0:1164:U:N3 | 1:0:1192:A:H2 | 2.07 | 0.44 |
| 1:0:1463:A:H2' | 1:0:1464:U:H6 | 1.82 | 0.44 |
| 1:0:1746:A:O4' | 1:0:1747:A:C2 | 2.70 | 0.44 |
| 1:0:2912:C:O2' | 1:0:2913:A:H5' | 2.18 | 0.44 |
| 1:0:363:A:O2' | 1:0:364:C:H5' | 2.18 | 0.44 |
| 1:0:622:G:P | 27:X:148:GLY:HA3 | 2.57 | 0.44 |
| 1:0:821:U:H5'' | 38:0:4004:HOH:O | 2.17 | 0.44 |
| 32:0:9500:SLD:N4S | 3:4:75:C:OP2 | 2.50 | 0.44 |
| 2:9:3088:G:OP1 | 25:V:130:HIS:NE2 | 2.40 | 0.44 |
| 5:B:52:VAL:C | 5:B:53:LEU:HD12 | 2.38 | 0.44 |
| 11:H:86:ARG:H | 11:H:86:ARG:HG2 | 1.44 | 0.44 |
| 13:J:34:VAL:CG2 | 13:J:47:ALA:HB2 | 2.48 | 0.44 |
| 14:K:101:ASP:C | 14:K:103:ALA:H | 2.20 | 0.44 |
| 18:O:109:ARG:NH1 | 18:O:119:TYR:CE2 | 2.85 | 0.44 |
| 25:V:110:GLN:HE21 | 25:V:110:GLN:HA | 1.82 | 0.44 |
| 25:V:80:ASP:O | 25:V:84:VAL:HG23 | 2.17 | 0.44 |
| 1:0:101:C:H2' | 1:0:102:A:C8 | 2.53 | 0.44 |
| 1:0:1299:G:N2 | 38:0:5591:HOH:O | 2.50 | 0.44 |
| 1:0:1432:U:H5' | 38:0:3181:HOH:O | 2.17 | 0.44 |
| 1:0:1514:C:O2' | 1:0:1515:A:H5' | 2.18 | 0.44 |
| 1:0:152:A:O2' | 1:0:153:C:H5' | 2.18 | 0.44 |
| 1:0:2241:C:H2' | 1:0:2242:U:H6 | 1.79 | 0.44 |
| 1:0:2509:A:OP2 | 1:0:2510:C:H5 | 2.01 | 0.44 |
| 1:0:2815:G:N7 | 12:I:80:LYS:NZ | 2.64 | 0.44 |
| 1:0:283:U:H5 | 1:0:284:C:H42 | 1.65 | 0.44 |
| 1:0:659:A:H5'' | 38:N:6799:HOH:O | 2.17 | 0.44 |
| 1:0:2091:G:O3' | 5:B:235:ARG:HD3 | 2.17 | 0.44 |
| 13:J:10:GLN:NE2 | 13:J:10:GLN:N | 2.31 | 0.44 |
| 13:J:113:ILE:HD12 | 13:J:128:ALA:HB2 | 2.00 | 0.44 |
| 1:0:1019:C:O2 | 19:P:94:GLN:NE2 | 2.51 | 0.44 |
| 25:V:13:MET:HE1 | 25:V:18:GLN:CA | 2.43 | 0.44 |
| 26:W:43:VAL:CG1 | 26:W:47:ALA:HB3 | 2.47 | 0.44 |
| 28:Y:30:GLU:HB3 | 28:Y:34:LYS:HE3 | 1.99 | 0.44 |
| 1:0:1283:G:O2' | 1:0:1284:G:H5' | 2.18 | 0.44 |
| 1:0:130:C:O2' | 1:0:131:A:N7 | 2.50 | 0.44 |
| 1:0:1759:A:N3 | 1:0:1818:C:H2' | 2.33 | 0.44 |
| 1:0:2064:U:H2' | 1:0:2065:C:H6 | 1.83 | 0.44 |
| 1:0:377:C:O2' | 1:0:378:A:H5' | 2.18 | 0.44 |
| 2:9:3078:G:N2 | 2:9:3103:A:OP2 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:A:56:ALA:O | 4:A:68:ILE:N | 2.49 | 0.44 |
| 7:D:173:GLU:O | 7:D:174:VAL:C | 2.56 | 0.44 |
| 8:E:7:ILE:HA | 8:E:8:PRO:HD3 | 1.90 | 0.44 |
| 9:F:50:VAL:CG1 | 9:F:60:VAL:HG11 | 2.46 | 0.44 |
| 11:H:72:VAL:HG13 | 11:H:72:VAL:O | 2.17 | 0.44 |
| 15:L:40:ILE:O | 15:L:40:ILE:HG13 | 2.18 | 0.44 |
| 25:V:7:LEU:HD12 | 25:V:53:ALA:HB2 | 2.00 | 0.44 |
| 1:0:818:A:O2' | 28:Y:13:ARG:HD3 | 2.17 | 0.44 |
| 1:0:1072:G:OP2 | 27:X:154:ARG:NH2 | 2.51 | 0.44 |
| 1:0:1118:A:H8 | 1:0:1119:G:H5'' | 1.82 | 0.44 |
| 1:0:1180:U:H2' | 1:0:1181:A:O4' | 2.18 | 0.44 |
| 1:0:1201:C:H2' | 1:0:1202:A:H5' | 1.99 | 0.44 |
| 1:0:1419:U:H2' | 1:0:1685:A:C2 | 2.53 | 0.44 |
| 1:0:1901:G:O2' | 1:0:1902:G:H5' | 2.18 | 0.44 |
| 1:0:2252:A:H2' | 1:0:2253:G:O4' | 2.18 | 0.44 |
| 1:0:2401:A:H5' | 38:0:3467:HOH:O | 2.17 | 0.44 |
| 1:0:2834:G:C4 | 1:0:2847:G:N2 | 2.85 | 0.44 |
| 1:0:2868:C:H2' | 1:0:2869:G:O4' | 2.18 | 0.44 |
| 1:0:2896:A:OP1 | 26:W:15:ARG:NH1 | 2.51 | 0.44 |
| 1:0:541:C:O2' | 1:0:542:A:H5'' | 2.18 | 0.44 |
| 1:0:612:U:H2' | 1:0:613:C:H6 | 1.83 | 0.44 |
| 1:0:60:A:H5' | 30:1:19:SER:HG | 1.83 | 0.44 |
| 5:B:148:PRO:HD2 | 38:B:8593:HOH:O | 2.18 | 0.44 |
| 10:G:12:ILE:HA | 38:G:8806:HOH:O | 2.18 | 0.44 |
| 11:H:26:LYS:CG | 11:H:28:ILE:H | 2.20 | 0.44 |
| 12:I:107:ASN:HD22 | 12:I:107:ASN:C | 2.20 | 0.44 |
| 14:K:121:ILE:HG12 | 14:K:141:GLU:HB2 | 1.99 | 0.44 |
| 15:L:153:THR:O | 15:L:156:ARG:HG3 | 2.17 | 0.44 |
| 25:V:7:LEU:CD1 | 25:V:53:ALA:HB2 | 2.48 | 0.44 |
| 27:X:184:GLU:OE2 | 27:X:204:ARG:HD2 | 2.17 | 0.44 |
| 1:0:177:A:H2' | 1:0:178:U:O4' | 2.18 | 0.44 |
| 1:0:1882:C:OP1 | 4:A:192:VAL:HG23 | 2.18 | 0.44 |
| 1:0:1936:C:O2' | 1:0:1937:U:H5' | 2.18 | 0.44 |
| 1:0:2807:U:OP2 | 5:B:28:SER:OG | 2.28 | 0.44 |
| 1:0:2872:U:H2' | 1:0:2873:C:H6 | 1.83 | 0.44 |
| 1:0:823:U:H2' | 1:0:824:G:O4' | 2.17 | 0.44 |
| 2:9:3053:G:O2' | 2:9:3054:A:H5' | 2.18 | 0.44 |
| 5:B:66:GLU:OE1 | 5:B:328:ARG:HD2 | 2.18 | 0.44 |
| 5:B:41:PHE:CE1 | 5:B:79:MET:HG3 | 2.53 | 0.44 |
| 6:C:133:ARG:NE | 6:C:138:VAL:HG22 | 2.33 | 0.44 |
| 6:C:156:LEU:HD12 | 6:C:156:LEU:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:D:136:ARG:HD2 | 7:D:155:HIS:O | 2.18 | 0.44 |
| 7:D:27:ILE:CG2 | 7:D:28:GLY:H | 2.18 | 0.44 |
| 8:E:69:ILE:HA | 8:E:72:MET:CE | 2.48 | 0.44 |
| 9:F:26:THR:HB | 9:F:102:GLY:O | 2.17 | 0.44 |
| 11:H:84:ARG:CZ | 11:H:135:TRP:CH2 | 3.00 | 0.44 |
| 16:M:104:ILE:O | 16:M:107:ASN:HB2 | 2.17 | 0.44 |
| 1:O:308:U:H5' | 22:S:97:ARG:NH2 | 2.33 | 0.44 |
| 38:J:408:HOH:O | 23:T:37:GLU:HB3 | 2.17 | 0.44 |
| 24:U:23:LEU:HD22 | 24:U:49:LEU:HD23 | 2.00 | 0.44 |
| 25:V:122:ARG:CG | 25:V:152:ALA:O | 2.66 | 0.44 |
| 25:V:5:VAL:HG11 | 25:V:153:MET:CE | 2.48 | 0.44 |
| 38:O:7167:HOH:O | 27:X:158:LYS:HD3 | 2.17 | 0.44 |
| 28:Y:56:MET:CE | 28:Y:63:LYS:HE3 | 2.48 | 0.44 |
| 1:O:102:A:H2' | 1:O:103:U:C6 | 2.53 | 0.43 |
| 1:O:1052:G:H2' | 1:O:1052:G:N3 | 2.33 | 0.43 |
| 1:O:1311:G:C2 | 1:O:1312:G:C8 | 3.05 | 0.43 |
| 1:O:1505:U:C6 | 1:O:1505:U:H5' | 2.48 | 0.43 |
| 1:O:1537:C:H1' | 38:O:7461:HOH:O | 2.18 | 0.43 |
| 1:O:1852:A:H2' | 1:O:1853:C:H6 | 1.83 | 0.43 |
| 1:O:2004:U:C2' | 1:O:2005:G:OP1 | 2.66 | 0.43 |
| 1:O:2595:U:O2' | 1:O:2596:A:H5' | 2.18 | 0.43 |
| 1:O:2719:A:C2 | 5:B:70:PRO:HG3 | 2.53 | 0.43 |
| 1:O:2880:A:H2' | 1:O:2881:C:O4' | 2.18 | 0.43 |
| 1:O:861:A:H2' | 1:O:862:U:H6 | 1.83 | 0.43 |
| 1:O:60:A:H5' | 30:1:19:SER:OG | 2.18 | 0.43 |
| 2:9:3039:U:H3' | 2:9:3040:C:H5'' | 1.99 | 0.43 |
| 6:C:19:PRO:HD2 | 6:C:240:LEU:HD21 | 2.00 | 0.43 |
| 7:D:55:LYS:O | 7:D:56:ARG:HB2 | 2.18 | 0.43 |
| 9:F:115:VAL:O | 9:F:118:LEU:N | 2.51 | 0.43 |
| 9:F:8:VAL:HG13 | 9:F:12:LEU:HD13 | 1.99 | 0.43 |
| 12:I:19:MET:HE1 | 12:I:132:LEU:CD2 | 2.47 | 0.43 |
| 13:J:78:LYS:HA | 13:J:79:PRO:HD3 | 1.85 | 0.43 |
| 13:J:81:ARG:HD3 | 13:J:87:ARG:NH1 | 2.33 | 0.43 |
| 15:L:87:MET:H | 15:L:87:MET:HG3 | 1.35 | 0.43 |
| 16:M:114:LYS:O | 16:M:117:ALA:HB3 | 2.18 | 0.43 |
| 20:Q:50:VAL:O | 20:Q:53:GLY:N | 2.51 | 0.43 |
| 1:O:305:A:C5 | 1:O:329:A:C2 | 3.06 | 0.43 |
| 4:A:36:ASP:CA | 4:A:83:GLY:HA3 | 2.47 | 0.43 |
| 4:A:95:PRO:HG2 | 4:A:98:GLU:HG2 | 2.00 | 0.43 |
| 7:D:77:ASP:HB3 | 7:D:78:GLU:H | 1.59 | 0.43 |
| 9:F:104:ALA:O | 9:F:108:LEU:HB3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:X:212:ARG:HD2 | 38:X:8610:HOH:O | 2.17 | 0.43 |
| 1:O:1114:A:H2' | 1:O:1115:U:H6 | 1.83 | 0.43 |
| 1:O:1116:U:O2' | 1:O:1118:A:C2 | 2.44 | 0.43 |
| 1:O:1278:A:P | 17:N:19:ARG:HH22 | 2.41 | 0.43 |
| 1:O:2502:C:H4' | 11:H:151:MET:CG | 2.43 | 0.43 |
| 1:O:2529:G:O2' | 1:O:2530:C:H5' | 2.18 | 0.43 |
| 1:O:2837:U:H1' | 5:B:307:ARG:HH12 | 1.83 | 0.43 |
| 1:O:602:A:O2' | 1:O:605:C:H4' | 2.19 | 0.43 |
| 1:O:1486:A:C5 | 30:1:2:LYS:HG3 | 2.53 | 0.43 |
| 4:A:66:ARG:CB | 4:A:66:ARG:NH1 | 2.81 | 0.43 |
| 1:O:2898:G:H4' | 5:B:288:GLY:HA2 | 1.99 | 0.43 |
| 8:E:101:GLU:HB2 | 8:E:116:THR:O | 2.17 | 0.43 |
| 11:H:26:LYS:CE | 11:H:28:ILE:HB | 2.47 | 0.43 |
| 12:I:97:ALA:O | 12:I:101:VAL:HG23 | 2.17 | 0.43 |
| 16:M:37:ARG:HD3 | 16:M:37:ARG:HA | 1.83 | 0.43 |
| 16:M:49:THR:CG2 | 16:M:56:ASP:HB2 | 2.36 | 0.43 |
| 18:O:114:LEU:HA | 18:O:118:GLN:NE2 | 2.34 | 0.43 |
| 19:P:40:HIS:HD2 | 19:P:60:THR:OG1 | 2.01 | 0.43 |
| 25:V:122:ARG:NH2 | 38:V:4276:HOH:O | 2.49 | 0.43 |
| 1:O:1805:G:O2' | 1:O:1806:G:H5' | 2.18 | 0.43 |
| 1:O:235:C:O2' | 1:O:236:A:H2' | 2.18 | 0.43 |
| 1:O:2758:G:O2' | 1:O:2759:C:H5' | 2.19 | 0.43 |
| 1:O:695:C:H2' | 1:O:696:C:C6 | 2.53 | 0.43 |
| 1:O:2434:A:O3' | 31:2:28:GLY:HA3 | 2.19 | 0.43 |
| 4:A:109:GLU:HG2 | 4:A:116:GLY:N | 2.33 | 0.43 |
| 5:B:41:PHE:CZ | 5:B:79:MET:HG3 | 2.53 | 0.43 |
| 5:B:62:ARG:HG2 | 5:B:65:MET:HE3 | 2.00 | 0.43 |
| 8:E:7:ILE:HD11 | 8:E:11:VAL:O | 2.19 | 0.43 |
| 1:O:2694:A:C4' | 8:E:91:PHE:HE1 | 2.23 | 0.43 |
| 11:H:47:GLU:HG2 | 11:H:133:ILE:CD1 | 2.49 | 0.43 |
| 11:H:58:HIS:CE1 | 11:H:59:ASN:ND2 | 2.86 | 0.43 |
| 15:L:95:LYS:HG2 | 15:L:99:ARG:HB3 | 1.99 | 0.43 |
| 18:O:103:THR:HA | 18:O:106:ARG:HH12 | 1.81 | 0.43 |
| 27:X:100:ARG:HE | 27:X:234:VAL:HG21 | 1.81 | 0.43 |
| 1:O:1461:U:H2' | 1:O:1462:C:H6 | 1.80 | 0.43 |
| 1:O:400:C:O2' | 1:O:401:C:H5' | 2.19 | 0.43 |
| 31:2:69:TYR:CE1 | 31:2:80:ARG:HD2 | 2.53 | 0.43 |
| 5:B:132:HIS:HB2 | 5:B:137:LEU:HD22 | 1.99 | 0.43 |
| 5:B:55:ASN:CB | 5:B:63:GLU:HA | 2.46 | 0.43 |
| 7:D:60:GLU:C | 7:D:62:ASP:N | 2.72 | 0.43 |
| 10:G:18:GLU:O | 10:G:21:ASP:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:2244:A:H5'' | 15:L:29:GLN:OE1 | 2.19 | 0.43 |
| 15:L:85:ARG:C | 15:L:87:MET:HG3 | 2.39 | 0.43 |
| 16:M:47:LEU:CD1 | 16:M:97:VAL:HG11 | 2.48 | 0.43 |
| 18:O:103:THR:O | 18:O:106:ARG:HB3 | 2.18 | 0.43 |
| 21:R:56:ASN:O | 30:1:8:LYS:HE2 | 2.18 | 0.43 |
| 27:X:144:ARG:NE | 38:X:8621:HOH:O | 2.50 | 0.43 |
| 27:X:203:VAL:CG1 | 27:X:228:VAL:HG22 | 2.46 | 0.43 |
| 1:O:1114:A:H2' | 1:O:1115:U:C6 | 2.54 | 0.43 |
| 1:O:1244:U:H4' | 1:O:1246:A:O4' | 2.19 | 0.43 |
| 1:O:1276:U:H3' | 17:N:19:ARG:HH11 | 1.83 | 0.43 |
| 1:O:2296:C:H2' | 1:O:2297:U:C6 | 2.53 | 0.43 |
| 5:B:180:ASP:O | 5:B:181:ILE:C | 2.57 | 0.43 |
| 7:D:128:LEU:C | 7:D:128:LEU:HD23 | 2.39 | 0.43 |
| 8:E:18:LEU:HD13 | 8:E:34:TRP:CG | 2.54 | 0.43 |
| 15:L:55:LYS:HB2 | 15:L:60:ILE:CD1 | 2.49 | 0.43 |
| 15:L:61:ILE:N | 15:L:61:ILE:HD12 | 2.33 | 0.43 |
| 38:O:5481:HOH:O | 15:L:86:MET:HE3 | 2.18 | 0.43 |
| 16:M:15:GLU:O | 16:M:17:ARG:HG3 | 2.19 | 0.43 |
| 26:W:9:VAL:HG13 | 26:W:88:GLU:CD | 2.38 | 0.43 |
| 27:X:200:THR:HG22 | 27:X:201:GLU:HG2 | 2.00 | 0.43 |
| 28:Y:58:GLY:HA3 | 38:Y:8442:HOH:O | 2.19 | 0.43 |
| 1:O:1755:A:H2' | 1:O:1756:G:O4' | 2.18 | 0.43 |
| 1:O:353:G:H2' | 1:O:354:A:H8 | 1.82 | 0.43 |
| 1:O:473:A:O2' | 1:O:474:C:H5' | 2.19 | 0.43 |
| 1:O:797:A:H5' | 28:Y:10:ARG:HG2 | 2.00 | 0.43 |
| 1:O:883:U:O2 | 1:O:883:U:H2' | 2.18 | 0.43 |
| 8:E:22:VAL:O | 8:E:28:SER:HA | 2.19 | 0.43 |
| 9:F:49:PHE:CD1 | 9:F:49:PHE:N | 2.87 | 0.43 |
| 10:G:12:ILE:O | 10:G:12:ILE:HG22 | 2.19 | 0.43 |
| 11:H:28:ILE:HG23 | 38:H:8390:HOH:O | 2.17 | 0.43 |
| 13:J:87:ARG:HB2 | 23:T:19:THR:HG23 | 2.01 | 0.43 |
| 22:S:3:GLN:HA | 22:S:4:PRO:HD3 | 1.89 | 0.43 |
| 27:X:151:SER:HB3 | 27:X:154:ARG:HB3 | 2.00 | 0.43 |
| 27:X:189:ASN:ND2 | 27:X:192:ASP:H | 2.16 | 0.43 |
| 1:O:2670:G:O2' | 1:O:2671:U:H5' | 2.18 | 0.43 |
| 1:O:440:C:H2' | 1:O:441:A:C8 | 2.54 | 0.43 |
| 1:O:999:C:O2' | 1:O:1000:C:H5' | 2.19 | 0.43 |
| 7:D:21:VAL:HA | 7:D:131:THR:O | 2.18 | 0.43 |
