



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1YJ9
Title : Crystal Structure Of The Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui Containing a three residue deletion in L22
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-13
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

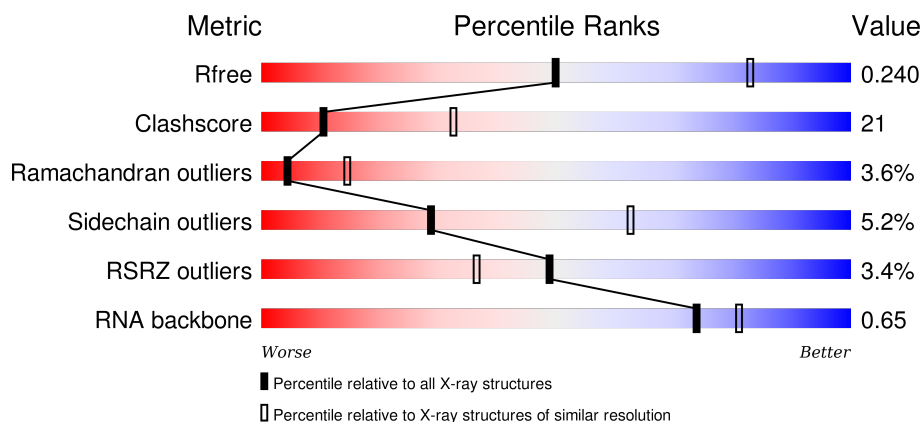
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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




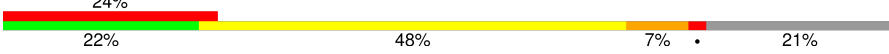

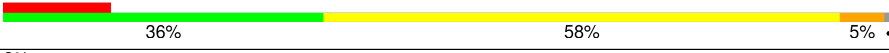
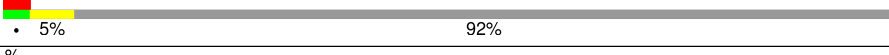
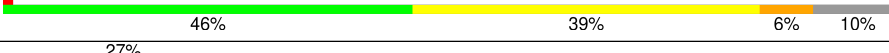



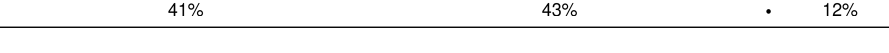
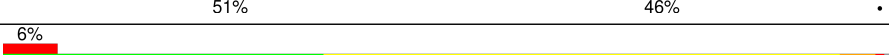


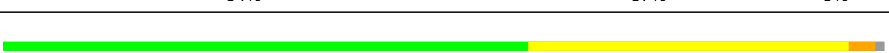

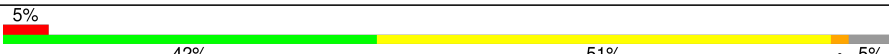
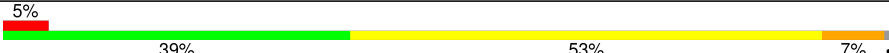




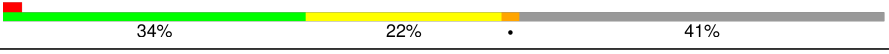

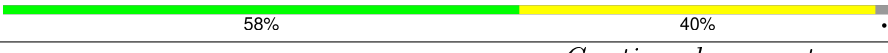

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 2393 (2.80-2.80) |
| Clashscore | 102246 | 2827 (2.80-2.80) |
| Ramachandran outliers | 100387 | 2782 (2.80-2.80) |
| Sidechain outliers | 100360 | 2784 (2.80-2.80) |
| RSRZ outliers | 91569 | 2404 (2.80-2.80) |
| RNA backbone | 2183 | 1091 (3.20-2.40) |

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>51%</div> <div>38%</div> <div>5%</div> <div>6%</div> </div> |
| 2 | 9 | 122 | <div>2%</div> <div>38%</div> <div>53%</div> <div>8%</div> <div>.</div> |
| 3 | A | 240 | <div>4%</div> <div>50%</div> <div>41%</div> <div>7%</div> <div>.</div> |
| 4 | B | 338 | <div>%</div> <div>43%</div> <div>49%</div> <div>8%</div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | C | 246 |  |
| 6 | D | 177 |  |
| 7 | E | 178 |  |
| 8 | F | 120 |  |
| 9 | G | 348 |  |
| 10 | H | 177 |  |
| 11 | I | 162 |  |
| 12 | J | 145 |  |
| 13 | K | 132 |  |
| 14 | L | 165 |  |
| 15 | M | 195 |  |
| 16 | N | 187 |  |
| 17 | O | 116 |  |
| 18 | P | 149 |  |
| 19 | Q | 96 |  |
| 20 | R | 152 |  |
| 21 | S | 85 |  |
| 22 | T | 120 |  |
| 23 | U | 66 |  |
| 24 | V | 71 |  |
| 25 | W | 154 |  |
| 26 | X | 92 |  |
| 27 | Y | 241 |  |
| 28 | Z | 83 |  |
| 29 | 1 | 57 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 30 | 2 | 50 | |
| 31 | 3 | 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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 32 | MG | 0 | 8038 | - | - | - | X |
| 32 | MG | 0 | 8064 | - | - | - | X |
| 33 | K | 0 | 8401 | - | - | - | X |
| 34 | NA | 0 | 8502 | - | - | - | X |
| 34 | NA | 0 | 8503 | - | - | - | X |
| 34 | NA | 0 | 8510 | - | - | - | X |
| 34 | NA | 0 | 8521 | - | - | - | X |
| 34 | NA | 0 | 8526 | - | - | - | X |
| 34 | NA | 0 | 8529 | - | - | - | X |
| 34 | NA | 0 | 8531 | - | - | - | X |
| 34 | NA | 0 | 8532 | - | - | - | X |
| 34 | NA | 0 | 8535 | - | - | - | X |
| 34 | NA | 0 | 8550 | - | - | - | X |
| 34 | NA | 0 | 8555 | - | - | - | X |
| 34 | NA | 0 | 8556 | - | - | - | X |
| 34 | NA | 0 | 8559 | - | - | - | X |
| 34 | NA | 0 | 8561 | - | - | - | X |
| 34 | NA | 0 | 8562 | - | - | - | X |
| 34 | NA | 0 | 8565 | - | - | - | X |
| 34 | NA | 0 | 8566 | - | - | - | X |
| 34 | NA | 0 | 8568 | - | - | - | X |
| 34 | NA | 0 | 8571 | - | - | - | X |
| 34 | NA | 0 | 8573 | - | - | - | X |
| 34 | NA | 0 | 8574 | - | - | - | X |
| 34 | NA | 0 | 8576 | - | - | - | X |
| 34 | NA | 0 | 8578 | - | - | - | X |
| 34 | NA | 0 | 8579 | - | - | - | X |
| 34 | NA | 0 | 8582 | - | - | - | X |
| 34 | NA | 9 | 8583 | - | - | - | X |
| 34 | NA | L | 8580 | - | - | - | X |
| 34 | NA | M | 8547 | - | - | - | X |
| 34 | NA | R | 8586 | - | - | - | X |
| 35 | CL | 0 | 8805 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 35 | CL | 0 | 8815 | - | - | - | X |
| 35 | CL | 0 | 8816 | - | - | - | X |
| 35 | CL | B | 8819 | - | - | - | X |
| 35 | CL | J | 8801 | - | - | X | - |
| 35 | CL | J | 8802 | - | - | X | - |
| 35 | CL | O | 8808 | - | - | - | X |

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99031 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 | 1 | 0 |
| | | | 59041 | 26358 | 10875 | 19062 | 2746 | | | |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|-------------|
| 0 | 628 | 1MA | A | MODIFIED RESIDUE | GB 55229667 |
| 0 | 2587 | OMU | U | MODIFIED RESIDUE | GB 55229667 |
| 0 | 2588 | OMG | G | MODIFIED RESIDUE | GB 55229667 |
| 0 | 2619 | UR3 | U | MODIFIED RESIDUE | GB 55229667 |
| 0 | 2621 | PSU | U | MODIFIED RESIDUE | GB 55229667 |

- 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 |
| | | | 2599 | 1160 | 471 | 847 | 121 | | | |

- Molecule 3 is a protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | A | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1753 | 1072 | 352 | 324 | 5 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | B | 337 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2625 | 1616 | 493 | 511 | 5 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | C | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1859 | 1131 | 344 | 383 | 1 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L5P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | D | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1094 | 685 | 195 | 210 | 4 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | E | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1357 | 840 | 224 | 289 | 4 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | F | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 551 | 141 | 197 | 1 | | | |

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | G | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 240 | 149 | 39 | 51 | 1 | | | |

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | H | 160 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1282 | 798 | 240 | 238 | 6 | | | |

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 11 | I | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 519 | 323 | 81 | 114 | 1 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | K | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 992 | 609 | 187 | 192 | 4 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| K | 44 | LEU | HIS | CONFLICT | UNP P22450 |

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | M | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1558 | 942 | 332 | 283 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| M | 13 | GLU | LYS | CONFLICT | GB 55231501 |

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18 | P | 143 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1136 | 683 | 229 | 224 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | R | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1123 | 699 | 204 | 216 | 4 | | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| R | ? | - | GLN | DELETION | UNP P10970 |
| R | ? | - | GLN | DELETION | UNP P10970 |
| R | ? | - | GLY | DELETION | UNP P10970 |

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | Z | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 578 | 346 | 116 | 111 | 5 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| Z | 10 | ARG | SER | CONFLICT | GB 55231162 |

- Molecule 29 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | 1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 431 | 258 | 86 | 83 | 4 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | 2 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 421 | 254 | 93 | 73 | 1 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | 3 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 458 | 153 | 137 | 7 | | | |

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 32 | 0 | 107 | Total | Mg | 0 | 0 |
| | | | 107 | 107 | | |
| 32 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | A | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 32 | T | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 2 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 9 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 33 | 0 | 2 | Total | K | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 34 | 0 | 74 | Total | Na | 0 | 0 |
| | | | 74 | 74 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 34 | J | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | Q | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | C | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | A | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | T | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | R | 2 | Total 2 | Na 2 | 0 | 0 |
| 34 | 9 | 2 | Total 2 | Na 2 | 0 | 0 |
| 34 | L | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | S | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | M | 1 | Total 1 | Na 1 | 0 | 0 |

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35 | 0 | 9 | Total 9 | Cl 9 | 0 | 0 |
| 35 | J | 3 | Total 3 | Cl 3 | 0 | 0 |
| 35 | Q | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | B | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | A | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | N | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | O | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | R | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | Y | 1 | Total 1 | Cl 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35 | L | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | 3 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | M | 1 | Total 1 | Cl 1 | 0 | 0 |

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 36 | O | 1 | Total 1 | Cd 1 | 0 | 0 |
| 36 | Z | 1 | Total 1 | Cd 1 | 0 | 0 |
| 36 | 1 | 1 | Total 1 | Cd 1 | 0 | 0 |
| 36 | 3 | 1 | Total 1 | Cd 1 | 0 | 0 |
| 36 | U | 1 | Total 1 | Cd 1 | 0 | 0 |

- Molecule 37 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 37 | 0 | 5866 | Total 5866 | O 5866 | 0 | 0 |
| 37 | 9 | 143 | Total 143 | O 143 | 0 | 0 |
| 37 | A | 119 | Total 119 | O 119 | 0 | 0 |
| 37 | B | 148 | Total 148 | O 148 | 0 | 0 |
| 37 | C | 180 | Total 180 | O 180 | 0 | 0 |
| 37 | D | 46 | Total 46 | O 46 | 0 | 0 |
| 37 | E | 45 | Total 45 | O 45 | 0 | 0 |
| 37 | F | 27 | Total 27 | O 27 | 0 | 0 |
| 37 | G | 19 | Total 19 | O 19 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 37 | H | 69 | Total 69 | O 69 | 0 | 0 |
| 37 | I | 9 | Total 9 | O 9 | 0 | 0 |
| 37 | J | 57 | Total 57 | O 57 | 0 | 0 |
| 37 | K | 54 | Total 54 | O 54 | 0 | 0 |
| 37 | L | 84 | Total 84 | O 84 | 0 | 0 |
| 37 | M | 130 | Total 130 | O 130 | 0 | 0 |
| 37 | N | 64 | Total 64 | O 64 | 0 | 0 |
| 37 | O | 45 | Total 45 | O 45 | 0 | 0 |
| 37 | P | 64 | Total 64 | O 64 | 0 | 0 |
| 37 | Q | 53 | Total 53 | O 53 | 0 | 0 |
| 37 | R | 58 | Total 58 | O 58 | 0 | 0 |
| 37 | S | 34 | Total 34 | O 34 | 0 | 0 |
| 37 | T | 32 | Total 32 | O 32 | 0 | 0 |
| 37 | U | 26 | Total 26 | O 26 | 0 | 0 |
| 37 | V | 14 | Total 14 | O 14 | 0 | 0 |
| 37 | W | 72 | Total 72 | O 72 | 0 | 0 |
| 37 | X | 24 | Total 24 | O 24 | 0 | 0 |
| 37 | Y | 104 | Total 104 | O 104 | 0 | 0 |
| 37 | Z | 34 | Total 34 | O 34 | 0 | 0 |
| 37 | 1 | 63 | Total 63 | O 63 | 0 | 0 |
| 37 | 2 | 32 | Total 32 | O 32 | 0 | 0 |

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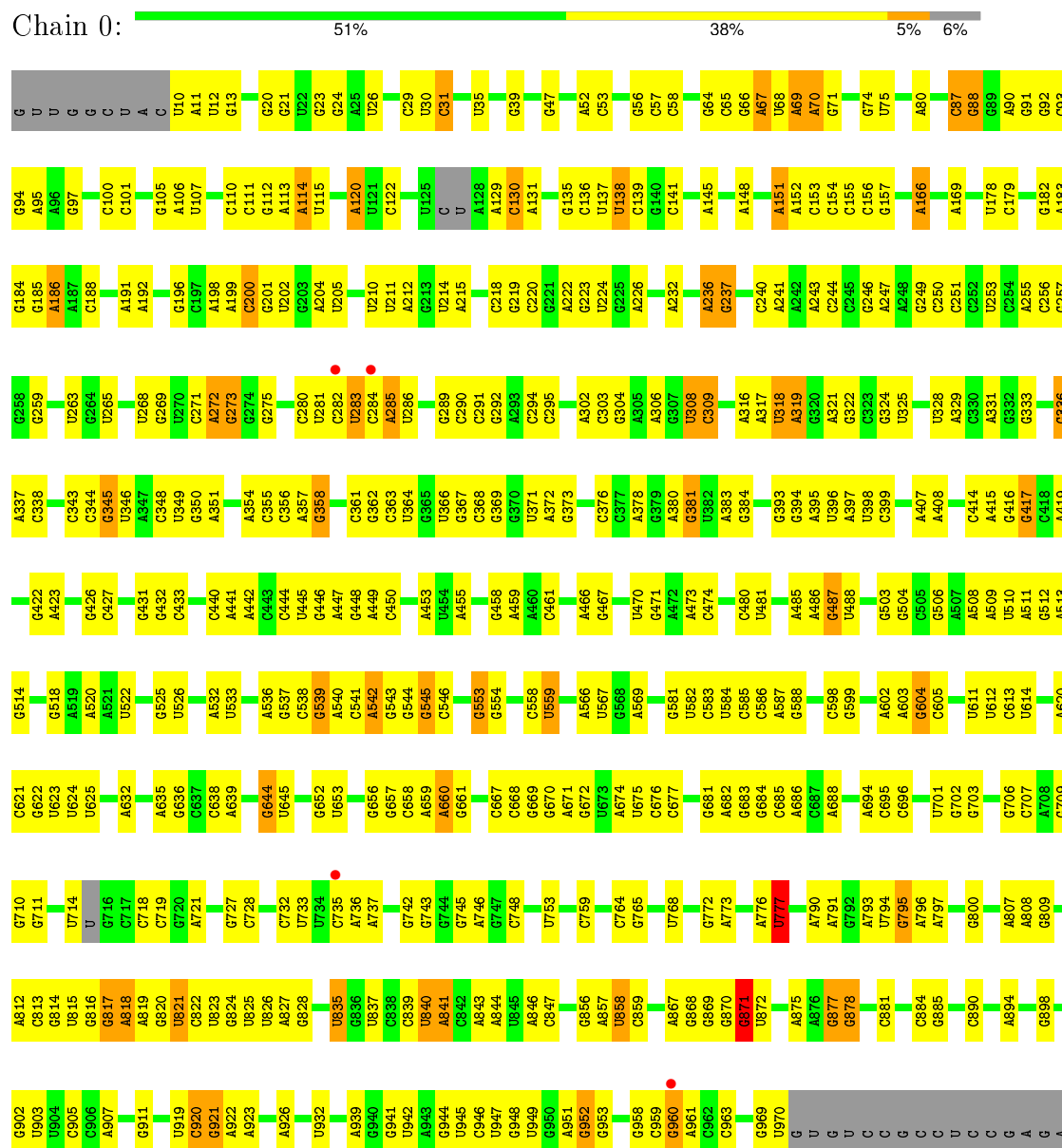
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 37 | 3 | 69 | Total | O | 0 | 0 |
| | | | 69 | 69 | | |

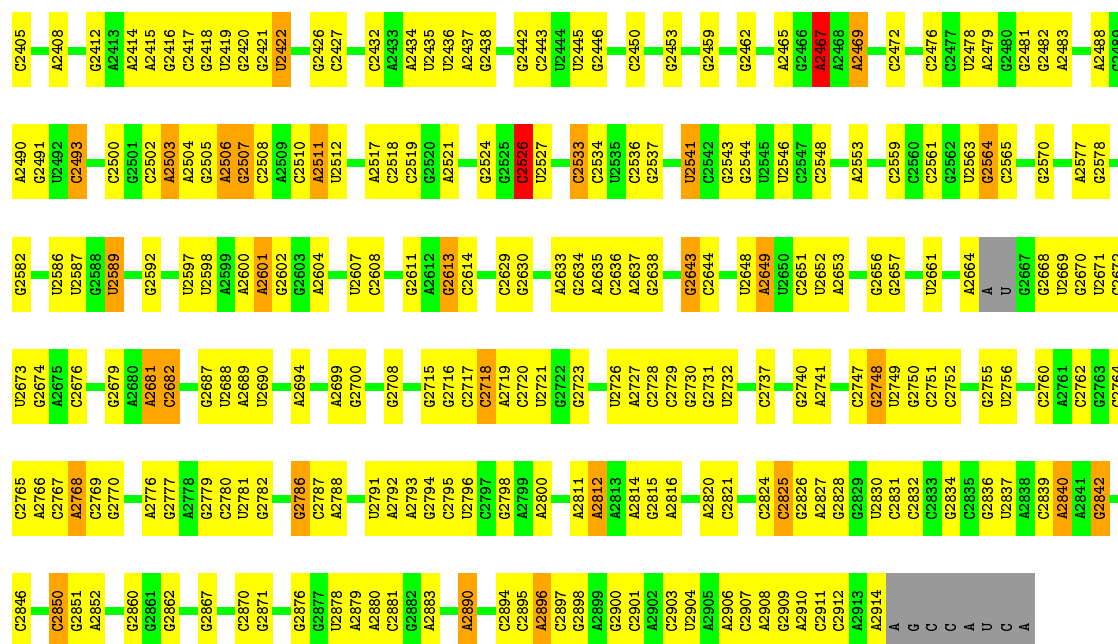
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

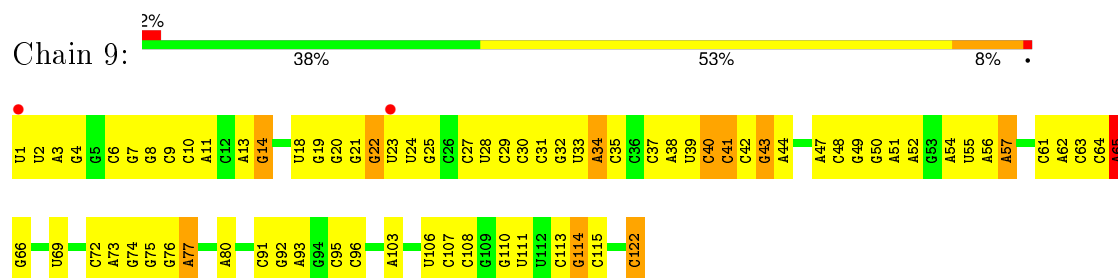
• Molecule 1: 23S Ribosomal RNA



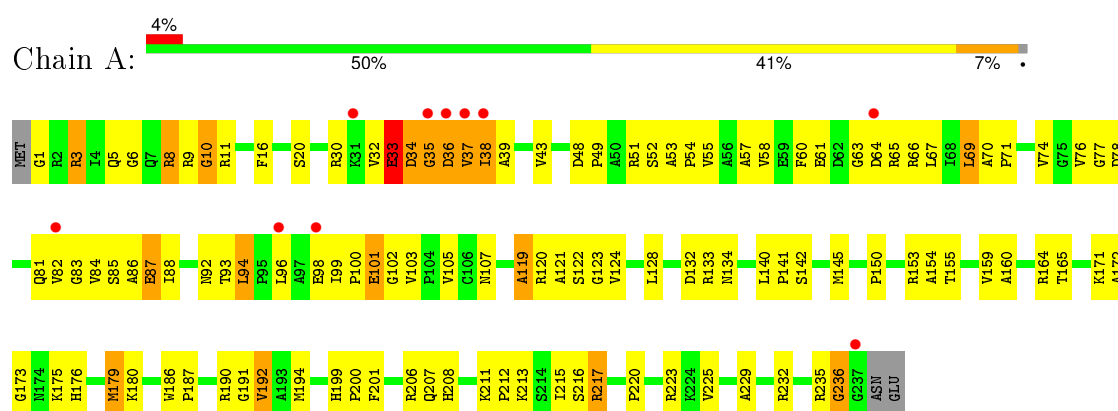




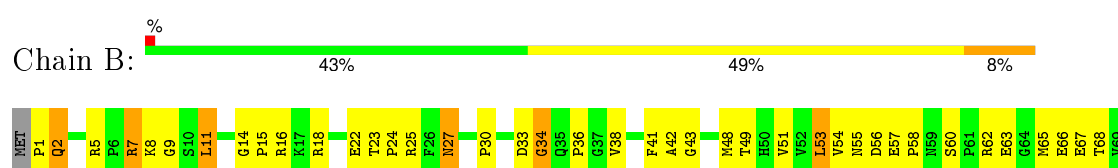
• Molecule 2: 5S Ribosomal RNA

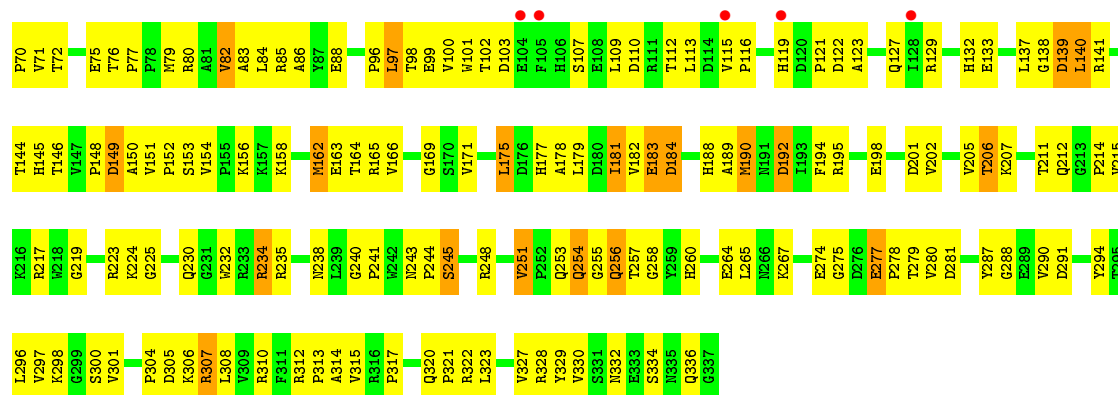


• Molecule 3: 50S ribosomal protein L2P



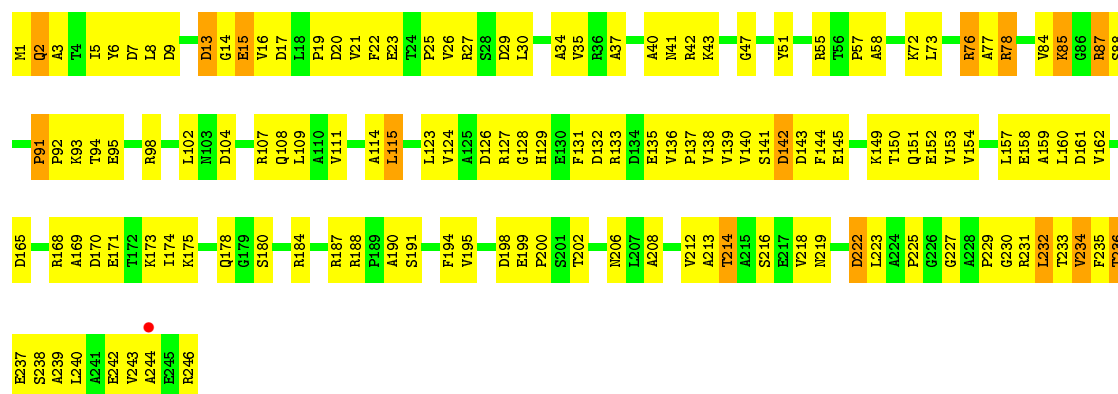
• Molecule 4: 50S ribosomal protein L3P





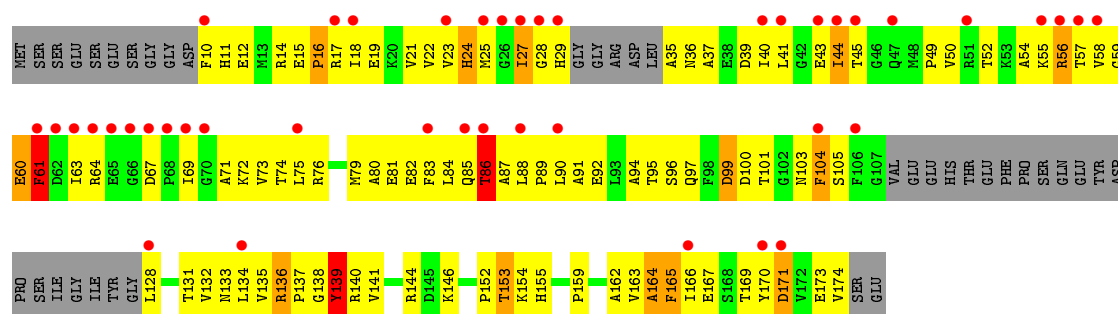
• Molecule 5: 50S ribosomal protein L4E

Chain C: 43% 50% 6%



• Molecule 6: 50S ribosomal protein L5P

Chain D: 24% 22% 48% 7% 21%

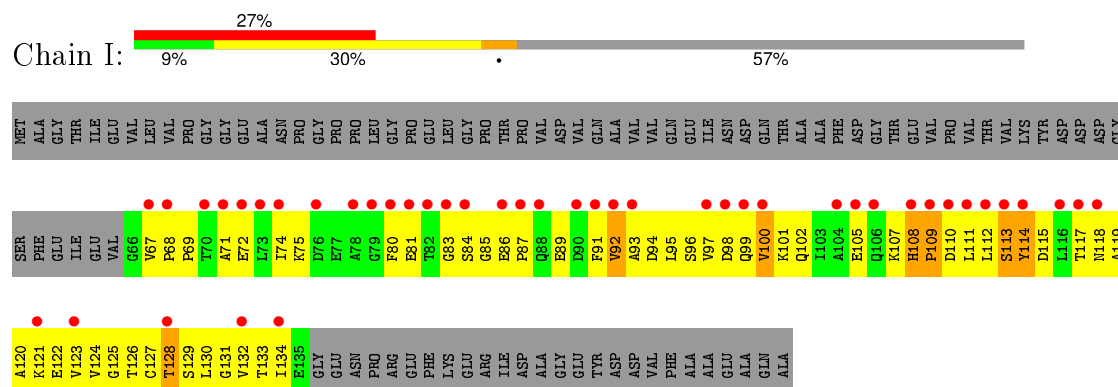


• Molecule 7: 50S ribosomal protein L6P

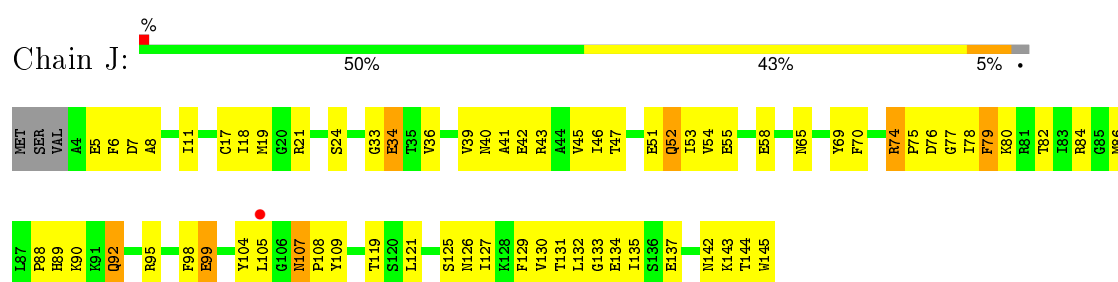
Chain E: 7% 46% 48%



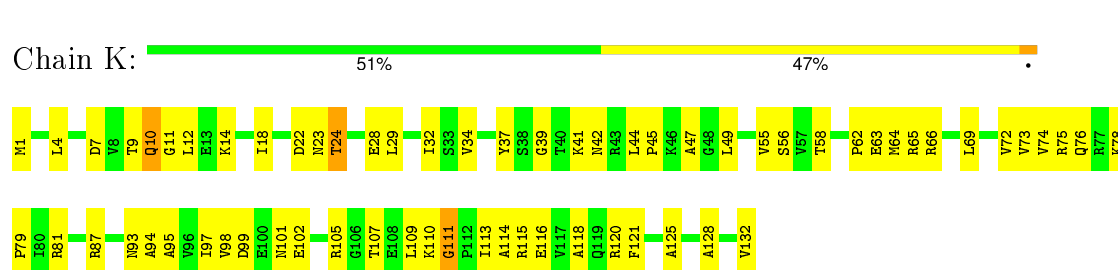
- Molecule 11: 50S RIBOSOMAL PROTEIN L11P



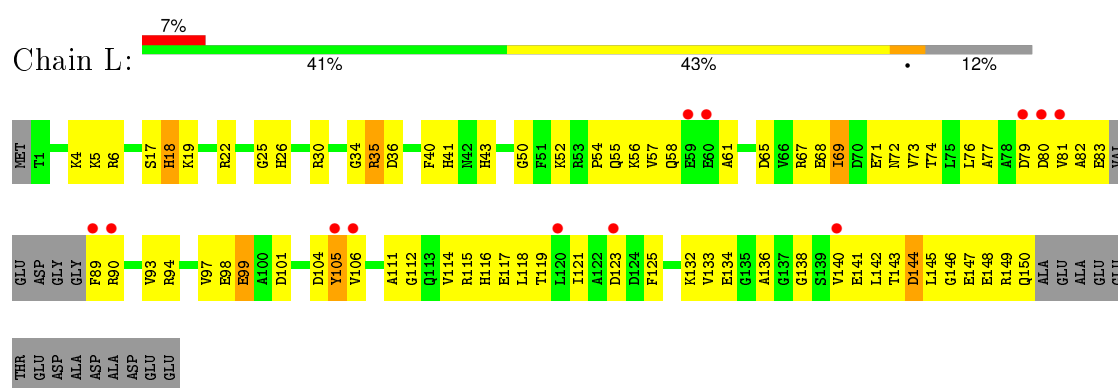
- Molecule 12: 50S ribosomal protein L13P



- Molecule 13: 50S ribosomal protein L14P

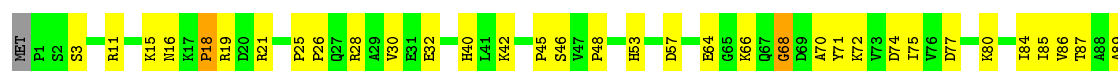


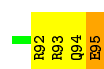
- Molecule 14: 50S ribosomal protein L15P



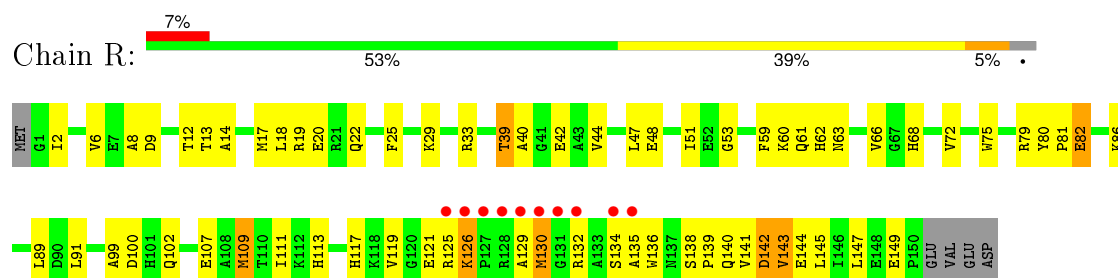
- Molecule 15: 50S Ribosomal Protein L15E



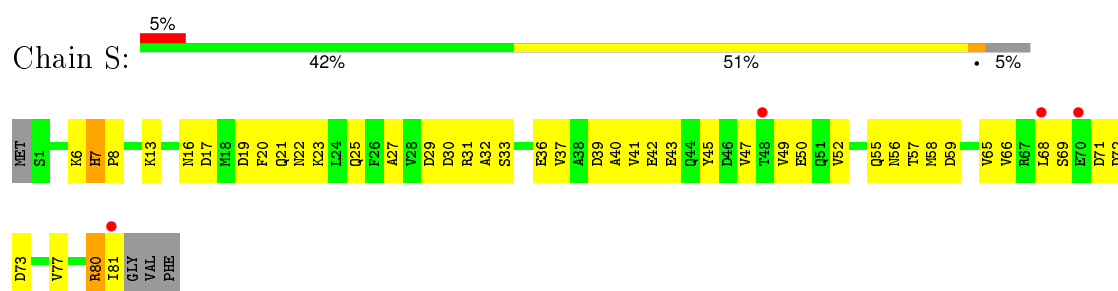




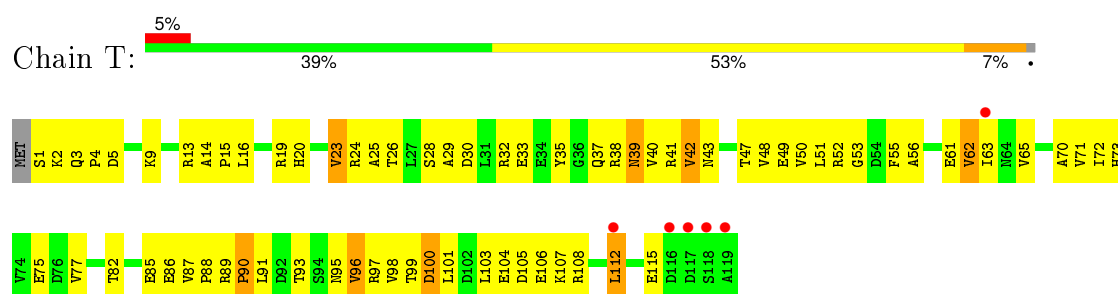
- Molecule 20: 50S ribosomal protein L22P



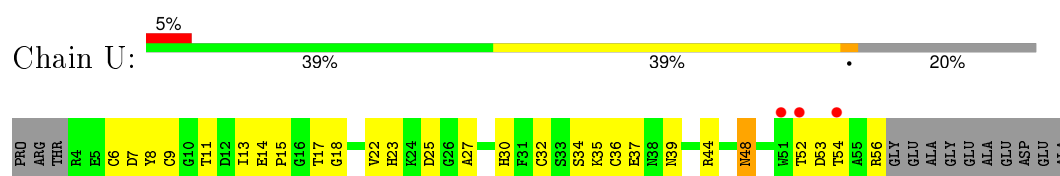
- Molecule 21: 50S ribosomal protein L23P



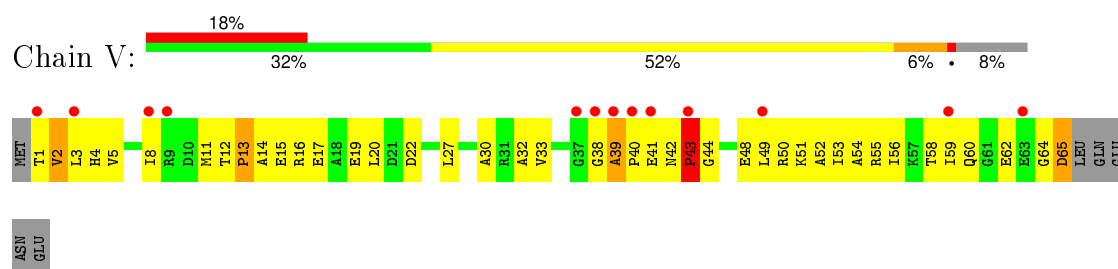
- Molecule 22: 50S ribosomal protein L24P



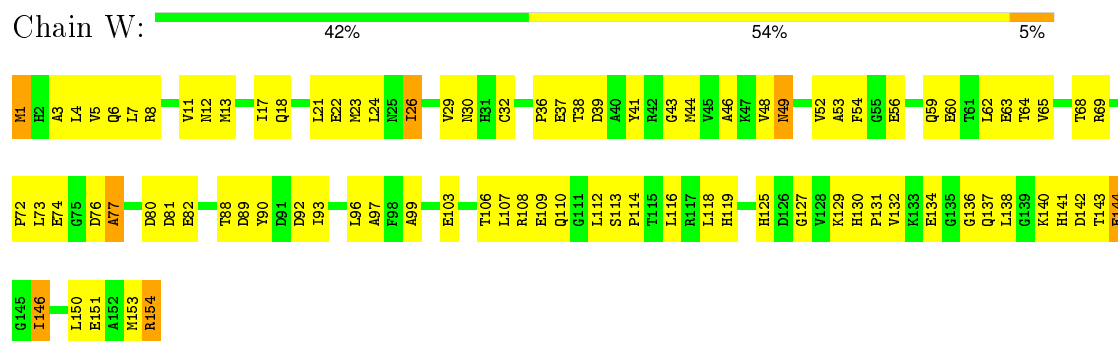
- Molecule 23: 50S ribosomal protein L24E



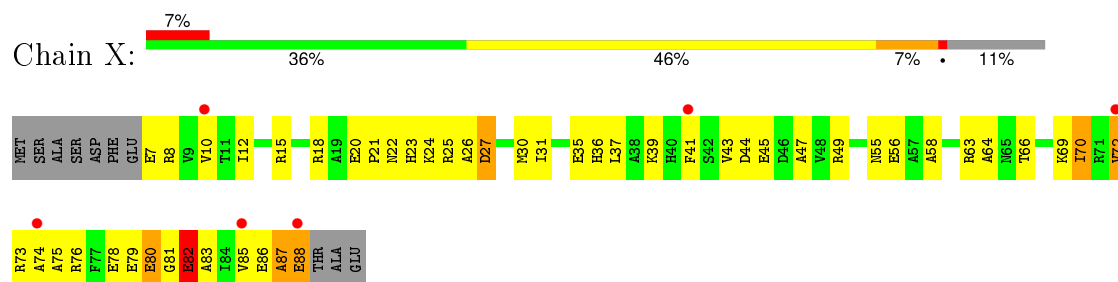
- Molecule 24: 50S ribosomal protein L29P



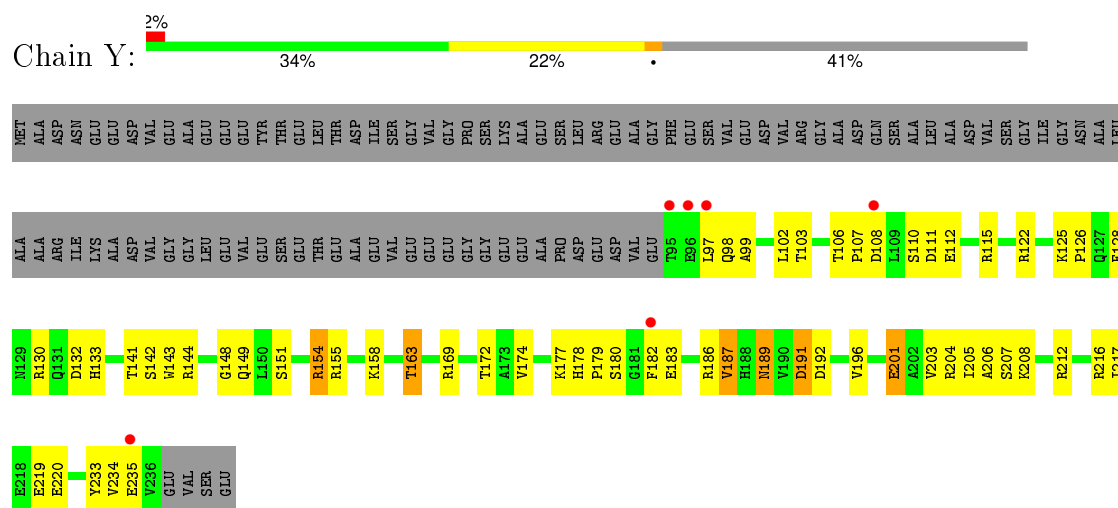
- Molecule 25: 50S ribosomal protein L30P



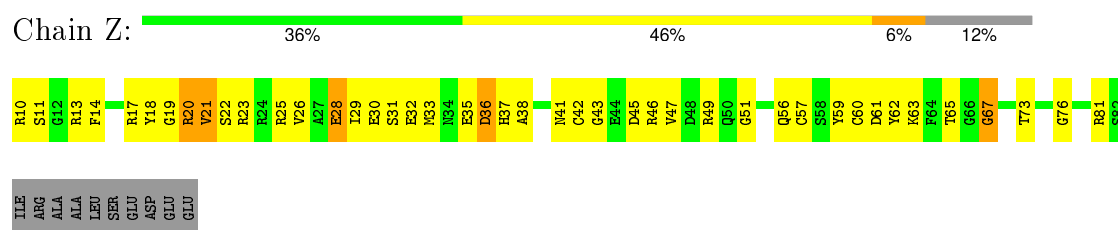
- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae



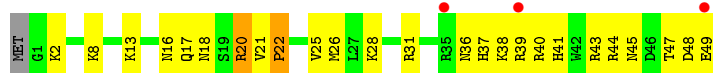
- Molecule 29: 50S ribosomal protein L37e

Chain 1:  58% 40%



- Molecule 30: 50S ribosomal protein L39e

Chain 2:  6% 48% 46%



- Molecule 31: 50S ribosomal protein L44E

Chain 3:  63% 34%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 213.08Å 300.75Å 575.48Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 29.94 – 2.80 49.56 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 89.3 (29.94-2.80) 89.2 (49.56-2.80) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.82 (at 2.81Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.184 , 0.242 0.185 , 0.240 | Depositor DCC |
| R_{free} test set | 3986 reflections (1.00%) | DCC |
| Wilson B-factor (Å ²) | 55.8 | Xtriage |
| Anisotropy | 0.325 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 63.5 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Outliers | 0 of 400940 reflections | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 99031 | wwPDB-VP |
| Average B, all atoms (Å ²) | 62.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, OMG, CL, NA, K, CD, OMU, UR3, 1MA, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | 0 | 0.42 | 0/65980 | 0.69 | 13/102903 (0.0%) |
| 2 | 9 | 0.38 | 0/2904 | 0.70 | 1/4526 (0.0%) |
| 3 | A | 0.35 | 0/1786 | 0.66 | 0/2408 |
| 4 | B | 0.35 | 0/2690 | 0.66 | 0/3652 |
| 5 | C | 0.39 | 0/1884 | 0.66 | 0/2551 |
| 6 | D | 0.33 | 0/1111 | 0.57 | 0/1498 |
| 7 | E | 0.35 | 0/1382 | 0.59 | 0/1880 |
| 8 | F | 0.34 | 0/901 | 0.59 | 0/1224 |
| 9 | G | 0.31 | 0/241 | 0.53 | 0/324 |
| 10 | H | 0.38 | 0/1302 | 0.70 | 1/1743 (0.1%) |
| 11 | I | 0.31 | 0/526 | 0.59 | 0/716 |
| 12 | J | 0.40 | 0/1136 | 0.61 | 0/1530 |
| 13 | K | 0.37 | 0/1001 | 0.69 | 0/1347 |
| 14 | L | 0.36 | 0/1130 | 0.65 | 0/1509 |
| 15 | M | 0.36 | 0/1582 | 0.62 | 1/2117 (0.0%) |
| 16 | N | 0.32 | 0/1474 | 0.64 | 0/1999 |
| 17 | O | 0.35 | 0/874 | 0.58 | 0/1181 |
| 18 | P | 0.37 | 0/1147 | 0.55 | 0/1528 |
| 19 | Q | 0.40 | 0/749 | 0.74 | 1/1005 (0.1%) |
| 20 | R | 0.42 | 0/1146 | 0.63 | 0/1544 |
| 21 | S | 0.36 | 0/648 | 0.59 | 0/875 |
| 22 | T | 0.34 | 0/958 | 0.64 | 0/1289 |
| 23 | U | 0.34 | 0/417 | 0.58 | 0/562 |
| 24 | V | 0.31 | 0/502 | 0.56 | 0/675 |
| 25 | W | 0.37 | 0/1219 | 0.65 | 0/1655 |
| 26 | X | 0.36 | 0/664 | 0.62 | 0/895 |
| 27 | Y | 0.38 | 0/1146 | 0.65 | 0/1536 |
| 28 | Z | 0.38 | 0/589 | 0.63 | 0/787 |
| 29 | 1 | 0.40 | 0/438 | 0.64 | 0/578 |
| 30 | 2 | 0.41 | 0/427 | 0.61 | 0/566 |
| 31 | 3 | 0.40 | 0/771 | 0.58 | 0/1024 |
| All | All | 0.40 | 0/98725 | 0.68 | 17/147627 (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 | 46 |
| 2 | 9 | 0 | 1 |
| All | All | 0 | 47 |

There are no bond length outliers.

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1 | 0 | 1942 | A | C5'-C4'-C3' | 7.17 | 127.47 | 116.00 |
| 1 | 0 | 1504 | A | C1'-O4'-C4' | -6.38 | 104.80 | 109.90 |
| 1 | 0 | 2291 | A | N9-C1'-C2' | 6.19 | 122.05 | 114.00 |
| 19 | Q | 68 | GLY | N-CA-C | -5.89 | 98.36 | 113.10 |
| 1 | 0 | 1504 | A | N9-C1'-C2' | 5.75 | 121.48 | 114.00 |
| 1 | 0 | 2467 | A | C1'-O4'-C4' | -5.72 | 105.32 | 109.90 |
| 2 | 9 | 65 | A | N9-C1'-C2' | 5.66 | 121.35 | 114.00 |
| 1 | 0 | 1971 | G | N9-C1'-C2' | 5.52 | 121.18 | 114.00 |
| 1 | 0 | 2313 | C | C5'-C4'-O4' | 5.45 | 115.64 | 109.10 |
| 1 | 0 | 871 | G | C5'-C4'-O4' | -5.39 | 102.63 | 109.10 |
| 1 | 0 | 2316 | G | C5'-C4'-C3' | -5.30 | 107.52 | 116.00 |
| 10 | H | 115 | GLY | N-CA-C | -5.23 | 100.01 | 113.10 |
| 1 | 0 | 840[A] | U | C5'-C4'-O4' | 5.15 | 115.28 | 109.10 |
| 1 | 0 | 840[B] | U | C5'-C4'-O4' | 5.15 | 115.28 | 109.10 |
| 15 | M | 194 | GLY | N-CA-C | 5.11 | 125.88 | 113.10 |
| 1 | 0 | 777 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 1 | 0 | 1261 | A | N9-C1'-C2' | 5.01 | 120.51 | 114.00 |

There are no chirality outliers.

All (47) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | 0 | 1039 | G | Sidechain |
| 1 | 0 | 1078 | A | Sidechain |
| 1 | 0 | 1131 | G | Sidechain |
| 1 | 0 | 1340 | G | Sidechain |
| 1 | 0 | 1351 | G | Sidechain |
| 1 | 0 | 1430 | G | Sidechain |
| 1 | 0 | 148 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | 0 | 1599 | U | Sidechain |
| 1 | 0 | 1635 | U | Sidechain |
| 1 | 0 | 1653 | A | Sidechain |
| 1 | 0 | 1684 | A | Sidechain |
| 1 | 0 | 1809 | G | Sidechain |
| 1 | 0 | 1829 | A | Sidechain |
| 1 | 0 | 1863 | G | Sidechain |
| 1 | 0 | 1877 | G | Sidechain |
| 1 | 0 | 1878 | G | Sidechain |
| 1 | 0 | 1972 | U | Sidechain |
| 1 | 0 | 2034 | U | Sidechain |
| 1 | 0 | 2101 | A | Sidechain |
| 1 | 0 | 2313 | C | Sidechain |
| 1 | 0 | 2315 | C | Sidechain |
| 1 | 0 | 2316 | G | 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 | 26 | U | Sidechain |
| 1 | 0 | 2630 | G | Sidechain |
| 1 | 0 | 2643 | G | Sidechain |
| 1 | 0 | 2842 | G | Sidechain |
| 1 | 0 | 333 | G | Sidechain |
| 1 | 0 | 398 | U | Sidechain |
| 1 | 0 | 458 | G | Sidechain |
| 1 | 0 | 471 | G | Sidechain |
| 1 | 0 | 481 | U | Sidechain |
| 1 | 0 | 518 | G | Sidechain |
| 1 | 0 | 768 | U | Sidechain |
| 1 | 0 | 795 | G | Sidechain |
| 1 | 0 | 815 | U | Sidechain |
| 1 | 0 | 817 | G | Sidechain |
| 1 | 0 | 818 | A | Sidechain |
| 1 | 0 | 867 | A | Sidechain |
| 1 | 0 | 881 | C | Sidechain |
| 1 | 0 | 919 | U | Sidechain |
| 1 | 0 | 952 | G | Sidechain |
| 2 | 9 | 65 | A | 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 | 59041 | 0 | 29817 | 1161 | 0 |
| 2 | 9 | 2599 | 0 | 1325 | 86 | 0 |
| 3 | A | 1753 | 0 | 1766 | 148 | 0 |
| 4 | B | 2625 | 0 | 2533 | 200 | 0 |
| 5 | C | 1859 | 0 | 1816 | 160 | 0 |
| 6 | D | 1094 | 0 | 1085 | 138 | 0 |
| 7 | E | 1357 | 0 | 1266 | 77 | 0 |
| 8 | F | 890 | 0 | 843 | 79 | 0 |
| 9 | G | 240 | 0 | 231 | 22 | 0 |
| 10 | H | 1282 | 0 | 1292 | 95 | 0 |
| 11 | I | 519 | 0 | 500 | 63 | 0 |
| 12 | J | 1120 | 0 | 1098 | 80 | 0 |
| 13 | K | 992 | 0 | 1031 | 77 | 0 |
| 14 | L | 1118 | 0 | 1076 | 81 | 0 |
| 15 | M | 1558 | 0 | 1566 | 98 | 0 |
| 16 | N | 1445 | 0 | 1401 | 147 | 0 |
| 17 | O | 865 | 0 | 873 | 62 | 0 |
| 18 | P | 1136 | 0 | 1123 | 71 | 0 |
| 19 | Q | 735 | 0 | 729 | 37 | 0 |
| 20 | R | 1123 | 0 | 1099 | 69 | 0 |
| 21 | S | 641 | 0 | 605 | 39 | 0 |
| 22 | T | 950 | 0 | 923 | 99 | 0 |
| 23 | U | 410 | 0 | 364 | 31 | 0 |
| 24 | V | 499 | 0 | 511 | 44 | 0 |
| 25 | W | 1196 | 0 | 1137 | 120 | 0 |
| 26 | X | 654 | 0 | 653 | 57 | 0 |
| 27 | Y | 1130 | 0 | 1133 | 66 | 0 |
| 28 | Z | 578 | 0 | 539 | 39 | 0 |
| 29 | 1 | 431 | 0 | 426 | 36 | 0 |
| 30 | 2 | 421 | 0 | 437 | 35 | 0 |
| 31 | 3 | 755 | 0 | 728 | 31 | 0 |
| 32 | 0 | 107 | 0 | 0 | 0 | 0 |
| 32 | 2 | 1 | 0 | 0 | 0 | 0 |
| 32 | 3 | 1 | 0 | 0 | 0 | 0 |
| 32 | 9 | 1 | 0 | 0 | 0 | 0 |
| 32 | A | 2 | 0 | 0 | 0 | 0 |
| 32 | B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | K | 1 | 0 | 0 | 0 | 0 |
| 32 | T | 1 | 0 | 0 | 0 | 0 |
| 32 | Y | 1 | 0 | 0 | 0 | 0 |
| 33 | 0 | 2 | 0 | 0 | 0 | 0 |
| 34 | 0 | 74 | 0 | 0 | 0 | 0 |
| 34 | 9 | 2 | 0 | 0 | 0 | 0 |
| 34 | A | 1 | 0 | 0 | 0 | 0 |
| 34 | C | 1 | 0 | 0 | 0 | 0 |
| 34 | J | 1 | 0 | 0 | 0 | 0 |
| 34 | L | 1 | 0 | 0 | 0 | 0 |
| 34 | M | 1 | 0 | 0 | 0 | 0 |
| 34 | Q | 1 | 0 | 0 | 0 | 0 |
| 34 | R | 2 | 0 | 0 | 0 | 0 |
| 34 | S | 1 | 0 | 0 | 0 | 0 |
| 34 | T | 1 | 0 | 0 | 0 | 0 |
| 35 | 0 | 9 | 0 | 0 | 1 | 0 |
| 35 | 3 | 1 | 0 | 0 | 0 | 0 |
| 35 | A | 1 | 0 | 0 | 0 | 0 |
| 35 | B | 1 | 0 | 0 | 0 | 0 |
| 35 | J | 3 | 0 | 0 | 4 | 0 |
| 35 | L | 1 | 0 | 0 | 0 | 0 |
| 35 | M | 1 | 0 | 0 | 0 | 0 |
| 35 | N | 1 | 0 | 0 | 1 | 0 |
| 35 | O | 1 | 0 | 0 | 0 | 0 |
| 35 | Q | 1 | 0 | 0 | 0 | 0 |
| 35 | R | 1 | 0 | 0 | 0 | 0 |
| 35 | Y | 1 | 0 | 0 | 0 | 0 |
| 36 | 1 | 1 | 0 | 0 | 0 | 0 |
| 36 | 3 | 1 | 0 | 0 | 0 | 0 |
| 36 | O | 1 | 0 | 0 | 0 | 0 |
| 36 | U | 1 | 0 | 0 | 0 | 0 |
| 36 | Z | 1 | 0 | 0 | 0 | 0 |
| 37 | 0 | 5866 | 0 | 0 | 246 | 0 |
| 37 | 1 | 63 | 0 | 0 | 8 | 0 |
| 37 | 2 | 32 | 0 | 0 | 2 | 0 |
| 37 | 3 | 69 | 0 | 0 | 8 | 0 |
| 37 | 9 | 143 | 0 | 0 | 12 | 0 |
| 37 | A | 119 | 0 | 0 | 21 | 0 |
| 37 | B | 148 | 0 | 0 | 31 | 0 |
| 37 | C | 180 | 0 | 0 | 34 | 0 |
| 37 | D | 46 | 0 | 0 | 17 | 0 |
| 37 | E | 45 | 0 | 0 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37 | F | 27 | 0 | 0 | 8 | 0 |
| 37 | G | 19 | 0 | 0 | 2 | 0 |
| 37 | H | 69 | 0 | 0 | 12 | 0 |
| 37 | I | 9 | 0 | 0 | 5 | 0 |
| 37 | J | 57 | 0 | 0 | 8 | 0 |
| 37 | K | 54 | 0 | 0 | 10 | 0 |
| 37 | L | 84 | 0 | 0 | 17 | 0 |
| 37 | M | 130 | 0 | 0 | 10 | 0 |
| 37 | N | 64 | 0 | 0 | 22 | 0 |
| 37 | O | 45 | 0 | 0 | 11 | 0 |
| 37 | P | 64 | 0 | 0 | 10 | 0 |
| 37 | Q | 53 | 0 | 0 | 7 | 0 |
| 37 | R | 58 | 0 | 0 | 5 | 0 |
| 37 | S | 34 | 0 | 0 | 3 | 0 |
| 37 | T | 32 | 0 | 0 | 9 | 0 |
| 37 | U | 26 | 0 | 0 | 3 | 0 |
| 37 | V | 14 | 0 | 0 | 5 | 0 |
| 37 | W | 72 | 0 | 0 | 12 | 0 |
| 37 | X | 24 | 0 | 0 | 5 | 0 |
| 37 | Y | 104 | 0 | 0 | 15 | 0 |
| 37 | Z | 34 | 0 | 0 | 3 | 0 |
| All | All | 99031 | 0 | 59926 | 3232 | 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 21.