| 12:I:4:ALA:O | 12:I:5:GLU:O | 2.36 | 0.43 |
| 13:J:90:PHE:CD1 | 13:J:90:PHE:N | 2.87 | 0.43 |
| 15:L:184:ARG:NH1 | 15:L:184:ARG:HB2 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:M:143:ARG:HA | 16:M:172:PHE:CE2 | 2.54 | 0.43 |
| 19:P:50:GLY:HA3 | 19:P:87:THR:OG1 | 2.19 | 0.43 |
| 22:S:87:VAL:HB | 22:S:88:PRO:HD2 | 2.00 | 0.43 |
| 1:O:1008:C:H2' | 1:O:1009:U:C6 | 2.53 | 0.43 |
| 1:O:111:C:H2' | 1:O:112:G:O4' | 2.19 | 0.43 |
| 1:O:1205:U:H2' | 1:O:1206:U:C5' | 2.49 | 0.43 |
| 1:O:1566:C:O2' | 1:O:1567:A:H5' | 2.19 | 0.43 |
| 1:O:2060:A:H2' | 1:O:2061:C:C6 | 2.54 | 0.43 |
| 1:O:2106:C:H1' | 1:O:2484:U:O2 | 2.19 | 0.43 |
| 1:O:2538:A:H4' | 1:O:2539:U:OP1 | 2.19 | 0.43 |
| 1:O:264:G:H1' | 1:O:265:U:H5 | 1.82 | 0.43 |
| 1:O:2661:U:H3 | 1:O:2812:A:H62 | 1.67 | 0.43 |
| 1:O:559:U:O2' | 1:O:560:C:H5' | 2.19 | 0.43 |
| 1:O:685:C:O2 | 1:O:748:C:H4' | 2.18 | 0.43 |
| 1:O:790:A:H2' | 1:O:791:A:O4' | 2.19 | 0.43 |
| 38:O:3070:HOH:O | 5:B:214:PRO:HD2 | 2.19 | 0.43 |
| 7:D:146:LYS:CE | 16:M:107:ASN:ND2 | 2.81 | 0.43 |
| 7:D:23:VAL:HG21 | 7:D:45:THR:CG2 | 2.49 | 0.43 |
| 13:J:125:ALA:C | 13:J:127:ALA:H | 2.21 | 0.43 |
| 13:J:29:LEU:HB3 | 13:J:55:VAL:CG1 | 2.42 | 0.43 |
| 15:L:122:GLU:HB2 | 15:L:126:HIS:O | 2.19 | 0.43 |
| 18:O:16:VAL:CG1 | 18:O:17:GLY:N | 2.82 | 0.43 |
| 1:O:2054:A:H2 | 20:Q:128:ARG:HH22 | 1.61 | 0.43 |
| 21:R:42:GLU:HG2 | 21:R:49:VAL:HG23 | 2.01 | 0.43 |
| 25:V:26:ILE:CG1 | 25:V:26:ILE:O | 2.66 | 0.43 |
| 26:W:26:ALA:O | 26:W:27:ASP:C | 2.57 | 0.43 |
| 28:Y:32:LYS:HB3 | 28:Y:32:LYS:HE2 | 1.90 | 0.43 |
| 1:O:1008:C:O2' | 1:O:1009:U:H5' | 2.19 | 0.43 |
| 1:O:1377:C:H5' | 1:O:1377:C:C6 | 2.51 | 0.43 |
| 1:O:1947:G:N2 | 1:O:1966:U:C2 | 2.87 | 0.43 |
| 1:O:250:C:O2' | 1:O:251:C:H5' | 2.18 | 0.43 |
| 1:O:2684:A:H2' | 1:O:2685:C:C6 | 2.54 | 0.43 |
| 1:O:354:A:H2' | 1:O:355:C:H6 | 1.83 | 0.43 |
| 4:A:103:VAL:HA | 4:A:104:PRO:HD3 | 1.84 | 0.43 |
| 1:O:1853:C:H5' | 4:A:228:ILE:O | 2.18 | 0.43 |
| 4:A:97:ALA:HB2 | 4:A:150:PRO:HB2 | 2.01 | 0.43 |
| 2:9:3056:A:O2' | 7:D:14:ARG:HD3 | 2.19 | 0.43 |
| 9:F:36:THR:OG1 | 38:F:3111:HOH:O | 2.22 | 0.43 |
| 11:H:111:MET:O | 11:H:114:PRO:HD3 | 2.19 | 0.43 |
| 1:O:392:U:H4' | 15:L:193:LYS:HB3 | 2.00 | 0.43 |
| 15:L:71:SER:HB2 | 15:L:92:THR:HG22 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:M:108:SER:HA | 16:M:109:PRO:HD3 | 1.80 | 0.43 |
| 18:O:135:ALA:HB1 | 18:O:139:ARG:HH12 | 1.84 | 0.43 |
| 19:P:93:ARG:HG3 | 19:P:93:ARG:NH1 | 2.34 | 0.43 |
| 1:O:123:U:H2' | 1:O:124:C:C6 | 2.54 | 0.42 |
| 1:O:1329:A:N1 | 36:O:8513:CL:CL | 2.88 | 0.42 |
| 1:O:152:A:H2' | 1:O:153:C:C6 | 2.54 | 0.42 |
| 1:O:1667:A:C8 | 1:O:1667:A:H5' | 2.50 | 0.42 |
| 1:O:2688:U:H2' | 1:O:2689:A:C8 | 2.54 | 0.42 |
| 5:B:205:VAL:O | 5:B:307:ARG:CD | 2.67 | 0.42 |
| 6:C:138:VAL:O | 6:C:234:VAL:HA | 2.19 | 0.42 |
| 6:C:7:ASP:C | 6:C:9:ASP:H | 2.22 | 0.42 |
| 7:D:151:ILE:HA | 7:D:152:PRO:HD3 | 1.89 | 0.42 |
| 14:K:133:VAL:HB | 38:K:8562:HOH:O | 2.19 | 0.42 |
| 38:O:4117:HOH:O | 15:L:87:MET:HE1 | 2.19 | 0.42 |
| 20:Q:89:LEU:HD23 | 20:Q:89:LEU:HA | 1.79 | 0.42 |
| 24:U:12:THR:HG23 | 24:U:14:ALA:N | 2.34 | 0.42 |
| 1:O:2105:C:H2' | 1:O:2106:C:C6 | 2.54 | 0.42 |
| 1:O:2544:G:H2' | 1:O:2545:U:O4' | 2.18 | 0.42 |
| 1:O:2708:G:H2' | 1:O:2709:G:O4' | 2.19 | 0.42 |
| 1:O:2730:G:O2' | 1:O:2731:G:H5' | 2.19 | 0.42 |
| 1:O:2840:A:H3' | 38:O:8528:HOH:O | 2.18 | 0.42 |
| 1:O:61:G:C2 | 1:O:62:C:C2 | 3.07 | 0.42 |
| 1:O:843:A:C2 | 1:O:846:A:C8 | 3.08 | 0.42 |
| 31:2:5:ARG:HG3 | 31:2:5:ARG:O | 2.20 | 0.42 |
| 5:B:238:ASN:ND2 | 5:B:240:GLY:N | 2.54 | 0.42 |
| 38:O:4962:HOH:O | 6:C:149:LYS:HE3 | 2.18 | 0.42 |
| 6:C:178:GLN:O | 6:C:179:GLY:C | 2.58 | 0.42 |
| 6:C:194:PHE:HA | 6:C:234:VAL:HG13 | 2.00 | 0.42 |
| 8:E:106:ASN:ND2 | 8:E:109:GLY:HA2 | 2.34 | 0.42 |
| 12:I:6:PHE:O | 12:I:8:ALA:N | 2.52 | 0.42 |
| 15:L:35:PRO:HD2 | 15:L:38:VAL:CG2 | 2.48 | 0.42 |
| 2:9:3007:G:H4' | 16:M:55:ASP:OD2 | 2.18 | 0.42 |
| 21:R:57:THR:CG2 | 21:R:58:MET:N | 2.82 | 0.42 |
| 25:V:154:ARG:HB3 | 25:V:154:ARG:HE | 1.50 | 0.42 |
| 25:V:29:VAL:O | 25:V:30:ASN:HB2 | 2.18 | 0.42 |
| 28:Y:27:ALA:O | 28:Y:28:ASP:C | 2.57 | 0.42 |
| 1:O:1139:U:H2' | 1:O:1140:C:H6 | 1.84 | 0.42 |
| 1:O:1328:A:N7 | 1:O:1329:A:C5 | 2.87 | 0.42 |
| 1:O:1342:C:O2' | 1:O:1343:C:H5' | 2.19 | 0.42 |
| 1:O:1433:G:O2' | 1:O:1434:A:H5' | 2.19 | 0.42 |
| 1:O:2347:C:H2' | 1:O:2348:C:H6 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2896:A:N3 | 1:0:2896:A:H2' | 2.34 | 0.42 |
| 1:0:525:G:H2' | 1:0:526:U:O4' | 2.18 | 0.42 |
| 1:0:639:A:H2' | 1:0:640:G:H8 | 1.83 | 0.42 |
| 1:0:776:A:H1' | 1:0:779:U:O4 | 2.19 | 0.42 |
| 4:A:88:ILE:CD1 | 4:A:100:PRO:HD3 | 2.47 | 0.42 |
| 7:D:133:ASN:HD22 | 7:D:133:ASN:HA | 1.66 | 0.42 |
| 38:9:8411:HOH:O | 7:D:68:PRO:HG3 | 2.20 | 0.42 |
| 8:E:101:GLU:OE2 | 8:E:115:ARG:HD3 | 2.19 | 0.42 |
| 11:H:46:VAL:CG1 | 11:H:146:TRP:HZ3 | 2.32 | 0.42 |
| 13:J:9:THR:HG22 | 13:J:78:LYS:HG2 | 2.01 | 0.42 |
| 16:M:34:LEU:HD22 | 16:M:129:ILE:CD1 | 2.49 | 0.42 |
| 38:0:7645:HOH:O | 16:M:4:PRO:HD2 | 2.19 | 0.42 |
| 24:U:39:ALA:C | 24:U:41:GLU:N | 2.72 | 0.42 |
| 1:0:1028:U:H5' | 1:0:1031:G:O4' | 2.19 | 0.42 |
| 1:0:1635:U:O2' | 1:0:1636:G:H5' | 2.19 | 0.42 |
| 1:0:1649:G:O2' | 1:0:1650:C:H5' | 2.18 | 0.42 |
| 1:0:1669:A:H2' | 1:0:1670:G:H8 | 1.84 | 0.42 |
| 1:0:2011:A:H5' | 1:0:2013:G:H1' | 2.00 | 0.42 |
| 1:0:2353:A:H4' | 1:0:2354:A:O5' | 2.19 | 0.42 |
| 1:0:2039:A:H4' | 1:0:2760:C:O2' | 2.20 | 0.42 |
| 1:0:301:G:O2' | 1:0:302:A:H5' | 2.19 | 0.42 |
| 1:0:565:A:H2' | 1:0:566:A:C8 | 2.54 | 0.42 |
| 1:0:675:U:O2' | 6:C:42:ARG:NH1 | 2.52 | 0.42 |
| 29:Z:25:LYS:CD | 30:1:49:GLU:H | 2.28 | 0.42 |
| 5:B:152:PRO:HD2 | 38:B:8645:HOH:O | 2.18 | 0.42 |
| 5:B:33:ASP:HB3 | 5:B:34:GLY:H | 1.71 | 0.42 |
| 6:C:40:ALA:HB3 | 6:C:100:LEU:HD12 | 2.02 | 0.42 |
| 7:D:166:ILE:O | 7:D:169:THR:N | 2.51 | 0.42 |
| 38:0:5879:HOH:O | 11:H:57:ARG:HG3 | 2.19 | 0.42 |
| 11:H:71:TYR:C | 11:H:73:GLN:N | 2.71 | 0.42 |
| 11:H:31:PHE:HE2 | 11:H:87:LYS:O | 2.02 | 0.42 |
| 12:I:142:ASN:O | 12:I:144:THR:N | 2.52 | 0.42 |
| 16:M:152:GLU:C | 16:M:154:LEU:N | 2.72 | 0.42 |
| 16:M:175:LEU:HA | 16:M:175:LEU:HD12 | 1.75 | 0.42 |
| 1:0:2053:G:H4' | 20:Q:136:TRP:CE2 | 2.55 | 0.42 |
| 27:X:235:GLU:N | 27:X:235:GLU:CD | 2.71 | 0.42 |
| 1:0:1517:U:H2' | 1:0:1518:A:C8 | 2.54 | 0.42 |
| 1:0:1714:C:H4' | 1:0:2745:C:O2 | 2.19 | 0.42 |
| 1:0:191:A:H2' | 1:0:237:G:O6 | 2.19 | 0.42 |
| 1:0:2039:A:H2' | 1:0:2040:C:C6 | 2.55 | 0.42 |
| 1:0:2651:C:H2' | 1:0:2652:U:O4' | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2824:C:H5'' | 1:0:2825:C:H5' | 2.01 | 0.42 |
| 1:0:307:G:C2 | 1:0:309:C:C4 | 3.06 | 0.42 |
| 1:0:317:A:H5' | 22:S:52:ARG:HD2 | 2.01 | 0.42 |
| 1:0:370:G:O2' | 1:0:371:U:H5' | 2.19 | 0.42 |
| 1:0:770:C:O2' | 1:0:771:G:H5' | 2.18 | 0.42 |
| 1:0:821:U:H2' | 1:0:822:C:C6 | 2.54 | 0.42 |
| 1:0:902:G:N7 | 14:K:18:HIS:CD2 | 2.85 | 0.42 |
| 5:B:83:ALA:HB2 | 5:B:101:TRP:CD2 | 2.54 | 0.42 |
| 7:D:54:ALA:O | 7:D:65:GLU:O | 2.37 | 0.42 |
| 9:F:4:VAL:HA | 9:F:76:PHE:CE1 | 2.54 | 0.42 |
| 11:H:48:LEU:CG | 11:H:157:ILE:HG21 | 2.48 | 0.42 |
| 12:I:45:VAL:HG22 | 12:I:46:ILE:N | 2.34 | 0.42 |
| 13:J:19:THR:HB | 13:J:94:ALA:HB2 | 2.01 | 0.42 |
| 14:K:124:ASP:OD1 | 14:K:149:ARG:NH2 | 2.53 | 0.42 |
| 15:L:137:ASP:O | 15:L:142:LYS:HE3 | 2.19 | 0.42 |
| 18:O:84:ALA:C | 18:O:86:ALA:H | 2.23 | 0.42 |
| 1:0:1200:A:H2' | 38:O:6645:HOH:O | 2.20 | 0.42 |
| 1:0:1217:G:H2' | 1:0:1218:U:H6 | 1.85 | 0.42 |
| 1:0:1320:U:H2' | 1:0:1321:A:C8 | 2.55 | 0.42 |
| 1:0:1574:C:H2' | 1:0:1575:C:C6 | 2.55 | 0.42 |
| 1:0:1996:U:H6 | 1:0:2586:U:O2 | 2.03 | 0.42 |
| 1:0:585:C:H2' | 1:0:586:C:C6 | 2.54 | 0.42 |
| 1:0:709:G:O2' | 17:N:25:VAL:CG1 | 2.67 | 0.42 |
| 1:0:846:A:O2' | 1:0:847:C:H5' | 2.19 | 0.42 |
| 1:0:920:C:H5' | 1:0:921:G:C4 | 2.55 | 0.42 |
| 1:0:1014:A:H5'' | 2:9:3101:G:O2' | 2.20 | 0.42 |
| 1:0:2670:G:H4' | 5:B:112:THR:HG22 | 2.02 | 0.42 |
| 5:B:132:HIS:CE1 | 5:B:171:VAL:CG2 | 3.03 | 0.42 |
| 6:C:200:PRO:HB3 | 6:C:212:VAL:HG23 | 2.01 | 0.42 |
| 7:D:95:THR:C | 7:D:97:GLN:N | 2.71 | 0.42 |
| 8:E:116:THR:HG22 | 8:E:151:LEU:HD22 | 2.00 | 0.42 |
| 8:E:15:GLN:NE2 | 8:E:40:VAL:O | 2.52 | 0.42 |
| 10:G:20:VAL:O | 10:G:24:VAL:HG23 | 2.20 | 0.42 |
| 12:I:130:VAL:HG12 | 12:I:131:THR:N | 2.32 | 0.42 |
| 38:O:4613:HOH:O | 15:L:79:LYS:HD3 | 2.20 | 0.42 |
| 1:0:2413:A:N7 | 16:M:109:PRO:CB | 2.81 | 0.42 |
| 16:M:69:TYR:HE2 | 16:M:183:ASP:OD2 | 2.03 | 0.42 |
| 18:O:103:THR:O | 18:O:107:GLU:HG3 | 2.20 | 0.42 |
| 19:P:42:LYS:HD2 | 19:P:42:LYS:HA | 1.93 | 0.42 |
| 1:0:92:G:H4' | 24:U:44:GLY:HA3 | 2.00 | 0.42 |
| 29:Z:25:LYS:HD2 | 30:1:48:ASP:HA | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1236:A:H2' | 1:0:1237:U:O4' | 2.20 | 0.42 |
| 1:0:1362:U:H5' | 38:0:4214:HOH:O | 2.19 | 0.42 |
| 1:0:1477:C:O2' | 1:0:1478:U:H5' | 2.19 | 0.42 |
| 1:0:1511:U:O2' | 1:0:1512:G:H5' | 2.19 | 0.42 |
| 1:0:1992:U:H2' | 1:0:1994:A:OP2 | 2.20 | 0.42 |
| 1:0:2004:U:H2' | 1:0:2005:G:OP1 | 2.19 | 0.42 |
| 1:0:1976:G:H1' | 1:0:2005:G:N2 | 2.35 | 0.42 |
| 1:0:2327:A:H2' | 1:0:2328:U:C6 | 2.55 | 0.42 |
| 1:0:2478:U:H2' | 1:0:2479:A:H8 | 1.85 | 0.42 |
| 1:0:255:A:H2' | 1:0:256:C:H6 | 1.83 | 0.42 |
| 1:0:35:U:O2' | 1:0:36:C:H5' | 2.20 | 0.42 |
| 1:0:424:C:H2' | 1:0:425:U:H6 | 1.85 | 0.42 |
| 1:0:424:C:H2' | 1:0:425:U:C6 | 2.53 | 0.42 |
| 1:0:750:A:O3' | 6:C:101:ASP:HB2 | 2.20 | 0.42 |
| 30:1:22:PRO:HG2 | 30:1:25:VAL:HG23 | 2.02 | 0.42 |
| 1:0:169:A:O2' | 31:2:48:ASN:ND2 | 2.53 | 0.42 |
| 4:A:16:PHE:HB3 | 38:A:8556:HOH:O | 2.20 | 0.42 |
| 5:B:183:GLU:OE1 | 5:B:183:GLU:HA | 2.20 | 0.42 |
| 14:K:40:PHE:C | 14:K:40:PHE:CD1 | 2.92 | 0.42 |
| 14:K:73:VAL:HG11 | 14:K:118:LEU:HD21 | 2.02 | 0.42 |
| 16:M:34:LEU:HA | 16:M:47:LEU:CD2 | 2.50 | 0.42 |
| 16:M:67:ALA:O | 16:M:69:TYR:N | 2.53 | 0.42 |
| 1:0:1597:A:O4' | 18:O:95:GLU:HG2 | 2.20 | 0.42 |
| 22:S:80:GLU:OE2 | 22:S:84:GLY:HA2 | 2.20 | 0.42 |
| 28:Y:13:ARG:NH1 | 28:Y:14:PHE:CZ | 2.87 | 0.42 |
| 28:Y:42:CYS:SG | 28:Y:43:GLY:N | 2.93 | 0.42 |
| 1:0:1276:U:H3' | 17:N:19:ARG:NH1 | 2.34 | 0.42 |
| 1:0:1666:C:H2' | 1:0:1667:A:C8 | 2.54 | 0.42 |
| 1:0:17:G:H2' | 1:0:18:C:C6 | 2.54 | 0.42 |
| 1:0:39:G:N2 | 1:0:444:C:C2 | 2.88 | 0.42 |
| 2:9:3031:C:H2' | 2:9:3032:G:O4' | 2.19 | 0.42 |
| 5:B:27:ASN:HB3 | 38:B:8641:HOH:O | 2.19 | 0.42 |
| 5:B:5:ARG:HD2 | 5:B:8:LYS:HZ1 | 1.82 | 0.42 |