All (3232) 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) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:127:ARG:NH2 | 5:C:225:PRO:HG2 | 1.66 | 1.09 |
| 5:C:236:THR:HG22 | 5:C:239:ALA:H | 0.95 | 1.08 |
| 1:0:1160:G:H5' | 1:0:1161:A:H5' | 1.13 | 1.07 |
| 4:B:264:GLU:HG2 | 4:B:267:LYS:HE2 | 1.36 | 1.04 |
| 29:1:25:LYS:HD2 | 30:2:49:GLU:H | 1.20 | 1.03 |
| 13:K:10:GLN:NE2 | 13:K:10:GLN:H | 1.58 | 1.02 |
| 1:0:871:G:H5' | 1:0:871:G:H8 | 1.21 | 1.01 |
| 24:V:12:THR:HG22 | 24:V:15:GLU:HG3 | 1.42 | 1.00 |
| 1:0:156:C:H5'' | 15:M:171:ARG:HD3 | 1.42 | 0.99 |
| 1:0:1559:A:H1' | 37:0:5655:HOH:O | 1.61 | 0.98 |
| 1:0:1119:G:H2' | 12:J:52:GLN:HE22 | 1.29 | 0.97 |
| 1:0:871:G:C8 | 1:0:871:G:H5' | 1.98 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:381:G:H5'' | 37:0:4123:HOH:O | 1.62 | 0.96 |
| 30:2:40:ARG:HD2 | 30:2:47:THR:HG22 | 1.46 | 0.96 |
| 2:9:76:G:H3' | 2:9:77:A:H5'' | 1.44 | 0.96 |
| 5:C:236:THR:HG22 | 5:C:239:ALA:N | 1.80 | 0.96 |
| 1:0:1242:A:H5' | 12:J:82:THR:HG23 | 1.44 | 0.96 |
| 30:2:20:ARG:HG3 | 30:2:20:ARG:HH11 | 1.29 | 0.95 |
| 6:D:54:ALA:HB2 | 6:D:69:ILE:HD12 | 1.48 | 0.95 |
| 2:9:6:C:H5'' | 16:N:37:ARG:NH1 | 1.82 | 0.95 |
| 25:W:4:LEU:HD22 | 25:W:52:VAL:HG21 | 1.45 | 0.95 |
| 28:Z:10:ARG:HA | 37:Z:8715:HOH:O | 1.67 | 0.95 |
| 13:K:10:GLN:N | 13:K:10:GLN:HE21 | 1.66 | 0.94 |
| 1:0:2270:G:H4' | 3:A:223:ARG:HH12 | 1.33 | 0.94 |
| 1:0:2717:C:H2' | 1:0:2718:C:H5'' | 1.46 | 0.94 |
| 5:C:233:THR:HG22 | 5:C:234:VAL:H | 1.33 | 0.94 |
| 1:0:396:U:H1' | 37:0:7397:HOH:O | 1.66 | 0.93 |
| 1:0:1474:C:H6 | 1:0:1474:C:H5' | 1.34 | 0.93 |
| 5:C:76:ARG:HB3 | 5:C:76:ARG:HH11 | 1.30 | 0.93 |
| 4:B:202:VAL:HG11 | 4:B:301:VAL:HG13 | 1.51 | 0.92 |
| 1:0:541:C:H2' | 1:0:542:A:H5'' | 1.51 | 0.92 |
| 1:0:1187:U:HO2' | 1:0:1189:A:H2 | 1.03 | 0.92 |
| 3:A:81:GLN:HB2 | 3:A:92:ASN:ND2 | 1.85 | 0.92 |
| 11:I:127:CYS:HB3 | 11:I:132:VAL:HB | 1.51 | 0.92 |
| 18:P:115:SER:H | 18:P:118:GLN:HE21 | 0.92 | 0.92 |
| 20:R:8:ALA:HB1 | 20:R:13:THR:HG21 | 1.51 | 0.92 |
| 1:0:1160:G:C5' | 1:0:1161:A:H5' | 1.99 | 0.92 |
| 3:A:211:LYS:HB3 | 3:A:212:PRO:HD2 | 1.52 | 0.92 |
| 12:J:74:ARG:HB3 | 12:J:74:ARG:HH11 | 1.35 | 0.91 |
| 16:N:97:VAL:HG12 | 16:N:127:LEU:HD11 | 1.53 | 0.91 |
| 6:D:94:ALA:HB3 | 6:D:97:GLN:HE21 | 1.34 | 0.91 |
| 28:Z:46:ARG:HD2 | 28:Z:59:TYR:HB2 | 1.53 | 0.91 |
| 1:0:1160:G:H5' | 1:0:1161:A:C5' | 2.01 | 0.90 |
| 18:P:115:SER:H | 18:P:118:GLN:NE2 | 1.69 | 0.90 |
| 26:X:37:LEU:HD13 | 26:X:85:VAL:HG21 | 1.52 | 0.90 |
| 11:I:95:LEU:HD22 | 11:I:99:GLN:HB3 | 1.49 | 0.90 |
| 22:T:71:VAL:HG11 | 22:T:90:PRO:HB3 | 1.53 | 0.90 |
| 14:L:79:ASP:HB3 | 37:L:8862:HOH:O | 1.70 | 0.90 |
| 4:B:238:ASN:HD22 | 4:B:240:GLY:H | 0.92 | 0.90 |
| 11:I:107:LYS:HD2 | 11:I:110:ASP:HB2 | 1.51 | 0.90 |
| 10:H:59:GLN:HE21 | 10:H:129:ARG:HE | 1.19 | 0.90 |
| 1:0:56:G:H5'' | 24:V:50:ARG:HH12 | 1.37 | 0.89 |
| 20:R:18:LEU:HB2 | 20:R:143:VAL:HG13 | 1.53 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:M:164:THR:HG23 | 15:M:167:GLY:H | 1.35 | 0.89 |
| 25:W:88:THR:HG22 | 25:W:89:ASP:H | 1.36 | 0.89 |
| 10:H:59:GLN:NE2 | 10:H:129:ARG:HE | 1.72 | 0.88 |
| 3:A:35:GLY:O | 3:A:36:ASP:HB3 | 1.72 | 0.88 |
| 25:W:6:GLN:HB2 | 25:W:26:ILE:HD12 | 1.55 | 0.88 |
| 1:O:2586:U:H3 | 1:O:2592:G:H22 | 1.20 | 0.87 |
| 1:O:1118:A:H3' | 1:O:1118:A:H8 | 1.39 | 0.87 |
| 6:D:57:THR:HG23 | 6:D:63:ILE:HA | 1.55 | 0.87 |
| 1:O:1835:U:H5 | 1:O:1840:A:N7 | 1.72 | 0.87 |
| 4:B:238:ASN:HD22 | 4:B:240:GLY:N | 1.73 | 0.86 |
| 4:B:217:ARG:HG3 | 4:B:257:THR:HG22 | 1.57 | 0.86 |
| 1:O:2717:C:C2' | 1:O:2718:C:H5'' | 2.06 | 0.86 |
| 18:P:115:SER:N | 18:P:118:GLN:HE21 | 1.74 | 0.85 |
| 6:D:146:LYS:NZ | 16:N:107:ASN:HD21 | 1.73 | 0.85 |
| 3:A:85:SER:HA | 37:A:8909:HOH:O | 1.74 | 0.85 |
| 14:L:77:ALA:HB3 | 37:L:8833:HOH:O | 1.75 | 0.85 |
| 24:V:1:THR:HG23 | 24:V:2:VAL:H | 1.40 | 0.85 |
| 4:B:238:ASN:ND2 | 4:B:240:GLY:H | 1.74 | 0.85 |
| 25:W:21:LEU:HD21 | 25:W:48:VAL:HG11 | 1.56 | 0.85 |
| 12:J:105:LEU:HA | 37:J:8866:HOH:O | 1.77 | 0.85 |
| 13:K:29:LEU:HB3 | 13:K:55:VAL:HG11 | 1.57 | 0.85 |
| 4:B:55:ASN:HB3 | 4:B:63:GLU:HA | 1.57 | 0.85 |
| 4:B:320:GLN:NE2 | 4:B:321:PRO:HD2 | 1.92 | 0.85 |
| 1:O:182:G:H5' | 37:O:4959:HOH:O | 1.77 | 0.85 |
| 1:O:1162:G:H1' | 11:I:112:LEU:HD11 | 1.59 | 0.85 |
| 1:O:21:G:H5' | 20:R:2:ILE:HA | 1.58 | 0.84 |
| 1:O:870:G:H2' | 1:O:871:G:H5'' | 1.57 | 0.84 |
| 10:H:41:LYS:HE2 | 10:H:45:ASP:HB3 | 1.59 | 0.84 |
| 10:H:168:VAL:HG13 | 37:H:213:HOH:O | 1.76 | 0.84 |
| 4:B:201:ASP:HB2 | 4:B:312:ARG:HD2 | 1.58 | 0.84 |
| 8:F:96:ALA:HA | 37:F:3111:HOH:O | 1.78 | 0.84 |
| 31:3:60:LYS:HG3 | 31:3:61:PRO:HD2 | 1.57 | 0.84 |
| 16:N:23:ARG:HD3 | 37:N:8842:HOH:O | 1.76 | 0.84 |
| 5:C:236:THR:HA | 37:C:8660:HOH:O | 1.77 | 0.83 |
| 10:H:49:GLN:HE21 | 10:H:140:TYR:HE2 | 1.25 | 0.83 |
| 5:C:236:THR:CG2 | 5:C:239:ALA:H | 1.86 | 0.83 |
| 1:O:1118:A:H3' | 1:O:1118:A:C8 | 2.13 | 0.83 |
| 10:H:102:LYS:HD3 | 10:H:122:LYS:HD3 | 1.58 | 0.83 |
| 12:J:107:ASN:ND2 | 12:J:109:TYR:H | 1.76 | 0.83 |
| 8:F:61:MET:HB3 | 15:M:19:GLN:OE1 | 1.79 | 0.82 |
| 18:P:59:ARG:NH2 | 18:P:66:GLN:HE22 | 1.77 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:H:62:HIS:HA | 10:H:65:LEU:HD23 | 1.59 | 0.82 |
| 7:E:20:ILE:HD11 | 7:E:40:VAL:HG11 | 1.62 | 0.82 |
| 1:0:1118:A:H62 | 1:0:1244:U:H3 | 1.27 | 0.82 |
| 30:2:41:HIS:HD2 | 30:2:44:ARG:H | 1.27 | 0.82 |
| 1:0:1205:U:H2' | 1:0:1206:U:H5' | 1.62 | 0.82 |
| 14:L:149:ARG:O | 14:L:150:GLN:HB2 | 1.79 | 0.82 |
| 1:0:1834:C:H2' | 1:0:1840:A:N6 | 1.94 | 0.82 |
| 3:A:94:LEU:HG | 3:A:99:ILE:HD11 | 1.59 | 0.82 |
| 4:B:98:THR:HG22 | 4:B:99:GLU:H | 1.45 | 0.82 |
| 1:0:541:C:C2' | 1:0:542:A:H5'' | 2.10 | 0.81 |
| 4:B:7:ARG:NH1 | 4:B:11:LEU:HD21 | 1.94 | 0.81 |
| 1:0:1184:C:H1' | 37:0:7238:HOH:O | 1.79 | 0.81 |
| 1:0:2506:A:HO2' | 1:0:2507:G:H8 | 1.28 | 0.81 |
| 14:L:121:ILE:HG12 | 14:L:141:GLU:HB2 | 1.61 | 0.81 |
| 37:0:5022:HOH:O | 13:K:39:GLY:HA2 | 1.80 | 0.81 |
| 24:V:39:ALA:H | 24:V:40:PRO:HD2 | 1.46 | 0.81 |
| 13:K:74:VAL:HG11 | 13:K:113:ILE:HG12 | 1.61 | 0.81 |
| 3:A:192:VAL:HG12 | 3:A:207:GLN:HB3 | 1.60 | 0.81 |
| 1:0:1751:G:H2' | 1:0:1752:G:H5'' | 1.60 | 0.81 |
| 13:K:98:VAL:HG11 | 13:K:102:GLU:HA | 1.61 | 0.81 |
| 22:T:52:ARG:HB2 | 22:T:95:ASN:HB3 | 1.63 | 0.81 |
| 6:D:25:MET:HE2 | 6:D:41:LEU:HG | 1.63 | 0.81 |
| 16:N:151:ASP:O | 16:N:154:LEU:HB2 | 1.81 | 0.81 |
| 6:D:136:ARG:HD2 | 6:D:155:HIS:O | 1.80 | 0.80 |
| 1:0:542:A:H5' | 1:0:542:A:H8 | 1.46 | 0.80 |
| 29:1:21:ARG:HD2 | 29:1:39:PHE:HB2 | 1.62 | 0.80 |
| 1:0:2756:U:H3 | 1:0:2896:A:H2 | 1.30 | 0.80 |
| 1:0:2908:A:H2' | 1:0:2909:G:O4' | 1.81 | 0.80 |
| 2:9:14:G:H5' | 2:9:14:G:H8 | 1.47 | 0.80 |
| 25:W:21:LEU:HD21 | 25:W:48:VAL:CG1 | 2.11 | 0.80 |
| 2:9:56:A:H2' | 2:9:57:A:H5'' | 1.64 | 0.80 |
| 4:B:41:PHE:HB3 | 4:B:190:MET:HE1 | 1.62 | 0.80 |
| 18:P:115:SER:OG | 18:P:118:GLN:HG3 | 1.82 | 0.79 |
| 6:D:25:MET:HE1 | 6:D:37:ALA:HB1 | 1.64 | 0.79 |
| 5:C:27:ARG:HG2 | 5:C:30:LEU:HD12 | 1.63 | 0.79 |
| 14:L:55:GLN:HA | 14:L:58:GLN:HE21 | 1.47 | 0.79 |
| 9:G:64:ASN:N | 9:G:64:ASN:HD22 | 1.79 | 0.79 |
| 1:0:2364:A:H5'' | 19:Q:15:LYS:HD3 | 1.64 | 0.79 |
| 13:K:81:ARG:HB2 | 13:K:87:ARG:HH11 | 1.46 | 0.79 |
| 5:C:140:VAL:HB | 37:C:8660:HOH:O | 1.82 | 0.79 |
| 37:0:5326:HOH:O | 15:M:58:GLN:HG3 | 1.82 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:S:22:ASN:ND2 | 21:S:68:LEU:HB2 | 1.98 | 0.79 |
| 5:C:2:GLN:HB3 | 37:C:8588:HOH:O | 1.83 | 0.79 |
| 1:0:1119:G:H2' | 12:J:52:GLN:NE2 | 1.97 | 0.79 |
| 1:0:1116:U:H3 | 1:0:1246:A:H62 | 1.27 | 0.79 |
| 37:0:5256:HOH:O | 9:G:12:ILE:HA | 1.82 | 0.79 |
| 4:B:177:HIS:O | 4:B:181:ILE:HG13 | 1.82 | 0.79 |
| 13:K:10:GLN:HE21 | 13:K:10:GLN:H | 0.84 | 0.79 |
| 9:G:27:ILE:HD13 | 9:G:71:LEU:HD23 | 1.63 | 0.79 |
| 21:S:57:THR:HG22 | 21:S:59:ASP:H | 1.47 | 0.79 |
| 1:0:877:G:H5' | 1:0:878:G:OP1 | 1.83 | 0.78 |
| 1:0:871:G:C5' | 1:0:871:G:H8 | 1.97 | 0.78 |
| 1:0:1206:U:H5' | 1:0:1206:U:H6 | 1.48 | 0.78 |
| 16:N:151:ASP:OD1 | 16:N:154:LEU:HD13 | 1.84 | 0.78 |
| 8:F:99:THR:HA | 37:F:3461:HOH:O | 1.82 | 0.78 |
| 13:K:118:ALA:HA | 13:K:125:ALA:HB2 | 1.64 | 0.78 |
| 1:0:1684:A:H1' | 30:2:43:ARG:HH22 | 1.49 | 0.78 |
| 16:N:169:PRO:O | 16:N:172:PHE:HB3 | 1.84 | 0.78 |
| 37:C:8572:HOH:O | 22:T:2:LYS:HE2 | 1.81 | 0.78 |
| 6:D:94:ALA:CB | 6:D:97:GLN:HE21 | 1.96 | 0.78 |
| 37:9:8671:HOH:O | 16:N:147:ILE:HB | 1.84 | 0.78 |
| 25:W:4:LEU:HD23 | 25:W:54:PHE:HB3 | 1.65 | 0.78 |
| 6:D:104:PHE:HE2 | 6:D:132:VAL:HB | 1.48 | 0.78 |
| 10:H:146:ALA:O | 10:H:149:VAL:HG12 | 1.84 | 0.78 |
| 4:B:304:PRO:HD2 | 4:B:307:ARG:HD2 | 1.65 | 0.77 |
| 31:3:25:VAL:HG22 | 31:3:68:LYS:HG3 | 1.64 | 0.77 |
| 29:1:10:LYS:HG3 | 37:1:2979:HOH:O | 1.84 | 0.77 |
| 1:0:272:A:H5' | 1:0:273:G:OP2 | 1.83 | 0.77 |
| 3:A:121:ALA:O | 3:A:124:VAL:HG22 | 1.84 | 0.77 |
| 10:H:165:ARG:HD3 | 37:H:238:HOH:O | 1.84 | 0.77 |
| 12:J:19:MET:HE3 | 12:J:132:LEU:HD11 | 1.64 | 0.77 |
| 26:X:43:VAL:HG12 | 26:X:44:ASP:H | 1.49 | 0.77 |
| 16:N:80:SER:HB2 | 37:N:8832:HOH:O | 1.83 | 0.77 |
| 1:0:21:G:C5' | 20:R:2:ILE:HA | 2.14 | 0.77 |
| 6:D:28:GLY:HA2 | 6:D:69:ILE:HG23 | 1.65 | 0.77 |
| 4:B:162:MET:HG3 | 4:B:310:ARG:HD3 | 1.67 | 0.77 |
| 6:D:99:ASP:CG | 6:D:100:ASP:H | 1.88 | 0.77 |
| 1:0:272:A:H3' | 37:0:7298:HOH:O | 1.85 | 0.77 |
| 8:F:91:VAL:HG12 | 8:F:92:GLY:H | 1.50 | 0.77 |
| 3:A:37:VAL:HG23 | 3:A:38:ILE:H | 1.49 | 0.77 |
| 8:F:63:ILE:HB | 8:F:64:PRO:HD3 | 1.65 | 0.77 |
| 1:0:1474:C:C6 | 1:0:1474:C:H5' | 2.20 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 24:V:12:THR:HG22 | 24:V:15:GLU:CG | 2.15 | 0.76 |
| 2:9:92:G:H2' | 2:9:93:A:C8 | 2.20 | 0.76 |
| 37:0:7226:HOH:O | 4:B:211:THR:HG21 | 1.85 | 0.76 |
| 3:A:223:ARG:HG3 | 37:A:8892:HOH:O | 1.85 | 0.76 |
| 27:Y:219:GLU:HG3 | 27:Y:220:GLU:N | 1.99 | 0.76 |
| 5:C:78:ARG:HH11 | 5:C:78:ARG:HG3 | 1.50 | 0.76 |
| 29:1:8:GLN:HE22 | 29:1:11:LYS:NZ | 1.84 | 0.76 |
| 27:Y:216:ARG:HD3 | 37:Y:8874:HOH:O | 1.86 | 0.76 |
| 21:S:22:ASN:HD21 | 21:S:68:LEU:HB2 | 1.51 | 0.76 |
| 1:0:559:U:H6 | 1:0:559:U:H5' | 1.50 | 0.76 |
| 16:N:7:LYS:HE3 | 19:Q:21:ARG:O | 1.86 | 0.76 |
| 37:0:4030:HOH:O | 30:2:38:LYS:HE3 | 1.84 | 0.76 |
| 8:F:110:ASP:O | 8:F:114:LYS:HG3 | 1.86 | 0.76 |
| 1:0:545:G:H8 | 1:0:545:G:H5' | 1.50 | 0.75 |
| 1:0:2426:G:H1' | 37:0:5876:HOH:O | 1.87 | 0.75 |
| 1:0:1979:G:H2' | 37:0:9091:HOH:O | 1.85 | 0.75 |
| 5:C:16:VAL:HG12 | 5:C:17:ASP:H | 1.52 | 0.75 |
| 4:B:312:ARG:HD3 | 4:B:315:VAL:HG13 | 1.68 | 0.75 |
| 26:X:43:VAL:HG11 | 26:X:82:GLU:HA | 1.66 | 0.75 |
| 5:C:25:PRO:HD2 | 37:C:8638:HOH:O | 1.84 | 0.75 |
| 1:0:1634:G:H3' | 37:0:3693:HOH:O | 1.85 | 0.75 |
| 1:0:1450:C:H4' | 1:0:1451:C:OP2 | 1.85 | 0.75 |
| 1:0:2243:C:H5'' | 37:0:3549:HOH:O | 1.86 | 0.75 |
| 1:0:282:C:H1' | 1:0:368:C:N4 | 2.01 | 0.75 |
| 6:D:104:PHE:CE2 | 6:D:132:VAL:HB | 2.22 | 0.75 |
| 14:L:61:ALA:HA | 37:L:8868:HOH:O | 1.85 | 0.75 |
| 1:0:1593:C:H5' | 18:P:116:SER:O | 1.86 | 0.75 |
| 1:0:506:G:H22 | 1:0:509:A:H5' | 1.51 | 0.75 |
| 1:0:1446:U:H2' | 21:S:55:GLN:NE2 | 2.02 | 0.75 |
| 1:0:1919:A:H4' | 37:0:4649:HOH:O | 1.86 | 0.75 |
| 14:L:138:GLY:HA3 | 37:L:8857:HOH:O | 1.86 | 0.75 |
| 6:D:174:VAL:HG12 | 37:D:6555:HOH:O | 1.87 | 0.74 |
| 14:L:80:ASP:HB2 | 14:L:90:ARG:O | 1.87 | 0.74 |
| 1:0:130:C:H2' | 37:0:9961:HOH:O | 1.86 | 0.74 |
| 1:0:154:C:H2' | 1:0:155:C:H6 | 1.52 | 0.74 |
| 29:1:25:LYS:HD2 | 30:2:49:GLU:N | 2.00 | 0.74 |
| 21:S:37:VAL:O | 21:S:41:VAL:HG23 | 1.87 | 0.74 |
| 2:9:75:G:H1 | 2:9:106:U:H3 | 1.34 | 0.74 |
| 6:D:99:ASP:HA | 37:D:5675:HOH:O | 1.88 | 0.74 |
| 1:0:2769:C:H2' | 1:0:2770:G:O4' | 1.87 | 0.74 |
| 1:0:2578:G:H5' | 1:0:2578:G:H8 | 1.52 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:V:56:ILE:O | 24:V:60:GLN:HG3 | 1.88 | 0.74 |
| 18:P:59:ARG:HH22 | 18:P:66:GLN:HE22 | 1.33 | 0.74 |
| 30:2:41:HIS:H | 30:2:45:ASN:HD22 | 1.31 | 0.74 |
| 8:F:46:GLU:O | 8:F:73:PRO:HD2 | 1.87 | 0.74 |
| 23:U:9:CYS:HA | 23:U:52:THR:HG23 | 1.69 | 0.74 |
| 1:0:821:U:H2' | 1:0:822:C:H6 | 1.51 | 0.74 |
| 25:W:72:PRO:HG2 | 25:W:77:ALA:HB3 | 1.68 | 0.74 |
| 1:0:2748:G:H5' | 37:0:7309:HOH:O | 1.87 | 0.74 |
| 7:E:43:ASP:HA | 37:E:5864:HOH:O | 1.87 | 0.74 |
| 1:0:200:C:H2' | 37:0:3243:HOH:O | 1.87 | 0.74 |
| 1:0:100:C:H4' | 22:T:16:LEU:HB2 | 1.67 | 0.74 |
| 20:R:129:ALA:O | 20:R:130:MET:HB2 | 1.87 | 0.74 |
| 6:D:99:ASP:HB3 | 6:D:103:ASN:H | 1.53 | 0.74 |
| 5:C:184:ARG:HG2 | 37:C:8673:HOH:O | 1.88 | 0.74 |
| 16:N:48:VAL:CG1 | 16:N:55:ASP:HB3 | 2.17 | 0.74 |
| 1:0:2004:U:H4' | 37:0:5105:HOH:O | 1.86 | 0.74 |
| 1:0:541:C:H2' | 1:0:542:A:C5' | 2.18 | 0.74 |
| 18:P:13:VAL:HG21 | 18:P:41:ARG:HG2 | 1.69 | 0.74 |
| 21:S:43:GLU:HB3 | 37:S:8543:HOH:O | 1.88 | 0.73 |
| 22:T:32:ARG:NH1 | 22:T:38:ARG:HH12 | 1.85 | 0.73 |
| 1:0:236:A:H4' | 1:0:237:G:OP1 | 1.87 | 0.73 |
| 21:S:57:THR:HG22 | 21:S:59:ASP:N | 2.03 | 0.73 |
| 37:B:8852:HOH:O | 12:J:104:TYR:HA | 1.87 | 0.73 |
| 1:0:794:U:H3 | 1:0:819:A:H61 | 1.35 | 0.73 |
| 16:N:119:GLN:O | 16:N:123:ILE:HG13 | 1.89 | 0.73 |
| 1:0:1835:U:C5 | 1:0:1840:A:N7 | 2.55 | 0.73 |
| 1:0:544:G:H2' | 1:0:545:G:H5'' | 1.70 | 0.73 |
| 4:B:179:LEU:O | 4:B:183:GLU:HG2 | 1.87 | 0.73 |
| 25:W:88:THR:HB | 37:W:6679:HOH:O | 1.89 | 0.73 |
| 9:G:23:ILE:O | 9:G:27:ILE:HG13 | 1.88 | 0.73 |
| 13:K:14:LYS:HB2 | 13:K:45:PRO:HG2 | 1.71 | 0.73 |
| 1:0:2332:A:H5' | 6:D:56:ARG:HH22 | 1.53 | 0.72 |
| 12:J:45:VAL:HG23 | 12:J:130:VAL:O | 1.89 | 0.72 |
| 4:B:132:HIS:HB2 | 4:B:137:LEU:HD22 | 1.71 | 0.72 |
| 13:K:32:ILE:HD11 | 13:K:56:SER:HB2 | 1.72 | 0.72 |
| 13:K:74:VAL:CG1 | 13:K:113:ILE:HG12 | 2.20 | 0.72 |
| 1:0:2840:A:OP1 | 4:B:211:THR:HG23 | 1.88 | 0.72 |
| 1:0:2851:G:O2' | 1:0:2852:A:H5' | 1.88 | 0.72 |
| 20:R:125:ARG:O | 20:R:126:LYS:HB2 | 1.89 | 0.72 |
| 4:B:235:ARG:HA | 37:B:8895:HOH:O | 1.89 | 0.72 |
| 1:0:2862:G:H4' | 4:B:336:GLN:O | 1.89 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1328:A:OP1 | 27:Y:169:ARG:HD2 | 1.89 | 0.72 |
| 29:1:45:ARG:HB3 | 37:1:988:HOH:O | 1.89 | 0.72 |
| 10:H:61:ARG:HH11 | 10:H:61:ARG:HG3 | 1.54 | 0.72 |
| 4:B:18:ARG:HG3 | 4:B:256:GLN:HG3 | 1.70 | 0.72 |
| 5:C:145:GLU:HG3 | 37:C:8578:HOH:O | 1.88 | 0.72 |
| 16:N:132:ASN:O | 16:N:135:VAL:HG12 | 1.88 | 0.72 |
| 1:0:2524:G:H21 | 1:0:2526:C:N4 | 1.86 | 0.72 |
| 1:0:2812:A:H2 | 1:0:2814:A:H62 | 1.35 | 0.72 |
| 25:W:130:HIS:O | 25:W:136:GLY:HA3 | 1.90 | 0.72 |
| 37:0:3789:HOH:O | 5:C:188:ARG:HD3 | 1.89 | 0.72 |
| 1:0:944:G:H21 | 25:W:44:MET:CE | 2.03 | 0.72 |
| 3:A:153:ARG:HH11 | 3:A:153:ARG:HB2 | 1.54 | 0.72 |
| 1:0:1234:U:N3 | 4:B:244:PRO:HB3 | 2.04 | 0.72 |
| 5:C:127:ARG:HH21 | 5:C:225:PRO:HG2 | 1.55 | 0.72 |
| 1:0:558:C:H2' | 1:0:559:U:H5' | 1.71 | 0.72 |
| 25:W:82:GLU:HB2 | 37:W:2749:HOH:O | 1.89 | 0.72 |
| 37:0:7197:HOH:O | 22:T:9:LYS:HB2 | 1.89 | 0.71 |
| 27:Y:141:THR:HG23 | 37:Y:8896:HOH:O | 1.89 | 0.71 |
| 5:C:246:ARG:NH1 | 5:C:246:ARG:HB3 | 2.04 | 0.71 |
| 23:U:14:GLU:OE1 | 23:U:15:PRO:HD2 | 1.90 | 0.71 |
| 5:C:242:GLU:HG3 | 37:C:8585:HOH:O | 1.90 | 0.71 |
| 6:D:54:ALA:HB1 | 37:D:4069:HOH:O | 1.89 | 0.71 |
| 8:F:91:VAL:HG12 | 8:F:92:GLY:N | 2.04 | 0.71 |
| 5:C:111:VAL:HB | 37:C:8522:HOH:O | 1.90 | 0.71 |
| 1:0:1080:C:H4' | 1:0:1081:A:OP1 | 1.89 | 0.71 |
| 1:0:1278:A:H4' | 1:0:1279:U:C4 | 2.25 | 0.71 |
| 5:C:132:ASP:HB2 | 5:C:161:ASP:HB3 | 1.73 | 0.71 |
| 25:W:64:THR:O | 25:W:68:THR:HG22 | 1.90 | 0.71 |
| 1:0:553:G:P | 27:Y:204:ARG:HH22 | 2.13 | 0.71 |
| 17:O:105:ASN:HD21 | 17:O:109:SER:H | 1.39 | 0.71 |
| 17:O:42:GLU:HB2 | 37:O:2176:HOH:O | 1.89 | 0.71 |
| 4:B:264:GLU:HG2 | 4:B:267:LYS:CE | 2.16 | 0.71 |
| 8:F:58:GLU:HA | 8:F:61:MET:HE2 | 1.72 | 0.71 |
| 3:A:192:VAL:CG1 | 3:A:207:GLN:HB3 | 2.20 | 0.71 |
| 1:0:506:G:H22 | 1:0:509:A:C5' | 2.04 | 0.71 |
| 18:P:64:GLU:HG2 | 37:P:169:HOH:O | 1.91 | 0.71 |
| 1:0:1733:A:H4' | 4:B:212:GLN:HA | 1.73 | 0.71 |
| 9:G:64:ASN:HD22 | 9:G:64:ASN:H | 1.38 | 0.71 |
| 22:T:106:GLU:HG3 | 37:T:4913:HOH:O | 1.88 | 0.71 |
| 1:0:2890:A:H1' | 23:U:56:ARG:NH2 | 2.06 | 0.71 |
| 1:0:1594:C:OP2 | 18:P:120:ARG:HD2 | 1.91 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:2:20:ARG:HH11 | 30:2:20:ARG:CG | 2.04 | 0.71 |
| 4:B:1:PRO:O | 4:B:2:GLN:HB2 | 1.90 | 0.71 |
| 27:Y:186:ARG:HH11 | 27:Y:186:ARG:HG2 | 1.55 | 0.71 |
| 5:C:236:THR:HG21 | 37:C:8578:HOH:O | 1.90 | 0.70 |
| 1:0:459:A:H4' | 37:0:9260:HOH:O | 1.90 | 0.70 |
| 1:0:2548:C:OP2 | 4:B:5:ARG:NH2 | 2.24 | 0.70 |
| 24:V:44:GLY:O | 24:V:48:GLU:HG2 | 1.91 | 0.70 |
| 3:A:217:ARG:HH11 | 3:A:217:ARG:HG3 | 1.55 | 0.70 |
| 4:B:305:ASP:O | 4:B:306:LYS:HB2 | 1.89 | 0.70 |
| 26:X:76:ARG:HH11 | 26:X:76:ARG:HG3 | 1.57 | 0.70 |
| 1:0:1120:U:H6 | 1:0:1120:U:H5' | 1.55 | 0.70 |
| 12:J:19:MET:HE1 | 12:J:132:LEU:HD21 | 1.72 | 0.70 |
| 1:0:285:A:H2' | 1:0:286:U:O4' | 1.90 | 0.70 |
| 1:0:902:G:N7 | 14:L:18:HIS:HD2 | 1.90 | 0.70 |
| 1:0:2850:C:H6 | 1:0:2850:C:H5' | 1.56 | 0.70 |
| 26:X:78:GLU:HG2 | 26:X:79:GLU:H | 1.55 | 0.70 |
| 4:B:332:ASN:HB3 | 37:B:8861:HOH:O | 1.91 | 0.70 |
| 18:P:115:SER:O | 18:P:117:SER:N | 2.23 | 0.70 |
| 12:J:107:ASN:HD21 | 12:J:109:TYR:HB2 | 1.57 | 0.70 |
| 1:0:2506:A:O2' | 1:0:2507:G:H8 | 1.73 | 0.70 |
| 1:0:447:A:P | 22:T:1:SER:HB2 | 2.32 | 0.70 |
| 3:A:217:ARG:HG2 | 3:A:229:ALA:HB2 | 1.74 | 0.70 |
| 4:B:195:ARG:HG2 | 4:B:323:LEU:HD22 | 1.74 | 0.70 |
| 1:0:1205:U:H2' | 1:0:1206:U:C5' | 2.21 | 0.70 |
| 22:T:48:VAL:HG13 | 22:T:97:ARG:O | 1.92 | 0.70 |
| 1:0:1679:C:H5' | 37:0:9135:HOH:O | 1.90 | 0.70 |
| 16:N:163:PHE:HZ | 16:N:171:HIS:HD1 | 1.38 | 0.70 |
| 2:9:73:A:H61 | 2:9:108:C:H42 | 1.39 | 0.70 |
| 10:H:49:GLN:HG3 | 10:H:140:TYR:CD2 | 2.27 | 0.70 |
| 1:0:1596:U:H2' | 1:0:1598:A:OP2 | 1.92 | 0.70 |
| 1:0:1118:A:H2' | 1:0:1120:U:H5'' | 1.75 | 0.69 |
| 12:J:19:MET:CE | 12:J:132:LEU:HD11 | 2.22 | 0.69 |
| 1:0:88:G:H5' | 1:0:88:G:H8 | 1.55 | 0.69 |
| 4:B:36:PRO:HG3 | 4:B:169:GLY:H | 1.56 | 0.69 |
| 1:0:2291:A:C8 | 1:0:2309:C:H5' | 2.26 | 0.69 |
| 2:9:56:A:C2' | 2:9:57:A:H5'' | 2.21 | 0.69 |
| 20:R:72:VAL:CG1 | 20:R:75:TRP:HB3 | 2.22 | 0.69 |
| 37:0:6135:HOH:O | 4:B:298:LYS:HD3 | 1.91 | 0.69 |
| 1:0:1926:G:H2' | 1:0:1927:A:C8 | 2.26 | 0.69 |
| 13:K:98:VAL:CG1 | 13:K:102:GLU:HA | 2.21 | 0.69 |
| 7:E:6:GLU:HA | 7:E:46:THR:HG22 | 1.72 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:22:VAL:HG22 | 6:D:74:THR:HG22 | 1.74 | 0.69 |
| 16:N:152:GLU:C | 16:N:154:LEU:H | 1.92 | 0.69 |
| 9:G:64:ASN:ND2 | 9:G:64:ASN:H | 1.91 | 0.69 |
| 17:O:32:ARG:HH21 | 17:O:35:LYS:CD | 2.05 | 0.69 |
| 1:O:2491:G:H1' | 37:O:6645:HOH:O | 1.92 | 0.69 |
| 22:T:35:TYR:CD2 | 22:T:112:LEU:HD22 | 2.28 | 0.69 |
| 27:Y:99:ALA:HB2 | 27:Y:233:TYR:CZ | 2.28 | 0.69 |
| 21:S:81:ILE:HG12 | 37:S:8536:HOH:O | 1.91 | 0.69 |
| 1:O:2363:G:O2' | 19:Q:11:ARG:HG3 | 1.93 | 0.69 |
| 1:O:2559:C:H4' | 37:O:7025:HOH:O | 1.92 | 0.69 |
| 16:N:11:ARG:HG3 | 16:N:14:ARG:NH1 | 2.07 | 0.69 |
| 26:X:72:VAL:HG22 | 26:X:85:VAL:HG12 | 1.75 | 0.69 |
| 22:T:28:SER:O | 22:T:32:ARG:HG3 | 1.91 | 0.69 |
| 24:V:5:VAL:HG23 | 37:V:2271:HOH:O | 1.93 | 0.69 |
| 15:M:46:LEU:HG | 37:M:8919:HOH:O | 1.92 | 0.69 |
| 1:O:1119:G:N2 | 1:O:1246:A:C2 | 2.60 | 0.69 |
| 21:S:33:SER:OG | 21:S:36:GLU:HG3 | 1.92 | 0.69 |
| 1:O:839:C:H4' | 1:O:840[A]:U:H5' | 1.73 | 0.69 |
| 29:1:42:SER:HB2 | 37:1:354:HOH:O | 1.92 | 0.69 |
| 14:L:73:VAL:HG21 | 14:L:116:HIS:CD2 | 2.27 | 0.69 |
| 1:O:839:C:H5'' | 1:O:840[B]:U:OP1 | 1.93 | 0.69 |
| 2:9:35:C:H5'' | 37:9:8659:HOH:O | 1.91 | 0.69 |
| 1:O:1130:U:H5' | 37:O:7441:HOH:O | 1.91 | 0.69 |
| 1:O:1589:G:N2 | 1:O:1605:G:H1' | 2.07 | 0.69 |
| 24:V:12:THR:HG23 | 24:V:14:ALA:H | 1.57 | 0.69 |
| 1:O:1180:U:H4' | 11:I:86:GLU:HG2 | 1.74 | 0.69 |
| 25:W:13:MET:HE1 | 25:W:18:GLN:HA | 1.73 | 0.69 |
| 3:A:36:ASP:HB2 | 3:A:84:VAL:N | 2.09 | 0.68 |
| 2:9:56:A:C3' | 2:9:57:A:H5'' | 2.23 | 0.68 |
| 4:B:119:HIS:O | 4:B:121:PRO:HD3 | 1.93 | 0.68 |
| 37:O:4504:HOH:O | 28:Z:51:GLY:HA3 | 1.93 | 0.68 |
| 27:Y:133:HIS:HD2 | 37:Y:8886:HOH:O | 1.76 | 0.68 |
| 15:M:80:GLY:O | 15:M:81:ARG:HD2 | 1.94 | 0.68 |
| 3:A:36:ASP:HA | 3:A:83:GLY:HA3 | 1.75 | 0.68 |
| 4:B:5:ARG:HD2 | 4:B:8:LYS:NZ | 2.09 | 0.68 |
| 1:O:1666:C:H2' | 1:O:1667:A:H8 | 1.59 | 0.68 |
| 17:O:32:ARG:HH21 | 17:O:35:LYS:HD2 | 1.57 | 0.68 |
| 9:G:63:ARG:N | 37:G:2569:HOH:O | 2.26 | 0.68 |
| 25:W:39:ASP:HB2 | 37:W:3580:HOH:O | 1.93 | 0.68 |
| 12:J:52:GLN:HG3 | 12:J:53:ILE:N | 2.09 | 0.68 |
| 13:K:74:VAL:HG13 | 13:K:113:ILE:HG23 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2392:C:H4' | 37:Q:2875:HOH:O | 1.91 | 0.68 |
| 1:0:1429:U:H1' | 20:R:132:ARG:NH1 | 2.09 | 0.68 |
| 21:S:33:SER:O | 21:S:37:VAL:HG23 | 1.94 | 0.68 |
| 22:T:101:LEU:HD13 | 22:T:112:LEU:HD11 | 1.76 | 0.68 |
| 28:Z:37:HIS:HB2 | 28:Z:47:VAL:HB | 1.75 | 0.68 |
| 1:0:1187:U:O2' | 1:0:1189:A:H2 | 1.75 | 0.68 |
| 10:H:12:ILE:HD12 | 10:H:57:THR:HG22 | 1.76 | 0.68 |
| 1:0:2502:C:C2' | 1:0:2503:A:H5' | 2.22 | 0.68 |
| 4:B:152:PRO:HD2 | 37:B:8931:HOH:O | 1.92 | 0.68 |
| 20:R:62:HIS:NE2 | 37:R:8831:HOH:O | 2.26 | 0.68 |
| 2:9:6:C:H5'' | 16:N:37:ARG:HH12 | 1.57 | 0.67 |
| 1:0:2570:G:H5'' | 37:0:4714:HOH:O | 1.93 | 0.67 |
| 27:Y:212:ARG:HD2 | 37:Y:8909:HOH:O | 1.94 | 0.67 |
| 16:N:86:LEU:HD12 | 16:N:125:ALA:HB2 | 1.75 | 0.67 |
| 1:0:1741:U:H5' | 1:0:1742:A:OP1 | 1.94 | 0.67 |
| 6:D:63:ILE:HG13 | 6:D:64:ARG:N | 2.08 | 0.67 |
| 14:L:104:ASP:O | 14:L:105:TYR:HB3 | 1.93 | 0.67 |
| 22:T:43:ASN:HD22 | 22:T:108:ARG:CZ | 2.07 | 0.67 |
| 11:I:68:PRO:HB2 | 11:I:69:PRO:HD2 | 1.76 | 0.67 |
| 17:O:44:ASN:OD1 | 17:O:65:LEU:HB2 | 1.93 | 0.67 |
| 16:N:83:LEU:HD13 | 16:N:175:LEU:HD23 | 1.75 | 0.67 |
| 31:3:65:THR:HG22 | 31:3:67:LEU:HG | 1.76 | 0.67 |
| 4:B:198:GLU:HA | 37:B:8958:HOH:O | 1.93 | 0.67 |
| 16:N:71:TRP:HE3 | 16:N:175:LEU:HD22 | 1.60 | 0.67 |
| 4:B:297:VAL:HB | 37:B:8905:HOH:O | 1.94 | 0.67 |
| 5:C:154:VAL:O | 5:C:158:GLU:HG3 | 1.95 | 0.67 |
| 1:0:870:G:C2' | 1:0:871:G:H5'' | 2.23 | 0.67 |
| 26:X:43:VAL:HG12 | 26:X:44:ASP:N | 2.08 | 0.67 |
| 1:0:583:C:H2' | 1:0:584:U:H6 | 1.60 | 0.67 |
| 17:O:49:GLU:OE1 | 17:O:72:LYS:HG3 | 1.94 | 0.67 |
| 12:J:74:ARG:O | 12:J:78:ILE:HG12 | 1.95 | 0.67 |
| 15:M:28:GLN:O | 15:M:32:ARG:HG3 | 1.94 | 0.67 |
| 4:B:84:LEU:HD23 | 4:B:178:ALA:HB1 | 1.77 | 0.67 |
| 22:T:48:VAL:HG11 | 22:T:96:VAL:HG13 | 1.76 | 0.67 |
| 1:0:1636:G:O2' | 1:0:1637:A:H5' | 1.94 | 0.67 |
| 24:V:64:GLY:O | 24:V:65:ASP:HB2 | 1.94 | 0.67 |
| 8:F:27:GLY:HA3 | 8:F:101:ALA:O | 1.95 | 0.67 |
| 3:A:5:GLN:HB3 | 37:A:8894:HOH:O | 1.94 | 0.67 |
| 5:C:16:VAL:HG12 | 5:C:17:ASP:N | 2.10 | 0.67 |
| 1:0:2526:C:O2' | 1:0:2527:U:H5' | 1.94 | 0.67 |
| 1:0:814:G:H4' | 37:0:9934:HOH:O | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:2346:C:O2' | 6:D:52:THR:HG21 | 1.95 | 0.67 |
| 14:L:148:GLU:HA | 37:L:8876:HOH:O | 1.95 | 0.67 |
| 2:9:14:G:C8 | 2:9:14:G:H5' | 2.28 | 0.67 |
| 1:O:840[B]:U:H5' | 37:O:4709:HOH:O | 1.95 | 0.67 |
| 1:O:1419:U:H2' | 1:O:1685:A:C2 | 2.30 | 0.67 |
| 17:O:87:THR:O | 17:O:91:GLN:HG3 | 1.95 | 0.67 |
| 8:F:79:GLN:HB2 | 8:F:82:ASP:OD2 | 1.96 | 0.66 |
| 1:O:308:U:H5' | 1:O:309:C:OP1 | 1.94 | 0.66 |
| 1:O:136:C:H2' | 1:O:137:U:O4' | 1.94 | 0.66 |
| 4:B:86:ALA:HA | 37:B:8880:HOH:O | 1.94 | 0.66 |
| 20:R:39:THR:HB | 20:R:42:GLU:HG3 | 1.76 | 0.66 |
| 1:O:2637:A:H5' | 37:O:9086:HOH:O | 1.94 | 0.66 |
| 1:O:1244:U:OP1 | 12:J:18:ILE:HD13 | 1.95 | 0.66 |
| 25:W:4:LEU:HD22 | 25:W:52:VAL:CG2 | 2.24 | 0.66 |
| 1:O:1043:C:H2' | 37:O:7091:HOH:O | 1.94 | 0.66 |
| 4:B:190:MET:HE2 | 4:B:194:PHE:CD1 | 2.30 | 0.66 |
| 1:O:1964:U:O2 | 1:O:1964:U:H2' | 1.94 | 0.66 |
| 11:I:111:LEU:HD22 | 11:I:122:GLU:OE1 | 1.95 | 0.66 |
| 10:H:59:GLN:HE21 | 10:H:129:ARG:NE | 1.91 | 0.66 |
| 2:9:64:C:H2' | 2:9:65:A:H5' | 1.78 | 0.66 |
| 11:I:94:ASP:OD1 | 11:I:133:THR:HB | 1.96 | 0.66 |
| 1:O:21:G:H4' | 20:R:2:ILE:HG22 | 1.78 | 0.66 |
| 1:O:1181:A:H2' | 1:O:1182:C:H5' | 1.76 | 0.66 |
| 7:E:11:VAL:HG12 | 7:E:12:ASP:N | 2.10 | 0.66 |
| 10:H:26:ILE:HA | 10:H:123:ILE:HG21 | 1.77 | 0.66 |
| 16:N:154:LEU:O | 16:N:155:GLU:HB3 | 1.95 | 0.66 |
| 25:W:38:THR:HG22 | 25:W:39:ASP:N | 2.09 | 0.66 |
| 1:O:1717:A:H5'' | 18:P:54:LYS:HB2 | 1.78 | 0.66 |
| 10:H:43:ALA:O | 10:H:170:ARG:NH1 | 2.28 | 0.66 |
| 6:D:135:VAL:HG21 | 6:D:139:TYR:CD1 | 2.31 | 0.66 |
| 1:O:1926:G:H2' | 1:O:1927:A:H8 | 1.60 | 0.66 |
| 15:M:134:ILE:HG23 | 15:M:141:ILE:HD13 | 1.77 | 0.66 |
| 13:K:22:ASP:HB2 | 37:K:5264:HOH:O | 1.96 | 0.66 |
| 30:2:40:ARG:CD | 30:2:47:THR:HG22 | 2.24 | 0.66 |
| 15:M:164:THR:HG23 | 15:M:167:GLY:N | 2.10 | 0.66 |
| 25:W:21:LEU:HD22 | 25:W:26:ILE:CD1 | 2.26 | 0.66 |
| 4:B:98:THR:HG22 | 4:B:99:GLU:N | 2.10 | 0.66 |
| 23:U:17:THR:HG22 | 23:U:18:GLY:N | 2.10 | 0.66 |
| 1:O:1589:G:H22 | 1:O:1605:G:H1' | 1.60 | 0.66 |
| 19:Q:26:PRO:O | 19:Q:30:VAL:HG23 | 1.95 | 0.66 |
| 5:C:76:ARG:CB | 5:C:76:ARG:HH11 | 2.08 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:134:LEU:HD11 | 6:D:166:ILE:HD11 | 1.76 | 0.66 |
| 3:A:88:ILE:HG22 | 3:A:88:ILE:O | 1.94 | 0.66 |
| 18:P:143:ALA:HA | 37:P:193:HOH:O | 1.95 | 0.66 |
| 25:W:88:THR:HG23 | 25:W:110:GLN:HB3 | 1.78 | 0.66 |
| 23:U:52:THR:HG22 | 23:U:54:THR:H | 1.60 | 0.66 |
| 10:H:12:ILE:HG22 | 10:H:12:ILE:O | 1.96 | 0.66 |
| 1:O:1362:U:H5' | 37:O:3068:HOH:O | 1.96 | 0.66 |
| 13:K:62:PRO:HG3 | 13:K:65:ARG:HH21 | 1.59 | 0.66 |
| 1:O:657:G:H2' | 1:O:658:C:H6 | 1.61 | 0.65 |
| 21:S:17:ASP:HB3 | 21:S:23:LYS:HB2 | 1.78 | 0.65 |
| 1:O:338:C:H4' | 5:C:174:ILE:CD1 | 2.26 | 0.65 |
| 1:O:1116:U:O2' | 1:O:1118:A:H2 | 1.80 | 0.65 |
| 25:W:21:LEU:HD13 | 25:W:26:ILE:HD11 | 1.79 | 0.65 |
| 1:O:681:G:N3 | 1:O:681:G:H5' | 2.11 | 0.65 |
| 1:O:111:C:O2' | 29:1:20:ARG:HG2 | 1.96 | 0.65 |
| 1:O:1319:G:H1' | 37:O:4492:HOH:O | 1.95 | 0.65 |
| 15:M:65:VAL:HG21 | 15:M:105:ALA:HB2 | 1.78 | 0.65 |
| 1:O:2053:G:H4' | 20:R:136:TRP:CE3 | 2.31 | 0.65 |
| 1:O:2301:A:H5'' | 1:O:2302:A:H5' | 1.78 | 0.65 |
| 5:C:236:THR:H | 5:C:239:ALA:HB3 | 1.61 | 0.65 |
| 3:A:81:GLN:HB2 | 3:A:92:ASN:HD21 | 1.62 | 0.65 |
| 1:O:1909:A:H2' | 1:O:1910:A:C8 | 2.31 | 0.65 |
| 16:N:4:PRO:HD2 | 37:N:8854:HOH:O | 1.94 | 0.65 |
| 1:O:1790:C:H2' | 1:O:1791:U:H6 | 1.60 | 0.65 |
| 6:D:21:VAL:HG13 | 6:D:132:VAL:HG22 | 1.76 | 0.65 |
| 6:D:166:ILE:HB | 37:D:6326:HOH:O | 1.96 | 0.65 |
| 24:V:27:LEU:HA | 24:V:49:LEU:HD13 | 1.79 | 0.65 |
| 12:J:74:ARG:CB | 12:J:74:ARG:HH11 | 2.06 | 0.65 |
| 1:O:2504:A:H4' | 10:H:74:ARG:HH11 | 1.61 | 0.65 |
| 5:C:246:ARG:HH11 | 5:C:246:ARG:HB3 | 1.59 | 0.65 |
| 16:N:166:ALA:HA | 37:N:8824:HOH:O | 1.95 | 0.65 |
| 16:N:37:ARG:HD3 | 35:N:8807:CL:CL | 2.33 | 0.65 |
| 1:O:450:C:OP1 | 5:C:184:ARG:NH2 | 2.30 | 0.65 |
| 20:R:72:VAL:HG11 | 20:R:75:TRP:HB3 | 1.78 | 0.65 |
| 17:O:14:LEU:HD23 | 17:O:102:ILE:HD11 | 1.77 | 0.65 |
| 4:B:162:MET:HE3 | 4:B:308:LEU:HD21 | 1.79 | 0.65 |
| 17:O:73:ASP:HA | 17:O:92:VAL:O | 1.97 | 0.65 |
| 1:O:1657:A:H2' | 1:O:1658:A:C8 | 2.32 | 0.65 |
| 8:F:36:THR:HG23 | 8:F:97:ALA:HB2 | 1.78 | 0.65 |
| 1:O:1525:G:H2' | 1:O:1526:A:C8 | 2.32 | 0.65 |
| 6:D:17:ARG:HG2 | 6:D:135:VAL:O | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:657:G:H2' | 1:0:658:C:C6 | 2.32 | 0.65 |
| 1:0:285:A:C2 | 1:0:368:C:H4' | 2.31 | 0.65 |
| 3:A:200:PRO:HD3 | 37:A:8818:HOH:O | 1.95 | 0.65 |
| 1:0:1701:A:H4' | 1:0:1702:U:H5'' | 1.79 | 0.65 |
| 15:M:102:GLU:OE1 | 15:M:164:THR:HG21 | 1.97 | 0.64 |
| 2:9:54:A:O2' | 2:9:55:U:H5' | 1.96 | 0.64 |
| 13:K:81:ARG:HD3 | 13:K:87:ARG:NH1 | 2.12 | 0.64 |
| 7:E:138:ILE:HG22 | 37:E:6457:HOH:O | 1.96 | 0.64 |
| 1:0:199:A:H5'' | 37:0:3331:HOH:O | 1.97 | 0.64 |
| 1:0:246:G:H5' | 37:0:5368:HOH:O | 1.97 | 0.64 |
| 1:0:157:G:H4' | 15:M:95:LYS:HE3 | 1.77 | 0.64 |
| 14:L:114:VAL:HG11 | 37:L:8877:HOH:O | 1.96 | 0.64 |
| 1:0:20:G:H21 | 20:R:117:HIS:HD2 | 1.44 | 0.64 |
| 25:W:52:VAL:HG22 | 25:W:53:ALA:H | 1.61 | 0.64 |
| 1:0:2272:G:H5' | 3:A:223:ARG:HB2 | 1.77 | 0.64 |
| 1:0:1428:C:O2' | 20:R:132:ARG:HB2 | 1.96 | 0.64 |
| 9:G:16:LYS:O | 9:G:20:VAL:HG23 | 1.98 | 0.64 |
| 1:0:2679:G:H2' | 1:0:2681:A:OP2 | 1.97 | 0.64 |
| 4:B:51:VAL:CG1 | 4:B:53:LEU:HD13 | 2.26 | 0.64 |
| 27:Y:187:VAL:HG12 | 27:Y:205:ILE:HA | 1.79 | 0.64 |
| 13:K:109:LEU:HD13 | 13:K:113:ILE:HD11 | 1.79 | 0.64 |
| 10:H:174:LEU:HA | 37:H:225:HOH:O | 1.97 | 0.64 |
| 3:A:94:LEU:N | 3:A:94:LEU:HD23 | 2.12 | 0.64 |
| 1:0:544:G:C2' | 1:0:545:G:H5'' | 2.28 | 0.64 |
| 12:J:126:ASN:HA | 35:J:8801:CL:CL | 2.35 | 0.64 |
| 14:L:143:THR:HG22 | 14:L:145:LEU:H | 1.61 | 0.64 |
| 1:0:1377:C:H6 | 1:0:1377:C:H5' | 1.63 | 0.64 |
| 5:C:107:ARG:NE | 37:C:8666:HOH:O | 2.29 | 0.64 |
| 25:W:6:GLN:HB2 | 25:W:26:ILE:CD1 | 2.28 | 0.64 |
| 1:0:447:A:OP1 | 22:T:2:LYS:HG2 | 1.98 | 0.64 |
| 1:0:1687:C:O2 | 29:1:9:GLY:HA2 | 1.97 | 0.64 |
| 1:0:2904:U:H4' | 26:X:8:ARG:NH1 | 2.13 | 0.64 |
| 25:W:110:GLN:HA | 25:W:110:GLN:HE21 | 1.62 | 0.64 |
| 4:B:62:ARG:HA | 4:B:65:MET:HE3 | 1.80 | 0.64 |
| 15:M:134:ILE:O | 15:M:136:PRO:HD3 | 1.98 | 0.64 |
| 11:I:118:ASN:HA | 11:I:121:LYS:CD | 2.27 | 0.64 |
| 4:B:83:ALA:HA | 4:B:100:VAL:O | 1.96 | 0.64 |
| 26:X:20:GLU:OE1 | 26:X:21:PRO:HD2 | 1.97 | 0.64 |
| 24:V:33:VAL:HG12 | 24:V:38:GLY:HA3 | 1.78 | 0.64 |
| 16:N:78:MET:HB2 | 16:N:79:PRO:HD3 | 1.79 | 0.64 |
| 1:0:1181:A:H5' | 11:I:89:GLU:OE2 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:I:80:PHE:CD2 | 11:I:92:VAL:HG12 | 2.33 | 0.64 |
| 25:W:110:GLN:HA | 25:W:110:GLN:NE2 | 2.13 | 0.64 |
| 4:B:162:MET:CE | 4:B:308:LEU:HD21 | 2.27 | 0.64 |
| 16:N:48:VAL:HG11 | 16:N:55:ASP:HB3 | 1.80 | 0.64 |
| 20:R:40:ALA:O | 20:R:44:VAL:HG23 | 1.98 | 0.64 |
| 25:W:59:GLN:HE22 | 25:W:97:ALA:HB3 | 1.63 | 0.64 |
| 3:A:33:GLU:O | 3:A:34:ASP:HB2 | 1.95 | 0.64 |
| 5:C:14:GLY:O | 5:C:15:GLU:HB3 | 1.97 | 0.64 |
| 2:9:1:U:H4' | 2:9:3:A:OP1 | 1.99 | 0.63 |
| 19:Q:66:LYS:HB2 | 19:Q:70:ALA:O | 1.98 | 0.63 |
| 1:0:621:C:H5' | 27:Y:132:ASP:OD2 | 1.98 | 0.63 |
| 1:0:1804:A:H2' | 1:0:1805:G:C8 | 2.33 | 0.63 |
| 29:1:25:LYS:O | 29:1:25:LYS:HG2 | 1.97 | 0.63 |
| 3:A:36:ASP:HB2 | 3:A:85:SER:H | 1.63 | 0.63 |
| 20:R:53:GLY:HA2 | 20:R:80:TYR:CD2 | 2.33 | 0.63 |
| 37:0:6147:HOH:O | 20:R:33:ARG:HG3 | 1.97 | 0.63 |
| 6:D:63:ILE:HG13 | 6:D:64:ARG:H | 1.60 | 0.63 |
| 28:Z:56:GLN:HG3 | 28:Z:62:TYR:O | 1.98 | 0.63 |
| 1:0:1804:A:H2' | 1:0:1805:G:H8 | 1.63 | 0.63 |
| 25:W:60:GLU:HG2 | 37:W:705:HOH:O | 1.98 | 0.63 |
| 16:N:165:ALA:HA | 37:N:8821:HOH:O | 1.96 | 0.63 |
| 1:0:1116:U:HO2' | 1:0:1118:A:H2 | 1.44 | 0.63 |
| 25:W:52:VAL:HG22 | 25:W:53:ALA:N | 2.13 | 0.63 |
| 1:0:56:G:H5'' | 24:V:50:ARG:NH1 | 2.11 | 0.63 |
| 12:J:75:PRO:HG2 | 12:J:105:LEU:HD21 | 1.80 | 0.63 |
| 10:H:49:GLN:HB3 | 10:H:170:ARG:CG | 2.29 | 0.63 |
| 1:0:2681:A:H4' | 1:0:2682:C:H5' | 1.80 | 0.63 |
| 1:0:653:U:H5'' | 37:O:7674:HOH:O | 1.96 | 0.63 |
| 1:0:2073:G:OP2 | 1:0:2490:A:H5' | 1.99 | 0.63 |
| 9:G:71:LEU:C | 9:G:73:ASP:H | 2.00 | 0.63 |
| 16:N:71:TRP:CE3 | 16:N:175:LEU:HD22 | 2.33 | 0.63 |
| 25:W:81:ASP:OD1 | 25:W:92:ASP:HB2 | 1.99 | 0.63 |
| 1:0:1506:U:H5' | 1:0:1506:U:H6 | 1.64 | 0.63 |
| 1:0:2827:A:H2' | 1:0:2828:G:O4' | 1.99 | 0.63 |
| 4:B:66:GLU:OE1 | 4:B:328:ARG:HD2 | 1.98 | 0.63 |
| 1:0:1603:A:H5' | 1:0:1605:G:O4' | 1.99 | 0.63 |
| 29:1:1:THR:HB | 37:1:6858:HOH:O | 1.99 | 0.63 |
| 4:B:24:PRO:O | 4:B:25:ARG:HD3 | 1.98 | 0.63 |
| 1:0:1168:C:H5' | 11:I:83:GLY:HA3 | 1.80 | 0.63 |
| 1:0:584:U:H3' | 37:0:5879:HOH:O | 1.98 | 0.63 |
| 1:0:753:U:H3' | 37:0:5320:HOH:O | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:115:LEU:HD21 | 5:C:243:VAL:HG13 | 1.81 | 0.63 |
| 5:C:237:GLU:HB2 | 37:C:8640:HOH:O | 1.97 | 0.63 |
| 14:L:140:VAL:HG23 | 37:L:8860:HOH:O | 1.97 | 0.63 |
| 20:R:99:ALA:HB1 | 20:R:109:MET:HE2 | 1.80 | 0.63 |
| 22:T:99:THR:O | 22:T:100:ASP:HB2 | 1.98 | 0.63 |
| 1:0:69:A:H5' | 1:0:69:A:H8 | 1.64 | 0.62 |
| 1:0:1197:G:H21 | 1:0:1202:A:H62 | 1.44 | 0.62 |
| 26:X:37:LEU:CD1 | 26:X:85:VAL:HG21 | 2.27 | 0.62 |
| 3:A:94:LEU:HG | 3:A:99:ILE:CD1 | 2.26 | 0.62 |
| 1:0:69:A:H5' | 1:0:69:A:C8 | 2.34 | 0.62 |
| 1:0:800:G:H4' | 37:0:6831:HOH:O | 1.98 | 0.62 |
| 1:0:1118:A:C3' | 1:0:1118:A:C8 | 2.78 | 0.62 |
| 14:L:90:ARG:HA | 14:L:119:THR:HB | 1.81 | 0.62 |
| 7:E:166:VAL:HG12 | 37:E:3134:HOH:O | 1.98 | 0.62 |
| 2:9:48:C:H4' | 16:N:141:ARG:HH21 | 1.64 | 0.62 |
| 1:0:2459:G:H3' | 37:0:6782:HOH:O | 1.97 | 0.62 |
| 5:C:3:ALA:HA | 37:C:8581:HOH:O | 1.98 | 0.62 |
| 1:0:1632:A:H2' | 1:0:1633:C:H5' | 1.82 | 0.62 |
| 1:0:1221:G:H8 | 37:0:5773:HOH:O | 1.82 | 0.62 |
| 7:E:37:ASP:OD1 | 12:J:125:SER:HB3 | 1.99 | 0.62 |
| 1:0:944:G:H21 | 25:W:44:MET:HE2 | 1.63 | 0.62 |
| 14:L:133:VAL:HB | 37:L:8860:HOH:O | 1.98 | 0.62 |
| 1:0:694:A:H2' | 1:0:695:C:H5' | 1.81 | 0.62 |
| 30:2:49:GLU:HB2 | 37:2:719:HOH:O | 1.98 | 0.62 |
| 1:0:2332:A:H5' | 6:D:56:ARG:NH2 | 2.15 | 0.62 |
| 3:A:43:VAL:O | 3:A:76:VAL:HG13 | 2.00 | 0.62 |
| 8:F:21:GLU:HA | 8:F:24:ARG:HD3 | 1.81 | 0.62 |
| 1:0:2256:G:O2' | 1:0:2257:G:H5' | 2.00 | 0.62 |