| 7:D:41:LEU:O | 7:D:44:ILE:HG22 | 2.20 | 0.42 |
| 7:D:81:GLU:O | 7:D:84:LEU:N | 2.52 | 0.42 |
| 8:E:3:VAL:HG22 | 8:E:49:ILE:HB | 2.01 | 0.42 |
| 9:F:21:GLU:O | 9:F:24:ARG:CG | 2.65 | 0.42 |
| 9:F:23:ALA:HB1 | 38:F:5413:HOH:O | 2.19 | 0.42 |
| 11:H:47:GLU:CB | 11:H:133:ILE:CD1 | 2.95 | 0.42 |
| 11:H:29:ALA:CB | 11:H:65:ARG:HH12 | 2.18 | 0.42 |
| 12:I:19:MET:CE | 12:I:78:ILE:HG22 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:K:12:THR:HG21 | 14:K:16:GLY:O | 2.19 | 0.42 |
| 15:L:49:ALA:C | 15:L:54:TYR:HB3 | 2.40 | 0.42 |
| 16:M:154:LEU:HG | 16:M:155:GLU:H | 1.84 | 0.42 |
| 16:M:157:PRO:HG3 | 38:M:8526:HOH:O | 2.19 | 0.42 |
| 23:T:37:GLU:O | 23:T:40:ALA:HB3 | 2.20 | 0.42 |
| 25:V:65:VAL:HA | 25:V:68:THR:HG22 | 2.01 | 0.42 |
| 1:O:1069:C:H2' | 1:O:1070:A:O4' | 2.20 | 0.42 |
| 1:O:1268:C:O2' | 1:O:1269:G:H5' | 2.19 | 0.42 |
| 1:O:1289:C:O2' | 1:O:1290:G:H5' | 2.20 | 0.42 |
| 1:O:1769:C:O2' | 1:O:1770:U:H5' | 2.20 | 0.42 |
| 1:O:1988:C:C2 | 1:O:2001:G:N2 | 2.88 | 0.42 |
| 1:O:2055:A:H4' | 20:Q:132:ARG:NH2 | 2.35 | 0.42 |
| 1:O:2406:U:C2 | 1:O:2407:G:C8 | 3.08 | 0.42 |
| 1:O:2869:G:H2' | 1:O:2870:C:C6 | 2.54 | 0.42 |
| 1:O:2895:C:H4' | 38:W:4132:HOH:O | 2.19 | 0.42 |
| 1:O:630:A:H5'' | 38:O:5660:HOH:O | 2.19 | 0.42 |
| 1:O:757:C:H2' | 1:O:758:A:C8 | 2.55 | 0.42 |
| 1:O:462:A:C8 | 30:1:37:HIS:CE1 | 3.08 | 0.42 |
| 11:H:147:ARG:HA | 11:H:150:LYS:HZ2 | 1.85 | 0.42 |
| 11:H:150:LYS:HA | 11:H:153:VAL:HG22 | 2.01 | 0.42 |
| 20:Q:19:ARG:HA | 20:Q:142:ASP:OD1 | 2.20 | 0.42 |
| 28:Y:57:CYS:C | 28:Y:59:HIS:N | 2.73 | 0.42 |
| 1:O:1184:C:O2' | 1:O:1185:U:OP2 | 2.35 | 0.42 |
| 1:O:1352:A:P | 6:C:92:PRO:HG3 | 2.60 | 0.42 |
| 1:O:1520:G:H2' | 1:O:1521:C:C6 | 2.54 | 0.42 |
| 1:O:185:G:H4' | 1:O:186:A:H4' | 2.01 | 0.42 |
| 1:O:1905:U:H2' | 1:O:1906:C:C6 | 2.54 | 0.42 |
| 1:O:2381:C:H4' | 31:2:80:ARG:NH1 | 2.34 | 0.42 |
| 1:O:2445:U:H2' | 1:O:2446:G:C8 | 2.55 | 0.42 |
| 1:O:2604:A:H5' | 38:O:6679:HOH:O | 2.19 | 0.42 |
| 1:O:2782:G:O6 | 1:O:2790:C:H5'' | 2.19 | 0.42 |
| 1:O:2866:U:H4' | 1:O:2867:G:H5' | 2.02 | 0.42 |
| 1:O:319:A:H2' | 1:O:320:G:C8 | 2.55 | 0.42 |
| 1:O:441:A:H1' | 1:O:442:A:N7 | 2.35 | 0.42 |
| 1:O:660:A:N6 | 1:O:746:A:O4' | 2.53 | 0.42 |
| 1:O:668:C:H2' | 1:O:669:G:C8 | 2.55 | 0.42 |
| 1:O:73:C:O2' | 1:O:74:A:H5' | 2.19 | 0.42 |
| 1:O:834:G:H5'' | 1:O:835:U:O5' | 2.19 | 0.42 |
| 4:A:130:THR:HG22 | 4:A:131:HIS:N | 2.33 | 0.42 |
| 4:A:65:ARG:NH1 | 4:A:65:ARG:HG2 | 2.35 | 0.42 |
| 6:C:21:VAL:C | 6:C:23:GLU:N | 2.72 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:C:114:ALA:HB1 | 6:C:223:LEU:HB3 | 2.01 | 0.42 |
| 8:E:15:GLN:HB2 | 8:E:20:ILE:HA | 2.02 | 0.42 |
| 18:O:59:ARG:O | 18:O:62:ALA:HB3 | 2.20 | 0.42 |
| 18:O:84:ALA:C | 18:O:86:ALA:N | 2.73 | 0.42 |
| 20:Q:29:LYS:CD | 38:Q:8542:HOH:O | 2.60 | 0.42 |
| 22:S:69:LYS:O | 22:S:71:VAL:HG23 | 2.20 | 0.42 |
| 1:O:1116:U:C2' | 1:O:1118:A:C2 | 3.03 | 0.41 |
| 1:O:1514:C:H2' | 1:O:1515:A:C8 | 2.55 | 0.41 |
| 1:O:1524:U:O2' | 1:O:1525:G:P | 2.78 | 0.41 |
| 1:O:2253:G:O2' | 1:O:2254:G:H5' | 2.21 | 0.41 |
| 1:O:2301:A:H5'' | 1:O:2302:A:H5' | 2.02 | 0.41 |
| 1:O:2389:U:H4' | 19:P:53:HIS:CD2 | 2.54 | 0.41 |
| 1:O:23:G:H1' | 1:O:520:A:N6 | 2.35 | 0.41 |
| 1:O:51:G:O2' | 1:O:52:A:H5' | 2.20 | 0.41 |
| 1:O:163:U:O3' | 1:O:896:C:H4' | 2.19 | 0.41 |
| 30:1:36:ASN:HB3 | 30:1:39:ARG:HG3 | 2.01 | 0.41 |
| 5:B:139:ASP:HB2 | 38:B:8532:HOH:O | 2.19 | 0.41 |
| 5:B:304:PRO:HD2 | 5:B:307:ARG:HH11 | 1.83 | 0.41 |
| 6:C:236:THR:HG21 | 38:C:8382:HOH:O | 2.20 | 0.41 |
| 7:D:140:ARG:HH11 | 7:D:140:ARG:HG3 | 1.84 | 0.41 |
| 11:H:75:SER:HB3 | 11:H:79:ALA:HB1 | 2.02 | 0.41 |
| 14:K:124:ASP:CG | 14:K:125:PHE:N | 2.73 | 0.41 |
| 15:L:133:LEU:O | 15:L:134:ILE:HD13 | 2.20 | 0.41 |
| 1:O:145:A:H4' | 15:L:137:ASP:OD2 | 2.20 | 0.41 |
| 15:L:87:MET:HE3 | 38:L:8596:HOH:O | 2.18 | 0.41 |
| 16:M:102:LEU:HG | 16:M:104:ILE:CG2 | 2.50 | 0.41 |
| 20:Q:123:GLN:HA | 20:Q:137:ASN:OD1 | 2.20 | 0.41 |
| 20:Q:44:VAL:HG13 | 20:Q:89:LEU:HD22 | 2.01 | 0.41 |
| 21:R:8:PRO:HD2 | 24:U:32:ALA:HA | 2.02 | 0.41 |
| 1:O:1044:C:H5'' | 38:O:3019:HOH:O | 2.19 | 0.41 |
| 1:O:1334:C:H2' | 1:O:1335:C:H6 | 1.85 | 0.41 |
| 1:O:1409:G:H5' | 38:O:4658:HOH:O | 2.19 | 0.41 |
| 1:O:2502:C:C4' | 11:H:151:MET:CG | 2.98 | 0.41 |
| 1:O:689:G:H2' | 1:O:690:G:H8 | 1.84 | 0.41 |
| 1:O:883:U:C2' | 1:O:883:U:O2 | 2.67 | 0.41 |
| 2:9:3011:A:O2' | 2:9:3012:C:H3' | 2.20 | 0.41 |
| 2:9:3036:C:C5 | 2:9:3037:C:C5 | 3.08 | 0.41 |
| 6:C:35:VAL:HG21 | 6:C:227:GLY:HA2 | 2.02 | 0.41 |
| 12:I:70:PHE:CD2 | 12:I:70:PHE:O | 2.73 | 0.41 |
| 14:K:90:ARG:HA | 14:K:119:THR:HB | 2.02 | 0.41 |
| 19:P:66:LYS:HB2 | 19:P:70:ALA:O | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:S:53:GLY:HA3 | 38:S:6384:HOH:O | 2.20 | 0.41 |
| 25:V:34:LEU:HD12 | 25:V:100:LEU:HD13 | 2.02 | 0.41 |
| 25:V:28:HIS:HD2 | 25:V:31:HIS:CE1 | 2.38 | 0.41 |
| 26:W:74:ALA:HB2 | 26:W:85:VAL:HG13 | 2.01 | 0.41 |
| 1:O:1735:C:H5' | 5:B:235:ARG:NH2 | 2.35 | 0.41 |
| 1:O:2737:C:H3' | 1:O:2738:G:H5'' | 2.02 | 0.41 |
| 1:O:2781:U:H2' | 1:O:2782:G:C5' | 2.50 | 0.41 |
| 1:O:294:C:H2' | 1:O:295:C:O4' | 2.20 | 0.41 |
| 1:O:876:A:N3 | 1:O:876:A:H2' | 2.35 | 0.41 |
| 2:9:3056:A:C3' | 2:9:3057:A:H5'' | 2.50 | 0.41 |
| 4:A:130:THR:HG22 | 4:A:131:HIS:O | 2.20 | 0.41 |
| 4:A:186:TRP:CG | 4:A:187:PRO:HA | 2.55 | 0.41 |
| 7:D:95:THR:OG1 | 7:D:174:VAL:HG22 | 2.20 | 0.41 |
| 1:O:251:C:H5' | 15:L:140:ALA:HA | 2.02 | 0.41 |
| 16:M:141:ARG:HB3 | 38:M:8569:HOH:O | 2.20 | 0.41 |
| 16:M:67:ALA:HA | 16:M:71:TRP:HB3 | 2.02 | 0.41 |
| 19:P:88:ALA:O | 19:P:90:HIS:N | 2.53 | 0.41 |
| 22:S:43:ASN:C | 22:S:45:GLY:H | 2.24 | 0.41 |
| 23:T:6:CYS:HA | 23:T:13:ILE:HD11 | 2.02 | 0.41 |
| 26:W:76:ARG:NH1 | 26:W:76:ARG:CG | 2.79 | 0.41 |
| 27:X:197:ASP:OD1 | 27:X:199:ASP:HB2 | 2.20 | 0.41 |
| 1:O:1150:A:N7 | 10:G:69:ARG:NH2 | 2.69 | 0.41 |
| 1:O:1365:C:H2' | 1:O:1366:C:H6 | 1.85 | 0.41 |
| 1:O:1586:G:H2' | 1:O:1587:U:H6 | 1.85 | 0.41 |
| 1:O:1711:A:O2' | 1:O:1712:A:H5' | 2.20 | 0.41 |
| 1:O:213:G:O2' | 1:O:214:U:OP2 | 2.37 | 0.41 |
| 1:O:2703:A:H2' | 1:O:2704:C:H6 | 1.85 | 0.41 |
| 1:O:2900:G:H2' | 1:O:2901:C:O4' | 2.20 | 0.41 |
| 1:O:311:C:H2' | 1:O:312:U:C6 | 2.56 | 0.41 |
| 1:O:474:C:O3' | 6:C:73:LEU:HD21 | 2.20 | 0.41 |
| 31:2:38:ARG:O | 31:2:42:ARG:HB2 | 2.20 | 0.41 |
| 1:O:1150:A:C2 | 10:G:20:VAL:HG21 | 2.55 | 0.41 |
| 11:H:82:LYS:HB2 | 11:H:82:LYS:NZ | 2.36 | 0.41 |
| 15:L:46:LEU:HB2 | 38:L:8611:HOH:O | 2.20 | 0.41 |
| 15:L:78:ASN:O | 15:L:79:LYS:HG2 | 2.20 | 0.41 |
| 2:9:3008:G:O6 | 16:M:11:ARG:NH1 | 2.54 | 0.41 |
| 16:M:24:LEU:O | 16:M:28:LYS:HG2 | 2.21 | 0.41 |
| 16:M:50:LEU:HA | 16:M:50:LEU:HD12 | 1.74 | 0.41 |
| 16:M:71:TRP:CE2 | 16:M:73:ALA:HB3 | 2.55 | 0.41 |
| 17:N:42:GLU:HB2 | 38:N:2176:HOH:O | 2.20 | 0.41 |
| 20:Q:34:GLU:HG2 | 20:Q:46:TYR:CZ | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:V:146:ILE:HG23 | 25:V:150:LEU:HD12 | 2.02 | 0.41 |
| 1:0:1666:C:C2' | 1:0:1667:A:C5' | 2.97 | 0.41 |
| 1:0:2135:A:O2' | 1:0:2136:G:H5' | 2.20 | 0.41 |
| 1:0:2501:G:H1' | 38:0:5452:HOH:O | 2.20 | 0.41 |
| 1:0:541:C:H2' | 1:0:542:A:H5' | 2.01 | 0.41 |
| 1:0:734:U:H2' | 1:0:736:A:OP2 | 2.21 | 0.41 |
| 1:0:736:A:H2' | 1:0:737:A:O4' | 2.20 | 0.41 |
| 1:0:946:C:H2' | 1:0:947:U:H6 | 1.85 | 0.41 |
| 6:C:187:ARG:HD2 | 6:C:188:ARG:N | 2.35 | 0.41 |
| 6:C:2:GLN:HB3 | 38:C:8342:HOH:O | 2.20 | 0.41 |
| 38:0:4776:HOH:O | 11:H:11:LYS:HE2 | 2.20 | 0.41 |
| 1:0:1003:U:O2' | 11:H:90:PHE:HE1 | 2.03 | 0.41 |
| 15:L:137:ASP:HA | 15:L:142:LYS:HE3 | 2.02 | 0.41 |
| 15:L:69:LYS:HD3 | 15:L:125:ARG:HA | 2.02 | 0.41 |
| 15:L:71:SER:CB | 15:L:92:THR:HG22 | 2.51 | 0.41 |
| 18:O:76:GLY:O | 18:O:79:SER:HB2 | 2.21 | 0.41 |
| 21:R:23:LYS:HE2 | 38:R:8333:HOH:O | 2.20 | 0.41 |
| 1:0:1192:A:H3' | 1:0:1193:A:H5' | 2.02 | 0.41 |
| 1:0:128:A:H3' | 1:0:128:A:C8 | 2.55 | 0.41 |
| 1:0:1323:G:C2 | 1:0:1324:G:C8 | 3.09 | 0.41 |
| 1:0:1375:A:C2' | 1:0:1376:G:H5' | 2.50 | 0.41 |
| 1:0:1473:U:O2' | 1:0:1474:C:H5'' | 2.20 | 0.41 |
| 1:0:1626:A:C2' | 1:0:1627:G:H5' | 2.51 | 0.41 |
| 1:0:168:C:C2' | 1:0:169:A:H5' | 2.50 | 0.41 |
| 1:0:1780:G:O2' | 1:0:1781:G:H5' | 2.20 | 0.41 |
| 1:0:2082:G:O2' | 1:0:2083:A:H5' | 2.20 | 0.41 |
| 1:0:2443:C:O3' | 14:K:56:LYS:HE3 | 2.20 | 0.41 |
| 1:0:2656:G:C2' | 1:0:2657:G:H5' | 2.50 | 0.41 |
| 1:0:2686:C:O2' | 1:0:2687:G:H5' | 2.21 | 0.41 |
| 31:2:70:ARG:HB3 | 38:2:8576:HOH:O | 2.20 | 0.41 |
| 38:0:3197:HOH:O | 4:A:11:ARG:HD3 | 2.20 | 0.41 |
| 9:F:58:GLU:CA | 9:F:61:MET:HG3 | 2.46 | 0.41 |
| 11:H:47:GLU:CG | 11:H:133:ILE:CD1 | 2.99 | 0.41 |
| 12:I:74:ARG:HD3 | 38:I:5061:HOH:O | 2.21 | 0.41 |
| 14:K:122:ALA:HB3 | 14:K:125:PHE:CZ | 2.56 | 0.41 |
| 16:M:180:LEU:O | 16:M:181:ASP:CB | 2.69 | 0.41 |
| 17:N:25:VAL:HG23 | 17:N:26:TRP:N | 2.36 | 0.41 |
| 20:Q:99:ALA:HB1 | 20:Q:109:MET:HE3 | 1.99 | 0.41 |
| 25:V:6:GLN:CB | 25:V:26:ILE:HD12 | 2.39 | 0.41 |
| 28:Y:57:CYS:C | 28:Y:59:HIS:H | 2.23 | 0.41 |
| 1:0:2478:U:O2' | 1:0:2479:A:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2551:C:O2' | 1:0:2552:C:H5' | 2.21 | 0.41 |
| 1:0:2599:A:C6 | 1:0:2600:A:N1 | 2.89 | 0.41 |
| 1:0:2831:C:H2' | 1:0:2832:C:H5' | 2.02 | 0.41 |
| 1:0:2833:C:H2' | 1:0:2834:G:H8 | 1.85 | 0.41 |
| 1:0:2898:G:H2' | 1:0:2899:A:H8 | 1.84 | 0.41 |
| 1:0:345:G:N2 | 1:0:346:U:H1' | 2.35 | 0.41 |
| 1:0:681:G:N3 | 1:0:681:G:H5' | 2.36 | 0.41 |
| 1:0:711:G:N2 | 1:0:718:C:C2 | 2.88 | 0.41 |
| 1:0:778:C:C4 | 1:0:779:U:C4 | 3.09 | 0.41 |
| 2:9:3034:A:H2' | 2:9:3035:C:O4' | 2.21 | 0.41 |
| 4:A:105:VAL:HG13 | 4:A:155:THR:O | 2.20 | 0.41 |
| 4:A:169:PHE:O | 4:A:170:VAL:HB | 2.21 | 0.41 |
| 4:A:194:MET:HE3 | 4:A:199:HIS:HB2 | 1.96 | 0.41 |
| 4:A:211:LYS:HB3 | 4:A:212:PRO:CD | 2.43 | 0.41 |
| 4:A:48:ASP:HA | 4:A:49:PRO:HD3 | 1.85 | 0.41 |
| 5:B:320:GLN:HG3 | 5:B:321:PRO:CD | 2.51 | 0.41 |
| 6:C:237:GLU:N | 38:C:8461:HOH:O | 2.53 | 0.41 |
| 1:0:166:A:N7 | 14:K:25:GLY:HA2 | 2.35 | 0.41 |
| 15:L:173:LEU:HD23 | 15:L:183:VAL:HG12 | 2.02 | 0.41 |
| 15:L:63:VAL:HG21 | 15:L:109:PHE:CE1 | 2.56 | 0.41 |
| 2:9:3007:G:OP1 | 16:M:23:ARG:NE | 2.53 | 0.41 |
| 20:Q:17:MET:HE1 | 20:Q:19:ARG:NH2 | 2.36 | 0.41 |
| 23:T:14:GLU:HA | 23:T:15:PRO:HD2 | 1.92 | 0.41 |
| 23:T:9:CYS:CA | 23:T:52:THR:HG23 | 2.46 | 0.41 |
| 24:U:42:ASN:O | 24:U:44:GLY:N | 2.53 | 0.41 |
| 1:0:138:U:OP2 | 1:0:139:C:H5 | 2.03 | 0.41 |
| 1:0:1525:G:H5' | 1:0:1526:A:OP2 | 2.20 | 0.41 |