| 22:T:71:VAL:HG13 | 22:T:91:LEU:O | 2.00 | 0.62 |
| 13:K:55:VAL:HG12 | 13:K:56:SER:N | 2.15 | 0.62 |
| 12:J:6:PHE:HB3 | 12:J:109:TYR:OH | 1.99 | 0.62 |
| 21:S:45:TYR:HE2 | 21:S:81:ILE:HD13 | 1.65 | 0.62 |
| 1:0:969:G:H1 | 1:0:999:C:N4 | 1.97 | 0.62 |
| 10:H:32:ALA:HB3 | 10:H:69:ARG:HH12 | 1.63 | 0.62 |
| 29:1:25:LYS:CD | 30:2:49:GLU:H | 2.03 | 0.62 |
| 1:0:1285:U:H4' | 25:W:74:GLU:OE1 | 2.00 | 0.62 |
| 1:0:1279:U:O2 | 1:0:1279:U:H2' | 2.00 | 0.62 |
| 6:D:159:PRO:O | 6:D:163:VAL:HG23 | 1.99 | 0.62 |
| 1:0:684:G:H5'' | 37:0:3862:HOH:O | 1.99 | 0.62 |
| 8:F:28:ALA:HB3 | 8:F:99:THR:HG23 | 1.82 | 0.62 |
| 23:U:9:CYS:HA | 23:U:52:THR:CG2 | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:2346:C:H6 | 1:0:2346:C:O5' | 1.83 | 0.62 |
| 16:N:128:ASP:HA | 37:N:8858:HOH:O | 2.00 | 0.62 |
| 1:0:1528:A:H2' | 1:0:1529:G:O4' | 1.99 | 0.62 |
| 8:F:107:ASP:O | 8:F:111:ILE:HG13 | 2.00 | 0.62 |
| 17:O:32:ARG:HB2 | 37:O:4656:HOH:O | 1.98 | 0.61 |
| 7:E:93:MET:O | 7:E:94:GLN:HG3 | 1.99 | 0.61 |
| 1:0:2897:C:H2' | 1:0:2898:G:H8 | 1.65 | 0.61 |
| 4:B:225:GLY:HA3 | 37:B:8866:HOH:O | 1.99 | 0.61 |
| 1:0:2251:G:H2' | 1:0:2252:A:C8 | 2.35 | 0.61 |
| 3:A:194:MET:CE | 3:A:199:HIS:HB2 | 2.29 | 0.61 |
| 14:L:93:VAL:HG12 | 14:L:97:VAL:HG23 | 1.82 | 0.61 |
| 4:B:149:ASP:HB2 | 37:B:8881:HOH:O | 2.00 | 0.61 |
| 8:F:38:LYS:NZ | 15:M:3:SER:HA | 2.14 | 0.61 |
| 13:K:101:ASN:HA | 37:K:6456:HOH:O | 2.00 | 0.61 |
| 22:T:26:THR:HA | 22:T:39:ASN:HB3 | 1.81 | 0.61 |
| 26:X:43:VAL:HG22 | 26:X:76:ARG:NH1 | 2.15 | 0.61 |
| 1:0:154:C:H2' | 1:0:155:C:C6 | 2.33 | 0.61 |
| 8:F:48:VAL:HG23 | 8:F:74:PHE:CB | 2.29 | 0.61 |
| 25:W:73:LEU:O | 25:W:74:GLU:HG3 | 2.01 | 0.61 |
| 37:O:6651:HOH:O | 15:M:178:LYS:HB2 | 2.01 | 0.61 |
| 3:A:220:PRO:HD2 | 3:A:223:ARG:HD3 | 1.82 | 0.61 |
| 1:0:1159:G:H21 | 1:0:1189:A:H8 | 1.48 | 0.61 |
| 26:X:72:VAL:HG22 | 26:X:85:VAL:CG1 | 2.30 | 0.61 |
| 15:M:31:TRP:HA | 15:M:34:GLU:HG3 | 1.81 | 0.61 |
| 1:0:1688:G:H4' | 29:1:8:GLN:HG3 | 1.83 | 0.61 |
| 1:0:1164:U:H3 | 1:0:1192:A:H2 | 1.48 | 0.61 |
| 14:L:136:ALA:HB3 | 37:L:8877:HOH:O | 1.99 | 0.61 |
| 4:B:51:VAL:HG22 | 4:B:330:VAL:HG22 | 1.81 | 0.61 |
| 4:B:54:VAL:HB | 37:B:8913:HOH:O | 2.00 | 0.61 |
| 3:A:211:LYS:HB2 | 37:A:8914:HOH:O | 2.00 | 0.61 |
| 14:L:133:VAL:HA | 37:L:8877:HOH:O | 2.00 | 0.61 |
| 1:0:2488:A:H61 | 1:0:2534:C:H42 | 1.48 | 0.61 |
| 1:0:1008:C:H5'' | 10:H:19:ARG:HH12 | 1.65 | 0.61 |
| 11:I:127:CYS:C | 11:I:129:SER:H | 2.03 | 0.61 |
| 4:B:313:PRO:HA | 37:B:8896:HOH:O | 2.01 | 0.61 |
| 10:H:30:LYS:H | 10:H:62:HIS:CD2 | 2.18 | 0.61 |
| 10:H:88:MET:HA | 10:H:139:ALA:HA | 1.83 | 0.61 |
| 7:E:132:THR:HB | 37:E:2227:HOH:O | 2.00 | 0.61 |
| 25:W:125:HIS:HD2 | 25:W:127:GLY:H | 1.47 | 0.61 |
| 4:B:217:ARG:HG3 | 4:B:257:THR:CG2 | 2.29 | 0.61 |
| 7:E:118:ILE:HG23 | 7:E:144:THR:HG21 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2414:A:H2' | 1:0:2415:A:C8 | 2.35 | 0.61 |
| 37:0:3868:HOH:O | 15:M:97:ILE:HB | 2.00 | 0.61 |
| 1:0:2895:C:H2' | 37:0:9379:HOH:O | 2.00 | 0.61 |
| 1:0:290:C:H2' | 1:0:291:C:H6 | 1.64 | 0.61 |
| 6:D:146:LYS:HE2 | 16:N:107:ASN:ND2 | 2.16 | 0.61 |
| 2:9:34:A:H2' | 2:9:35:C:O4' | 2.00 | 0.61 |
| 1:0:447:A:OP2 | 22:T:1:SER:HB2 | 2.00 | 0.61 |
| 23:U:9:CYS:CA | 23:U:52:THR:HG23 | 2.29 | 0.61 |
| 1:0:856:G:H2' | 37:0:5225:HOH:O | 2.00 | 0.61 |
| 3:A:191:GLY:HA2 | 3:A:194:MET:HE2 | 1.83 | 0.61 |
| 4:B:129:ARG:O | 4:B:133:GLU:HG3 | 2.00 | 0.61 |
| 26:X:31:ILE:O | 26:X:35:GLU:HG3 | 1.99 | 0.61 |
| 13:K:49:LEU:HD21 | 13:K:74:VAL:O | 2.00 | 0.60 |
| 16:N:110:THR:HG22 | 37:N:8848:HOH:O | 2.01 | 0.60 |
| 6:D:55:LYS:O | 6:D:56:ARG:HB2 | 2.01 | 0.60 |
| 16:N:43:VAL:O | 16:N:84:THR:HG21 | 2.01 | 0.60 |
| 27:Y:234:VAL:HG12 | 27:Y:235:GLU:N | 2.16 | 0.60 |
| 18:P:135:ALA:HB1 | 18:P:139:ARG:HH12 | 1.66 | 0.60 |
| 16:N:149:GLU:HA | 16:N:152:GLU:HB2 | 1.83 | 0.60 |
| 1:0:2502:C:H2' | 1:0:2503:A:H5' | 1.83 | 0.60 |
| 21:S:73:ASP:O | 21:S:77:VAL:HG23 | 2.01 | 0.60 |
| 1:0:2421:G:H3' | 1:0:2422:U:H5'' | 1.83 | 0.60 |
| 1:0:1691:A:H5'' | 37:0:9946:HOH:O | 2.01 | 0.60 |
| 1:0:1422:U:H2' | 1:0:1423:C:C6 | 2.37 | 0.60 |
| 5:C:127:ARG:HH11 | 5:C:127:ARG:HG2 | 1.65 | 0.60 |
| 4:B:162:MET:HG3 | 4:B:310:ARG:CD | 2.29 | 0.60 |
| 19:Q:28:ARG:HG2 | 37:Q:4350:HOH:O | 2.00 | 0.60 |
| 3:A:105:VAL:HG13 | 3:A:155:THR:O | 2.02 | 0.60 |
| 1:0:1845:A:OP2 | 3:A:190:ARG:NH1 | 2.35 | 0.60 |
| 1:0:2094:G:H4' | 4:B:245:SER:HB3 | 1.82 | 0.60 |
| 1:0:506:G:H5' | 37:0:5722:HOH:O | 2.00 | 0.60 |
| 14:L:134:GLU:HG3 | 37:L:8860:HOH:O | 2.01 | 0.60 |
| 4:B:154:VAL:HG12 | 4:B:156:LYS:HG2 | 1.84 | 0.60 |
| 1:0:2690:U:O2' | 7:E:111:LYS:HE3 | 2.01 | 0.60 |
| 7:E:172:PRO:HB3 | 37:E:6931:HOH:O | 2.02 | 0.60 |
| 12:J:133:GLY:O | 12:J:137:GLU:HG3 | 2.01 | 0.60 |
| 1:0:714:U:H3' | 37:0:6721:HOH:O | 2.00 | 0.60 |
| 22:T:38:ARG:HH11 | 22:T:38:ARG:HG3 | 1.67 | 0.60 |
| 15:M:122:GLN:OE1 | 15:M:127:LYS:HE2 | 2.01 | 0.60 |
| 7:E:20:ILE:HD11 | 7:E:40:VAL:CG1 | 2.31 | 0.60 |
| 1:0:545:G:C8 | 1:0:545:G:H5' | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:140:LEU:HA | 37:B:8880:HOH:O | 2.01 | 0.60 |
| 7:E:7:ILE:HD11 | 7:E:11:VAL:C | 2.22 | 0.60 |
| 10:H:66:GLU:HA | 37:H:235:HOH:O | 2.01 | 0.60 |
| 1:O:1311:G:O6 | 5:C:173:LYS:HE3 | 2.02 | 0.60 |
| 4:B:279:THR:OG1 | 4:B:290:VAL:HB | 2.01 | 0.60 |
| 6:D:40:ILE:O | 6:D:44:ILE:HG22 | 2.02 | 0.60 |
| 2:9:114:G:O6 | 16:N:11:ARG:HD3 | 2.01 | 0.60 |
| 7:E:125:GLU:HB2 | 7:E:132:THR:CG2 | 2.30 | 0.60 |
| 5:C:20:ASP:HB2 | 37:C:8601:HOH:O | 2.00 | 0.60 |
| 5:C:78:ARG:HG3 | 5:C:78:ARG:NH1 | 2.16 | 0.60 |
| 8:F:56:PRO:CG | 15:M:44:THR:HA | 2.31 | 0.60 |
| 11:I:113:SER:HB2 | 11:I:118:ASN:HB2 | 1.83 | 0.60 |
| 29:1:28:HIS:HD2 | 29:1:30:LYS:H | 1.49 | 0.60 |
| 27:Y:106:THR:HG23 | 27:Y:107:PRO:HD2 | 1.82 | 0.60 |
| 1:O:709:G:O2' | 17:O:25:VAL:HG12 | 2.02 | 0.60 |
| 7:E:126:ILE:HB | 7:E:131:LEU:HD23 | 1.83 | 0.60 |
| 6:D:25:MET:CE | 6:D:41:LEU:HG | 2.31 | 0.60 |
| 16:N:154:LEU:HD12 | 16:N:156:GLU:O | 2.01 | 0.60 |
| 4:B:132:HIS:HB2 | 4:B:137:LEU:CD2 | 2.32 | 0.60 |
| 1:O:1803:C:H2' | 1:O:1804:A:C8 | 2.36 | 0.60 |
| 1:O:2676:C:H4' | 12:J:70:PHE:CE1 | 2.37 | 0.60 |
| 28:Z:60:CYS:O | 28:Z:61:ASP:HB2 | 2.02 | 0.59 |
| 16:N:67:ALA:HA | 16:N:71:TRP:HB3 | 1.84 | 0.59 |
| 29:1:28:HIS:O | 29:1:32:LYS:N | 2.35 | 0.59 |
| 20:R:25:PHE:CE2 | 20:R:29:LYS:HE2 | 2.37 | 0.59 |
| 1:O:1878:G:H1' | 37:O:5905:HOH:O | 2.02 | 0.59 |
| 1:O:1523:G:H2' | 1:O:1524:U:O4' | 2.02 | 0.59 |
| 1:O:354:A:H2' | 1:O:355:C:C6 | 2.36 | 0.59 |
| 12:J:52:GLN:HG3 | 12:J:53:ILE:H | 1.65 | 0.59 |
| 4:B:55:ASN:ND2 | 4:B:67:GLU:OE2 | 2.35 | 0.59 |
| 8:F:100:ASP:HB3 | 37:F:5691:HOH:O | 2.01 | 0.59 |
| 29:1:8:GLN:HE22 | 29:1:11:LYS:HZ2 | 1.50 | 0.59 |
| 27:Y:187:VAL:HG22 | 27:Y:192:ASP:HB2 | 1.83 | 0.59 |
| 1:O:1213:C:O2' | 1:O:1214:G:H5' | 2.01 | 0.59 |
| 1:O:1535:G:H2' | 1:O:1536:C:C6 | 2.37 | 0.59 |
| 1:O:1189:A:H1' | 1:O:1209:C:O4' | 2.02 | 0.59 |
| 12:J:74:ARG:NH1 | 12:J:76:ASP:HB2 | 2.17 | 0.59 |
| 1:O:558:C:H2' | 1:O:559:U:C5' | 2.32 | 0.59 |
| 15:M:60:VAL:C | 15:M:61:ILE:HD12 | 2.23 | 0.59 |
| 25:W:151:GLU:O | 25:W:154:ARG:HB3 | 2.02 | 0.59 |
| 11:I:120:ALA:O | 11:I:124:VAL:HG23 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:N:139:TRP:HA | 16:N:139:TRP:HE3 | 1.67 | 0.59 |
| 14:L:94:ARG:HA | 14:L:106:VAL:HG21 | 1.84 | 0.59 |
| 13:K:81:ARG:HB2 | 13:K:87:ARG:NH1 | 2.17 | 0.59 |
| 1:O:2769:C:O2' | 1:O:2770:G:H5' | 2.03 | 0.59 |
| 1:O:2719:A:C2 | 4:B:70:PRO:HG3 | 2.37 | 0.59 |
| 4:B:141:ARG:HD2 | 4:B:163:GLU:OE2 | 2.03 | 0.59 |
| 2:9:38:A:H2' | 2:9:39:U:C6 | 2.37 | 0.59 |
| 28:Z:46:ARG:CD | 28:Z:59:TYR:HB2 | 2.29 | 0.59 |
| 4:B:307:ARG:HB2 | 4:B:307:ARG:HH11 | 1.66 | 0.59 |
| 13:K:37:TYR:HB3 | 37:K:7169:HOH:O | 2.02 | 0.59 |
| 1:O:1342:C:C2' | 1:O:1343:C:H5' | 2.32 | 0.59 |
| 25:W:21:LEU:HD22 | 25:W:26:ILE:HD11 | 1.85 | 0.59 |
| 16:N:113:SER:HB2 | 37:N:8856:HOH:O | 2.01 | 0.59 |
| 4:B:102:THR:HG23 | 4:B:182:VAL:HG12 | 1.85 | 0.59 |
| 22:T:24:ARG:HH11 | 22:T:24:ARG:HG2 | 1.66 | 0.59 |
| 27:Y:130:ARG:HB2 | 27:Y:142:SER:O | 2.01 | 0.59 |
| 11:I:108:HIS:N | 11:I:109:PRO:HD2 | 2.17 | 0.59 |
| 1:O:671:A:O2' | 1:O:672:G:H2' | 2.01 | 0.59 |
| 22:T:87:VAL:HB | 37:T:5545:HOH:O | 2.03 | 0.59 |
| 1:O:87:C:H2' | 30:2:28:LYS:O | 2.02 | 0.59 |
| 4:B:85:ARG:NH1 | 37:B:8935:HOH:O | 2.36 | 0.59 |
| 17:O:88:LYS:HB3 | 37:O:7061:HOH:O | 2.01 | 0.59 |
| 1:O:2740:G:H2' | 1:O:2741:A:O4' | 2.03 | 0.59 |
| 1:O:871:G:C8 | 1:O:871:G:C5' | 2.76 | 0.59 |
| 1:O:1189:A:H3' | 37:O:7449:HOH:O | 2.03 | 0.59 |
| 12:J:39:VAL:HG12 | 12:J:40:ASN:CG | 2.23 | 0.59 |
| 13:K:113:ILE:HD12 | 13:K:128:ALA:HB2 | 1.83 | 0.59 |
| 2:9:13:A:O2' | 2:9:14:G:H5'' | 2.02 | 0.59 |
| 1:O:2521:A:OP2 | 10:H:6:ALA:HB3 | 2.03 | 0.59 |
| 24:V:13:PRO:O | 24:V:17:GLU:HG3 | 2.02 | 0.59 |
| 6:D:101:THR:HG22 | 6:D:101:THR:O | 2.03 | 0.59 |
| 25:W:65:VAL:HA | 25:W:68:THR:HG22 | 1.83 | 0.59 |
| 5:C:170:ASP:O | 5:C:171:GLU:HG3 | 2.03 | 0.59 |
| 1:O:837:U:H4' | 37:O:3192:HOH:O | 2.02 | 0.59 |
| 6:D:50:VAL:O | 6:D:71:ALA:HA | 2.03 | 0.59 |
| 6:D:86:THR:C | 6:D:89:PRO:HD2 | 2.22 | 0.59 |
| 10:H:49:GLN:HB3 | 10:H:170:ARG:HG3 | 1.84 | 0.59 |
| 13:K:65:ARG:HD3 | 37:K:5358:HOH:O | 2.02 | 0.59 |
| 1:O:711:G:H1' | 37:O:6868:HOH:O | 2.03 | 0.59 |
| 12:J:90:LYS:HB2 | 35:J:8802:CL:CL | 2.39 | 0.59 |
| 31:3:3:MET:HG3 | 31:3:4:PRO:HD2 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 14:L:143:THR:HG22 | 14:L:144:ASP:N | 2.18 | 0.58 |
| 1:O:1819:G:H2' | 1:O:1820:G:H4' | 1.83 | 0.58 |
| 3:A:134:ASN:O | 3:A:150:PRO:HD3 | 2.02 | 0.58 |
| 1:O:1874:U:OP1 | 3:A:51:ARG:HD2 | 2.03 | 0.58 |
| 1:O:2716:G:H5'' | 4:B:206:THR:HG21 | 1.85 | 0.58 |
| 4:B:267:LYS:HE3 | 4:B:300:SER:O | 2.03 | 0.58 |
| 17:O:105:ASN:ND2 | 17:O:109:SER:H | 2.00 | 0.58 |
| 27:Y:186:ARG:NH1 | 27:Y:186:ARG:HG2 | 2.18 | 0.58 |
| 1:O:1666:C:H2' | 1:O:1667:A:C8 | 2.37 | 0.58 |
| 10:H:57:THR:HG23 | 10:H:131:GLN:HA | 1.85 | 0.58 |
| 20:R:39:THR:HG23 | 20:R:107:GLU:O | 2.02 | 0.58 |
| 5:C:3:ALA:O | 5:C:15:GLU:HB2 | 2.03 | 0.58 |
| 1:O:2880:A:H2' | 1:O:2881:C:H5' | 1.85 | 0.58 |
| 1:O:1537:C:H1' | 37:O:6368:HOH:O | 2.02 | 0.58 |
| 30:2:48:ASP:O | 30:2:49:GLU:HB2 | 2.02 | 0.58 |
| 25:W:7:LEU:HD12 | 25:W:53:ALA:HB2 | 1.85 | 0.58 |
| 15:M:164:THR:CG2 | 15:M:167:GLY:H | 2.10 | 0.58 |
| 16:N:163:PHE:O | 16:N:164:ASP:O | 2.20 | 0.58 |
| 1:O:80:A:H3' | 22:T:43:ASN:OD1 | 2.02 | 0.58 |
| 2:9:64:C:C2' | 2:9:65:A:H5' | 2.34 | 0.58 |
| 4:B:51:VAL:HG12 | 4:B:53:LEU:HD13 | 1.83 | 0.58 |
| 7:E:10:ASP:HA | 37:E:6017:HOH:O | 2.03 | 0.58 |
| 28:Z:26:VAL:O | 28:Z:30:GLU:HG3 | 2.02 | 0.58 |
| 1:O:1500:U:P | 18:P:41:ARG:HH22 | 2.26 | 0.58 |
| 1:O:1735:C:OP2 | 4:B:234:ARG:HG3 | 2.03 | 0.58 |
| 1:O:1850:U:H2' | 1:O:1851:G:H8 | 1.68 | 0.58 |
| 1:O:1778:A:H2' | 1:O:1779:A:H5' | 1.84 | 0.58 |
| 1:O:2635:A:O2' | 1:O:2636:C:H5' | 2.04 | 0.58 |
| 5:C:133:ARG:HE | 5:C:138:VAL:HG22 | 1.69 | 0.58 |
| 3:A:199:HIS:CD2 | 3:A:201:PHE:H | 2.21 | 0.58 |
| 37:O:9986:HOH:O | 15:M:9:ARG:HG3 | 2.04 | 0.58 |
| 25:W:1:MET:H2 | 25:W:37:GLU:HG3 | 1.68 | 0.58 |
| 4:B:264:GLU:CG | 4:B:267:LYS:HE2 | 2.24 | 0.58 |
| 10:H:42:ASP:HB2 | 10:H:45:ASP:OD1 | 2.04 | 0.58 |
| 8:F:28:ALA:CB | 8:F:99:THR:HG23 | 2.34 | 0.58 |
| 8:F:56:PRO:HG2 | 15:M:44:THR:HA | 1.85 | 0.58 |
| 37:O:3784:HOH:O | 22:T:82:THR:HA | 2.02 | 0.58 |
| 1:O:952:G:OP1 | 19:Q:42:LYS:HE2 | 2.02 | 0.58 |
| 7:E:5:LEU:HD21 | 7:E:66:GLN:HG3 | 1.86 | 0.58 |
| 4:B:329:TYR:HE2 | 23:U:15:PRO:HG2 | 1.69 | 0.58 |
| 22:T:48:VAL:HG13 | 22:T:97:ARG:C | 2.23 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:2053:G:OP1 | 20:R:138:SER:HB3 | 2.04 | 0.58 |
| 7:E:125:GLU:HB2 | 7:E:132:THR:HG23 | 1.86 | 0.58 |
| 7:E:81:GLU:HG2 | 7:E:134:SER:HB3 | 1.86 | 0.58 |
| 16:N:139:TRP:CE3 | 16:N:139:TRP:HA | 2.36 | 0.58 |
| 4:B:275:GLY:O | 4:B:291:ASP:HA | 2.03 | 0.58 |
| 1:O:1641:A:H2' | 1:O:1642:A:H5' | 1.84 | 0.58 |
| 17:O:78:ALA:O | 17:O:98:LEU:HD13 | 2.04 | 0.58 |
| 10:H:44:ASP:HA | 10:H:170:ARG:HH12 | 1.68 | 0.58 |
| 7:E:137:ASP:OD1 | 7:E:139:GLU:HB2 | 2.04 | 0.58 |
| 3:A:8:ARG:HG2 | 37:A:8849:HOH:O | 2.02 | 0.58 |
| 1:O:1183:C:N4 | 1:O:1184:C:H41 | 2.02 | 0.58 |
| 15:M:57:LYS:NZ | 15:M:144:ASP:HB2 | 2.19 | 0.58 |
| 1:O:2524:G:H21 | 1:O:2526:C:H41 | 1.52 | 0.58 |
| 11:I:118:ASN:HA | 11:I:121:LYS:HD2 | 1.85 | 0.58 |
| 27:Y:112:GLU:HA | 27:Y:112:GLU:OE1 | 2.04 | 0.58 |
| 1:O:419:A:H1' | 1:O:1921:A:C2 | 2.38 | 0.58 |
| 1:O:1060:C:H5' | 1:O:1060:C:H6 | 1.69 | 0.58 |
| 7:E:85:GLU:HG3 | 7:E:169:THR:OG1 | 2.04 | 0.58 |
| 5:C:2:GLN:HA | 5:C:17:ASP:HA | 1.86 | 0.58 |
| 1:O:1766:U:O2 | 1:O:1778:A:H5' | 2.04 | 0.58 |
| 1:O:841:A:P | 37:O:6689:HOH:O | 2.61 | 0.58 |
| 25:W:137:GLN:HE21 | 25:W:141:HIS:HE1 | 1.52 | 0.57 |
| 1:O:796:A:HO2' | 28:Z:10:ARG:N | 2.02 | 0.57 |
| 6:D:88:LEU:HB2 | 6:D:89:PRO:HD3 | 1.87 | 0.57 |
| 3:A:179:MET:HG2 | 3:A:186:TRP:CB | 2.34 | 0.57 |
| 7:E:126:ILE:HB | 7:E:131:LEU:CD2 | 2.34 | 0.57 |
| 27:Y:126:PRO:HG2 | 27:Y:128:PHE:CE1 | 2.38 | 0.57 |
| 1:O:214:U:H5' | 37:O:5924:HOH:O | 2.03 | 0.57 |
| 4:B:144:THR:HB | 37:B:8925:HOH:O | 2.04 | 0.57 |
| 1:O:1624:A:H5' | 1:O:1626:A:O4' | 2.04 | 0.57 |
| 4:B:62:ARG:HG2 | 4:B:65:MET:HE3 | 1.86 | 0.57 |
| 1:O:282:C:H2' | 1:O:283:U:O4' | 2.05 | 0.57 |
| 1:O:960:G:N3 | 1:O:960:G:H3' | 2.19 | 0.57 |
| 1:O:1561:U:H5' | 37:O:7201:HOH:O | 2.04 | 0.57 |
| 4:B:56:ASP:OD1 | 4:B:322:ARG:HB3 | 2.04 | 0.57 |
| 4:B:22:GLU:HG2 | 37:B:8851:HOH:O | 2.04 | 0.57 |
| 3:A:88:ILE:HD13 | 3:A:100:PRO:HD3 | 1.87 | 0.57 |
| 27:Y:115:ARG:NE | 37:Y:8857:HOH:O | 2.37 | 0.57 |
| 16:N:27:LEU:HD22 | 16:N:50:LEU:HD22 | 1.86 | 0.57 |
| 1:O:1015:C:H2' | 1:O:1016:U:H6 | 1.70 | 0.57 |
| 1:O:1400:C:H4' | 26:X:56:GLU:HG2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2467:A:H2' | 37:0:5254:HOH:O | 2.03 | 0.57 |
| 8:F:19:ALA:O | 8:F:22:VAL:HG22 | 2.04 | 0.57 |
| 8:F:50:VAL:HG21 | 8:F:63:ILE:HG21 | 1.85 | 0.57 |
| 23:U:14:GLU:O | 23:U:17:THR:HB | 2.05 | 0.57 |
| 1:0:1201:C:H2' | 1:0:1202:A:H5' | 1.87 | 0.57 |
| 1:0:316:A:N3 | 1:0:336:G:O2' | 2.36 | 0.57 |
| 28:Z:46:ARG:O | 28:Z:57:CYS:HA | 2.05 | 0.57 |
| 1:0:657:G:OP1 | 5:C:27:ARG:NH2 | 2.37 | 0.57 |
| 20:R:125:ARG:HH12 | 20:R:134:SER:HB2 | 1.70 | 0.57 |
| 24:V:64:GLY:O | 24:V:65:ASP:CB | 2.53 | 0.57 |
| 2:9:48:C:H4' | 16:N:141:ARG:NH2 | 2.18 | 0.57 |
| 26:X:25:ARG:NH1 | 37:X:3861:HOH:O | 2.38 | 0.57 |
| 1:0:2338:G:OP1 | 6:D:97:GLN:HG2 | 2.05 | 0.57 |
| 12:J:19:MET:CE | 12:J:132:LEU:HD21 | 2.34 | 0.57 |
| 1:0:583:C:H2' | 1:0:584:U:C6 | 2.40 | 0.57 |
| 1:0:585:C:H6 | 37:0:5879:HOH:O | 1.88 | 0.57 |
| 11:I:108:HIS:N | 11:I:109:PRO:CD | 2.67 | 0.57 |
| 1:0:232:A:H4' | 37:0:5867:HOH:O | 2.05 | 0.57 |
| 3:A:211:LYS:HB3 | 3:A:212:PRO:CD | 2.30 | 0.57 |
| 10:H:29:SER:HA | 10:H:62:HIS:HD2 | 1.70 | 0.57 |
| 30:2:39:ARG:HG2 | 37:2:3143:HOH:O | 2.05 | 0.57 |
| 3:A:153:ARG:HD3 | 37:A:8826:HOH:O | 2.05 | 0.57 |
| 1:0:2751:C:H3' | 37:0:7037:HOH:O | 2.03 | 0.57 |
| 4:B:27:ASN:H | 4:B:27:ASN:HD22 | 1.51 | 0.57 |
| 1:0:263:U:C4 | 8:F:54:VAL:HG13 | 2.38 | 0.57 |
| 15:M:24:GLN:NE2 | 15:M:27:ARG:HH11 | 2.03 | 0.57 |
| 24:V:42:ASN:HB3 | 37:V:7247:HOH:O | 2.03 | 0.57 |
| 17:O:32:ARG:NH2 | 17:O:35:LYS:HD2 | 2.20 | 0.57 |
| 1:0:1164:U:C1' | 1:0:1166:A:H5' | 2.34 | 0.57 |
| 1:0:2344:G:N3 | 1:0:2344:G:H2' | 2.19 | 0.57 |
| 1:0:2694:A:H4' | 7:E:91:PHE:HE1 | 1.70 | 0.57 |
| 5:C:7:ASP:OD2 | 5:C:9:ASP:HB2 | 2.05 | 0.57 |
| 26:X:18:ARG:NH1 | 37:X:4132:HOH:O | 2.37 | 0.57 |
| 8:F:2:VAL:HG22 | 8:F:57:GLU:OE1 | 2.05 | 0.57 |
| 1:0:2472:C:O2' | 1:0:2634:G:H4' | 2.04 | 0.57 |
| 1:0:702:G:O2' | 1:0:703:G:H5' | 2.05 | 0.57 |
| 31:3:38:ARG:HB3 | 31:3:42:ARG:HH12 | 1.70 | 0.57 |
| 12:J:105:LEU:HD23 | 37:J:8866:HOH:O | 2.05 | 0.57 |
| 1:0:1751:G:C2' | 1:0:1752:G:H5'' | 2.34 | 0.57 |
| 1:0:2050:G:OP1 | 20:R:79:ARG:HB3 | 2.05 | 0.57 |
| 1:0:732:C:H2' | 1:0:733:U:H6 | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:N:170:GLU:HA | 16:N:173:ASP:OD2 | 2.04 | 0.57 |
| 1:O:2563:U:H2' | 1:O:2565:C:O5' | 2.05 | 0.57 |
| 24:V:49:LEU:O | 24:V:53:ILE:HG13 | 2.04 | 0.57 |
| 8:F:22:VAL:HG23 | 8:F:104:ALA:HB2 | 1.87 | 0.57 |
| 1:O:2670:G:O2' | 1:O:2671:U:H5' | 2.05 | 0.57 |
| 1:O:1508:C:H5' | 21:S:21:GLN:NE2 | 2.20 | 0.57 |
| 25:W:88:THR:HG23 | 25:W:110:GLN:NE2 | 2.20 | 0.56 |
| 1:O:558:C:O2' | 1:O:559:U:H5'' | 2.05 | 0.56 |
| 2:9:69:U:OP1 | 16:N:4:PRO:HG3 | 2.04 | 0.56 |
| 7:E:84:MET:HG2 | 7:E:168:ILE:HD13 | 1.86 | 0.56 |
| 1:O:120:A:H2' | 1:O:120:A:N3 | 2.20 | 0.56 |
| 6:D:36:ASN:HA | 37:D:7500:HOH:O | 2.05 | 0.56 |
| 37:O:3401:HOH:O | 3:A:236:GLY:HA3 | 2.03 | 0.56 |
| 7:E:3:VAL:HG22 | 7:E:49:ILE:HB | 1.87 | 0.56 |
| 1:O:2737:C:OP2 | 18:P:61:ARG:NH2 | 2.37 | 0.56 |
| 2:9:11:A:P | 19:Q:19:ARG:HH21 | 2.28 | 0.56 |
| 6:D:54:ALA:HB2 | 6:D:69:ILE:CD1 | 2.30 | 0.56 |
| 12:J:74:ARG:HH12 | 12:J:76:ASP:HB2 | 1.71 | 0.56 |
| 6:D:21:VAL:HA | 6:D:131:THR:O | 2.05 | 0.56 |
| 10:H:49:GLN:NE2 | 10:H:140:TYR:HE2 | 2.00 | 0.56 |
| 14:L:149:ARG:O | 14:L:150:GLN:CB | 2.52 | 0.56 |
| 18:P:134:VAL:O | 18:P:137:LEU:HB3 | 2.04 | 0.56 |
| 21:S:19:ASP:O | 21:S:20:PHE:HD2 | 1.88 | 0.56 |
| 1:O:2359:G:H3' | 37:O:5484:HOH:O | 2.05 | 0.56 |
| 1:O:1333:U:H2' | 1:O:1334:C:C6 | 2.41 | 0.56 |
| 1:O:1711:A:O2' | 1:O:1712:A:H5' | 2.05 | 0.56 |
| 6:D:64:ARG:HG2 | 6:D:67:ASP:HB3 | 1.87 | 0.56 |
| 25:W:54:PHE:CZ | 25:W:140:LYS:HB2 | 2.41 | 0.56 |
| 12:J:74:ARG:HD3 | 37:J:8859:HOH:O | 2.04 | 0.56 |
| 1:O:1834:C:H2' | 1:O:1840:A:H62 | 1.67 | 0.56 |
| 23:U:52:THR:HG22 | 23:U:54:THR:N | 2.20 | 0.56 |
| 4:B:329:TYR:CE2 | 23:U:15:PRO:HG2 | 2.39 | 0.56 |
| 1:O:1164:U:O4' | 1:O:1166:A:H5' | 2.05 | 0.56 |
| 3:A:101:GLU:O | 3:A:103:VAL:HG23 | 2.06 | 0.56 |
| 17:O:14:LEU:CD2 | 17:O:102:ILE:HD11 | 2.34 | 0.56 |
| 8:F:48:VAL:HG23 | 8:F:74:PHE:HB3 | 1.86 | 0.56 |
| 17:O:41:ALA:HA | 37:O:5104:HOH:O | 2.06 | 0.56 |
| 1:O:1971:G:H2' | 37:O:3091:HOH:O | 2.04 | 0.56 |
| 1:O:1007:A:H2' | 10:H:22:TYR:CZ | 2.40 | 0.56 |
| 1:O:2715:G:N2 | 4:B:264:GLU:OE1 | 2.36 | 0.56 |
| 3:A:153:ARG:NH1 | 3:A:153:ARG:HB2 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:105:VAL:CG1 | 3:A:154:ALA:HB1 | 2.35 | 0.56 |
| 11:I:80:PHE:HB2 | 11:I:93:ALA:HB2 | 1.88 | 0.56 |
| 10:H:69:ARG:HB3 | 37:H:235:HOH:O | 2.05 | 0.56 |
| 5:C:136:VAL:HA | 5:C:137:PRO:C | 2.25 | 0.56 |
| 12:J:107:ASN:C | 12:J:107:ASN:HD22 | 2.08 | 0.56 |
| 16:N:24:LEU:HD13 | 19:Q:26:PRO:HB3 | 1.87 | 0.56 |
| 4:B:102:THR:CG2 | 4:B:182:VAL:HG12 | 2.36 | 0.56 |
| 6:D:64:ARG:NE | 6:D:67:ASP:HB3 | 2.20 | 0.56 |
| 15:M:99:ARG:HG2 | 37:M:8857:HOH:O | 2.05 | 0.56 |
| 2:9:49:G:H5'' | 37:9:8671:HOH:O | 2.04 | 0.56 |
| 3:A:217:ARG:CG | 3:A:217:ARG:HH11 | 2.18 | 0.56 |
| 1:0:1180:U:H2' | 1:0:1181:A:C8 | 2.39 | 0.56 |
| 13:K:62:PRO:HG3 | 13:K:65:ARG:NH2 | 2.19 | 0.56 |
| 1:0:1701:A:H4' | 1:0:1702:U:C5' | 2.36 | 0.56 |
| 8:F:57:GLU:HB2 | 15:M:23:LEU:HD11 | 1.88 | 0.56 |
| 17:O:27:GLY:O | 17:O:31:GLU:HG3 | 2.06 | 0.56 |
| 4:B:294:TYR:HE2 | 37:B:8951:HOH:O | 1.87 | 0.56 |
| 1:0:2816:A:H4' | 37:0:3702:HOH:O | 2.05 | 0.56 |
| 1:0:797:A:C4' | 28:Z:10:ARG:N | 2.68 | 0.56 |
| 8:F:56:PRO:HG2 | 15:M:43:PRO:O | 2.05 | 0.56 |
| 27:Y:189:ASN:HA | 27:Y:217:ILE:HD11 | 1.88 | 0.56 |
| 3:A:199:HIS:HD2 | 3:A:201:PHE:H | 1.54 | 0.56 |
| 2:9:44:A:O4' | 6:D:76:ARG:NE | 2.37 | 0.56 |
| 14:L:54:PRO:HG2 | 14:L:57:VAL:HG21 | 1.87 | 0.56 |
| 1:0:922:A:N7 | 1:0:2281:C:H5' | 2.21 | 0.56 |
| 12:J:19:MET:HE2 | 12:J:79:PHE:HA | 1.87 | 0.56 |
| 20:R:125:ARG:HA | 20:R:140:GLN:OE1 | 2.06 | 0.56 |
| 1:0:2661:U:H3 | 1:0:2812:A:H62 | 1.52 | 0.56 |
| 1:0:1504:A:H5'' | 37:0:5392:HOH:O | 2.06 | 0.56 |
| 1:0:1477:C:H5' | 1:0:1868:G:C5' | 2.36 | 0.56 |
| 12:J:92:GLN:HB3 | 37:J:8829:HOH:O | 2.06 | 0.56 |
| 1:0:2270:G:H4' | 3:A:223:ARG:NH1 | 2.13 | 0.56 |
| 12:J:41:ALA:HB3 | 37:J:8866:HOH:O | 2.05 | 0.56 |
| 1:0:820:G:C6 | 3:A:171:LYS:HB2 | 2.40 | 0.56 |
| 17:O:32:ARG:HD2 | 37:O:3240:HOH:O | 2.05 | 0.56 |
| 14:L:115:ARG:O | 14:L:116:HIS:ND1 | 2.39 | 0.56 |
| 1:0:1702:U:H5' | 37:0:3224:HOH:O | 2.05 | 0.56 |
| 1:0:2256:G:C2' | 1:0:2257:G:H5' | 2.36 | 0.56 |
| 1:0:638:C:H2' | 1:0:639:A:C8 | 2.41 | 0.56 |
| 1:0:1299:G:O6 | 14:L:6:ARG:HD3 | 2.06 | 0.56 |
| 1:0:2768:A:O2' | 1:0:2769:C:H5' | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:31:C:H4' | 37:0:7197:HOH:O | 2.06 | 0.56 |
| 14:L:73:VAL:HG21 | 14:L:116:HIS:HD2 | 1.67 | 0.56 |
| 1:0:2694:A:H4' | 7:E:91:PHE:CE1 | 2.40 | 0.56 |
| 1:0:2265:U:H2' | 1:0:2266:A:C8 | 2.41 | 0.56 |
| 6:D:23:VAL:HG23 | 6:D:23:VAL:O | 2.06 | 0.56 |
| 1:0:1176:C:H1' | 37:0:3728:HOH:O | 2.06 | 0.56 |
| 4:B:202:VAL:HG11 | 4:B:301:VAL:CG1 | 2.32 | 0.55 |
| 28:Z:57:CYS:SG | 28:Z:59:TYR:HB3 | 2.46 | 0.55 |
| 20:R:91:LEU:HD22 | 20:R:143:VAL:HG22 | 1.88 | 0.55 |
| 13:K:113:ILE:HG22 | 13:K:114:ALA:O | 2.04 | 0.55 |
| 1:0:282:C:O2' | 1:0:283:U:H5' | 2.06 | 0.55 |
| 13:K:34:VAL:HB | 37:K:7169:HOH:O | 2.05 | 0.55 |
| 16:N:13:ARG:NH1 | 16:N:13:ARG:O | 2.38 | 0.55 |
| 5:C:139:VAL:HG13 | 37:C:8657:HOH:O | 2.06 | 0.55 |
| 1:0:793:A:H5'' | 18:P:83:LYS:HG2 | 1.87 | 0.55 |
| 19:Q:64:GLU:HA | 19:Q:64:GLU:OE1 | 2.06 | 0.55 |
| 18:P:59:ARG:HH22 | 18:P:66:GLN:NE2 | 2.01 | 0.55 |
| 5:C:7:ASP:O | 5:C:9:ASP:N | 2.38 | 0.55 |
| 10:H:72:ALA:HB2 | 10:H:156:ALA:HB2 | 1.88 | 0.55 |
| 31:3:16:GLU:HB2 | 37:3:8864:HOH:O | 2.06 | 0.55 |
| 6:D:170:TYR:O | 6:D:171:ASP:HB3 | 2.05 | 0.55 |
| 1:0:90:A:H2' | 1:0:91:G:O4' | 2.05 | 0.55 |
| 5:C:165:ASP:OD2 | 5:C:191:SER:HB2 | 2.06 | 0.55 |
| 1:0:2831:C:H2' | 1:0:2832:C:H5' | 1.88 | 0.55 |
| 4:B:320:GLN:HE21 | 4:B:321:PRO:HD2 | 1.71 | 0.55 |
| 10:H:61:ARG:HG3 | 10:H:61:ARG:NH1 | 2.20 | 0.55 |
| 37:0:3554:HOH:O | 22:T:9:LYS:HD3 | 2.06 | 0.55 |
| 26:X:78:GLU:HG2 | 26:X:79:GLU:N | 2.22 | 0.55 |
| 4:B:109:LEU:HD11 | 4:B:113:LEU:HD12 | 1.87 | 0.55 |
| 5:C:5:ILE:HG22 | 5:C:6:TYR:N | 2.22 | 0.55 |
| 3:A:105:VAL:HG11 | 3:A:154:ALA:HB1 | 1.89 | 0.55 |
| 1:0:263:U:O4 | 8:F:54:VAL:HG13 | 2.06 | 0.55 |
| 16:N:170:GLU:O | 16:N:174:GLU:HG3 | 2.07 | 0.55 |
| 8:F:12:LEU:HD23 | 8:F:12:LEU:O | 2.06 | 0.55 |
| 16:N:22:GLN:HG2 | 16:N:26:LEU:CD2 | 2.36 | 0.55 |
| 2:9:6:C:OP1 | 16:N:37:ARG:NH1 | 2.37 | 0.55 |
| 16:N:37:ARG:NH2 | 37:N:8830:HOH:O | 2.39 | 0.55 |
| 8:F:58:GLU:CD | 15:M:27:ARG:HH22 | 2.09 | 0.55 |
| 1:0:558:C:H5' | 37:0:5056:HOH:O | 2.07 | 0.55 |
| 1:0:280:C:H2' | 1:0:281:U:O4' | 2.07 | 0.55 |
| 4:B:132:HIS:CE1 | 4:B:171:VAL:HG23 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:F:48:VAL:HG12 | 8:F:97:ALA:CB | 2.36 | 0.55 |
| 1:0:1702:U:H5'' | 37:0:6988:HOH:O | 2.05 | 0.55 |
| 22:T:99:THR:O | 22:T:100:ASP:CB | 2.54 | 0.55 |
| 19:Q:94:GLN:O | 19:Q:95:GLU:HB2 | 2.06 | 0.55 |
| 1:0:2427:C:OP2 | 31:3:84:ARG:HD2 | 2.05 | 0.55 |
| 1:0:1826:C:H3' | 37:0:7325:HOH:O | 2.06 | 0.55 |
| 11:I:96:SER:H | 11:I:99:GLN:HB2 | 1.71 | 0.55 |
| 25:W:65:VAL:HA | 25:W:68:THR:CG2 | 2.36 | 0.55 |
| 22:T:49:GLU:OE2 | 22:T:97:ARG:HD2 | 2.06 | 0.55 |
| 11:I:67:VAL:CG1 | 11:I:68:PRO:HD2 | 2.37 | 0.55 |
| 20:R:39:THR:HG22 | 20:R:42:GLU:H | 1.72 | 0.55 |
| 5:C:37:ALA:O | 5:C:41:ASN:ND2 | 2.39 | 0.55 |
| 5:C:240:LEU:O | 5:C:240:LEU:HD23 | 2.06 | 0.55 |
| 21:S:57:THR:C | 21:S:59:ASP:H | 2.10 | 0.55 |
| 25:W:77:ALA:HA | 37:W:6694:HOH:O | 2.06 | 0.55 |
| 22:T:101:LEU:HB2 | 22:T:103:LEU:HD21 | 1.87 | 0.55 |
| 13:K:66:ARG:HG2 | 13:K:66:ARG:HH11 | 1.71 | 0.55 |
| 3:A:200:PRO:HG2 | 3:A:225:VAL:HG21 | 1.87 | 0.55 |
| 1:0:1058:A:H2' | 1:0:1060:C:H5'' | 1.87 | 0.55 |
| 15:M:72:ALA:HB2 | 15:M:93:ARG:HG2 | 1.89 | 0.55 |
| 8:F:69:GLU:O | 8:F:70:LYS:HG2 | 2.07 | 0.55 |
| 1:0:797:A:H4' | 28:Z:10:ARG:N | 2.22 | 0.55 |
| 15:M:96:ASP:OD1 | 15:M:99:ARG:HD3 | 2.06 | 0.55 |
| 4:B:145:HIS:HD2 | 4:B:146:THR:O | 1.90 | 0.55 |
| 28:Z:22:SER:O | 28:Z:26:VAL:HG23 | 2.07 | 0.55 |
| 1:0:2780:C:H1' | 7:E:143:GLN:HE21 | 1.71 | 0.55 |
| 15:M:190:ASN:HB2 | 37:M:8820:HOH:O | 2.07 | 0.55 |
| 1:0:1593:C:OP1 | 18:P:117:SER:HB3 | 2.06 | 0.55 |
| 1:0:2769:C:C2' | 1:0:2770:G:H5' | 2.37 | 0.55 |
| 22:T:32:ARG:NH1 | 22:T:38:ARG:NH1 | 2.55 | 0.55 |
| 13:K:14:LYS:CB | 13:K:45:PRO:HG2 | 2.35 | 0.55 |
| 16:N:73:ALA:HB1 | 16:N:74:PRO:CD | 2.37 | 0.55 |
| 8:F:111:ILE:O | 8:F:115:VAL:HG23 | 2.06 | 0.55 |
| 1:0:1756:G:H1' | 37:0:6047:HOH:O | 2.07 | 0.55 |
| 7:E:18:LEU:HD13 | 7:E:34:TRP:CD1 | 2.42 | 0.55 |
| 20:R:12:THR:HG22 | 20:R:149:GLU:OE1 | 2.06 | 0.55 |
| 12:J:95:ARG:O | 12:J:99:GLU:HB2 | 2.07 | 0.55 |
| 1:0:1044:C:H5 | 37:0:6383:HOH:O | 1.89 | 0.55 |
| 1:0:1116:U:H3 | 1:0:1246:A:N6 | 2.02 | 0.55 |
| 1:0:1189:A:H1' | 1:0:1209:C:C1' | 2.37 | 0.55 |
| 4:B:171:VAL:O | 4:B:175:LEU:HB2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:153:ARG:CB | 3:A:153:ARG:HH11 | 2.19 | 0.55 |
| 27:Y:107:PRO:HB3 | 27:Y:182:PHE:CE2 | 2.42 | 0.55 |
| 1:0:2111:G:H1' | 37:0:8867:HOH:O | 2.07 | 0.55 |
| 25:W:88:THR:HG22 | 25:W:89:ASP:N | 2.15 | 0.54 |
| 13:K:49:LEU:HD23 | 13:K:73:VAL:O | 2.07 | 0.54 |
| 22:T:48:VAL:HG11 | 22:T:96:VAL:CG1 | 2.36 | 0.54 |
| 1:0:2415:A:O2' | 16:N:29:SER:HB3 | 2.07 | 0.54 |
| 16:N:33:ARG:NH1 | 16:N:103:ASP:OD2 | 2.39 | 0.54 |
| 23:U:39:ASN:ND2 | 23:U:44:ARG:HH11 | 2.04 | 0.54 |
| 1:0:945:U:H2' | 1:0:946:C:C6 | 2.43 | 0.54 |
| 5:C:47:GLY:HA2 | 5:C:92:PRO:HB2 | 1.88 | 0.54 |
| 1:0:2361:A:H5' | 37:0:4877:HOH:O | 2.05 | 0.54 |
| 3:A:37:VAL:HG23 | 3:A:38:ILE:N | 2.21 | 0.54 |
| 4:B:162:MET:HG3 | 4:B:310:ARG:CZ | 2.38 | 0.54 |
| 1:0:1701:A:H5' | 37:0:6068:HOH:O | 2.07 | 0.54 |
| 1:0:2755:G:H1' | 37:0:4482:HOH:O | 2.07 | 0.54 |
| 1:0:65:C:O2' | 1:0:66:G:H5' | 2.07 | 0.54 |
| 15:M:66:SER:HB3 | 15:M:128:TRP:CD1 | 2.43 | 0.54 |
| 17:O:52:ALA:HB1 | 17:O:74:VAL:HG11 | 1.90 | 0.54 |
| 1:0:2546:U:H4' | 37:B:8886:HOH:O | 2.06 | 0.54 |
| 1:0:449:A:N7 | 5:C:43:LYS:HG2 | 2.22 | 0.54 |
| 1:0:1168:C:H5'' | 11:I:83:GLY:H | 1.72 | 0.54 |
| 20:R:9:ASP:O | 20:R:13:THR:HG22 | 2.06 | 0.54 |
| 10:H:49:GLN:HB2 | 10:H:170:ARG:HD2 | 1.89 | 0.54 |
| 12:J:107:ASN:HD22 | 12:J:108:PRO:N | 2.05 | 0.54 |
| 1:0:544:G:C3' | 1:0:545:G:H5'' | 2.37 | 0.54 |
| 1:0:2316:G:H4' | 37:0:5876:HOH:O | 2.08 | 0.54 |
| 1:0:1342:C:O2' | 1:0:1343:C:H5' | 2.07 | 0.54 |
| 1:0:2793:A:H5' | 37:0:4360:HOH:O | 2.08 | 0.54 |
| 16:N:47:LEU:CD1 | 16:N:97:VAL:HG11 | 2.38 | 0.54 |
| 22:T:55:PHE:CD2 | 22:T:77:VAL:HG13 | 2.42 | 0.54 |
| 20:R:22:GLN:CG | 20:R:140:GLN:HE21 | 2.21 | 0.54 |
| 8:F:21:GLU:O | 8:F:24:ARG:HG2 | 2.07 | 0.54 |
| 22:T:25:ALA:O | 22:T:39:ASN:HB2 | 2.08 | 0.54 |
| 1:0:732:C:H2' | 1:0:733:U:C6 | 2.43 | 0.54 |
| 3:A:140:LEU:HB3 | 3:A:141:PRO:HD2 | 1.88 | 0.54 |
| 1:0:2604:A:H5' | 37:0:5579:HOH:O | 2.06 | 0.54 |
| 1:0:2469:A:H1' | 37:0:3045:HOH:O | 2.06 | 0.54 |
| 25:W:65:VAL:HG12 | 25:W:116:LEU:HD13 | 1.90 | 0.54 |
| 4:B:140:LEU:HD23 | 37:B:8880:HOH:O | 2.06 | 0.54 |
| 1:0:111:C:H2' | 1:0:112:G:O4' | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:N:38:LYS:HD2 | 16:N:114:LYS:HE3 | 1.88 | 0.54 |
| 8:F:30:LYS:HA | 37:F:5719:HOH:O | 2.06 | 0.54 |
| 1:0:2504:A:H2' | 1:0:2505:G:O4' | 2.08 | 0.54 |
| 1:0:2837:U:H1' | 4:B:307:ARG:HH12 | 1.73 | 0.54 |
| 1:0:1882:C:H4' | 37:0:4269:HOH:O | 2.08 | 0.54 |
| 1:0:2044:G:OP1 | 26:X:23:HIS:HE1 | 1.91 | 0.54 |
| 1:0:2434:A:O3' | 31:3:28:GLY:HA3 | 2.08 | 0.54 |
| 25:W:65:VAL:CG1 | 25:W:116:LEU:HD13 | 2.38 | 0.54 |
| 16:N:72:GLU:HB3 | 16:N:171:HIS:HE1 | 1.73 | 0.54 |
| 18:P:16:VAL:HG12 | 18:P:17:GLY:N | 2.22 | 0.54 |
| 3:A:194:MET:HE2 | 3:A:199:HIS:HB2 | 1.89 | 0.54 |
| 5:C:21:VAL:HG23 | 5:C:22:PHE:CD1 | 2.42 | 0.54 |
| 29:1:28:HIS:ND1 | 29:1:31:LYS:HE2 | 2.22 | 0.54 |
| 26:X:70:ILE:O | 26:X:70:ILE:HG23 | 2.08 | 0.54 |
| 20:R:14:ALA:HB3 | 20:R:147:LEU:HB2 | 1.89 | 0.54 |
| 10:H:135:GLN:HG3 | 37:H:236:HOH:O | 2.07 | 0.54 |
| 1:0:399:C:H5' | 15:M:179:GLY:O | 2.08 | 0.54 |
| 18:P:80:ARG:HG2 | 18:P:87:ARG:CZ | 2.38 | 0.54 |
| 8:F:53:ASP:OD1 | 8:F:80:GLN:HB2 | 2.08 | 0.54 |
| 21:S:52:VAL:HG22 | 21:S:66:VAL:HG22 | 1.89 | 0.54 |
| 3:A:96:LEU:HD22 | 3:A:128:LEU:HD13 | 1.89 | 0.54 |
| 1:0:2718:C:H6 | 1:0:2718:C:H5' | 1.73 | 0.54 |
| 25:W:68:THR:HG23 | 25:W:69:ARG:HG2 | 1.90 | 0.54 |
| 11:I:113:SER:CB | 11:I:118:ASN:HB2 | 2.38 | 0.54 |
| 1:0:947:U:O2' | 1:0:948:G:H5' | 2.07 | 0.54 |
| 4:B:82:VAL:O | 4:B:82:VAL:HG12 | 2.06 | 0.54 |
| 1:0:1787:C:H4' | 1:0:2883:A:O4' | 2.08 | 0.54 |
| 1:0:1972:U:H2' | 1:0:1973:A:H5' | 1.90 | 0.54 |
| 1:0:1617:C:C4 | 1:0:1643:C:H4' | 2.43 | 0.54 |
| 2:9:122:C:H5' | 37:9:8628:HOH:O | 2.07 | 0.54 |
| 24:V:11:MET:HB3 | 24:V:15:GLU:HB2 | 1.88 | 0.54 |
| 1:0:542:A:H2' | 1:0:543:G:O4' | 2.08 | 0.54 |
| 23:U:17:THR:CG2 | 23:U:18:GLY:N | 2.71 | 0.54 |
| 37:0:6155:HOH:O | 29:1:30:LYS:HE2 | 2.08 | 0.54 |
| 15:M:107:ARG:HD2 | 37:M:8875:HOH:O | 2.08 | 0.54 |
| 1:0:1847:A:OP1 | 3:A:175:LYS:HG3 | 2.08 | 0.54 |
| 6:D:154:LYS:HD2 | 6:D:154:LYS:H | 1.71 | 0.54 |
| 24:V:4:HIS:O | 24:V:8:ILE:HG13 | 2.07 | 0.54 |
| 10:H:100:GLU:HB3 | 10:H:124:VAL:HG11 | 1.88 | 0.54 |
| 28:Z:11:SER:CB | 28:Z:23:ARG:HB2 | 2.38 | 0.54 |
| 1:0:2824:C:H5'' | 1:0:2825:C:H5' | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:86:ALA:HB1 | 3:A:92:ASN:HD22 | 1.72 | 0.54 |
| 4:B:212:GLN:HB2 | 4:B:257:THR:HG21 | 1.88 | 0.54 |
| 4:B:7:ARG:CZ | 4:B:11:LEU:HD21 | 2.38 | 0.54 |
| 29:1:8:GLN:HE22 | 29:1:11:LYS:HZ1 | 1.56 | 0.54 |
| 1:0:819:A:HO2' | 1:0:821:U:H6 | 1.56 | 0.54 |
| 1:0:1701:A:H5'' | 1:0:1702:U:H3' | 1.90 | 0.54 |
| 27:Y:234:VAL:HG12 | 27:Y:235:GLU:H | 1.73 | 0.54 |
| 5:C:26:VAL:N | 37:C:8558:HOH:O | 2.41 | 0.54 |
| 2:9:76:G:C3' | 2:9:77:A:H5'' | 2.29 | 0.53 |
| 6:D:95:THR:OG1 | 6:D:174:VAL:HG13 | 2.08 | 0.53 |
| 26:X:87:ALA:O | 26:X:88:GLU:CB | 2.56 | 0.53 |
| 16:N:176:ARG:HE | 16:N:180:LEU:HD21 | 1.73 | 0.53 |
| 1:0:2795:C:O2' | 1:0:2796:U:H5' | 2.07 | 0.53 |
| 16:N:64:SER:C | 16:N:66:LEU:H | 2.11 | 0.53 |
| 5:C:95:GLU:HG3 | 37:C:8684:HOH:O | 2.06 | 0.53 |
| 1:0:1614:G:H2' | 37:0:4429:HOH:O | 2.07 | 0.53 |
| 13:K:75:ARG:NH2 | 37:K:4172:HOH:O | 2.41 | 0.53 |
| 10:H:49:GLN:HG3 | 10:H:140:TYR:CE2 | 2.43 | 0.53 |
| 30:2:41:HIS:CD2 | 30:2:44:ARG:H | 2.17 | 0.53 |
| 12:J:130:VAL:HG11 | 12:J:135:ILE:HG13 | 1.90 | 0.53 |
| 25:W:1:MET:N | 25:W:37:GLU:HG3 | 2.22 | 0.53 |
| 5:C:1:MET:HG2 | 5:C:2:GLN:H | 1.73 | 0.53 |
| 1:0:542:A:H5' | 1:0:542:A:C8 | 2.35 | 0.53 |
| 5:C:218:VAL:HG12 | 37:C:8633:HOH:O | 2.07 | 0.53 |
| 22:T:48:VAL:HG12 | 22:T:49:GLU:N | 2.23 | 0.53 |
| 22:T:51:LEU:HD11 | 22:T:97:ARG:HB2 | 1.91 | 0.53 |
| 3:A:107:ASN:N | 3:A:119:ALA:O | 2.38 | 0.53 |
| 1:0:2597:U:H2' | 1:0:2598:U:H5' | 1.89 | 0.53 |
| 11:I:119:ALA:O | 11:I:123:VAL:HG23 | 2.07 | 0.53 |
| 1:0:324:G:O2' | 1:0:325:U:H5' | 2.08 | 0.53 |
| 20:R:47:LEU:O | 20:R:51:ILE:HG13 | 2.09 | 0.53 |
| 1:0:2036:C:O4' | 13:K:44:LEU:HG | 2.08 | 0.53 |
| 1:0:719:C:O2' | 17:O:112:ARG:NH2 | 2.41 | 0.53 |
| 1:0:870:G:OP2 | 3:A:3:ARG:HD3 | 2.09 | 0.53 |
| 4:B:7:ARG:HD3 | 4:B:9:GLY:O | 2.08 | 0.53 |
| 9:G:12:ILE:HG22 | 9:G:17:GLN:NE2 | 2.23 | 0.53 |
| 1:0:88:G:H1' | 37:0:6850:HOH:O | 2.08 | 0.53 |
| 17:O:44:ASN:HB3 | 17:O:67:SER:O | 2.08 | 0.53 |
| 1:0:2252:A:C5 | 1:0:2253:G:H1' | 2.44 | 0.53 |
| 1:0:1505:U:H6 | 1:0:1505:U:H5' | 1.71 | 0.53 |
| 10:H:79:GLU:C | 10:H:80:LEU:HD23 | 2.29 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:2237:G:H1' | 37:0:4653:HOH:O | 2.08 | 0.53 |
| 7:E:116:THR:HG22 | 7:E:151:LEU:HD22 | 1.91 | 0.53 |
| 25:W:4:LEU:O | 25:W:32:CYS:HA | 2.09 | 0.53 |
| 1:0:1185:U:H5' | 37:0:7238:HOH:O | 2.08 | 0.53 |
| 26:X:85:VAL:HG12 | 26:X:86:GLU:N | 2.23 | 0.53 |
| 22:T:55:PHE:HB2 | 37:T:6384:HOH:O | 2.08 | 0.53 |
| 1:0:2578:G:C8 | 1:0:2578:G:H5' | 2.40 | 0.53 |
| 1:0:677:C:H4' | 5:C:246:ARG:NH2 | 2.23 | 0.53 |
| 8:F:48:VAL:HG12 | 8:F:97:ALA:HB2 | 1.89 | 0.53 |
| 1:0:67:A:H5'' | 1:0:69:A:C8 | 2.43 | 0.53 |
| 1:0:1632:A:C2' | 1:0:1633:C:H5' | 2.39 | 0.53 |
| 1:0:1334:C:H2' | 1:0:1335:C:H6 | 1.74 | 0.53 |
| 1:0:2314:G:C2' | 1:0:2315:C:H5' | 2.39 | 0.53 |
| 31:3:30:GLN:HB3 | 37:3:8852:HOH:O | 2.08 | 0.53 |
| 3:A:36:ASP:CB | 3:A:85:SER:H | 2.22 | 0.53 |
| 6:D:44:ILE:O | 6:D:44:ILE:HG12 | 2.08 | 0.53 |
| 9:G:23:ILE:HG22 | 9:G:27:ILE:HD11 | 1.90 | 0.53 |
| 3:A:121:ALA:H | 3:A:124:VAL:CG2 | 2.20 | 0.53 |
| 6:D:55:LYS:O | 6:D:56:ARG:CB | 2.56 | 0.53 |
| 20:R:39:THR:HB | 20:R:42:GLU:CG | 2.38 | 0.53 |
| 1:0:635:A:H2' | 1:0:636:G:H5'' | 1.89 | 0.53 |
| 14:L:17:SER:C | 14:L:19:LYS:H | 2.12 | 0.53 |
| 1:0:2276:U:H2' | 1:0:2277:U:C6 | 2.43 | 0.53 |
| 11:I:133:THR:HG22 | 11:I:134:ILE:N | 2.24 | 0.53 |
| 1:0:2748:G:H2' | 37:0:7309:HOH:O | 2.08 | 0.53 |
| 10:H:27:PRO:HD3 | 10:H:123:ILE:CG2 | 2.39 | 0.53 |
| 1:0:338:C:H5'' | 37:0:3599:HOH:O | 2.08 | 0.53 |
| 17:O:38:ARG:NH1 | 37:O:7674:HOH:O | 2.42 | 0.53 |
| 1:0:2672:C:OP2 | 4:B:25:ARG:NH1 | 2.40 | 0.53 |
| 1:0:290:C:H2' | 1:0:291:C:C6 | 2.43 | 0.53 |
| 7:E:80:TRP:O | 7:E:134:SER:HA | 2.08 | 0.53 |
| 23:U:6:CYS:C | 23:U:8:TYR:H | 2.12 | 0.53 |