| 1:0:1616:A:H2' | 1:0:1618:G:C8 | 2.55 | 0.41 |
| 1:0:2381:C:H4' | 31:2:80:ARG:CZ | 2.51 | 0.41 |
| 1:0:2688:U:H2' | 1:0:2689:A:H8 | 1.85 | 0.41 |
| 1:0:2737:C:H3' | 1:0:2738:G:C5' | 2.51 | 0.41 |
| 1:0:329:A:OP2 | 6:C:206:ASN:HB2 | 2.21 | 0.41 |
| 1:0:380:A:H5'' | 15:L:48:ARG:NH2 | 2.35 | 0.41 |
| 1:0:716:G:O2' | 1:0:717:C:H5' | 2.21 | 0.41 |
| 1:0:952:G:N3 | 1:0:2302:A:H2' | 2.35 | 0.41 |
| 31:2:55:VAL:O | 31:2:56:PRO:C | 2.58 | 0.41 |
| 4:A:123:GLY:HA3 | 4:A:162:GLY:HA2 | 2.03 | 0.41 |
| 4:A:36:ASP:HB2 | 4:A:85:ASP:H | 1.86 | 0.41 |
| 5:B:26:PHE:CE1 | 5:B:310:ARG:HB3 | 2.55 | 0.41 |
| 1:0:1003:U:O2 | 11:H:90:PHE:HZ | 2.03 | 0.41 |
| 12:I:24:SER:HA | 12:I:86:MET:SD | 2.61 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:I:74:ARG:C | 12:I:76:ASP:N | 2.74 | 0.41 |
| 15:L:59:GLY:HA3 | 15:L:141:ILE:CD1 | 2.50 | 0.41 |
| 16:M:35:VAL:HG12 | 16:M:37:ARG:HG2 | 2.02 | 0.41 |
| 24:U:5:VAL:HG23 | 38:U:2271:HOH:O | 2.20 | 0.41 |
| 25:V:139:GLY:O | 25:V:141:HIS:CD2 | 2.74 | 0.41 |
| 4:A:75:GLY:HA2 | 28:Y:63:LYS:O | 2.21 | 0.41 |
| 1:0:1165:G:OP1 | 1:0:1165:G:H3' | 2.21 | 0.41 |
| 1:0:1196:C:C2' | 1:0:1197:G:H5' | 2.51 | 0.41 |
| 1:0:1224:G:H2' | 1:0:1225:C:C6 | 2.55 | 0.41 |
| 1:0:1269:G:H2' | 1:0:1270:U:H6 | 1.86 | 0.41 |
| 1:0:1748:U:H4' | 38:0:8399:HOH:O | 2.21 | 0.41 |
| 1:0:2042:U:H2' | 1:0:2043:U:C6 | 2.56 | 0.41 |
| 1:0:2281:C:C2' | 1:0:2282:U:H5' | 2.49 | 0.41 |
| 1:0:2506:A:O2' | 1:0:2507:G:P | 2.79 | 0.41 |
| 1:0:331:A:C6 | 1:0:332:G:C4 | 3.08 | 0.41 |
| 1:0:358:G:O2' | 1:0:359:U:OP2 | 2.39 | 0.41 |
| 1:0:701:U:C2 | 1:0:744:G:C2 | 3.08 | 0.41 |
| 1:0:61:G:OP1 | 30:1:17:GLN:HG2 | 2.21 | 0.41 |
| 7:D:15:GLU:HA | 7:D:16:PRO:HD3 | 1.95 | 0.41 |
| 7:D:24:HIS:HB2 | 7:D:72:LYS:CB | 2.51 | 0.41 |
| 11:H:127:GLY:O | 11:H:128:ALA:CB | 2.66 | 0.41 |
| 14:K:73:VAL:HG21 | 14:K:116:HIS:CD2 | 2.56 | 0.41 |
| 14:K:98:GLU:O | 14:K:99:GLU:HB2 | 2.21 | 0.41 |
| 15:L:35:PRO:HD2 | 15:L:38:VAL:HG21 | 2.01 | 0.41 |
| 18:O:98:ILE:O | 18:O:98:ILE:HD13 | 2.20 | 0.41 |
| 24:U:59:ILE:O | 24:U:63:GLU:HG2 | 2.21 | 0.41 |
| 27:X:126:PRO:HG2 | 27:X:128:PHE:CZ | 2.56 | 0.41 |
| 27:X:130:ARG:HB2 | 27:X:142:SER:O | 2.20 | 0.41 |
| 1:0:1562:C:H2' | 1:0:1562:C:O2 | 2.21 | 0.41 |
| 1:0:1697:G:O2' | 1:0:1698:U:H5' | 2.20 | 0.41 |
| 1:0:2134:G:C6 | 1:0:2258:A:C8 | 3.09 | 0.41 |
| 1:0:2385:G:H2' | 1:0:2386:U:C6 | 2.55 | 0.41 |
| 1:0:2664:A:OP1 | 1:0:2664:A:H8 | 2.04 | 0.41 |
| 1:0:291:C:H2' | 1:0:292:G:O4' | 2.21 | 0.41 |
| 1:0:818:A:H2 | 28:Y:13:ARG:HA | 1.86 | 0.41 |
| 1:0:899:C:H5' | 38:0:4153:HOH:O | 2.21 | 0.41 |
| 1:0:926:A:H5' | 14:K:39:GLU:OE2 | 2.20 | 0.41 |
| 5:B:168:GLY:O | 5:B:169:GLY:O | 2.39 | 0.41 |
| 5:B:254:GLN:HG2 | 5:B:255:GLY:H | 1.85 | 0.41 |
| 5:B:310:ARG:HD2 | 38:B:8663:HOH:O | 2.21 | 0.41 |
| 6:C:7:ASP:O | 6:C:9:ASP:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:D:23:VAL:O | 7:D:23:VAL:CG2 | 2.69 | 0.41 |
| 7:D:57:THR:CG2 | 7:D:63:ILE:HG22 | 2.48 | 0.41 |
| 11:H:140:PRO:HA | 11:H:142:VAL:CG1 | 2.50 | 0.41 |
| 11:H:55:GLN:NE2 | 11:H:124:ARG:NE | 2.59 | 0.41 |
| 12:I:107:ASN:HD22 | 12:I:108:PRO:N | 2.19 | 0.41 |
| 23:T:31:PHE:CG | 23:T:37:GLU:HG2 | 2.56 | 0.41 |
| 25:V:133:LYS:HG3 | 38:V:5904:HOH:O | 2.20 | 0.41 |
| 25:V:139:GLY:O | 25:V:141:HIS:HD2 | 2.03 | 0.41 |
| 25:V:35:VAL:HA | 25:V:36:PRO:HD3 | 1.85 | 0.41 |
| 26:W:7:GLU:HA | 26:W:75:ALA:HA | 2.03 | 0.41 |
| 27:X:163:THR:HG23 | 38:X:8529:HOH:O | 2.20 | 0.41 |
| 29:Z:10:LYS:HG3 | 38:Z:2979:HOH:O | 2.20 | 0.41 |
| 1:O:1021:G:O2' | 1:O:1022:A:H5' | 2.21 | 0.41 |
| 1:O:10:U:O2' | 1:O:11:A:H8 | 2.03 | 0.41 |
| 1:O:1269:G:O2' | 1:O:1270:U:H5' | 2.21 | 0.41 |
| 1:O:1427:A:H61 | 1:O:1440:U:H1' | 1.85 | 0.41 |
| 1:O:1552:G:H2' | 1:O:1553:C:H6 | 1.84 | 0.41 |
| 1:O:1616:A:H5'' | 1:O:1617:C:OP1 | 2.21 | 0.41 |
| 1:O:1679:C:H5' | 38:O:3303:HOH:O | 2.20 | 0.41 |
| 1:O:1896:G:C6 | 1:O:1897:U:C4 | 3.08 | 0.41 |
| 1:O:2284:G:H5' | 38:O:3431:HOH:O | 2.20 | 0.41 |
| 1:O:2531:U:H2' | 1:O:2532:A:O4' | 2.20 | 0.41 |
| 1:O:255:A:H2' | 1:O:256:C:O4' | 2.21 | 0.41 |
| 1:O:2539:U:C5 | 32:O:9500:SLD:H7 | 2.56 | 0.41 |
| 1:O:968:G:O2' | 1:O:969:G:H5' | 2.20 | 0.41 |
| 2:9:3103:A:O2' | 2:9:3104:A:H5' | 2.21 | 0.41 |
| 4:A:93:THR:HG23 | 4:A:154:ALA:O | 2.21 | 0.41 |
| 4:A:217:ARG:HG3 | 4:A:217:ARG:HH11 | 1.84 | 0.41 |
| 6:C:37:ALA:O | 6:C:41:ASN:ND2 | 2.54 | 0.41 |
| 9:F:60:VAL:O | 9:F:61:MET:C | 2.59 | 0.41 |
| 12:I:131:THR:CG2 | 12:I:134:GLU:HG3 | 2.51 | 0.41 |
| 15:L:115:LEU:HD13 | 15:L:115:LEU:C | 2.41 | 0.41 |
| 16:M:25:ARG:O | 16:M:28:LYS:HB2 | 2.21 | 0.41 |
| 16:M:71:TRP:CZ2 | 16:M:73:ALA:HB3 | 2.56 | 0.41 |
| 18:O:115:SER:C | 18:O:117:SER:N | 2.74 | 0.41 |
| 18:O:132:ASP:O | 18:O:133:SER:HB3 | 2.20 | 0.41 |
| 25:V:105:THR:HA | 25:V:109:GLU:OE1 | 2.20 | 0.41 |
| 25:V:108:ARG:HE | 25:V:114:PRO:CG | 2.33 | 0.41 |
| 25:V:132:VAL:HG23 | 25:V:138:LEU:O | 2.21 | 0.41 |
| 26:W:75:ALA:O | 26:W:83:ALA:HA | 2.21 | 0.41 |
| 1:O:1242:A:H5' | 12:I:82:THR:CG2 | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1472:C:H6 | 1:0:1472:C:O5' | 2.04 | 0.40 |
| 1:0:1624:A:H4' | 1:0:1626:A:H5'' | 2.03 | 0.40 |
| 1:0:1853:C:H4' | 4:A:217:ARG:HH22 | 1.87 | 0.40 |
| 1:0:210:U:H2' | 1:0:211:U:C6 | 2.56 | 0.40 |
| 1:0:2120:U:H2' | 1:0:2121:G:O4' | 2.22 | 0.40 |
| 1:0:244:C:H6 | 1:0:244:C:O5' | 2.04 | 0.40 |
| 1:0:2472:C:O2' | 1:0:2634:G:H4' | 2.21 | 0.40 |
| 1:0:2548:C:OP2 | 5:B:5:ARG:NH2 | 2.54 | 0.40 |
| 1:0:860:U:H2' | 1:0:861:A:C8 | 2.56 | 0.40 |
| 5:B:30:PRO:HB2 | 5:B:39:GLN:NE2 | 2.35 | 0.40 |
| 6:C:127:ARG:HD2 | 6:C:229:PRO:O | 2.20 | 0.40 |
| 12:I:40:ASN:OD1 | 12:I:106:GLY:HA2 | 2.21 | 0.40 |
| 13:J:82:ARG:HH21 | 13:J:115:ARG:HG2 | 1.86 | 0.40 |
| 14:K:125:PHE:CE2 | 14:K:140:VAL:HG22 | 2.56 | 0.40 |
| 15:L:67:ILE:HG21 | 15:L:97:ILE:HG23 | 2.03 | 0.40 |
| 19:P:11:ARG:HD3 | 38:P:5620:HOH:O | 2.20 | 0.40 |
| 20:Q:57:VAL:HG21 | 20:Q:81:PRO:HD2 | 2.03 | 0.40 |
| 22:S:48:VAL:CG1 | 22:S:96:VAL:HG13 | 2.51 | 0.40 |
| 22:S:89:ARG:HG3 | 22:S:89:ARG:O | 2.21 | 0.40 |
| 24:U:42:ASN:N | 24:U:43:PRO:HD3 | 2.36 | 0.40 |
| 1:0:56:G:C5' | 24:U:50:ARG:HH12 | 2.25 | 0.40 |
| 1:0:1001:U:O2' | 1:0:1002:G:H5' | 2.21 | 0.40 |
| 1:0:1159:G:H1 | 1:0:1208:C:H42 | 1.69 | 0.40 |
| 1:0:1314:U:H2' | 38:O:6761:HOH:O | 2.20 | 0.40 |
| 1:0:1767:A:O2' | 1:0:1768:C:H5' | 2.21 | 0.40 |
| 1:0:2001:G:C2' | 1:0:2002:C:H5' | 2.52 | 0.40 |
| 1:0:2890:A:H1' | 23:T:56:ARG:HH21 | 1.80 | 0.40 |
| 1:0:485:A:O2' | 1:0:487:G:H5' | 2.22 | 0.40 |
| 1:0:558:C:C2' | 1:0:559:U:C5' | 2.99 | 0.40 |
| 1:0:816:G:C6 | 1:0:817:G:N1 | 2.89 | 0.40 |
| 1:0:834:G:H3' | 1:0:835:U:H4' | 2.04 | 0.40 |
| 2:9:3072:C:O2' | 2:9:3073:G:H5' | 2.21 | 0.40 |
| 4:A:55:VAL:HG11 | 4:A:67:LEU:HD13 | 2.02 | 0.40 |
| 5:B:84:LEU:HD13 | 5:B:84:LEU:C | 2.41 | 0.40 |
| 6:C:185:LYS:HD3 | 6:C:186:TYR:CE1 | 2.56 | 0.40 |
| 11:H:118:PRO:HD2 | 38:H:8341:HOH:O | 2.20 | 0.40 |
| 11:H:74:ASN:ND2 | 11:H:141:ASN:OD1 | 2.55 | 0.40 |
| 11:H:82:LYS:CB | 11:H:82:LYS:NZ | 2.85 | 0.40 |
| 12:I:14:ALA:HB1 | 12:I:44:ALA:HB2 | 2.02 | 0.40 |
| 13:J:72:VAL:O | 13:J:95:ALA:HA | 2.21 | 0.40 |
| 15:L:97:ILE:CD1 | 15:L:127:LYS:HD2 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:L:74:ARG:HD3 | 15:L:91:ILE:HD12 | 2.04 | 0.40 |
| 16:M:154:LEU:CG | 16:M:155:GLU:H | 2.34 | 0.40 |
| 17:N:105:ASN:HD21 | 17:N:109:SER:H | 1.68 | 0.40 |
| 22:S:113:GLU:O | 22:S:114:SER:C | 2.58 | 0.40 |
| 27:X:117:LEU:HA | 27:X:174:VAL:HG11 | 2.03 | 0.40 |
| 1:O:1434:A:H2' | 1:O:1436:C:C5 | 2.56 | 0.40 |
| 1:O:1897:U:O2' | 1:O:1898:G:H5' | 2.21 | 0.40 |
| 1:O:2050:G:OP1 | 20:Q:79:ARG:HB3 | 2.21 | 0.40 |
| 1:O:2852:A:H5'' | 38:O:6132:HOH:O | 2.21 | 0.40 |
| 1:O:514:G:H8 | 1:O:514:G:O5' | 2.04 | 0.40 |
| 1:O:873:G:H2' | 1:O:875:A:N7 | 2.37 | 0.40 |
| 30:1:41:HIS:CD2 | 30:1:44:ARG:H | 2.34 | 0.40 |
| 31:2:84:ARG:HH11 | 31:2:84:ARG:HG3 | 1.86 | 0.40 |
| 2:9:3013:A:H3' | 2:9:3014:G:H5' | 2.02 | 0.40 |
| 2:9:3067:C:H2' | 2:9:3068:G:H8 | 1.86 | 0.40 |
| 4:A:107:ASN:OD1 | 4:A:116:GLY:HA3 | 2.21 | 0.40 |
| 4:A:211:LYS:HD3 | 38:A:8623:HOH:O | 2.20 | 0.40 |
| 5:B:209:LYS:HE2 | 38:B:8579:HOH:O | 2.21 | 0.40 |
| 6:C:219:ASN:N | 6:C:222:ASP:OD1 | 2.52 | 0.40 |
| 7:D:58:VAL:CG1 | 7:D:59:GLY:N | 2.83 | 0.40 |
| 7:D:94:ALA:O | 7:D:95:THR:O | 2.39 | 0.40 |
| 8:E:21:THR:HG23 | 8:E:30:THR:OG1 | 2.21 | 0.40 |
| 28:Y:50:ALA:HB3 | 28:Y:54:ILE:CG2 | 2.49 | 0.40 |
| 1:O:1331:A:O2' | 1:O:1332:C:H5' | 2.21 | 0.40 |
| 1:O:1497:G:O2' | 1:O:1498:G:H5' | 2.22 | 0.40 |
| 1:O:1572:A:H2' | 1:O:1573:A:C8 | 2.55 | 0.40 |
| 1:O:1682:A:H5'' | 38:O:3430:HOH:O | 2.21 | 0.40 |
| 1:O:1743:G:H1' | 38:O:5797:HOH:O | 2.22 | 0.40 |
| 1:O:2124:G:H2' | 1:O:2125:G:C8 | 2.57 | 0.40 |
| 1:O:2134:G:N2 | 1:O:2242:U:C2 | 2.90 | 0.40 |
| 1:O:230:C:H2' | 1:O:231:G:C8 | 2.57 | 0.40 |
| 1:O:2546:U:H2' | 1:O:2547:C:C6 | 2.57 | 0.40 |
| 1:O:2653:A:H2' | 1:O:2654:C:C6 | 2.57 | 0.40 |
| 1:O:2658:G:H4' | 1:O:2842:G:C8 | 2.56 | 0.40 |
| 1:O:422:G:H2' | 1:O:423:A:H8 | 1.85 | 0.40 |
| 1:O:929:A:H8 | 1:O:929:A:O5' | 2.04 | 0.40 |
| 31:2:11:CYS:SG | 31:2:14:CYS:HB2 | 2.61 | 0.40 |
| 31:2:34:LYS:HB2 | 31:2:37:ASP:OD2 | 2.20 | 0.40 |
| 2:9:3045:A:H2' | 2:9:3046:C:C6 | 2.55 | 0.40 |
| 5:B:108:GLU:HB3 | 5:B:111:ARG:HD2 | 2.04 | 0.40 |
| 8:E:100:ASP:HB2 | 38:E:2789:HOH:O | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 14:K:146:GLY:C | 14:K:148:GLU:H | 2.25 | 0.40 |
| 15:L:183:VAL:HG12 | 15:L:184:ARG:N | 2.37 | 0.40 |
| 15:L:66:ALA:HB2 | 15:L:128:TRP:NE1 | 2.37 | 0.40 |
| 17:N:26:TRP:CE3 | 17:N:26:TRP:HA | 2.57 | 0.40 |
| 22:S:32:ARG:HH12 | 22:S:38:ARG:HH12 | 1.67 | 0.40 |
| 22:S:48:VAL:HG13 | 22:S:96:VAL:HG13 | 2.03 | 0.40 |
| 1:O:775:G:OP1 | 29:Z:16:HIS:HE1 | 2.03 | 0.40 |
| 1:O:1211:G:O2' | 1:O:1212:C:H5' | 2.21 | 0.40 |
| 1:O:1235:G:C1' | 12:I:63:ILE:HG23 | 2.51 | 0.40 |
| 1:O:1345:A:H2' | 1:O:1346:U:H6 | 1.85 | 0.40 |
| 1:O:1609:C:H2' | 1:O:1610:G:H8 | 1.87 | 0.40 |
| 1:O:1792:C:H2' | 1:O:1793:C:C6 | 2.56 | 0.40 |
| 1:O:2011:A:O4' | 1:O:2013:G:C8 | 2.75 | 0.40 |
| 1:O:2255:A:N1 | 1:O:2256:G:C4 | 2.90 | 0.40 |
| 1:O:2659:U:H4' | 20:Q:76:ASP:HB3 | 2.04 | 0.40 |
| 1:O:473:A:OP1 | 29:Z:51:GLN:NE2 | 2.55 | 0.40 |
| 1:O:675:U:H2' | 1:O:676:C:H5' | 2.03 | 0.40 |
| 1:O:870:G:C3' | 1:O:871:G:H5'' | 2.52 | 0.40 |
| 1:O:1675:C:H5'' | 30:1:5:LYS:HD2 | 2.04 | 0.40 |
| 31:2:55:VAL:HG22 | 38:2:8509:HOH:O | 2.22 | 0.40 |
| 4:A:105:VAL:HG11 | 4:A:154:ALA:CB | 2.52 | 0.40 |