| 10:H:114:ASP:HB2 | 37:H:199:HOH:O | 2.07 | 0.53 |
| 9:G:19:GLU:HG2 | 9:G:66:LEU:HD12 | 1.90 | 0.53 |
| 21:S:7:HIS:CD2 | 21:S:27:ALA:HB3 | 2.44 | 0.53 |
| 6:D:18:ILE:HG12 | 6:D:134:LEU:CD2 | 2.39 | 0.53 |
| 1:0:2896:A:H5'' | 37:0:5883:HOH:O | 2.08 | 0.53 |
| 18:P:20:ARG:NH1 | 18:P:54:LYS:HD3 | 2.22 | 0.53 |
| 27:Y:107:PRO:HB3 | 27:Y:182:PHE:CD2 | 2.44 | 0.53 |
| 5:C:136:VAL:HG22 | 5:C:137:PRO:HA | 1.90 | 0.53 |
| 28:Z:73:THR:O | 28:Z:76:GLY:N | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:2533:C:H6 | 1:0:2533:C:H5' | 1.74 | 0.53 |
| 1:0:656:G:H5' | 17:O:3:THR:HB | 1.91 | 0.53 |
| 5:C:198:ASP:C | 5:C:199:GLU:HG3 | 2.29 | 0.53 |
| 1:0:1120:U:H5' | 1:0:1120:U:C6 | 2.40 | 0.53 |
| 10:H:30:LYS:H | 10:H:62:HIS:HD2 | 1.55 | 0.53 |
| 6:D:99:ASP:CG | 6:D:100:ASP:N | 2.59 | 0.53 |
| 29:1:10:LYS:N | 37:1:2979:HOH:O | 2.41 | 0.53 |
| 4:B:150:ALA:O | 4:B:152:PRO:HD3 | 2.09 | 0.53 |
| 1:0:1527:A:H1' | 1:0:1528:A:C8 | 2.43 | 0.53 |
| 18:P:135:ALA:HB1 | 18:P:139:ARG:NH1 | 2.24 | 0.53 |
| 1:0:1874:U:H2' | 3:A:120:ARG:HG3 | 1.91 | 0.53 |
| 1:0:2028:U:H2' | 1:0:2029:C:C6 | 2.43 | 0.53 |
| 1:0:1762:C:H4' | 37:0:4456:HOH:O | 2.08 | 0.53 |
| 1:0:122:C:H5'' | 37:0:3387:HOH:O | 2.08 | 0.53 |
| 1:0:1132:A:N6 | 1:0:1229:C:H2' | 2.24 | 0.53 |
| 26:X:87:ALA:O | 26:X:88:GLU:HB3 | 2.09 | 0.53 |
| 11:I:95:LEU:HD23 | 11:I:99:GLN:OE1 | 2.08 | 0.53 |
| 1:0:1790:C:H2' | 1:0:1791:U:C6 | 2.43 | 0.53 |
| 4:B:51:VAL:HG13 | 4:B:327:VAL:HG13 | 1.92 | 0.53 |
| 1:0:2405:C:H5' | 37:0:6375:HOH:O | 2.08 | 0.53 |
| 27:Y:203:VAL:HG22 | 37:Y:8875:HOH:O | 2.09 | 0.53 |
| 24:V:16:ARG:HB2 | 37:V:874:HOH:O | 2.09 | 0.53 |
| 1:0:2786:G:H2' | 37:0:6957:HOH:O | 2.08 | 0.53 |
| 1:0:2798:G:H3' | 37:0:4196:HOH:O | 2.08 | 0.53 |
| 1:0:2445:U:H2' | 1:0:2446:G:C8 | 2.44 | 0.53 |
| 21:S:42:GLU:HG2 | 21:S:49:VAL:HG23 | 1.91 | 0.53 |
| 37:0:5256:HOH:O | 9:G:12:ILE:HG23 | 2.10 | 0.52 |
| 37:0:6839:HOH:O | 20:R:33:ARG:HD3 | 2.08 | 0.52 |
| 1:0:1333:U:H2' | 1:0:1334:C:H6 | 1.74 | 0.52 |
| 1:0:1391:G:H2' | 1:0:1392:A:H5' | 1.91 | 0.52 |
| 15:M:152:ALA:HB1 | 37:M:8941:HOH:O | 2.07 | 0.52 |
| 1:0:138:U:OP2 | 1:0:139:C:H5 | 1.92 | 0.52 |
| 1:0:1477:C:H5' | 1:0:1868:G:H5'' | 1.92 | 0.52 |
| 3:A:69:LEU:HB3 | 37:A:8871:HOH:O | 2.08 | 0.52 |
| 1:0:660:A:H4' | 1:0:661:G:O5' | 2.09 | 0.52 |
| 4:B:253:GLN:HA | 37:B:8924:HOH:O | 2.10 | 0.52 |
| 31:3:69:TYR:O | 31:3:77:ALA:HA | 2.09 | 0.52 |
| 1:0:1268:C:H2' | 1:0:1269:G:H8 | 1.74 | 0.52 |
| 1:0:1119:G:H5' | 12:J:52:GLN:HE21 | 1.74 | 0.52 |
| 20:R:13:THR:HG23 | 37:R:8856:HOH:O | 2.08 | 0.52 |
| 16:N:86:LEU:O | 16:N:90:LEU:HG | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:41:LEU:HA | 6:D:44:ILE:HG22 | 1.91 | 0.52 |
| 12:J:127:ILE:N | 35:J:8801:CL:CL | 2.75 | 0.52 |
| 1:0:1882:C:O2' | 1:0:2012:U:OP 2 | 2.25 | 0.52 |
| 23:U:23:HIS:HB2 | 23:U:27:ALA:HB3 | 1.90 | 0.52 |
| 1:0:1815:A:H2' | 1:0:1816:C:O4' | 2.09 | 0.52 |
| 20:R:82:GLU:O | 20:R:86:LYS:HG3 | 2.09 | 0.52 |
| 27:Y:178:HIS:CG | 27:Y:179:PRO:HD2 | 2.45 | 0.52 |
| 5:C:236:THR:O | 5:C:237:GLU:C | 2.47 | 0.52 |
| 6:D:146:LYS:CE | 16:N:107:ASN:HD21 | 2.21 | 0.52 |
| 1:0:2910:A:H5'' | 37:0:3932:HOH:O | 2.09 | 0.52 |
| 8:F:50:VAL:CG2 | 8:F:63:ILE:HG21 | 2.39 | 0.52 |
| 4:B:254:GLN:HG2 | 4:B:255:GLY:N | 2.24 | 0.52 |
| 11:I:117:THR:O | 11:I:121:LYS:HG3 | 2.09 | 0.52 |
| 37:0:7477:HOH:O | 5:C:94:THR:HG21 | 2.09 | 0.52 |
| 5:C:34:ALA:HA | 5:C:102:LEU:CD2 | 2.39 | 0.52 |
| 1:0:513:A:N3 | 37:0:3459:HOH:O | 2.33 | 0.52 |
| 31:3:42:ARG:HH11 | 31:3:42:ARG:HB2 | 1.75 | 0.52 |
| 18:P:38:GLU:HA | 18:P:41:ARG:NH1 | 2.24 | 0.52 |
| 26:X:69:LYS:O | 26:X:70:ILE:HB | 2.10 | 0.52 |
| 1:0:2015:A:H2' | 1:0:2016:U:O4' | 2.08 | 0.52 |
| 16:N:58:LEU:HD12 | 16:N:58:LEU:N | 2.24 | 0.52 |
| 1:0:2776:A:H2' | 1:0:2777:G:O4' | 2.09 | 0.52 |
| 2:9:29:C:H2' | 2:9:30:C:H5' | 1.91 | 0.52 |
| 5:C:84:VAL:O | 5:C:85:LYS:HB2 | 2.09 | 0.52 |
| 8:F:34:ASN:HA | 15:M:4:ALA:HB2 | 1.92 | 0.52 |
| 27:Y:180:SER:HA | 37:Y:8844:HOH:O | 2.08 | 0.52 |
| 1:0:256:C:H2' | 1:0:257:G:O4' | 2.09 | 0.52 |
| 1:0:440:C:O2' | 1:0:441:A:H5' | 2.09 | 0.52 |
| 1:0:536:A:H3' | 37:0:4850:HOH:O | 2.10 | 0.52 |
| 5:C:127:ARG:HG2 | 5:C:127:ARG:NH1 | 2.25 | 0.52 |
| 6:D:84:LEU:C | 6:D:86:THR:H | 2.13 | 0.52 |
| 25:W:13:MET:HE3 | 25:W:17:ILE:HG22 | 1.92 | 0.52 |
| 1:0:1741:U:O2' | 1:0:2723:G:H4' | 2.10 | 0.52 |
| 19:Q:28:ARG:HD3 | 19:Q:92:ARG:HH12 | 1.73 | 0.52 |
| 4:B:53:LEU:HD12 | 4:B:327:VAL:HA | 1.91 | 0.52 |
| 5:C:26:VAL:HG21 | 5:C:123:LEU:HD11 | 1.91 | 0.52 |
| 1:0:1762:C:H2' | 1:0:1763:C:H6 | 1.75 | 0.52 |
| 5:C:219:ASN:O | 5:C:222:ASP:OD1 | 2.28 | 0.52 |
| 3:A:52:SER:HB2 | 3:A:164:ARG:HH11 | 1.74 | 0.52 |
| 25:W:48:VAL:HG12 | 25:W:48:VAL:O | 2.10 | 0.52 |
| 16:N:143:ARG:HA | 16:N:172:PHE:CD2 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2768:A:H2' | 1:0:2769:C:O4' | 2.09 | 0.52 |
| 17:O:49:GLU:HG2 | 37:O:5191:HOH:O | 2.09 | 0.52 |
| 26:X:80:GLU:HG2 | 26:X:80:GLU:O | 2.08 | 0.52 |
| 4:B:223:ARG:HG3 | 4:B:232:TRP:O | 2.10 | 0.52 |
| 5:C:131:PHE:CD2 | 5:C:232:LEU:HD22 | 2.45 | 0.52 |
| 1:0:1187:U:H2' | 37:0:6675:HOH:O | 2.09 | 0.52 |
| 1:0:2721:U:H4' | 13:K:87:ARG:HG3 | 1.92 | 0.52 |
| 1:0:2837:U:H2' | 37:0:6615:HOH:O | 2.10 | 0.52 |
| 1:0:820:G:C5 | 3:A:171:LYS:HB2 | 2.44 | 0.52 |
| 1:0:821:U:H2' | 1:0:822:C:C6 | 2.39 | 0.52 |
| 16:N:159:TYR:HB2 | 37:N:8828:HOH:O | 2.09 | 0.52 |
| 22:T:41:ARG:NH1 | 22:T:42:VAL:O | 2.43 | 0.52 |
| 5:C:235:PHE:CE2 | 5:C:243:VAL:HG21 | 2.44 | 0.52 |
| 1:0:625:U:H5' | 37:0:9987:HOH:O | 2.10 | 0.52 |
| 4:B:82:VAL:HG12 | 4:B:101:TRP:CE3 | 2.45 | 0.52 |
| 21:S:50:GLU:CG | 21:S:69:SER:HA | 2.40 | 0.52 |
| 22:T:23:VAL:C | 22:T:93:THR:HG21 | 2.30 | 0.52 |
| 1:0:2478:U:O2' | 1:0:2479:A:H5' | 2.09 | 0.52 |
| 28:Z:46:ARG:HA | 37:Z:8730:HOH:O | 2.10 | 0.52 |
| 6:D:146:LYS:HZ1 | 16:N:107:ASN:HD21 | 1.54 | 0.52 |
| 1:0:1495:C:H1' | 1:0:1573:A:H1' | 1.91 | 0.52 |
| 16:N:43:VAL:HG13 | 16:N:118:ILE:HD11 | 1.91 | 0.52 |
| 1:0:289:G:O2' | 1:0:290:C:H5' | 2.09 | 0.52 |
| 16:N:22:GLN:HG2 | 16:N:26:LEU:HD22 | 1.90 | 0.52 |
| 7:E:24:GLY:HA3 | 7:E:76:VAL:HB | 1.90 | 0.52 |
| 1:0:1771:U:O2' | 1:0:1773:G:N7 | 2.38 | 0.52 |
| 7:E:77:THR:OG1 | 7:E:78:GLU:N | 2.42 | 0.52 |
| 1:0:1441:G:H5' | 20:R:130:MET:HE2 | 1.92 | 0.52 |
| 3:A:103:VAL:O | 3:A:105:VAL:HG23 | 2.10 | 0.52 |
| 1:0:2256:G:H2' | 1:0:2257:G:C5' | 2.40 | 0.52 |
| 1:0:2481:G:C3' | 1:0:2482:G:H5'' | 2.40 | 0.52 |
| 16:N:82:TYR:CD2 | 16:N:82:TYR:C | 2.84 | 0.52 |
| 14:L:142:LEU:HG | 14:L:146:GLY:HA3 | 1.92 | 0.52 |
| 18:P:127:GLY:HA3 | 37:P:152:HOH:O | 2.08 | 0.52 |
| 1:0:2443:C:H3' | 37:0:3275:HOH:O | 2.09 | 0.52 |
| 1:0:2064:U:H4' | 1:0:2653:A:OP1 | 2.09 | 0.52 |
| 1:0:1428:C:O2 | 20:R:132:ARG:HD3 | 2.10 | 0.51 |
| 22:T:38:ARG:NH1 | 22:T:38:ARG:HG3 | 2.25 | 0.51 |
| 4:B:72:THR:HB | 37:B:8905:HOH:O | 2.09 | 0.51 |
| 5:C:21:VAL:C | 5:C:23:GLU:H | 2.13 | 0.51 |
| 1:0:1398:G:H2' | 1:0:1399:A:C8 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:114:ALA:HB1 | 5:C:223:LEU:HB3 | 1.91 | 0.51 |
| 1:O:685:C:O2 | 1:O:748:C:H4' | 2.09 | 0.51 |
| 27:Y:196:VAL:HG13 | 27:Y:201:GLU:HG3 | 1.91 | 0.51 |
| 3:A:84:VAL:O | 3:A:98:GLU:HG3 | 2.10 | 0.51 |
| 2:9:57:A:O2' | 6:D:152:PRO:HD2 | 2.10 | 0.51 |
| 22:T:48:VAL:CG1 | 22:T:96:VAL:HG22 | 2.39 | 0.51 |
| 27:Y:205:ILE:O | 27:Y:206:ALA:C | 2.49 | 0.51 |
| 4:B:154:VAL:CG1 | 4:B:156:LYS:HG2 | 2.40 | 0.51 |
| 3:A:39:ALA:HB3 | 3:A:61:GLU:OE2 | 2.10 | 0.51 |
| 1:O:2629:C:H41 | 3:A:206:ARG:HH21 | 1.56 | 0.51 |
| 4:B:43:GLY:HA3 | 4:B:76:THR:HG22 | 1.92 | 0.51 |
| 7:E:103:VAL:HG22 | 7:E:115:ARG:HB3 | 1.92 | 0.51 |
| 1:O:1120:U:H6 | 1:O:1120:U:C5' | 2.22 | 0.51 |
| 1:O:396:U:OP2 | 31:3:38:ARG:HD2 | 2.10 | 0.51 |
| 16:N:152:GLU:OE1 | 16:N:152:GLU:HA | 2.10 | 0.51 |
| 6:D:138:GLY:N | 37:D:7597:HOH:O | 2.42 | 0.51 |
| 6:D:140:ARG:O | 6:D:144:ARG:HG2 | 2.11 | 0.51 |
| 1:O:100:C:C4' | 22:T:16:LEU:HB2 | 2.39 | 0.51 |
| 10:H:157:TYR:C | 10:H:157:TYR:HD1 | 2.14 | 0.51 |
| 1:O:74:G:H1' | 37:O:9872:HOH:O | 2.09 | 0.51 |
| 1:O:188:C:H5'' | 15:M:163:LEU:HD21 | 1.91 | 0.51 |
| 31:3:70:ARG:HD3 | 37:3:8868:HOH:O | 2.09 | 0.51 |
| 25:W:21:LEU:HB3 | 25:W:26:ILE:HG12 | 1.93 | 0.51 |
| 1:O:2420:G:O2' | 1:O:2421:G:H5' | 2.10 | 0.51 |
| 1:O:138:U:H5'' | 1:O:139:C:OP2 | 2.10 | 0.51 |
| 10:H:157:TYR:CD1 | 10:H:157:TYR:C | 2.83 | 0.51 |
| 4:B:48:MET:N | 37:B:8858:HOH:O | 2.44 | 0.51 |
| 1:O:2815:G:N7 | 12:J:80:LYS:NZ | 2.59 | 0.51 |
| 3:A:53:ALA:HB3 | 37:A:8898:HOH:O | 2.10 | 0.51 |
| 16:N:47:LEU:HD11 | 16:N:97:VAL:HG11 | 1.93 | 0.51 |
| 12:J:108:PRO:HG2 | 12:J:109:TYR:HD1 | 1.75 | 0.51 |
| 24:V:39:ALA:C | 24:V:41:GLU:H | 2.14 | 0.51 |
| 1:O:2768:A:H5'' | 37:O:4229:HOH:O | 2.11 | 0.51 |
| 1:O:1734:C:OP1 | 4:B:234:ARG:HD3 | 2.11 | 0.51 |
| 1:O:318:U:O2' | 1:O:338:C:H2' | 2.11 | 0.51 |
| 1:O:736:A:H2' | 1:O:737:A:O4' | 2.10 | 0.51 |
| 1:O:1703:G:H21 | 18:P:57:ASN:HD21 | 1.57 | 0.51 |
| 1:O:1562:C:N4 | 37:O:5655:HOH:O | 2.44 | 0.51 |
| 14:L:104:ASP:O | 14:L:105:TYR:CB | 2.58 | 0.51 |
| 21:S:32:ALA:HA | 21:S:36:GLU:OE1 | 2.10 | 0.51 |
| 1:O:746:A:C6 | 17:O:65:LEU:HD13 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 31:3:65:THR:CG2 | 31:3:67:LEU:HG | 2.39 | 0.51 |
| 1:0:1973:A:H2' | 1:0:1974:G:O4' | 2.10 | 0.51 |
| 1:0:2597:U:H5'' | 37:0:3625:HOH:O | 2.11 | 0.51 |
| 1:0:1029:U:O2' | 1:0:1273:C:OP1 | 2.26 | 0.51 |
| 1:0:105:G:O2' | 1:0:106:A:H5' | 2.10 | 0.51 |
| 1:0:581:G:O2' | 1:0:582:U:H5' | 2.11 | 0.51 |
| 1:0:1215:A:O3' | 1:0:1216:G:H4' | 2.11 | 0.51 |
| 25:W:11:VAL:O | 25:W:12:ASN:HB2 | 2.11 | 0.51 |
| 5:C:127:ARG:HD2 | 5:C:229:PRO:O | 2.11 | 0.51 |
| 4:B:66:GLU:O | 4:B:67:GLU:HG3 | 2.11 | 0.51 |
| 19:Q:26:PRO:HG3 | 37:Q:2847:HOH:O | 2.11 | 0.51 |
| 7:E:149:GLU:OE1 | 7:E:167:TYR:HA | 2.11 | 0.51 |
| 28:Z:11:SER:HB3 | 28:Z:23:ARG:HB2 | 1.92 | 0.51 |
| 1:0:453:A:H4' | 1:0:455:A:N7 | 2.26 | 0.51 |
| 1:0:1072:G:OP2 | 27:Y:154:ARG:NH2 | 2.40 | 0.51 |
| 1:0:1313:A:H5' | 27:Y:208:LYS:O | 2.11 | 0.51 |
| 3:A:9:ARG:HG2 | 3:A:16:PHE:CD2 | 2.45 | 0.51 |
| 12:J:39:VAL:HG12 | 12:J:40:ASN:ND2 | 2.26 | 0.51 |
| 7:E:20:ILE:O | 7:E:30:THR:HA | 2.10 | 0.51 |
| 22:T:50:VAL:HG12 | 22:T:56:ALA:HA | 1.93 | 0.51 |
| 9:G:71:LEU:C | 9:G:73:ASP:N | 2.65 | 0.51 |
| 5:C:107:ARG:CZ | 37:C:8666:HOH:O | 2.59 | 0.51 |
| 23:U:30:HIS:HD2 | 37:U:6215:HOH:O | 1.93 | 0.51 |
| 22:T:73:HIS:HD2 | 22:T:88:PRO:CG | 2.24 | 0.51 |
| 37:0:3089:HOH:O | 13:K:9:THR:HA | 2.10 | 0.51 |
| 24:V:12:THR:CG2 | 24:V:15:GLU:HG3 | 2.29 | 0.51 |
| 25:W:7:LEU:CD1 | 25:W:53:ALA:HB2 | 2.41 | 0.51 |
| 12:J:75:PRO:HG2 | 12:J:105:LEU:CD2 | 2.40 | 0.51 |
| 13:K:29:LEU:HB3 | 13:K:55:VAL:CG1 | 2.34 | 0.51 |
| 1:0:1439:C:OP1 | 30:2:41:HIS:HE1 | 1.93 | 0.51 |
| 15:M:122:GLN:O | 15:M:122:GLN:HG3 | 2.11 | 0.51 |
| 7:E:84:MET:HE3 | 7:E:131:LEU:HD13 | 1.92 | 0.51 |
| 1:0:243:A:H61 | 1:0:269:G:H1' | 1.76 | 0.51 |
| 28:Z:36:ASP:HB3 | 28:Z:45:ASP:HB3 | 1.93 | 0.51 |
| 16:N:143:ARG:HG2 | 16:N:172:PHE:CE2 | 2.45 | 0.51 |
| 4:B:310:ARG:HB3 | 37:B:8949:HOH:O | 2.09 | 0.51 |
| 23:U:14:GLU:OE1 | 23:U:15:PRO:CD | 2.59 | 0.51 |
| 25:W:18:GLN:O | 25:W:22:GLU:HG3 | 2.11 | 0.51 |
| 13:K:65:ARG:O | 13:K:66:ARG:HB2 | 2.11 | 0.51 |
| 1:0:1882:C:H2' | 1:0:1883:U:H6 | 1.76 | 0.51 |
| 22:T:23:VAL:O | 22:T:93:THR:HG21 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:I:101:LYS:O | 11:I:105:GLU:HG3 | 2.11 | 0.51 |
| 1:O:1761:U:H5' | 18:P:81:LYS:O | 2.11 | 0.51 |
| 1:O:226:A:H1' | 1:O:393:G:C5 | 2.46 | 0.51 |
| 25:W:107:LEU:O | 25:W:112:LEU:HB2 | 2.11 | 0.51 |
| 20:R:111:ILE:HG23 | 20:R:145:LEU:CD1 | 2.40 | 0.51 |
| 1:O:2338:G:H4' | 6:D:105:SER:O | 2.11 | 0.50 |
| 6:D:89:PRO:C | 6:D:91:ALA:H | 2.14 | 0.50 |
| 6:D:146:LYS:CE | 16:N:107:ASN:ND2 | 2.74 | 0.50 |
| 10:H:169:GLU:OE1 | 10:H:169:GLU:HA | 2.11 | 0.50 |
| 1:O:1439:C:O5' | 1:O:1439:C:H6 | 1.94 | 0.50 |
| 14:L:149:ARG:NH2 | 37:L:8890:HOH:O | 2.44 | 0.50 |
| 3:A:100:PRO:HG2 | 3:A:103:VAL:HG21 | 1.92 | 0.50 |
| 27:Y:235:GLU:CD | 27:Y:235:GLU:N | 2.64 | 0.50 |
| 15:M:61:ILE:CG2 | 15:M:62:VAL:N | 2.73 | 0.50 |
| 1:O:1266:U:H4' | 27:Y:115:ARG:HH21 | 1.76 | 0.50 |
| 1:O:110:C:H3' | 37:O:5423:HOH:O | 2.11 | 0.50 |
| 1:O:152:A:O2' | 1:O:153:C:H5' | 2.11 | 0.50 |
| 1:O:558:C:C2' | 1:O:559:U:C5' | 2.89 | 0.50 |
| 5:C:132:ASP:O | 5:C:161:ASP:HB2 | 2.11 | 0.50 |
| 16:N:5:ARG:HG2 | 19:Q:18:PRO:HB3 | 1.92 | 0.50 |
| 26:X:7:GLU:HG2 | 26:X:8:ARG:N | 2.26 | 0.50 |
| 2:9:1:U:O3' | 2:9:3:A:H5' | 2.11 | 0.50 |
| 1:O:1504:A:H5' | 37:O:4218:HOH:O | 2.11 | 0.50 |
| 27:Y:106:THR:HG22 | 27:Y:107:PRO:O | 2.11 | 0.50 |
| 3:A:58:VAL:O | 3:A:65:ARG:HD2 | 2.12 | 0.50 |
| 4:B:88:GLU:O | 4:B:88:GLU:HG3 | 2.11 | 0.50 |
| 1:O:2727:A:H2' | 1:O:2728:C:H5' | 1.93 | 0.50 |
| 5:C:159:ALA:O | 5:C:160:LEU:HG | 2.11 | 0.50 |
| 26:X:73:ARG:O | 26:X:85:VAL:HG13 | 2.11 | 0.50 |
| 25:W:108:ARG:HE | 25:W:114:PRO:CG | 2.24 | 0.50 |
| 13:K:109:LEU:CD1 | 13:K:113:ILE:HD11 | 2.41 | 0.50 |
| 22:T:55:PHE:O | 22:T:56:ALA:C | 2.48 | 0.50 |
| 27:Y:219:GLU:HG3 | 27:Y:220:GLU:H | 1.76 | 0.50 |
| 12:J:130:VAL:CG1 | 12:J:135:ILE:HG13 | 2.41 | 0.50 |
| 14:L:57:VAL:O | 14:L:57:VAL:HG12 | 2.11 | 0.50 |
| 13:K:18:ILE:HG22 | 13:K:93:ASN:HB2 | 1.93 | 0.50 |
| 1:O:2248:C:H3' | 37:O:5240:HOH:O | 2.10 | 0.50 |
| 14:L:36:ASP:HB2 | 37:L:8839:HOH:O | 2.09 | 0.50 |
| 27:Y:174:VAL:O | 27:Y:177:LYS:HB2 | 2.12 | 0.50 |
| 1:O:2089:A:O2' | 1:O:2090:G:H5' | 2.11 | 0.50 |
| 4:B:195:ARG:N | 4:B:198:GLU:OE1 | 2.43 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:9:55:U:H4' | 2:9:56:A:C8 | 2.46 | 0.50 |
| 1:0:1450:C:O2' | 1:0:1494:A:H5' | 2.11 | 0.50 |
| 1:0:1441:G:O2' | 1:0:1442:A:H5' | 2.11 | 0.50 |
| 1:0:1595:G:O2' | 1:0:1596:U:H5' | 2.11 | 0.50 |
| 7:E:11:VAL:HG12 | 7:E:12:ASP:H | 1.76 | 0.50 |
| 5:C:7:ASP:C | 5:C:9:ASP:H | 2.15 | 0.50 |
| 1:0:1655:G:H3' | 37:0:6195:HOH:O | 2.11 | 0.50 |
| 24:V:3:LEU:HD23 | 24:V:52:ALA:HB1 | 1.94 | 0.50 |
| 27:Y:219:GLU:CG | 27:Y:220:GLU:N | 2.74 | 0.50 |
| 1:0:1328:A:N7 | 1:0:1329:G:C5 | 2.80 | 0.50 |
| 16:N:67:ALA:C | 16:N:69:TYR:H | 2.14 | 0.50 |
| 1:0:1937:U:O2' | 1:0:1938:G:H5' | 2.12 | 0.50 |
| 13:K:23:ASN:HD21 | 13:K:107:THR:H | 1.59 | 0.50 |
| 1:0:1053:G:OP1 | 10:H:15:PRO:HG3 | 2.11 | 0.50 |
| 5:C:140:VAL:HG12 | 5:C:141:SER:N | 2.27 | 0.50 |
| 6:D:21:VAL:HG23 | 6:D:80:ALA:HB1 | 1.94 | 0.50 |
| 13:K:55:VAL:HG12 | 13:K:56:SER:H | 1.75 | 0.50 |
| 4:B:312:ARG:HG2 | 4:B:313:PRO:N | 2.26 | 0.50 |
| 2:9:57:A:H5' | 37:9:8717:HOH:O | 2.11 | 0.50 |
| 6:D:144:ARG:CZ | 37:D:3839:HOH:O | 2.59 | 0.50 |
| 1:0:1166:A:OP2 | 1:0:1174:A:H4' | 2.12 | 0.50 |
| 2:9:28:U:H5'' | 16:N:40:ASN:HD21 | 1.77 | 0.50 |
| 24:V:19:GLU:O | 24:V:22:ASP:HB2 | 2.12 | 0.50 |
| 1:0:1649:G:H1' | 37:0:4882:HOH:O | 2.11 | 0.50 |
| 15:M:71:SER:O | 15:M:73:ARG:NH1 | 2.44 | 0.50 |
| 1:0:2132:C:H1' | 15:M:124:GLY:HA3 | 1.94 | 0.50 |
| 1:0:1025:C:H5' | 25:W:23:MET:O | 2.12 | 0.50 |
| 1:0:1783:A:O2' | 1:0:1784:U:H5' | 2.11 | 0.50 |
| 2:9:61:C:H2' | 2:9:62:A:H8 | 1.77 | 0.50 |
| 14:L:68:GLU:HB2 | 37:L:8873:HOH:O | 2.10 | 0.50 |
| 5:C:1:MET:HG2 | 5:C:2:GLN:NE2 | 2.26 | 0.50 |
| 4:B:217:ARG:CG | 4:B:257:THR:HG22 | 2.36 | 0.50 |
| 37:0:9348:HOH:O | 18:P:81:LYS:HG2 | 2.11 | 0.50 |
| 1:0:1811:A:H2' | 1:0:1812:G:H5' | 1.94 | 0.50 |
| 26:X:75:ALA:O | 26:X:83:ALA:HA | 2.11 | 0.50 |
| 13:K:24:THR:HB | 13:K:64:MET:HE1 | 1.94 | 0.50 |
| 6:D:94:ALA:HB3 | 6:D:97:GLN:NE2 | 2.15 | 0.50 |
| 8:F:91:VAL:CG1 | 8:F:92:GLY:H | 2.23 | 0.50 |
| 14:L:145:LEU:O | 14:L:145:LEU:HD23 | 2.11 | 0.50 |
| 25:W:125:HIS:CD2 | 25:W:127:GLY:H | 2.29 | 0.50 |
| 5:C:165:ASP:O | 5:C:168:ARG:HB3 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:827:A:H2' | 1:0:828:G:O4' | 2.12 | 0.50 |
| 7:E:16:ASP:O | 7:E:17:HIS:HB2 | 2.11 | 0.50 |
| 1:0:2377:U:H6 | 1:0:2377:U:O5' | 1.94 | 0.50 |
| 19:Q:46:SER:O | 19:Q:48:PRO:HD3 | 2.11 | 0.50 |
| 25:W:8:ARG:HB3 | 37:W:1427:HOH:O | 2.12 | 0.50 |
| 1:0:2404:G:O5' | 19:Q:68:GLY:HA3 | 2.12 | 0.50 |
| 13:K:49:LEU:HD21 | 13:K:74:VAL:C | 2.32 | 0.50 |
| 6:D:39:ASP:HB2 | 37:D:5583:HOH:O | 2.12 | 0.50 |
| 6:D:138:GLY:O | 6:D:140:ARG:N | 2.45 | 0.50 |
| 22:T:16:LEU:O | 22:T:19:ARG:HB2 | 2.12 | 0.50 |
| 7:E:45:ASP:OD2 | 7:E:46:THR:HG23 | 2.12 | 0.50 |
| 1:0:1805:G:O2' | 1:0:1806:G:H5' | 2.12 | 0.50 |
| 1:0:354:A:H2' | 1:0:355:C:H6 | 1.76 | 0.50 |
| 1:0:1015:C:H2' | 1:0:1016:U:C6 | 2.47 | 0.50 |