| 4:A:165:THR:O | 4:A:165:THR:HG22 | 2.20 | 0.40 |
| 4:A:94:LEU:N | 4:A:94:LEU:CD2 | 2.83 | 0.40 |
| 5:B:185:GLY:HA2 | 38:B:8647:HOH:O | 2.21 | 0.40 |
| 5:B:5:ARG:HA | 5:B:6:PRO:HD3 | 2.00 | 0.40 |
| 7:D:18:ILE:HG12 | 7:D:134:LEU:HD21 | 2.04 | 0.40 |
| 9:F:22:VAL:CG2 | 9:F:104:ALA:HB2 | 2.52 | 0.40 |
| 11:H:57:ARG:HH11 | 11:H:57:ARG:HG3 | 1.86 | 0.40 |
| 11:H:58:HIS:CE1 | 11:H:59:ASN:HD21 | 2.40 | 0.40 |
| 12:I:75:PRO:HG2 | 12:I:105:LEU:CD2 | 2.49 | 0.40 |
| 15:L:169:ARG:HD2 | 38:L:8593:HOH:O | 2.21 | 0.40 |
| 16:M:119:GLN:HE21 | 16:M:129:ILE:CG2 | 2.34 | 0.40 |
| 16:M:37:ARG:HD3 | 36:M:8507:CL:CL | 2.58 | 0.40 |
| 18:O:11:ALA:HB2 | 18:O:18:LYS:HA | 2.03 | 0.40 |
| 23:T:49:LEU:HD13 | 23:T:51:TRP:CZ2 | 2.57 | 0.40 |
| 1:O:588:G:O6 | 25:V:154:ARG:NH1 | 2.55 | 0.40 |
| 28:Y:20:LEU:O | 28:Y:21:LYS:C | 2.59 | 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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4 | A | 235/239 (98%) | 207 (88%) | 24 (10%) | 4 (2%) | 10 | 42 |
| 5 | B | 335/337 (99%) | 300 (90%) | 28 (8%) | 7 (2%) | 8 | 36 |
| 6 | C | 244/246 (99%) | 213 (87%) | 28 (12%) | 3 (1%) | 14 | 51 |
| 7 | D | 134/176 (76%) | 96 (72%) | 26 (19%) | 12 (9%) | 1 | 4 |
| 8 | E | 170/177 (96%) | 157 (92%) | 12 (7%) | 1 (1%) | 27 | 67 |
| 9 | F | 117/119 (98%) | 102 (87%) | 12 (10%) | 3 (3%) | 6 | 30 |
| 10 | G | 25/348 (7%) | 22 (88%) | 2 (8%) | 1 (4%) | 3 | 18 |
| 11 | H | 152/167 (91%) | 132 (87%) | 16 (10%) | 4 (3%) | 6 | 30 |
| 12 | I | 140/145 (97%) | 127 (91%) | 10 (7%) | 3 (2%) | 8 | 36 |
| 13 | J | 130/132 (98%) | 117 (90%) | 11 (8%) | 2 (2%) | 11 | 45 |
| 14 | K | 141/164 (86%) | 116 (82%) | 23 (16%) | 2 (1%) | 12 | 47 |
| 15 | L | 192/194 (99%) | 167 (87%) | 20 (10%) | 5 (3%) | 6 | 30 |
| 16 | M | 184/186 (99%) | 153 (83%) | 24 (13%) | 7 (4%) | 3 | 20 |
| 17 | N | 113/115 (98%) | 106 (94%) | 6 (5%) | 1 (1%) | 19 | 59 |
| 18 | O | 141/148 (95%) | 129 (92%) | 11 (8%) | 1 (1%) | 24 | 64 |
| 19 | P | 93/95 (98%) | 88 (95%) | 3 (3%) | 2 (2%) | 7 | 34 |
| 20 | Q | 148/154 (96%) | 134 (90%) | 14 (10%) | 0 | 100 | 100 |
| 21 | R | 79/84 (94%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 22 | S | 117/119 (98%) | 103 (88%) | 12 (10%) | 2 (2%) | 10 | 42 |
| 23 | T | 51/66 (77%) | 47 (92%) | 3 (6%) | 1 (2%) | 8 | 37 |
| 24 | U | 63/70 (90%) | 57 (90%) | 4 (6%) | 2 (3%) | 4 | 24 |
| 25 | V | 152/154 (99%) | 140 (92%) | 11 (7%) | 1 (1%) | 24 | 64 |
| 26 | W | 80/91 (88%) | 71 (89%) | 7 (9%) | 2 (2%) | 6 | 31 |
| 27 | X | 140/240 (58%) | 134 (96%) | 6 (4%) | 0 | 100 | 100 |
| 28 | Y | 71/73 (97%) | 58 (82%) | 10 (14%) | 3 (4%) | 3 | 17 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 29 | Z | 54/56 (96%) | 50 (93%) | 4 (7%) | 0 | 100 | 100 |
| 30 | 1 | 42/48 (88%) | 40 (95%) | 2 (5%) | 0 | 100 | 100 |
| 31 | 2 | 90/92 (98%) | 82 (91%) | 6 (7%) | 2 (2%) | 7 | 34 |
| All | All | 3633/4235 (86%) | 3224 (89%) | 338 (9%) | 71 (2%) | 8 | 37 |

All (71) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | B | 139 | ASP |
| 7 | D | 93 | LEU |
| 7 | D | 95 | THR |
| 7 | D | 137 | PRO |
| 7 | D | 173 | GLU |
| 9 | F | 101 | ALA |
| 11 | H | 138 | PRO |
| 11 | H | 162 | SER |
| 12 | I | 5 | GLU |
| 16 | M | 139 | TRP |
| 16 | M | 154 | LEU |
| 16 | M | 162 | ASP |
| 16 | M | 164 | ASP |
| 16 | M | 183 | ASP |
| 28 | Y | 20 | LEU |
| 28 | Y | 81 | LYS |
| 31 | 2 | 56 | PRO |
| 5 | B | 34 | GLY |
| 5 | B | 107 | SER |
| 5 | B | 169 | GLY |
| 6 | C | 8 | LEU |
| 7 | D | 11 | HIS |
| 7 | D | 16 | PRO |
| 7 | D | 20 | LYS |
| 7 | D | 61 | PHE |
| 7 | D | 147 | ALA |
| 10 | G | 72 | ASP |
| 11 | H | 164 | ALA |
| 12 | I | 89 | HIS |
| 12 | I | 143 | LYS |
| 14 | K | 80 | ASP |
| 15 | L | 148 | SER |
| 16 | M | 181 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | O | 116 | SER |
| 22 | S | 53 | GLY |
| 24 | U | 43 | PRO |
| 28 | Y | 28 | ASP |
| 31 | 2 | 57 | GLY |
| 4 | A | 34 | ASP |
| 4 | A | 132 | ASP |
| 5 | B | 184 | ASP |
| 7 | D | 171 | ASP |
| 11 | H | 40 | PRO |
| 13 | J | 119 | GLN |
| 14 | K | 105 | TYR |
| 15 | L | 18 | GLY |
| 15 | L | 140 | ALA |
| 26 | W | 77 | PHE |
| 4 | A | 62 | ASP |
| 5 | B | 185 | GLY |
| 17 | N | 20 | SER |
| 23 | T | 7 | ASP |
| 26 | W | 70 | ILE |
| 5 | B | 2 | GLN |
| 6 | C | 145 | GLU |
| 7 | D | 36 | ASN |
| 7 | D | 60 | GLU |
| 9 | F | 61 | MET |
| 9 | F | 64 | PRO |
| 13 | J | 126 | SER |
| 15 | L | 15 | PRO |
| 16 | M | 68 | GLU |
| 25 | V | 77 | ALA |
| 4 | A | 37 | VAL |
| 15 | L | 71 | SER |
| 22 | S | 44 | ALA |
| 8 | E | 44 | GLY |
| 24 | U | 40 | PRO |
| 19 | P | 18 | PRO |
| 6 | C | 19 | PRO |
| 19 | P | 54 | 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 | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 4 | A | 179/181 (99%) | 168 (94%) | 11 (6%) | 20 | 57 |
| 5 | B | 282/282 (100%) | 264 (94%) | 18 (6%) | 19 | 55 |
| 6 | C | 193/193 (100%) | 178 (92%) | 15 (8%) | 14 | 45 |
| 7 | D | 117/147 (80%) | 108 (92%) | 9 (8%) | 14 | 46 |
| 8 | E | 152/155 (98%) | 146 (96%) | 6 (4%) | 35 | 73 |
| 9 | F | 92/92 (100%) | 91 (99%) | 1 (1%) | 76 | 92 |
| 10 | G | 27/283 (10%) | 27 (100%) | 0 | 100 | 100 |
| 11 | H | 122/122 (100%) | 111 (91%) | 11 (9%) | 10 | 38 |
| 12 | I | 118/121 (98%) | 110 (93%) | 8 (7%) | 17 | 52 |
| 13 | J | 106/106 (100%) | 102 (96%) | 4 (4%) | 36 | 73 |
| 14 | K | 113/126 (90%) | 108 (96%) | 5 (4%) | 31 | 69 |
| 15 | L | 166/166 (100%) | 157 (95%) | 9 (5%) | 24 | 62 |
| 16 | M | 149/149 (100%) | 141 (95%) | 8 (5%) | 24 | 62 |
| 17 | N | 93/93 (100%) | 90 (97%) | 3 (3%) | 42 | 78 |
| 18 | O | 113/116 (97%) | 109 (96%) | 4 (4%) | 39 | 75 |
| 19 | P | 79/79 (100%) | 75 (95%) | 4 (5%) | 26 | 64 |
| 20 | Q | 117/121 (97%) | 114 (97%) | 3 (3%) | 49 | 81 |
| 21 | R | 71/73 (97%) | 69 (97%) | 2 (3%) | 47 | 80 |
| 22 | S | 105/105 (100%) | 100 (95%) | 5 (5%) | 28 | 66 |
| 23 | T | 44/52 (85%) | 44 (100%) | 0 | 100 | 100 |
| 24 | U | 51/56 (91%) | 49 (96%) | 2 (4%) | 35 | 73 |
| 25 | V | 130/130 (100%) | 122 (94%) | 8 (6%) | 20 | 56 |
| 26 | W | 66/73 (90%) | 62 (94%) | 4 (6%) | 20 | 57 |
| 27 | X | 120/195 (62%) | 113 (94%) | 7 (6%) | 22 | 59 |
| 28 | Y | 56/56 (100%) | 52 (93%) | 4 (7%) | 16 | 50 |
| 29 | Z | 46/46 (100%) | 45 (98%) | 1 (2%) | 55 | 84 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 30 | 1 | 42/44 (96%) | 41 (98%) | 1 (2%) | 52 83 |
| 31 | 2 | 79/79 (100%) | 75 (95%) | 4 (5%) | 26 64 |
| All | All | 3028/3441 (88%) | 2871 (95%) | 157 (5%) | 25 63 |

All (157) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 3 | ARG |
| 4 | A | 33 | GLU |
| 4 | A | 36 | ASP |
| 4 | A | 55 | VAL |
| 4 | A | 68 | ILE |
| 4 | A | 69 | LEU |
| 4 | A | 94 | LEU |
| 4 | A | 131 | HIS |
| 4 | A | 153 | ARG |
| 4 | A | 179 | MET |
| 4 | A | 217 | ARG |
| 5 | B | 7 | ARG |
| 5 | B | 11 | LEU |
| 5 | B | 27 | ASN |
| 5 | B | 33 | ASP |
| 5 | B | 63 | GLU |
| 5 | B | 97 | LEU |
| 5 | B | 98 | THR |
| 5 | B | 103 | ASP |
| 5 | B | 162 | MET |
| 5 | B | 234 | ARG |
| 5 | B | 245 | SER |
| 5 | B | 251 | VAL |
| 5 | B | 254 | GLN |
| 5 | B | 256 | GLN |
| 5 | B | 264 | GLU |
| 5 | B | 304 | PRO |
| 5 | B | 307 | ARG |
| 5 | B | 312 | ARG |
| 6 | C | 2 | GLN |
| 6 | C | 27 | ARG |
| 6 | C | 67 | GLN |
| 6 | C | 76 | ARG |
| 6 | C | 78 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | C | 115 | LEU |
| 6 | C | 136 | VAL |
| 6 | C | 180 | SER |
| 6 | C | 187 | ARG |
| 6 | C | 214 | THR |
| 6 | C | 222 | ASP |
| 6 | C | 223 | LEU |
| 6 | C | 234 | VAL |
| 6 | C | 236 | THR |
| 6 | C | 240 | LEU |
| 7 | D | 24 | HIS |
| 7 | D | 61 | PHE |
| 7 | D | 99 | ASP |
| 7 | D | 100 | ASP |
| 7 | D | 131 | THR |
| 7 | D | 133 | ASN |
| 7 | D | 136 | ARG |
| 7 | D | 137 | PRO |
| 7 | D | 149 | ARG |
| 8 | E | 7 | ILE |
| 8 | E | 12 | ASP |
| 8 | E | 15 | GLN |
| 8 | E | 54 | ASP |
| 8 | E | 102 | VAL |
| 8 | E | 164 | ASP |
| 9 | F | 64 | PRO |
| 11 | H | 18 | GLU |
| 11 | H | 59 | ASN |
| 11 | H | 61 | LEU |
| 11 | H | 72 | VAL |
| 11 | H | 73 | GLN |
| 11 | H | 82 | LYS |
| 11 | H | 86 | ARG |
| 11 | H | 94 | ARG |
| 11 | H | 109 | ASP |
| 11 | H | 142 | VAL |
| 11 | H | 150 | LYS |
| 12 | I | 46 | ILE |
| 12 | I | 47 | THR |
| 12 | I | 52 | GLN |
| 12 | I | 74 | ARG |
| 12 | I | 79 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | I | 107 | ASN |
| 12 | I | 127 | ILE |
| 12 | I | 131 | THR |
| 13 | J | 10 | GLN |
| 13 | J | 49 | LEU |
| 13 | J | 56 | SER |
| 13 | J | 98 | VAL |
| 14 | K | 30 | ARG |
| 14 | K | 35 | ARG |
| 14 | K | 80 | ASP |
| 14 | K | 83 | GLU |
| 14 | K | 117 | GLU |
| 15 | L | 38 | VAL |
| 15 | L | 46 | LEU |
| 15 | L | 68 | ARG |
| 15 | L | 87 | MET |
| 15 | L | 93 | ARG |
| 15 | L | 99 | ARG |
| 15 | L | 159 | THR |
| 15 | L | 164 | THR |
| 15 | L | 170 | CYS |
| 16 | M | 26 | LEU |
| 16 | M | 47 | LEU |
| 16 | M | 49 | THR |
| 16 | M | 80 | SER |
| 16 | M | 127 | LEU |
| 16 | M | 128 | ASP |
| 16 | M | 152 | GLU |
| 16 | M | 163 | PHE |
| 17 | N | 3 | THR |
| 17 | N | 98 | LEU |
| 17 | N | 111 | VAL |
| 18 | O | 52 | LYS |
| 18 | O | 81 | LYS |
| 18 | O | 91 | LYS |
| 18 | O | 98 | ILE |
| 19 | P | 11 | ARG |
| 19 | P | 16 | ASN |
| 19 | P | 57 | ASP |
| 19 | P | 95 | GLU |
| 20 | Q | 13 | THR |
| 20 | Q | 39 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | Q | 82 | GLU |
| 21 | R | 10 | VAL |
| 21 | R | 80 | ARG |
| 22 | S | 23 | VAL |
| 22 | S | 26 | THR |
| 22 | S | 39 | ASN |
| 22 | S | 48 | VAL |
| 22 | S | 73 | HIS |
| 24 | U | 22 | ASP |
| 24 | U | 65 | ASP |
| 25 | V | 35 | VAL |
| 25 | V | 52 | VAL |
| 25 | V | 73 | LEU |
| 25 | V | 122 | ARG |
| 25 | V | 128 | VAL |
| 25 | V | 142 | ASP |
| 25 | V | 146 | ILE |
| 25 | V | 154 | ARG |
| 26 | W | 15 | ARG |
| 26 | W | 27 | ASP |
| 26 | W | 49 | ARG |
| 26 | W | 72 | VAL |
| 27 | X | 115 | ARG |
| 27 | X | 154 | ARG |
| 27 | X | 163 | THR |
| 27 | X | 189 | ASN |
| 27 | X | 203 | VAL |
| 27 | X | 204 | ARG |
| 27 | X | 235 | GLU |
| 28 | Y | 11 | THR |
| 28 | Y | 42 | CYS |
| 28 | Y | 64 | ILE |
| 28 | Y | 68 | CYS |
| 29 | Z | 36 | SER |
| 30 | 1 | 18 | ASN |
| 31 | 2 | 42 | ARG |
| 31 | 2 | 56 | PRO |
| 31 | 2 | 65 | THR |
| 31 | 2 | 74 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 47 | HIS |
| 4 | A | 92 | ASN |
| 4 | A | 125 | ASN |
| 4 | A | 127 | GLN |
| 4 | A | 176 | HIS |
| 4 | A | 199 | HIS |
| 5 | B | 27 | ASN |
| 5 | B | 145 | HIS |
| 5 | B | 238 | ASN |
| 5 | B | 256 | GLN |
| 5 | B | 260 | HIS |
| 5 | B | 320 | GLN |
| 5 | B | 332 | ASN |
| 6 | C | 2 | GLN |
| 6 | C | 39 | GLN |
| 6 | C | 129 | HIS |
| 7 | D | 47 | GLN |
| 7 | D | 85 | GLN |
| 7 | D | 103 | ASN |
| 7 | D | 133 | ASN |
| 8 | E | 106 | ASN |
| 8 | E | 143 | GLN |
| 10 | G | 17 | GLN |
| 10 | G | 64 | ASN |
| 11 | H | 35 | ASN |
| 11 | H | 45 | GLN |
| 11 | H | 55 | GLN |
| 11 | H | 58 | HIS |
| 11 | H | 59 | ASN |
| 11 | H | 69 | ASN |
| 11 | H | 74 | ASN |
| 11 | H | 80 | ASN |
| 11 | H | 91 | HIS |
| 11 | H | 129 | ASN |
| 11 | H | 130 | HIS |
| 11 | H | 137 | ASN |
| 11 | H | 166 | ASN |
| 12 | I | 52 | GLN |
| 12 | I | 107 | ASN |
| 13 | J | 10 | GLN |
| 14 | K | 18 | HIS |
| 14 | K | 41 | HIS |
| 15 | L | 26 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | L | 58 | GLN |
| 15 | L | 176 | GLN |
| 16 | M | 40 | ASN |
| 16 | M | 107 | ASN |
| 16 | M | 119 | GLN |
| 16 | M | 132 | ASN |
| 16 | M | 153 | GLN |
| 17 | N | 53 | GLN |
| 18 | O | 50 | GLN |
| 18 | O | 66 | GLN |
| 18 | O | 73 | HIS |
| 18 | O | 118 | GLN |
| 19 | P | 16 | ASN |
| 19 | P | 40 | HIS |
| 20 | Q | 61 | GLN |
| 20 | Q | 94 | ASN |
| 20 | Q | 98 | ASN |
| 20 | Q | 113 | HIS |
| 20 | Q | 117 | HIS |
| 21 | R | 53 | ASN |
| 22 | S | 39 | ASN |
| 22 | S | 73 | HIS |
| 23 | T | 39 | ASN |
| 24 | U | 60 | GLN |
| 25 | V | 27 | HIS |
| 25 | V | 28 | HIS |
| 25 | V | 59 | GLN |
| 25 | V | 87 | HIS |
| 25 | V | 110 | GLN |
| 25 | V | 119 | HIS |
| 25 | V | 125 | HIS |
| 25 | V | 141 | HIS |
| 26 | W | 23 | HIS |
| 26 | W | 36 | HIS |
| 27 | X | 134 | HIS |
| 27 | X | 149 | GLN |
| 27 | X | 189 | ASN |
| 28 | Y | 70 | GLN |
| 29 | Z | 8 | GLN |
| 29 | Z | 16 | HIS |
| 29 | Z | 28 | HIS |
| 30 | 1 | 16 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 1 | 18 | ASN |
| 30 | 1 | 41 | HIS |
| 30 | 1 | 45 | ASN |
| 31 | 2 | 13 | HIS |
| 31 | 2 | 30 | GLN |
| 31 | 2 | 48 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 0 | 2745/2922 (93%) | 241 (8%) | 25 (0%) |
| 2 | 9 | 121/122 (99%) | 18 (14%) | 3 (2%) |
| 3 | 4 | 2/3 (66%) | 1 (50%) | 0 |
| All | All | 2868/3047 (94%) | 260 (9%) | 28 (0%) |

All (260) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 31 | C |
| 1 | 0 | 60 | A |
| 1 | 0 | 67 | A |
| 1 | 0 | 69 | A |
| 1 | 0 | 70 | A |
| 1 | 0 | 71 | G |
| 1 | 0 | 87 | C |
| 1 | 0 | 88 | G |
| 1 | 0 | 114 | A |
| 1 | 0 | 115 | U |
| 1 | 0 | 120 | A |
| 1 | 0 | 130 | C |
| 1 | 0 | 141 | C |
| 1 | 0 | 151 | A |
| 1 | 0 | 166 | A |
| 1 | 0 | 169 | A |
| 1 | 0 | 186 | A |
| 1 | 0 | 191 | A |
| 1 | 0 | 192 | A |
| 1 | 0 | 200 | U |
| 1 | 0 | 219 | G |
| 1 | 0 | 237 | G |
| 1 | 0 | 271 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 272 | A |
| 1 | 0 | 273 | G |
| 1 | 0 | 283 | U |
| 1 | 0 | 284 | C |
| 1 | 0 | 285 | A |
| 1 | 0 | 308 | U |
| 1 | 0 | 309 | C |
| 1 | 0 | 317 | A |
| 1 | 0 | 336 | G |
| 1 | 0 | 337 | A |
| 1 | 0 | 345 | G |
| 1 | 0 | 358 | G |
| 1 | 0 | 381 | G |
| 1 | 0 | 397 | A |
| 1 | 0 | 417 | G |
| 1 | 0 | 461 | C |
| 1 | 0 | 487 | G |
| 1 | 0 | 498 | A |
| 1 | 0 | 510 | U |
| 1 | 0 | 511 | A |
| 1 | 0 | 514 | G |
| 1 | 0 | 537 | G |
| 1 | 0 | 538 | C |
| 1 | 0 | 539 | G |
| 1 | 0 | 542 | A |
| 1 | 0 | 545 | G |
| 1 | 0 | 553 | G |
| 1 | 0 | 559 | U |
| 1 | 0 | 581 | G |
| 1 | 0 | 588 | G |
| 1 | 0 | 604 | G |
| 1 | 0 | 605 | C |
| 1 | 0 | 620 | A |
| 1 | 0 | 632 | A |
| 1 | 0 | 644 | G |
| 1 | 0 | 660 | A |
| 1 | 0 | 688 | A |
| 1 | 0 | 701 | U |
| 1 | 0 | 717 | C |
| 1 | 0 | 759 | C |
| 1 | 0 | 777 | U |
| 1 | 0 | 809 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 821 | U |
| 1 | 0 | 835 | U |
| 1 | 0 | 840 | U |
| 1 | 0 | 868 | G |
| 1 | 0 | 869 | G |
| 1 | 0 | 871 | G |
| 1 | 0 | 872 | U |
| 1 | 0 | 875 | A |
| 1 | 0 | 877 | G |
| 1 | 0 | 878 | G |
| 1 | 0 | 882 | A |
| 1 | 0 | 884 | C |
| 1 | 0 | 898 | G |
| 1 | 0 | 905 | C |
| 1 | 0 | 920 | C |
| 1 | 0 | 921 | G |
| 1 | 0 | 923 | A |
| 1 | 0 | 938 | G |
| 1 | 0 | 953 | G |
| 1 | 0 | 960 | G |
| 1 | 0 | 961 | A |
| 1 | 0 | 1006 | A |
| 1 | 0 | 1008 | C |
| 1 | 0 | 1029 | U |
| 1 | 0 | 1045 | G |
| 1 | 0 | 1059 | G |
| 1 | 0 | 1060 | C |
| 1 | 0 | 1072 | G |
| 1 | 0 | 1081 | A |
| 1 | 0 | 1088 | A |
| 1 | 0 | 1109 | U |
| 1 | 0 | 1110 | G |
| 1 | 0 | 1119 | G |
| 1 | 0 | 1130 | U |
| 1 | 0 | 1137 | G |
| 1 | 0 | 1151 | G |
| 1 | 0 | 1162 | G |
| 1 | 0 | 1164 | U |
| 1 | 0 | 1165 | G |
| 1 | 0 | 1166 | A |
| 1 | 0 | 1174 | A |
| 1 | 0 | 1175 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 1185 | U |
| 1 | 0 | 1192 | A |
| 1 | 0 | 1193 | A |
| 1 | 0 | 1206 | U |
| 1 | 0 | 1216 | G |
| 1 | 0 | 1237 | U |
| 1 | 0 | 1238 | C |
| 1 | 0 | 1239 | G |
| 1 | 0 | 1279 | U |
| 1 | 0 | 1289 | C |
| 1 | 0 | 1331 | A |
| 1 | 0 | 1342 | C |
| 1 | 0 | 1353 | C |
| 1 | 0 | 1360 | C |
| 1 | 0 | 1377 | C |
| 1 | 0 | 1407 | A |
| 1 | 0 | 1451 | C |
| 1 | 0 | 1460 | G |
| 1 | 0 | 1474 | C |
| 1 | 0 | 1485 | A |
| 1 | 0 | 1488 | U |
| 1 | 0 | 1505 | U |
| 1 | 0 | 1506 | U |
| 1 | 0 | 1524 | U |
| 1 | 0 | 1525 | G |
| 1 | 0 | 1526 | A |
| 1 | 0 | 1528 | A |
| 1 | 0 | 1564 | C |
| 1 | 0 | 1580 | A |
| 1 | 0 | 1592 | G |
| 1 | 0 | 1625 | U |
| 1 | 0 | 1626 | A |
| 1 | 0 | 1633 | C |
| 1 | 0 | 1634 | G |
| 1 | 0 | 1656 | A |
| 1 | 0 | 1667 | A |
| 1 | 0 | 1682 | A |
| 1 | 0 | 1684 | A |
| 1 | 0 | 1685 | A |
| 1 | 0 | 1692 | C |
| 1 | 0 | 1701 | A |
| 1 | 0 | 1722 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 1723 | G |
| 1 | 0 | 1725 | C |
| 1 | 0 | 1731 | C |
| 1 | 0 | 1732 | A |
| 1 | 0 | 1752 | G |
| 1 | 0 | 1778 | A |
| 1 | 0 | 1798 | C |
| 1 | 0 | 1819 | G |
| 1 | 0 | 1820 | G |
| 1 | 0 | 1829 | A |
| 1 | 0 | 1856 | C |
| 1 | 0 | 1879 | U |
| 1 | 0 | 1904 | A |
| 1 | 0 | 1919 | A |
| 1 | 0 | 1942 | A |
| 1 | 0 | 1971 | G |
| 1 | 0 | 1973 | A |
| 1 | 0 | 1974 | G |
| 1 | 0 | 1978 | A |
| 1 | 0 | 1979 | G |
| 1 | 0 | 1980 | U |
| 1 | 0 | 1996 | U |
| 1 | 0 | 2005 | G |
| 1 | 0 | 2008 | U |
| 1 | 0 | 2011 | A |
| 1 | 0 | 2012 | U |
| 1 | 0 | 2013 | G |
| 1 | 0 | 2033 | G |
| 1 | 0 | 2034 | U |
| 1 | 0 | 2063 | U |
| 1 | 0 | 2064 | U |
| 1 | 0 | 2072 | G |
| 1 | 0 | 2073 | G |
| 1 | 0 | 2074 | A |
| 1 | 0 | 2096 | A |
| 1 | 0 | 2101 | A |
| 1 | 0 | 2102 | G |
| 1 | 0 | 2110 | G |
| 1 | 0 | 2238 | A |
| 1 | 0 | 2243 | C |
| 1 | 0 | 2258 | A |
| 1 | 0 | 2271 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 2272 | G |
| 1 | 0 | 2317 | C |
| 1 | 0 | 2320 | U |
| 1 | 0 | 2321 | A |
| 1 | 0 | 2354 | A |
| 1 | 0 | 2361 | A |
| 1 | 0 | 2369 | A |
| 1 | 0 | 2422 | U |
| 1 | 0 | 2462 | G |
| 1 | 0 | 2467 | A |
| 1 | 0 | 2476 | C |
| 1 | 0 | 2483 | A |
| 1 | 0 | 2507 | G |
| 1 | 0 | 2511 | A |
| 1 | 0 | 2533 | C |
| 1 | 0 | 2537 | G |
| 1 | 0 | 2540 | G |
| 1 | 0 | 2541 | U |
| 1 | 0 | 2553 | A |
| 1 | 0 | 2564 | G |
| 1 | 0 | 2589 | U |
| 1 | 0 | 2601 | A |
| 1 | 0 | 2602 | G |
| 1 | 0 | 2608 | C |
| 1 | 0 | 2613 | G |
| 1 | 0 | 2634 | G |
| 1 | 0 | 2637 | A |
| 1 | 0 | 2649 | A |
| 1 | 0 | 2650 | U |
| 1 | 0 | 2664 | A |
| 1 | 0 | 2681 | A |
| 1 | 0 | 2682 | C |
| 1 | 0 | 2726 | U |
| 1 | 0 | 2747 | C |
| 1 | 0 | 2748 | G |
| 1 | 0 | 2749 | U |
| 1 | 0 | 2750 | G |
| 1 | 0 | 2768 | A |
| 1 | 0 | 2786 | G |
| 1 | 0 | 2792 | A |
| 1 | 0 | 2800 | A |
| 1 | 0 | 2811 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 2812 | A |
| 1 | 0 | 2825 | C |
| 1 | 0 | 2850 | C |
| 1 | 0 | 2876 | G |
| 1 | 0 | 2890 | A |
| 1 | 0 | 2896 | A |
| 1 | 0 | 2903 | C |
| 1 | 0 | 2914 | A |
| 2 | 9 | 3002 | U |
| 2 | 9 | 3007 | G |
| 2 | 9 | 3014 | G |
| 2 | 9 | 3022 | G |
| 2 | 9 | 3023 | U |
| 2 | 9 | 3024 | U |
| 2 | 9 | 3025 | G |
| 2 | 9 | 3026 | C |
| 2 | 9 | 3040 | C |
| 2 | 9 | 3041 | C |
| 2 | 9 | 3043 | G |
| 2 | 9 | 3044 | A |
| 2 | 9 | 3052 | A |
| 2 | 9 | 3057 | A |
| 2 | 9 | 3066 | G |
| 2 | 9 | 3077 | A |
| 2 | 9 | 3114 | G |
| 2 | 9 | 3122 | C |
| 3 | 4 | 76 | A |

All (28) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 129 | A |
| 1 | 0 | 284 | C |
| 1 | 0 | 338 | C |
| 1 | 0 | 603 | A |
| 1 | 0 | 604 | G |
| 1 | 0 | 834 | G |
| 1 | 0 | 871 | G |
| 1 | 0 | 877 | G |
| 1 | 0 | 1080 | C |
| 1 | 0 | 1164 | U |
| 1 | 0 | 1237 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 1352 | A |
| 1 | 0 | 1450 | C |
| 1 | 0 | 1563 | G |
| 1 | 0 | 1667 | A |
| 1 | 0 | 1856 | C |
| 1 | 0 | 1979 | G |
| 1 | 0 | 2011 | A |
| 1 | 0 | 2313 | C |
| 1 | 0 | 2320 | U |
| 1 | 0 | 2467 | A |
| 1 | 0 | 2536 | C |
| 1 | 0 | 2649 | A |
| 1 | 0 | 2718 | C |
| 1 | 0 | 2791 | U |
| 2 | 9 | 3024 | U |
| 2 | 9 | 3065 | A |
| 2 | 9 | 3103 | A |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 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 |
| 32 | SLD | 0 | 9500 | - | 37,39,39 | 4.57 | 16 (43%) | 47,53,53 | 2.64 | 17 (36%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 32 | SLD | 0 | 9500 | - | - | 0/23/51/51 | 0/3/3/3 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 32 | 0 | 9500 | SLD | C9S-C8S | -9.92 | 1.35 | 1.50 |
| 32 | 0 | 9500 | SLD | C9S-C0S | -5.74 | 1.43 | 1.51 |
| 32 | 0 | 9500 | SLD | O1-C7 | -3.60 | 1.41 | 1.46 |
| 32 | 0 | 9500 | SLD | C3-C12 | 2.80 | 1.46 | 1.41 |
| 32 | 0 | 9500 | SLD | F1-C11 | 3.50 | 1.44 | 1.35 |
| 32 | 0 | 9500 | SLD | O1-C6 | 3.61 | 1.40 | 1.35 |
| 32 | 0 | 9500 | SLD | C7S-C5S | 3.68 | 1.57 | 1.49 |
| 32 | 0 | 9500 | SLD | C1S-N2S | 3.77 | 1.45 | 1.38 |
| 32 | 0 | 9500 | SLD | C12-C2B | 4.51 | 1.54 | 1.47 |
| 32 | 0 | 9500 | SLD | C3-C1 | 5.16 | 1.47 | 1.38 |
| 32 | 0 | 9500 | SLD | C4-C11 | 5.25 | 1.46 | 1.37 |
| 32 | 0 | 9500 | SLD | C1-C2 | 5.65 | 1.50 | 1.39 |
| 32 | 0 | 9500 | SLD | C6S-C1S | 7.27 | 1.58 | 1.44 |
| 32 | 0 | 9500 | SLD | C6-N1 | 9.16 | 1.45 | 1.36 |
| 32 | 0 | 9500 | SLD | C5S-N4S | 9.71 | 1.45 | 1.32 |
| 32 | 0 | 9500 | SLD | C12-C11 | 14.47 | 1.53 | 1.39 |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32 | 0 | 9500 | SLD | O3-C6-N1 | -8.71 | 122.04 | 128.97 |
| 32 | 0 | 9500 | SLD | C5-N1-C6 | -5.57 | 108.17 | 111.26 |
| 32 | 0 | 9500 | SLD | C7-O1-C6 | -2.93 | 107.83 | 110.22 |
| 32 | 0 | 9500 | SLD | O1-C6-N1 | -2.85 | 108.18 | 109.97 |
| 32 | 0 | 9500 | SLD | CAS-N5S-C0S | -2.41 | 118.28 | 122.85 |
| 32 | 0 | 9500 | SLD | C7-C8-N2 | -2.37 | 106.40 | 111.95 |
| 32 | 0 | 9500 | SLD | C1-C2-N1 | -2.17 | 116.91 | 120.18 |
| 32 | 0 | 9500 | SLD | C3-C12-C11 | 2.10 | 117.72 | 115.97 |
| 32 | 0 | 9500 | SLD | C8-N2-C9 | 2.28 | 126.33 | 122.76 |
| 32 | 0 | 9500 | SLD | O2S-C0S-C9S | 2.92 | 126.61 | 121.04 |
| 32 | 0 | 9500 | SLD | F1-C11-C12 | 2.93 | 121.61 | 118.15 |
| 32 | 0 | 9500 | SLD | CAS-C5B-C4B | 3.05 | 122.35 | 113.08 |
| 32 | 0 | 9500 | SLD | O1-C7-C5 | 3.14 | 107.91 | 104.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|------|------|-------------|------|------------------------|---------------------|
| 32 | 0 | 9500 | SLD | C5B-CAS-N5S | 3.16 | 121.40 | 112.19 |
| 32 | 0 | 9500 | SLD | C2-N1-C6 | 4.78 | 131.36 | 125.86 |
| 32 | 0 | 9500 | SLD | C3S-N4S-C5S | 5.04 | 123.64 | 118.82 |
| 32 | 0 | 9500 | SLD | O1-C6-O3 | 6.53 | 129.77 | 122.40 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32 | 0 | 9500 | SLD | 4 | 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 | 0 | 2754/2922 (94%) | -0.44 | 32 (1%) 79 53 | 35, 63, 107, 150 | 0 |
| 2 | 9 | 122/122 (100%) | -0.02 | 5 (4%) 37 15 | 52, 80, 106, 150 | 0 |
| 3 | 4 | 3/3 (100%) | -0.43 | 0 100 100 | 49, 49, 51, 51 | 0 |
| 4 | A | 237/239 (99%) | -0.48 | 3 (1%) 77 51 | 44, 69, 101, 121 | 0 |
| 5 | B | 337/337 (100%) | -0.38 | 2 (0%) 89 71 | 42, 72, 98, 108 | 0 |
| 6 | C | 246/246 (100%) | -0.54 | 0 100 100 | 36, 63, 87, 99 | 0 |
| 7 | D | 140/176 (79%) | 0.32 | 9 (6%) 19 6 | 70, 115, 131, 137 | 0 |
| 8 | E | 172/177 (97%) | -0.28 | 3 (1%) 70 41 | 61, 84, 102, 107 | 0 |
| 9 | F | 119/119 (100%) | -0.07 | 2 (1%) 70 41 | 70, 88, 112, 118 | 0 |
| 10 | G | 29/348 (8%) | 0.09 | 1 (3%) 45 19 | 85, 105, 113, 117 | 0 |
| 11 | H | 156/167 (93%) | -0.30 | 2 (1%) 77 51 | 51, 72, 100, 108 | 0 |
| 12 | I | 142/145 (97%) | -0.51 | 0 100 100 | 50, 66, 85, 102 | 0 |
| 13 | J | 132/132 (100%) | -0.38 | 0 100 100 | 53, 71, 89, 96 | 0 |
| 14 | K | 145/164 (88%) | -0.29 | 2 (1%) 75 49 | 39, 83, 117, 129 | 0 |
| 15 | L | 194/194 (100%) | -0.63 | 0 100 100 | 47, 62, 79, 90 | 0 |
| 16 | M | 186/186 (100%) | -0.04 | 6 (3%) 47 20 | 58, 81, 120, 133 | 0 |
| 17 | N | 115/115 (100%) | -0.35 | 1 (0%) 84 62 | 56, 72, 90, 94 | 0 |
| 18 | O | 143/148 (96%) | -0.49 | 0 100 100 | 50, 72, 87, 94 | 0 |
| 19 | P | 95/95 (100%) | -0.48 | 1 (1%) 80 55 | 51, 62, 75, 88 | 0 |
| 20 | Q | 150/154 (97%) | -0.53 | 0 100 100 | 46, 61, 81, 88 | 0 |
| 21 | R | 81/84 (96%) | -0.35 | 1 (1%) 79 53 | 59, 76, 95, 103 | 0 |
| 22 | S | 119/119 (100%) | -0.34 | 3 (2%) 57 29 | 55, 74, 97, 113 | 0 |
| 23 | T | 53/66 (80%) | -0.31 | 0 100 100 | 57, 73, 92, 99 | 0 |
| 24 | U | 65/70 (92%) | 0.11 | 5 (7%) 13 4 | 68, 91, 123, 129 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 25 | V | 154/154 (100%) | -0.54 | 0 100 100 | 51, 64, 82, 94 | 0 |
| 26 | W | 82/91 (90%) | -0.25 | 2 (2%) 59 30 | 58, 75, 99, 117 | 0 |
| 27 | X | 142/240 (59%) | -0.60 | 1 (0%) 87 68 | 43, 61, 82, 101 | 0 |
| 28 | Y | 73/73 (100%) | -0.28 | 0 100 100 | 62, 76, 95, 104 | 0 |
| 29 | Z | 56/56 (100%) | -0.71 | 0 100 100 | 42, 52, 58, 68 | 0 |
| 30 | 1 | 46/48 (95%) | -0.15 | 2 (4%) 35 13 | 49, 77, 105, 117 | 0 |
| 31 | 2 | 92/92 (100%) | -0.19 | 2 (2%) 62 33 | 53, 73, 87, 98 | 0 |
| All | All | 6580/7282 (90%) | -0.38 | 85 (1%) 77 51 | 35, 69, 108, 150 | 0 |

All (85) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | 9 | 3001 | U | 6.1 |
| 1 | 0 | 2250 | G | 5.8 |
| 22 | S | 116 | ASP | 4.8 |
| 2 | 9 | 3025 | G | 4.7 |
| 24 | U | 1 | THR | 4.5 |
| 2 | 9 | 3023 | U | 4.4 |
| 1 | 0 | 2237 | G | 4.3 |
| 2 | 9 | 3002 | U | 4.2 |
| 1 | 0 | 735 | C | 4.1 |
| 7 | D | 66 | GLY | 3.7 |
| 7 | D | 10 | PHE | 3.7 |
| 31 | 2 | 56 | PRO | 3.7 |
| 14 | K | 80 | ASP | 3.7 |
| 24 | U | 38 | GLY | 3.6 |
| 24 | U | 40 | PRO | 3.6 |
| 1 | 0 | 2249 | G | 3.4 |
| 19 | P | 95 | GLU | 3.3 |
| 24 | U | 39 | ALA | 3.3 |
| 17 | N | 1 | SER | 3.2 |
| 30 | 1 | 35 | ARG | 3.1 |
| 1 | 0 | 960 | G | 3.1 |
| 1 | 0 | 1951 | G | 3.1 |
| 1 | 0 | 2251 | G | 3.0 |
| 7 | D | 43 | GLU | 2.9 |
| 7 | D | 12 | GLU | 2.9 |
| 1 | 0 | 362 | G | 2.9 |
| 1 | 0 | 970 | U | 2.8 |
| 8 | E | 10 | ASP | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | 0 | 1181 | A | 2.8 |
| 1 | 0 | 1199 | A | 2.7 |
| 4 | A | 133 | ARG | 2.7 |
| 1 | 0 | 365 | G | 2.7 |
| 7 | D | 57 | THR | 2.6 |
| 1 | 0 | 2664 | A | 2.6 |
| 1 | 0 | 1527 | A | 2.6 |
| 7 | D | 47 | GLN | 2.6 |
| 7 | D | 128 | LEU | 2.6 |
| 16 | M | 185 | GLU | 2.6 |
| 1 | 0 | 128 | A | 2.5 |
| 16 | M | 162 | ASP | 2.5 |
| 16 | M | 152 | GLU | 2.5 |
| 1 | 0 | 2253 | G | 2.5 |
| 26 | W | 80 | GLU | 2.5 |
| 7 | D | 63 | ILE | 2.5 |
| 11 | H | 35 | ASN | 2.5 |
| 1 | 0 | 736 | A | 2.5 |
| 1 | 0 | 1279 | U | 2.5 |
| 27 | X | 108 | ASP | 2.4 |
| 16 | M | 160 | SER | 2.4 |
| 16 | M | 56 | ASP | 2.4 |
| 24 | U | 37 | GLY | 2.4 |
| 31 | 2 | 55 | VAL | 2.4 |
| 30 | 1 | 36 | ASN | 2.4 |
| 22 | S | 115 | GLU | 2.4 |
| 10 | G | 72 | ASP | 2.3 |
| 1 | 0 | 2344 | G | 2.3 |
| 4 | A | 237 | GLY | 2.3 |
| 1 | 0 | 1130 | U | 2.3 |
| 5 | B | 118 | ASP | 2.3 |
| 1 | 0 | 1172 | G | 2.3 |
| 1 | 0 | 2254 | G | 2.3 |
| 7 | D | 170 | TYR | 2.3 |
| 1 | 0 | 1950 | G | 2.3 |
| 8 | E | 45 | ASP | 2.3 |
| 9 | F | 119 | ARG | 2.3 |
| 1 | 0 | 1525 | G | 2.3 |
| 1 | 0 | 1198 | U | 2.3 |
| 1 | 0 | 1171 | A | 2.3 |
| 5 | B | 83 | ALA | 2.2 |
| 1 | 0 | 2239 | C | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | R | 1 | SER | 2.2 |
| 22 | S | 117 | ASP | 2.2 |
| 9 | F | 100 | ASP | 2.1 |
| 2 | 9 | 3024 | U | 2.1 |
| 1 | 0 | 2508 | C | 2.1 |
| 14 | K | 150 | GLN | 2.1 |
| 1 | 0 | 1175 | G | 2.1 |
| 4 | A | 31 | LYS | 2.1 |
| 26 | W | 88 | GLU | 2.1 |
| 11 | H | 167 | ALA | 2.1 |
| 8 | E | 16 | ASP | 2.1 |
| 1 | 0 | 2252 | A | 2.0 |
| 1 | 0 | 1173 | A | 2.0 |
| 16 | M | 184 | ILE | 2.0 |
| 1 | 0 | 2509 | A | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35 | NA | 9 | 8351 | 1/1 | 0.33 | 0.25 | 94,94,94,94 | 0 |
| 35 | NA | Q | 8386 | 1/1 | 0.43 | 0.64 | 107,107,107,107 | 0 |
| 35 | NA | 0 | 8384 | 1/1 | 0.48 | 0.62 | 85,85,85,85 | 0 |
| 35 | NA | 0 | 8363 | 1/1 | 0.49 | 0.62 | 83,83,83,83 | 0 |
| 35 | NA | R | 8312 | 1/1 | 0.53 | 0.92 | 84,84,84,84 | 0 |
| 35 | NA | 0 | 8329 | 1/1 | 0.56 | 1.24 | 98,98,98,98 | 0 |
| 35 | NA | 0 | 8371 | 1/1 | 0.65 | 0.72 | 69,69,69,69 | 0 |
| 33 | MG | 0 | 8049 | 1/1 | 0.66 | 0.33 | 90,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35 | NA | H | 8322 | 1/1 | 0.70 | 0.41 | 78,78,78,78 | 0 |
| 35 | NA | 0 | 8324 | 1/1 | 0.71 | 0.39 | 58,58,58,58 | 0 |
| 35 | NA | 0 | 8361 | 1/1 | 0.73 | 0.36 | 77,77,77,77 | 0 |
| 34 | K | 0 | 8201 | 1/1 | 0.75 | 0.12 | 141,141,141,141 | 0 |
| 33 | MG | 0 | 8024 | 1/1 | 0.76 | 0.62 | 98,98,98,98 | 0 |
| 35 | NA | 0 | 8368 | 1/1 | 0.77 | 0.36 | 69,69,69,69 | 0 |
| 35 | NA | 0 | 8340 | 1/1 | 0.77 | 0.37 | 69,69,69,69 | 0 |
| 35 | NA | 0 | 8385 | 1/1 | 0.78 | 0.36 | 73,73,73,73 | 0 |
| 35 | NA | 0 | 8341 | 1/1 | 0.78 | 0.34 | 60,60,60,60 | 0 |
| 35 | NA | 9 | 8383 | 1/1 | 0.78 | 0.38 | 67,67,67,67 | 0 |
| 33 | MG | 0 | 8114 | 1/1 | 0.79 | 0.69 | 95,95,95,95 | 0 |
| 35 | NA | 0 | 8352 | 1/1 | 0.80 | 0.33 | 61,61,61,61 | 0 |
| 35 | NA | 0 | 8382 | 1/1 | 0.80 | 0.17 | 89,89,89,89 | 0 |
| 37 | CD | N | 8405 | 1/1 | 0.80 | 0.23 | 150,150,150,150 | 0 |
| 35 | NA | 0 | 8332 | 1/1 | 0.80 | 0.37 | 50,50,50,50 | 0 |
| 35 | NA | 0 | 8362 | 1/1 | 0.81 | 0.25 | 79,79,79,79 | 0 |
| 35 | NA | 0 | 8323 | 1/1 | 0.81 | 0.44 | 66,66,66,66 | 0 |
| 35 | NA | 0 | 8326 | 1/1 | 0.81 | 0.30 | 73,73,73,73 | 0 |
| 34 | K | 0 | 8202 | 1/1 | 0.81 | 0.77 | 92,92,92,92 | 0 |
| 35 | NA | 0 | 8307 | 1/1 | 0.82 | 0.32 | 71,71,71,71 | 0 |
| 36 | CL | 0 | 8505 | 1/1 | 0.82 | 0.44 | 99,99,99,99 | 0 |
| 33 | MG | A | 8105 | 1/1 | 0.82 | 0.30 | 52,52,52,52 | 0 |
| 35 | NA | 0 | 8366 | 1/1 | 0.82 | 0.36 | 82,82,82,82 | 0 |
| 33 | MG | 0 | 8113 | 1/1 | 0.83 | 0.10 | 60,60,60,60 | 0 |
| 35 | NA | 0 | 8365 | 1/1 | 0.83 | 0.43 | 47,47,47,47 | 0 |
| 36 | CL | K | 8510 | 1/1 | 0.83 | 0.25 | 104,104,104,104 | 0 |
| 35 | NA | 0 | 8378 | 1/1 | 0.84 | 0.75 | 65,65,65,65 | 0 |
| 33 | MG | 0 | 8102 | 1/1 | 0.84 | 0.38 | 91,91,91,91 | 0 |
| 35 | NA | 0 | 8316 | 1/1 | 0.84 | 0.21 | 52,52,52,52 | 0 |
| 35 | NA | 0 | 8369 | 1/1 | 0.84 | 0.35 | 96,96,96,96 | 0 |
| 35 | NA | 0 | 8360 | 1/1 | 0.84 | 0.41 | 69,69,69,69 | 0 |
| 36 | CL | 0 | 8515 | 1/1 | 0.85 | 0.30 | 100,100,100,100 | 0 |
| 33 | MG | 0 | 8071 | 1/1 | 0.85 | 0.07 | 104,104,104,104 | 0 |
| 33 | MG | 0 | 8013 | 1/1 | 0.85 | 0.17 | 60,60,60,60 | 0 |
| 33 | MG | 0 | 8092 | 1/1 | 0.86 | 0.37 | 111,111,111,111 | 0 |
| 35 | NA | 0 | 8350 | 1/1 | 0.86 | 0.28 | 57,57,57,57 | 0 |
| 33 | MG | 0 | 8066 | 1/1 | 0.86 | 0.17 | 105,105,105,105 | 0 |
| 35 | NA | 0 | 8313 | 1/1 | 0.86 | 0.21 | 89,89,89,89 | 0 |
| 33 | MG | 0 | 8046 | 1/1 | 0.87 | 0.15 | 86,86,86,86 | 0 |
| 35 | NA | 0 | 8381 | 1/1 | 0.87 | 0.31 | 69,69,69,69 | 0 |
| 35 | NA | 0 | 8325 | 1/1 | 0.87 | 0.28 | 64,64,64,64 | 0 |
| 36 | CL | P | 8511 | 1/1 | 0.87 | 0.37 | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35 | NA | 0 | 8364 | 1/1 | 0.88 | 0.24 | 66,66,66,66 | 0 |
| 33 | MG | 0 | 8085 | 1/1 | 0.88 | 0.22 | 92,92,92,92 | 0 |
| 36 | CL | B | 8519 | 1/1 | 0.88 | 0.38 | 95,95,95,95 | 0 |
| 35 | NA | 0 | 8374 | 1/1 | 0.88 | 0.14 | 77,77,77,77 | 0 |
| 35 | NA | 0 | 8328 | 1/1 | 0.88 | 0.22 | 55,55,55,55 | 0 |
| 33 | MG | 0 | 8011 | 1/1 | 0.88 | 0.19 | 50,50,50,50 | 0 |
| 33 | MG | 0 | 8022 | 1/1 | 0.88 | 0.58 | 83,83,83,83 | 0 |
| 33 | MG | 0 | 8045 | 1/1 | 0.89 | 0.25 | 91,91,91,91 | 0 |
| 36 | CL | N | 8508 | 1/1 | 0.89 | 0.22 | 116,116,116,116 | 0 |
| 35 | NA | 0 | 8333 | 1/1 | 0.89 | 0.26 | 40,40,40,40 | 0 |
| 33 | MG | S | 8073 | 1/1 | 0.89 | 0.14 | 71,71,71,71 | 0 |
| 33 | MG | 0 | 8003 | 1/1 | 0.89 | 0.15 | 51,51,51,51 | 0 |
| 33 | MG | 0 | 8076 | 1/1 | 0.89 | 0.16 | 102,102,102,102 | 0 |
| 35 | NA | 0 | 8370 | 1/1 | 0.90 | 0.40 | 76,76,76,76 | 0 |
| 36 | CL | I | 8502 | 1/1 | 0.90 | 0.11 | 93,93,93,93 | 0 |
| 36 | CL | A | 8509 | 1/1 | 0.90 | 0.72 | 89,89,89,89 | 0 |
| 35 | NA | 0 | 8311 | 1/1 | 0.90 | 0.26 | 73,73,73,73 | 0 |
| 35 | NA | P | 8348 | 1/1 | 0.90 | 0.09 | 68,68,68,68 | 0 |
| 33 | MG | 0 | 8028 | 1/1 | 0.90 | 0.17 | 57,57,57,57 | 0 |
| 36 | CL | 2 | 8504 | 1/1 | 0.90 | 0.49 | 100,100,100,100 | 0 |
| 35 | NA | 0 | 8375 | 1/1 | 0.91 | 0.69 | 81,81,81,81 | 0 |
| 35 | NA | Q | 8337 | 1/1 | 0.91 | 0.26 | 64,64,64,64 | 0 |
| 35 | NA | 0 | 8357 | 1/1 | 0.91 | 0.26 | 61,61,61,61 | 0 |
| 33 | MG | 0 | 8097 | 1/1 | 0.91 | 0.30 | 53,53,53,53 | 0 |
| 36 | CL | I | 8501 | 1/1 | 0.91 | 0.18 | 99,99,99,99 | 0 |
| 33 | MG | 0 | 8104 | 1/1 | 0.92 | 0.14 | 66,66,66,66 | 0 |
| 33 | MG | 0 | 8111 | 1/1 | 0.92 | 0.12 | 75,75,75,75 | 0 |
| 35 | NA | 0 | 8310 | 1/1 | 0.92 | 0.20 | 46,46,46,46 | 0 |
| 33 | MG | 0 | 8107 | 1/1 | 0.92 | 0.09 | 55,55,55,55 | 0 |
| 33 | MG | 0 | 8100 | 1/1 | 0.92 | 0.19 | 97,97,97,97 | 0 |
| 36 | CL | Q | 8506 | 1/1 | 0.92 | 0.23 | 80,80,80,80 | 0 |
| 33 | MG | 0 | 8081 | 1/1 | 0.92 | 0.08 | 67,67,67,67 | 0 |
| 36 | CL | 0 | 8513 | 1/1 | 0.92 | 0.24 | 74,74,74,74 | 0 |
| 33 | MG | 0 | 8103 | 1/1 | 0.92 | 0.42 | 97,97,97,97 | 0 |
| 35 | NA | 0 | 8377 | 1/1 | 0.92 | 0.58 | 75,75,75,75 | 0 |
| 33 | MG | 0 | 8054 | 1/1 | 0.93 | 0.19 | 45,45,45,45 | 0 |
| 35 | NA | 0 | 8336 | 1/1 | 0.93 | 0.13 | 63,63,63,63 | 0 |
| 35 | NA | 0 | 8330 | 1/1 | 0.93 | 0.11 | 61,61,61,61 | 0 |
| 35 | NA | C | 8304 | 1/1 | 0.93 | 0.38 | 51,51,51,51 | 0 |
| 36 | CL | 0 | 8503 | 1/1 | 0.93 | 0.30 | 82,82,82,82 | 0 |
| 33 | MG | 0 | 8115 | 1/1 | 0.93 | 0.12 | 73,73,73,73 | 0 |
| 35 | NA | 0 | 8308 | 1/1 | 0.93 | 0.25 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35 | NA | 0 | 8372 | 1/1 | 0.93 | 0.74 | 72,72,72,72 | 0 |
| 33 | MG | 0 | 8112 | 1/1 | 0.93 | 0.15 | 64,64,64,64 | 0 |
| 33 | MG | 9 | 8095 | 1/1 | 0.93 | 0.36 | 106,106,106,106 | 0 |
| 35 | NA | 0 | 8353 | 1/1 | 0.93 | 0.14 | 43,43,43,43 | 0 |
| 32 | SLD | 0 | 9500 | 37/37 | 0.93 | 0.21 | 46,50,53,59 | 0 |
| 33 | MG | 0 | 8082 | 1/1 | 0.93 | 0.16 | 79,79,79,79 | 0 |
| 35 | NA | 0 | 8354 | 1/1 | 0.93 | 0.41 | 58,58,58,58 | 0 |
| 33 | MG | 0 | 8108 | 1/1 | 0.93 | 0.27 | 102,102,102,102 | 0 |
| 33 | MG | 0 | 8099 | 1/1 | 0.93 | 0.23 | 80,80,80,80 | 0 |
| 33 | MG | 0 | 8116 | 1/1 | 0.94 | 0.17 | 84,84,84,84 | 0 |
| 35 | NA | 0 | 8321 | 1/1 | 0.94 | 0.42 | 67,67,67,67 | 0 |
| 33 | MG | J | 8069 | 1/1 | 0.94 | 0.05 | 87,87,87,87 | 0 |
| 36 | CL | 0 | 8514 | 1/1 | 0.94 | 0.13 | 75,75,75,75 | 0 |
| 33 | MG | 0 | 8035 | 1/1 | 0.94 | 0.06 | 69,69,69,69 | 0 |
| 33 | MG | 0 | 8062 | 1/1 | 0.94 | 0.09 | 90,90,90,90 | 0 |
| 35 | NA | 0 | 8317 | 1/1 | 0.94 | 0.11 | 57,57,57,57 | 0 |
| 35 | NA | 0 | 8373 | 1/1 | 0.94 | 0.24 | 57,57,57,57 | 0 |
| 33 | MG | 0 | 8067 | 1/1 | 0.94 | 0.12 | 81,81,81,81 | 0 |
| 36 | CL | M | 8507 | 1/1 | 0.94 | 0.24 | 86,86,86,86 | 0 |
| 33 | MG | 0 | 8020 | 1/1 | 0.94 | 0.19 | 53,53,53,53 | 0 |
| 35 | NA | 0 | 8356 | 1/1 | 0.94 | 0.96 | 73,73,73,73 | 0 |
| 35 | NA | 0 | 8359 | 1/1 | 0.94 | 0.15 | 81,81,81,81 | 0 |
| 35 | NA | 0 | 8338 | 1/1 | 0.94 | 0.08 | 66,66,66,66 | 0 |
| 33 | MG | 0 | 8064 | 1/1 | 0.94 | 0.37 | 39,39,39,39 | 0 |
| 33 | MG | 0 | 8029 | 1/1 | 0.95 | 0.07 | 60,60,60,60 | 0 |
| 35 | NA | 0 | 8335 | 1/1 | 0.95 | 0.17 | 83,83,83,83 | 0 |
| 35 | NA | 0 | 8334 | 1/1 | 0.95 | 0.20 | 48,48,48,48 | 0 |
| 33 | MG | 0 | 8053 | 1/1 | 0.95 | 0.29 | 63,63,63,63 | 0 |
| 33 | MG | 0 | 8072 | 1/1 | 0.95 | 0.33 | 78,78,78,78 | 0 |
| 36 | CL | I | 8521 | 1/1 | 0.95 | 0.25 | 69,69,69,69 | 0 |
| 33 | MG | 0 | 8034 | 1/1 | 0.95 | 0.10 | 46,46,46,46 | 0 |
| 36 | CL | 0 | 8517 | 1/1 | 0.95 | 0.33 | 82,82,82,82 | 0 |
| 33 | MG | 0 | 8051 | 1/1 | 0.95 | 0.19 | 97,97,97,97 | 0 |
| 35 | NA | 0 | 8303 | 1/1 | 0.95 | 0.49 | 55,55,55,55 | 0 |
| 33 | MG | 0 | 8018 | 1/1 | 0.95 | 0.09 | 57,57,57,57 | 0 |
| 33 | MG | 0 | 8101 | 1/1 | 0.95 | 0.14 | 94,94,94,94 | 0 |
| 33 | MG | 0 | 8087 | 1/1 | 0.95 | 0.07 | 82,82,82,82 | 0 |
| 35 | NA | 0 | 8339 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 33 | MG | B | 8055 | 1/1 | 0.95 | 0.06 | 71,71,71,71 | 0 |
| 33 | MG | 0 | 8090 | 1/1 | 0.95 | 0.33 | 81,81,81,81 | 0 |
| 35 | NA | 0 | 8376 | 1/1 | 0.95 | 0.46 | 79,79,79,79 | 0 |
| 33 | MG | 0 | 8016 | 1/1 | 0.96 | 0.07 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 33 | MG | 0 | 8026 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |
| 33 | MG | 0 | 8001 | 1/1 | 0.96 | 0.17 | 46,46,46,46 | 0 |
| 35 | NA | 0 | 8367 | 1/1 | 0.96 | 0.25 | 85,85,85,85 | 0 |
| 33 | MG | 0 | 8042 | 1/1 | 0.96 | 0.15 | 61,61,61,61 | 0 |
| 33 | MG | 0 | 8008 | 1/1 | 0.96 | 0.16 | 52,52,52,52 | 0 |
| 35 | NA | L | 8347 | 1/1 | 0.96 | 0.13 | 55,55,55,55 | 0 |
| 33 | MG | 0 | 8075 | 1/1 | 0.96 | 0.09 | 77,77,77,77 | 0 |
| 33 | MG | 0 | 8031 | 1/1 | 0.96 | 0.12 | 54,54,54,54 | 0 |
| 33 | MG | 0 | 8060 | 1/1 | 0.96 | 0.15 | 63,63,63,63 | 0 |
| 36 | CL | J | 8512 | 1/1 | 0.96 | 0.21 | 67,67,67,67 | 0 |
| 33 | MG | 0 | 8044 | 1/1 | 0.96 | 0.27 | 59,59,59,59 | 0 |
| 36 | CL | L | 8518 | 1/1 | 0.96 | 0.10 | 69,69,69,69 | 0 |
| 35 | NA | A | 8345 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 33 | MG | 0 | 8096 | 1/1 | 0.96 | 0.09 | 70,70,70,70 | 0 |
| 33 | MG | 9 | 8052 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 33 | MG | 0 | 8110 | 1/1 | 0.96 | 0.12 | 56,56,56,56 | 0 |
| 33 | MG | X | 8109 | 1/1 | 0.96 | 0.17 | 66,66,66,66 | 0 |
| 35 | NA | 0 | 8301 | 1/1 | 0.96 | 0.12 | 59,59,59,59 | 0 |
| 35 | NA | 0 | 8306 | 1/1 | 0.96 | 0.38 | 59,59,59,59 | 0 |
| 33 | MG | 0 | 8009 | 1/1 | 0.96 | 0.18 | 44,44,44,44 | 0 |
| 33 | MG | 0 | 8057 | 1/1 | 0.96 | 0.08 | 53,53,53,53 | 0 |
| 35 | NA | 0 | 8302 | 1/1 | 0.96 | 0.16 | 55,55,55,55 | 0 |
| 35 | NA | 0 | 8343 | 1/1 | 0.96 | 0.14 | 48,48,48,48 | 0 |
| 35 | NA | 0 | 8358 | 1/1 | 0.96 | 0.28 | 109,109,109,109 | 0 |
| 33 | MG | 0 | 8040 | 1/1 | 0.96 | 0.08 | 88,88,88,88 | 0 |
| 33 | MG | 0 | 8088 | 1/1 | 0.96 | 0.22 | 40,40,40,40 | 0 |
| 36 | CL | 0 | 8516 | 1/1 | 0.96 | 0.26 | 64,64,64,64 | 0 |
| 33 | MG | 0 | 8079 | 1/1 | 0.96 | 0.12 | 53,53,53,53 | 0 |
| 33 | MG | 0 | 8043 | 1/1 | 0.97 | 0.07 | 64,64,64,64 | 0 |
| 33 | MG | 0 | 8019 | 1/1 | 0.97 | 0.15 | 43,43,43,43 | 0 |
| 35 | NA | 0 | 8305 | 1/1 | 0.97 | 0.08 | 42,42,42,42 | 0 |
| 33 | MG | 0 | 8086 | 1/1 | 0.97 | 0.06 | 62,62,62,62 | 0 |
| 33 | MG | 2 | 8078 | 1/1 | 0.97 | 0.04 | 65,65,65,65 | 0 |
| 36 | CL | 0 | 8522 | 1/1 | 0.97 | 0.63 | 92,92,92,92 | 0 |
| 35 | NA | 0 | 8355 | 1/1 | 0.97 | 0.40 | 77,77,77,77 | 0 |
| 33 | MG | 0 | 8050 | 1/1 | 0.97 | 0.14 | 68,68,68,68 | 0 |
| 35 | NA | 0 | 8318 | 1/1 | 0.97 | 0.23 | 48,48,48,48 | 0 |
| 36 | CL | X | 8520 | 1/1 | 0.97 | 0.28 | 57,57,57,57 | 0 |
| 33 | MG | 0 | 8070 | 1/1 | 0.97 | 0.07 | 63,63,63,63 | 0 |
| 33 | MG | 0 | 8002 | 1/1 | 0.97 | 0.09 | 51,51,51,51 | 0 |
| 33 | MG | 0 | 8025 | 1/1 | 0.97 | 0.06 | 59,59,59,59 | 0 |
| 35 | NA | K | 8380 | 1/1 | 0.97 | 0.36 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35 | NA | 0 | 8327 | 1/1 | 0.97 | 0.10 | 46,46,46,46 | 0 |
| 33 | MG | 0 | 8089 | 1/1 | 0.97 | 0.07 | 82,82,82,82 | 0 |
| 35 | NA | 0 | 8314 | 1/1 | 0.97 | 0.23 | 53,53,53,53 | 0 |
| 33 | MG | 0 | 8004 | 1/1 | 0.97 | 0.19 | 50,50,50,50 | 0 |
| 33 | MG | 4 | 8063 | 1/1 | 0.97 | 0.11 | 62,62,62,62 | 0 |
| 33 | MG | 0 | 8106 | 1/1 | 0.97 | 0.26 | 78,78,78,78 | 0 |
| 35 | NA | 0 | 8344 | 1/1 | 0.97 | 0.12 | 48,48,48,48 | 0 |
| 35 | NA | 0 | 8379 | 1/1 | 0.97 | 0.24 | 48,48,48,48 | 0 |
| 33 | MG | 0 | 8036 | 1/1 | 0.97 | 0.06 | 52,52,52,52 | 0 |
| 33 | MG | 0 | 8117 | 1/1 | 0.98 | 0.07 | 45,45,45,45 | 0 |
| 33 | MG | 0 | 8007 | 1/1 | 0.98 | 0.12 | 47,47,47,47 | 0 |
| 33 | MG | 0 | 8027 | 1/1 | 0.98 | 0.08 | 65,65,65,65 | 0 |
| 33 | MG | 0 | 8037 | 1/1 | 0.98 | 0.07 | 54,54,54,54 | 0 |
| 33 | MG | 0 | 8083 | 1/1 | 0.98 | 0.07 | 65,65,65,65 | 0 |
| 33 | MG | 0 | 8048 | 1/1 | 0.98 | 0.06 | 66,66,66,66 | 0 |
| 33 | MG | 0 | 8077 | 1/1 | 0.98 | 0.13 | 54,54,54,54 | 0 |
| 35 | NA | 0 | 8349 | 1/1 | 0.98 | 0.44 | 69,69,69,69 | 0 |
| 35 | NA | 0 | 8331 | 1/1 | 0.98 | 0.12 | 60,60,60,60 | 0 |
| 33 | MG | 0 | 8041 | 1/1 | 0.98 | 0.24 | 68,68,68,68 | 0 |
| 33 | MG | 0 | 8059 | 1/1 | 0.98 | 0.06 | 60,60,60,60 | 0 |
| 33 | MG | 0 | 8039 | 1/1 | 0.98 | 0.10 | 53,53,53,53 | 0 |
| 33 | MG | 0 | 8006 | 1/1 | 0.98 | 0.28 | 60,60,60,60 | 0 |
| 33 | MG | 0 | 8084 | 1/1 | 0.98 | 0.05 | 70,70,70,70 | 0 |
| 33 | MG | 0 | 8032 | 1/1 | 0.98 | 0.08 | 52,52,52,52 | 0 |
| 33 | MG | 0 | 8014 | 1/1 | 0.98 | 0.18 | 46,46,46,46 | 0 |
| 33 | MG | 0 | 8098 | 1/1 | 0.98 | 0.06 | 50,50,50,50 | 0 |
| 35 | NA | 0 | 8315 | 1/1 | 0.98 | 0.19 | 70,70,70,70 | 0 |
| 33 | MG | 0 | 8047 | 1/1 | 0.98 | 0.10 | 90,90,90,90 | 0 |
| 33 | MG | 0 | 8058 | 1/1 | 0.98 | 0.11 | 61,61,61,61 | 0 |
| 37 | CD | Y | 8403 | 1/1 | 0.98 | 0.07 | 84,84,84,84 | 0 |
| 35 | NA | 0 | 8319 | 1/1 | 0.98 | 0.18 | 41,41,41,41 | 0 |
| 35 | NA | H | 8309 | 1/1 | 0.98 | 0.25 | 49,49,49,49 | 0 |
| 33 | MG | 0 | 8033 | 1/1 | 0.98 | 0.11 | 48,48,48,48 | 0 |
| 35 | NA | 0 | 8320 | 1/1 | 0.98 | 0.20 | 40,40,40,40 | 0 |
| 33 | MG | 0 | 8074 | 1/1 | 0.98 | 0.07 | 51,51,51,51 | 0 |
| 33 | MG | 0 | 8093 | 1/1 | 0.98 | 0.10 | 63,63,63,63 | 0 |
| 35 | NA | 0 | 8342 | 1/1 | 0.98 | 0.14 | 42,42,42,42 | 0 |
| 35 | NA | I | 8346 | 1/1 | 0.99 | 0.08 | 45,45,45,45 | 0 |
| 37 | CD | Z | 8402 | 1/1 | 0.99 | 0.07 | 89,89,89,89 | 0 |
| 37 | CD | T | 8401 | 1/1 | 0.99 | 0.07 | 83,83,83,83 | 0 |
| 33 | MG | 0 | 8038 | 1/1 | 0.99 | 0.19 | 56,56,56,56 | 0 |
| 33 | MG | 0 | 8094 | 1/1 | 0.99 | 0.07 | 97,97,97,97 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 33 | MG | 0 | 8056 | 1/1 | 0.99 | 0.09 | 60,60,60,60 | 0 |
| 33 | MG | 0 | 8061 | 1/1 | 0.99 | 0.05 | 45,45,45,45 | 0 |
| 33 | MG | 0 | 8023 | 1/1 | 0.99 | 0.06 | 46,46,46,46 | 0 |
| 33 | MG | 0 | 8030 | 1/1 | 0.99 | 0.16 | 48,48,48,48 | 0 |
| 33 | MG | A | 8065 | 1/1 | 0.99 | 0.15 | 55,55,55,55 | 0 |
| 33 | MG | 0 | 8068 | 1/1 | 0.99 | 0.06 | 64,64,64,64 | 0 |
| 37 | CD | 2 | 8404 | 1/1 | 0.99 | 0.09 | 90,90,90,90 | 0 |
| 33 | MG | 0 | 8012 | 1/1 | 0.99 | 0.06 | 42,42,42,42 | 0 |
| 33 | MG | 0 | 8080 | 1/1 | 0.99 | 0.08 | 52,52,52,52 | 0 |
| 33 | MG | 0 | 8017 | 1/1 | 0.99 | 0.15 | 43,43,43,43 | 0 |
| 33 | MG | 0 | 8010 | 1/1 | 0.99 | 0.10 | 47,47,47,47 | 0 |
| 33 | MG | 0 | 8015 | 1/1 | 0.99 | 0.11 | 60,60,60,60 | 0 |
| 33 | MG | 0 | 8005 | 1/1 | 0.99 | 0.10 | 58,58,58,58 | 0 |
| 33 | MG | 0 | 8021 | 1/1 | 0.99 | 0.18 | 54,54,54,54 | 0 |
| 33 | MG | 0 | 8091 | 1/1 | 0.99 | 0.06 | 65,65,65,65 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.