| 23:U:13:ILE:HG12 | 23:U:32:CYS:HB3 | 1.92 | 0.50 |
| 1:0:2320:U:H4' | 1:0:2321:A:O4' | 2.12 | 0.50 |
| 6:D:81:GLU:C | 6:D:83:PHE:H | 2.15 | 0.50 |
| 1:0:1276:U:H3' | 17:O:19:ARG:NH1 | 2.26 | 0.50 |
| 10:H:73:ASN:HB2 | 10:H:88:MET:CE | 2.42 | 0.49 |
| 20:R:44:VAL:O | 20:R:48:GLU:HG3 | 2.11 | 0.49 |
| 1:0:969:G:H1 | 1:0:999:C:H42 | 1.60 | 0.49 |
| 8:F:38:LYS:HZ3 | 15:M:3:SER:HA | 1.77 | 0.49 |
| 5:C:20:ASP:O | 5:C:23:GLU:HB2 | 2.12 | 0.49 |
| 1:0:1299:G:N7 | 14:L:6:ARG:NH1 | 2.60 | 0.49 |
| 1:0:2115:U:H2' | 1:0:2116:U:C6 | 2.47 | 0.49 |
| 1:0:2764:C:H2' | 1:0:2765:C:H6 | 1.76 | 0.49 |
| 12:J:34:GLU:HA | 12:J:34:GLU:OE1 | 2.11 | 0.49 |
| 1:0:1393:A:H2' | 1:0:1394:C:C6 | 2.47 | 0.49 |
| 37:O:4720:HOH:O | 15:M:14:ASN:HB3 | 2.12 | 0.49 |
| 1:0:383:A:H2' | 1:0:384:G:O4' | 2.12 | 0.49 |
| 25:W:21:LEU:HD22 | 25:W:26:ILE:HD13 | 1.94 | 0.49 |
| 8:F:50:VAL:HG13 | 8:F:60:VAL:HG11 | 1.94 | 0.49 |
| 1:0:130:C:O2' | 1:0:131:A:N7 | 2.45 | 0.49 |
| 16:N:73:ALA:HB1 | 16:N:74:PRO:HD2 | 1.94 | 0.49 |
| 7:E:12:ASP:HA | 37:E:1750:HOH:O | 2.11 | 0.49 |
| 15:M:134:ILE:CG2 | 15:M:141:ILE:HD13 | 2.41 | 0.49 |
| 1:0:2300:A:H4' | 1:0:2301:A:O5' | 2.12 | 0.49 |
| 3:A:194:MET:HE3 | 3:A:199:HIS:HB2 | 1.92 | 0.49 |
| 2:9:43:G:H5' | 37:9:8611:HOH:O | 2.11 | 0.49 |
| 3:A:120:ARG:HA | 3:A:159:VAL:HG21 | 1.93 | 0.49 |
| 18:P:105:LEU:CD2 | 18:P:137:LEU:HD21 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1470:A:OP1 | 15:M:93:ARG:HD2 | 2.12 | 0.49 |
| 1:0:2587:OMU:H6 | 1:0:2587:OMU:O5' | 2.12 | 0.49 |
| 6:D:58:VAL:CG1 | 6:D:60:GLU:HG2 | 2.42 | 0.49 |
| 27:Y:172:THR:N | 37:Y:8848:HOH:O | 2.45 | 0.49 |
| 31:3:40:ARG:HD3 | 37:3:8856:HOH:O | 2.12 | 0.49 |
| 1:0:1139:U:H2' | 1:0:1140:C:C6 | 2.47 | 0.49 |
| 1:0:1568:G:O2' | 1:0:1569:U:H5' | 2.12 | 0.49 |
| 4:B:248:ARG:O | 4:B:251:VAL:HG13 | 2.11 | 0.49 |
| 24:V:1:THR:HG23 | 24:V:2:VAL:N | 2.18 | 0.49 |
| 15:M:28:GLN:HA | 15:M:31:TRP:HB2 | 1.94 | 0.49 |
| 14:L:144:ASP:O | 14:L:147:GLU:HG3 | 2.13 | 0.49 |
| 5:C:235:PHE:HE2 | 5:C:243:VAL:HG21 | 1.76 | 0.49 |
| 16:N:29:SER:OG | 16:N:101:VAL:HG21 | 2.12 | 0.49 |
| 19:Q:64:GLU:HG3 | 19:Q:74:ASP:OD2 | 2.12 | 0.49 |
| 28:Z:67:GLY:HA3 | 28:Z:73:THR:CG2 | 2.42 | 0.49 |
| 1:0:470:U:O2' | 29:1:16:HIS:HD2 | 1.94 | 0.49 |
| 26:X:81:GLY:O | 26:X:82:GLU:HB3 | 2.12 | 0.49 |
| 1:0:2840:A:H3' | 37:0:7417:HOH:O | 2.11 | 0.49 |
| 25:W:65:VAL:CA | 25:W:68:THR:HG22 | 2.42 | 0.49 |
| 25:W:38:THR:CG2 | 25:W:39:ASP:N | 2.75 | 0.49 |
| 1:0:1525:G:N2 | 1:0:1526:A:H2' | 2.27 | 0.49 |
| 1:0:2780:C:H2' | 1:0:2781:U:C6 | 2.48 | 0.49 |
| 1:0:361:C:H2' | 1:0:362:G:O4' | 2.13 | 0.49 |
| 1:0:669:G:O2' | 1:0:670:G:H5' | 2.12 | 0.49 |
| 1:0:1768:C:H2' | 1:0:1769:C:O4' | 2.12 | 0.49 |
| 24:V:55:ARG:O | 24:V:59:ILE:HG12 | 2.12 | 0.49 |
| 16:N:112:GLY:HA2 | 16:N:137:ALA:HB2 | 1.93 | 0.49 |
| 1:0:522:U:O2' | 1:0:1366:C:H5' | 2.12 | 0.49 |
| 1:0:1167:G:H4' | 11:I:130:LEU:HD22 | 1.95 | 0.49 |
| 16:N:127:LEU:HB2 | 37:N:8853:HOH:O | 2.12 | 0.49 |
| 25:W:108:ARG:HE | 25:W:114:PRO:HG3 | 1.76 | 0.49 |
| 1:0:506:G:H3' | 37:0:3569:HOH:O | 2.11 | 0.49 |
| 7:E:81:GLU:HB3 | 37:E:4761:HOH:O | 2.12 | 0.49 |
| 1:0:2036:C:C1' | 13:K:44:LEU:HG | 2.42 | 0.49 |
| 14:L:81:VAL:HG12 | 14:L:81:VAL:O | 2.13 | 0.49 |
| 29:1:52:SER:HA | 37:1:4248:HOH:O | 2.12 | 0.49 |
| 1:0:602:A:O2' | 1:0:605:C:H4' | 2.11 | 0.49 |
| 25:W:129:LYS:HG2 | 37:W:1990:HOH:O | 2.12 | 0.49 |
| 37:0:6801:HOH:O | 3:A:211:LYS:HG2 | 2.10 | 0.49 |
| 15:M:164:THR:CG2 | 15:M:167:GLY:N | 2.73 | 0.49 |
| 1:0:1205:U:C2' | 1:0:1206:U:H5' | 2.40 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:V:39:ALA:N | 24:V:40:PRO:HD2 | 2.22 | 0.49 |
| 6:D:39:ASP:O | 6:D:43:GLU:HG3 | 2.13 | 0.49 |
| 1:0:545:G:H2' | 1:0:546:C:O4' | 2.12 | 0.49 |
| 3:A:171:LYS:HB3 | 28:Z:18:TYR:HE2 | 1.78 | 0.49 |
| 1:0:2851:G:C2' | 1:0:2852:A:H5' | 2.42 | 0.49 |
| 16:N:11:ARG:NH2 | 37:N:8817:HOH:O | 2.45 | 0.49 |
| 20:R:117:HIS:HA | 37:R:8826:HOH:O | 2.11 | 0.49 |
| 1:0:2676:C:H4' | 12:J:70:PHE:HE1 | 1.76 | 0.49 |
| 2:9:28:U:H5'' | 16:N:40:ASN:ND2 | 2.28 | 0.49 |
| 27:Y:151:SER:HB3 | 27:Y:154:ARG:HB3 | 1.94 | 0.49 |
| 1:0:1925:G:H5'' | 31:3:29:ARG:HH22 | 1.76 | 0.49 |
| 8:F:52:GLU:HG3 | 8:F:77:VAL:O | 2.11 | 0.49 |
| 7:E:154:ILE:HD11 | 7:E:157:LYS:HE2 | 1.94 | 0.49 |
| 11:I:128:THR:O | 11:I:128:THR:HG22 | 2.12 | 0.49 |
| 4:B:138:GLY:O | 4:B:139:ASP:O | 2.29 | 0.49 |
| 1:0:2507:G:H2' | 1:0:2510:C:H42 | 1.78 | 0.49 |
| 3:A:192:VAL:HB | 37:A:8884:HOH:O | 2.11 | 0.49 |
| 30:2:36:ASN:C | 30:2:38:LYS:H | 2.15 | 0.49 |
| 1:0:1603:A:H5'' | 1:0:1605:G:H5' | 1.93 | 0.49 |
| 1:0:1850:U:H2' | 1:0:1851:G:C8 | 2.47 | 0.49 |
| 1:0:1561:U:H2' | 37:0:3944:HOH:O | 2.11 | 0.49 |
| 1:0:1972:U:H2' | 1:0:1973:A:C5' | 2.43 | 0.49 |
| 1:0:2072:G:H4' | 37:0:6811:HOH:O | 2.12 | 0.49 |
| 1:0:363:C:H2' | 1:0:364:U:C6 | 2.47 | 0.49 |
| 1:0:1468:G:H5'' | 37:0:7227:HOH:O | 2.11 | 0.49 |
| 1:0:1289:C:O2' | 1:0:1290:G:H5' | 2.13 | 0.49 |
| 5:C:72:LYS:HG2 | 5:C:77:ALA:HA | 1.95 | 0.49 |
| 5:C:195:VAL:HA | 5:C:213:ALA:O | 2.13 | 0.49 |
| 1:0:1486:A:C4 | 30:2:2:LYS:HG3 | 2.47 | 0.49 |
| 1:0:1600:G:H4' | 37:0:5444:HOH:O | 2.11 | 0.49 |
| 1:0:1066:U:H2' | 1:0:1067:A:C8 | 2.47 | 0.49 |
| 20:R:100:ASP:C | 20:R:102:GLN:H | 2.14 | 0.49 |
| 4:B:62:ARG:HA | 4:B:65:MET:CE | 2.43 | 0.49 |
| 30:2:41:HIS:CD2 | 30:2:43:ARG:H | 2.31 | 0.49 |
| 13:K:49:LEU:HA | 13:K:73:VAL:HG12 | 1.93 | 0.49 |
| 1:0:1825:U:O2' | 1:0:1826:C:H5' | 2.12 | 0.49 |
| 2:9:18:U:OP2 | 6:D:154:LYS:HE2 | 2.12 | 0.49 |
| 24:V:4:HIS:HB3 | 37:V:6622:HOH:O | 2.13 | 0.49 |
| 3:A:61:GLU:C | 3:A:63:GLY:H | 2.14 | 0.49 |
| 1:0:2577:A:H5' | 37:0:7522:HOH:O | 2.12 | 0.49 |
| 1:0:1661:A:H2' | 1:0:1662:C:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:894:A:C2 | 5:C:87:ARG:NH2 | 2.81 | 0.49 |
| 25:W:36:PRO:HD2 | 25:W:41:TYR:CE1 | 2.48 | 0.49 |
| 1:0:303:C:H2' | 1:0:304:G:O4' | 2.13 | 0.49 |
| 5:C:230:GLY:N | 37:C:8547:HOH:O | 2.42 | 0.49 |
| 18:P:121:ASP:O | 18:P:125:LYS:HG3 | 2.13 | 0.49 |
| 1:0:525:G:H2' | 1:0:526:U:O4' | 2.12 | 0.49 |
| 26:X:43:VAL:HG12 | 26:X:47:ALA:HB3 | 1.93 | 0.49 |
| 1:0:1496:A:H5' | 1:0:1572:A:H1' | 1.95 | 0.49 |
| 37:O:4773:HOH:O | 10:H:61:ARG:HG3 | 2.12 | 0.49 |
| 17:O:44:ASN:HA | 17:O:65:LEU:O | 2.13 | 0.49 |
| 24:V:27:LEU:CA | 24:V:49:LEU:HD13 | 2.43 | 0.49 |
| 8:F:48:VAL:CG2 | 8:F:74:PHE:HB3 | 2.42 | 0.49 |
| 3:A:43:VAL:O | 3:A:76:VAL:HG22 | 2.12 | 0.49 |
| 1:0:2582:G:O3' | 13:K:41:LYS:HA | 2.13 | 0.49 |
| 1:0:343:C:O2' | 1:0:344:C:H5' | 2.12 | 0.49 |
| 1:0:445:U:H2' | 1:0:446:G:H8 | 1.78 | 0.49 |
| 24:V:39:ALA:O | 24:V:41:GLU:N | 2.42 | 0.49 |
| 5:C:27:ARG:NH2 | 17:O:4:ASN:ND2 | 2.61 | 0.49 |
| 20:R:129:ALA:O | 20:R:130:MET:CB | 2.61 | 0.49 |
| 1:0:2002:C:H2' | 1:0:2003:U:H5' | 1.95 | 0.49 |
| 1:0:816:G:H5' | 1:0:1598:A:H4' | 1.94 | 0.49 |
| 3:A:199:HIS:HD2 | 3:A:201:PHE:HB2 | 1.77 | 0.49 |
| 15:M:61:ILE:HD12 | 15:M:61:ILE:N | 2.28 | 0.49 |
| 31:3:11:CYS:HB2 | 31:3:20:HIS:CE1 | 2.48 | 0.49 |
| 17:O:50:ARG:HD2 | 17:O:51:TYR:CE1 | 2.48 | 0.49 |
| 15:M:153:ASP:HB2 | 37:M:8910:HOH:O | 2.13 | 0.49 |
| 25:W:46:ALA:O | 25:W:49:ASN:HB2 | 2.13 | 0.49 |
| 1:0:1513:C:O2' | 1:0:1514:C:H5' | 2.12 | 0.49 |
| 1:0:1250:C:O2' | 1:0:1251:C:H5' | 2.12 | 0.49 |
| 13:K:132:VAL:HG11 | 23:U:22:VAL:HG22 | 1.95 | 0.49 |
| 1:0:1119:G:N2 | 1:0:1246:A:H2 | 2.08 | 0.48 |
| 11:I:129:SER:O | 11:I:130:LEU:HD23 | 2.13 | 0.48 |
| 15:M:99:ARG:HD2 | 15:M:167:GLY:HA2 | 1.95 | 0.48 |
| 7:E:20:ILE:CD1 | 7:E:40:VAL:HG11 | 2.37 | 0.48 |
| 4:B:162:MET:HG3 | 4:B:310:ARG:NH1 | 2.28 | 0.48 |
| 16:N:115:VAL:HG23 | 16:N:116:PHE:H | 1.77 | 0.48 |
| 5:C:132:ASP:O | 5:C:133:ARG:HB2 | 2.12 | 0.48 |
| 2:9:73:A:H61 | 2:9:108:C:N4 | 2.08 | 0.48 |
| 1:0:661:G:C5 | 1:0:686:A:C2 | 3.01 | 0.48 |
| 3:A:57:ALA:HA | 3:A:67:LEU:HD23 | 1.95 | 0.48 |
| 12:J:54:VAL:HG12 | 12:J:58:GLU:HG3 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:415:A:O2' | 1:0:416:G:H5' | 2.13 | 0.48 |
| 1:0:321:A:O2' | 1:0:322:G:H5' | 2.12 | 0.48 |
| 5:C:5:ILE:HG23 | 37:C:8640:HOH:O | 2.13 | 0.48 |
| 1:0:797:A:H5' | 28:Z:10:ARG:N | 2.27 | 0.48 |
| 3:A:86:ALA:HB1 | 3:A:92:ASN:ND2 | 2.29 | 0.48 |
| 10:H:167:LYS:HE2 | 10:H:169:GLU:OE1 | 2.13 | 0.48 |
| 15:M:57:LYS:HG2 | 15:M:58:GLN:H | 1.77 | 0.48 |
| 22:T:40:VAL:HG22 | 22:T:41:ARG:N | 2.28 | 0.48 |
| 4:B:23:THR:HG22 | 4:B:25:ARG:HE | 1.78 | 0.48 |
| 3:A:191:GLY:HA2 | 3:A:194:MET:CE | 2.42 | 0.48 |
| 12:J:80:LYS:HE2 | 12:J:98:PHE:CZ | 2.48 | 0.48 |
| 13:K:64:MET:HE1 | 13:K:105:ARG:HE | 1.78 | 0.48 |
| 28:Z:33:MET:SD | 28:Z:49:ARG:HD2 | 2.53 | 0.48 |
| 1:0:485:A:N3 | 1:0:487:G:H5'' | 2.28 | 0.48 |
| 18:P:103:THR:HA | 18:P:106:ARG:NH1 | 2.27 | 0.48 |
| 26:X:30:MET:HE1 | 26:X:55:ASN:HA | 1.95 | 0.48 |
| 1:0:94:G:N2 | 37:0:4913:HOH:O | 2.38 | 0.48 |
| 1:0:380:A:H2' | 37:0:6998:HOH:O | 2.13 | 0.48 |
| 1:0:23:G:C6 | 1:0:24:G:N1 | 2.81 | 0.48 |
| 25:W:29:VAL:O | 25:W:30:ASN:HB2 | 2.12 | 0.48 |
| 1:0:2505:G:O2' | 1:0:2506:A:H5' | 2.14 | 0.48 |
| 21:S:57:THR:CG2 | 21:S:58:MET:N | 2.77 | 0.48 |
| 26:X:76:ARG:NH1 | 26:X:76:ARG:HG3 | 2.26 | 0.48 |
| 1:0:1377:C:H5' | 1:0:1377:C:C6 | 2.45 | 0.48 |
| 2:9:39:U:H3' | 2:9:40:C:H5'' | 1.94 | 0.48 |
| 1:0:2443:C:O3' | 14:L:56:LYS:HE3 | 2.13 | 0.48 |
| 12:J:34:GLU:O | 12:J:36:VAL:HG23 | 2.13 | 0.48 |
| 18:P:3:LEU:HA | 18:P:6:GLN:OE1 | 2.13 | 0.48 |
| 1:0:503:G:H2' | 1:0:504:G:H8 | 1.78 | 0.48 |
| 1:0:2372:A:H2' | 1:0:2373:U:C6 | 2.48 | 0.48 |
| 1:0:539:G:H2' | 1:0:540:A:C8 | 2.48 | 0.48 |
| 16:N:37:ARG:NE | 37:N:8830:HOH:O | 2.46 | 0.48 |
| 26:X:86:GLU:O | 26:X:87:ALA:O | 2.32 | 0.48 |
| 6:D:146:LYS:HZ3 | 16:N:107:ASN:HD21 | 1.56 | 0.48 |
| 4:B:314:ALA:HB3 | 4:B:317:PRO:HG3 | 1.95 | 0.48 |
| 2:9:73:A:N6 | 2:9:108:C:H42 | 2.09 | 0.48 |
| 1:0:1342:C:H2' | 1:0:1343:C:H5' | 1.96 | 0.48 |
| 1:0:1762:C:H2' | 1:0:1763:C:C6 | 2.48 | 0.48 |
| 26:X:30:MET:HE1 | 26:X:58:ALA:HB3 | 1.95 | 0.48 |
| 26:X:10:VAL:HG11 | 26:X:36:HIS:HE1 | 1.78 | 0.48 |
| 1:0:2561:C:OP1 | 7:E:153:ARG:NH2 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:N:93:GLN:HG2 | 37:N:8853:HOH:O | 2.14 | 0.48 |
| 14:L:76:LEU:HB3 | 14:L:79:ASP:OD2 | 2.14 | 0.48 |
| 7:E:21:THR:HG23 | 7:E:30:THR:OG1 | 2.13 | 0.48 |
| 11:I:68:PRO:CB | 11:I:69:PRO:HD2 | 2.42 | 0.48 |
| 4:B:23:THR:HB | 4:B:25:ARG:HH21 | 1.79 | 0.48 |
| 12:J:42:GLU:O | 12:J:131:THR:HG23 | 2.13 | 0.48 |
| 1:O:1545:C:H2' | 1:O:1546:G:O4' | 2.14 | 0.48 |
| 1:O:371:U:H2' | 1:O:372:A:H8 | 1.79 | 0.48 |
| 25:W:144:GLU:HG3 | 25:W:144:GLU:O | 2.14 | 0.48 |
| 29:1:5:THR:HB | 29:1:6:PRO:CD | 2.43 | 0.48 |
| 17:O:79:VAL:HA | 37:O:6810:HOH:O | 2.13 | 0.48 |
| 1:O:1155:G:H2' | 1:O:1156:C:C6 | 2.48 | 0.48 |
| 1:O:215:A:P | 14:L:52:LYS:HZ3 | 2.36 | 0.48 |
| 1:O:1297:U:H1' | 37:O:3185:HOH:O | 2.13 | 0.48 |
| 18:P:98:ILE:HD12 | 18:P:102:ARG:NE | 2.28 | 0.48 |
| 1:O:807:A:H2' | 1:O:808:A:C8 | 2.49 | 0.48 |
| 16:N:152:GLU:C | 16:N:154:LEU:N | 2.63 | 0.48 |
| 2:9:91:C:H2' | 2:9:92:G:O4' | 2.14 | 0.48 |
| 25:W:76:ASP:O | 25:W:77:ALA:C | 2.52 | 0.48 |
| 11:I:67:VAL:HG13 | 11:I:68:PRO:HD2 | 1.94 | 0.48 |
| 8:F:115:VAL:O | 8:F:118:LEU:N | 2.47 | 0.48 |
| 1:O:1398:G:O2' | 1:O:1399:A:H5' | 2.13 | 0.48 |
| 4:B:139:ASP:CB | 4:B:165:ARG:HE | 2.26 | 0.48 |
| 5:C:109:LEU:HD12 | 5:C:109:LEU:O | 2.13 | 0.48 |
| 1:O:667:C:H2' | 1:O:668:C:H6 | 1.77 | 0.48 |
| 6:D:27:ILE:HG22 | 6:D:28:GLY:N | 2.28 | 0.48 |
| 5:C:233:THR:HG22 | 5:C:234:VAL:N | 2.14 | 0.48 |
| 24:V:50:ARG:HD3 | 37:V:2826:HOH:O | 2.12 | 0.48 |
| 15:M:57:LYS:HZ2 | 15:M:144:ASP:HB2 | 1.78 | 0.48 |
| 20:R:61:GLN:CD | 37:R:8831:HOH:O | 2.51 | 0.48 |
| 19:Q:30:VAL:HG12 | 19:Q:30:VAL:O | 2.14 | 0.48 |
| 14:L:125:PHE:CZ | 14:L:140:VAL:HG13 | 2.49 | 0.48 |
| 1:O:1884:G:O6 | 3:A:190:ARG:HD2 | 2.13 | 0.48 |
| 12:J:33:GLY:O | 12:J:34:GLU:C | 2.52 | 0.48 |
| 12:J:17:CYS:HA | 12:J:119:THR:O | 2.14 | 0.48 |
| 1:O:2047:C:H5' | 37:O:9623:HOH:O | 2.12 | 0.48 |
| 1:O:682:A:H2' | 1:O:683:G:O4' | 2.13 | 0.48 |
| 1:O:1923:G:H4' | 31:3:31:THR:O | 2.13 | 0.48 |
| 1:O:2081:A:H4' | 12:J:69:TYR:CE1 | 2.49 | 0.48 |
| 2:9:6:C:C5' | 16:N:37:ARG:NH1 | 2.67 | 0.48 |
| 1:O:1189:A:O2' | 1:O:1208:C:H2' | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:N:34:LEU:HD13 | 16:N:47:LEU:CD2 | 2.44 | 0.48 |
| 4:B:201:ASP:CB | 4:B:312:ARG:HD2 | 2.38 | 0.48 |
| 1:0:581:G:H4' | 1:0:1254:C:O2' | 2.13 | 0.48 |
| 1:0:224:U:H1' | 37:0:9698:HOH:O | 2.14 | 0.48 |
| 1:0:2389:U:H4' | 19:Q:53:HIS:CD2 | 2.49 | 0.48 |
| 1:0:624:U:H5'' | 37:0:9327:HOH:O | 2.14 | 0.48 |
| 6:D:146:LYS:NZ | 16:N:107:ASN:ND2 | 2.53 | 0.48 |
| 9:G:23:ILE:HD13 | 9:G:67:LEU:HD23 | 1.96 | 0.48 |
| 1:0:1234:U:C4 | 4:B:244:PRO:HB3 | 2.48 | 0.48 |
| 1:0:1165:G:H4' | 1:0:1166:A:OP2 | 2.14 | 0.48 |
| 27:Y:235:GLU:CD | 27:Y:235:GLU:H | 2.17 | 0.48 |
| 5:C:129:HIS:CE1 | 5:C:231:ARG:HA | 2.49 | 0.48 |
| 5:C:26:VAL:HG21 | 5:C:123:LEU:CD1 | 2.44 | 0.48 |
| 1:0:656:G:OP2 | 17:O:37:ARG:HD2 | 2.14 | 0.48 |
| 3:A:65:ARG:C | 3:A:66:ARG:HG3 | 2.33 | 0.48 |
| 1:0:2500:C:H1' | 37:0:4465:HOH:O | 2.14 | 0.48 |
| 4:B:14:GLY:HA2 | 4:B:15:PRO:C | 2.34 | 0.48 |
| 5:C:142:ASP:OD1 | 5:C:236:THR:HG23 | 2.13 | 0.48 |
| 25:W:4:LEU:CD2 | 25:W:54:PHE:HB3 | 2.41 | 0.48 |
| 1:0:1184:C:O2' | 1:0:1185:U:OP2 | 2.23 | 0.48 |
| 11:I:127:CYS:C | 11:I:129:SER:N | 2.67 | 0.48 |
| 3:A:35:GLY:HA3 | 37:A:8887:HOH:O | 2.13 | 0.48 |
| 12:J:41:ALA:N | 37:J:8866:HOH:O | 2.46 | 0.48 |
| 4:B:63:GLU:HG3 | 4:B:63:GLU:O | 2.14 | 0.48 |
| 1:0:1205:U:C2' | 1:0:1206:U:C5' | 2.90 | 0.48 |
| 2:9:57:A:C8 | 6:D:141:VAL:HG21 | 2.49 | 0.48 |
| 15:M:54:TYR:CG | 15:M:55:LYS:N | 2.82 | 0.48 |
| 4:B:211:THR:HA | 4:B:255:GLY:O | 2.14 | 0.48 |
| 12:J:45:VAL:HG21 | 12:J:129:PHE:CD1 | 2.49 | 0.48 |
| 15:M:59:GLY:C | 15:M:141:ILE:HD11 | 2.34 | 0.48 |
| 1:0:2672:C:O2' | 1:0:2673:U:H5' | 2.14 | 0.48 |
| 1:0:2266:A:OP2 | 15:M:90:ARG:NH2 | 2.47 | 0.48 |
| 37:0:4785:HOH:O | 5:C:219:ASN:HB2 | 2.14 | 0.48 |
| 1:0:2629:C:N4 | 3:A:206:ARG:HH21 | 2.12 | 0.48 |
| 1:0:835:U:H3' | 37:0:9181:HOH:O | 2.13 | 0.48 |
| 1:0:210:U:O2' | 1:0:211:U:H5' | 2.14 | 0.48 |
| 1:0:1656:A:H5' | 37:0:4205:HOH:O | 2.13 | 0.48 |
| 1:0:2906:A:H5' | 1:0:2907:C:O4' | 2.14 | 0.48 |
| 1:0:422:G:H2' | 1:0:423:A:H8 | 1.79 | 0.48 |
| 8:F:105:ASP:O | 8:F:109:GLU:HB2 | 2.13 | 0.48 |
| 14:L:72:ASN:O | 14:L:76:LEU:HG | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 25:W:6:GLN:CB | 25:W:26:ILE:HD12 | 2.36 | 0.47 |
| 1:0:317:A:H4' | 37:0:3570:HOH:O | 2.13 | 0.47 |
| 8:F:91:VAL:CG1 | 8:F:92:GLY:N | 2.75 | 0.47 |
| 1:0:1572:A:H2' | 1:0:1573:A:C8 | 2.49 | 0.47 |
| 1:0:553:G:H2' | 1:0:554:G:H5' | 1.96 | 0.47 |
| 2:9:114:G:H2' | 2:9:115:C:C6 | 2.49 | 0.47 |
| 1:0:2256:G:H2' | 1:0:2257:G:H5' | 1.96 | 0.47 |
| 1:0:710:G:H5' | 17:O:25:VAL:CG1 | 2.43 | 0.47 |
| 4:B:96:PRO:HG3 | 37:B:8935:HOH:O | 2.14 | 0.47 |
| 18:P:83:LYS:NZ | 37:P:201:HOH:O | 2.47 | 0.47 |
| 18:P:7:LYS:HD3 | 18:P:21:VAL:CG2 | 2.45 | 0.47 |
| 10:H:87:LYS:HB2 | 10:H:87:LYS:NZ | 2.29 | 0.47 |
| 19:Q:3:SER:HB3 | 37:Q:5998:HOH:O | 2.13 | 0.47 |
| 13:K:4:LEU:HD21 | 13:K:120:ARG:HD2 | 1.96 | 0.47 |
| 18:P:126:ALA:C | 18:P:128:GLY:H | 2.17 | 0.47 |
| 7:E:101:GLU:HB3 | 7:E:117:THR:HA | 1.96 | 0.47 |
| 11:I:95:LEU:CD2 | 11:I:99:GLN:HB3 | 2.34 | 0.47 |
| 4:B:238:ASN:ND2 | 4:B:240:GLY:N | 2.47 | 0.47 |
| 6:D:135:VAL:HG22 | 6:D:136:ARG:N | 2.29 | 0.47 |
| 25:W:38:THR:HG22 | 25:W:39:ASP:H | 1.77 | 0.47 |
| 2:9:3:A:H2 | 2:9:21:G:N3 | 2.12 | 0.47 |
| 5:C:232:LEU:HA | 37:C:8505:HOH:O | 2.14 | 0.47 |
| 18:P:94:TRP:CZ2 | 18:P:98:ILE:HG13 | 2.49 | 0.47 |
| 1:0:2105:C:H2' | 1:0:2106:C:C6 | 2.49 | 0.47 |
| 37:0:5264:HOH:O | 9:G:65:THR:HG23 | 2.12 | 0.47 |
| 1:0:1372:A:H3' | 37:0:6959:HOH:O | 2.13 | 0.47 |
| 1:0:1200:A:H3' | 37:0:5546:HOH:O | 2.14 | 0.47 |
| 8:F:10:ALA:O | 8:F:13:GLU:HB3 | 2.13 | 0.47 |
| 2:9:33:U:H2' | 37:9:8651:HOH:O | 2.12 | 0.47 |
| 5:C:150:THR:O | 5:C:152:GLU:N | 2.47 | 0.47 |
| 8:F:26:THR:HG21 | 8:F:102:GLY:C | 2.34 | 0.47 |
| 18:P:138:GLU:C | 18:P:140:TYR:H | 2.17 | 0.47 |
| 5:C:246:ARG:NE | 37:C:8633:HOH:O | 2.46 | 0.47 |
| 25:W:38:THR:HG21 | 37:W:5390:HOH:O | 2.15 | 0.47 |
| 13:K:62:PRO:CG | 13:K:65:ARG:HH21 | 2.27 | 0.47 |
| 27:Y:189:ASN:ND2 | 27:Y:192:ASP:H | 2.12 | 0.47 |
| 1:0:2050:G:H5'' | 20:R:80:TYR:O | 2.14 | 0.47 |
| 22:T:47:THR:HB | 22:T:100:ASP:HB3 | 1.95 | 0.47 |
| 1:0:2421:G:H3' | 1:0:2422:U:C5' | 2.39 | 0.47 |
| 1:0:2072:G:C6 | 1:0:2533:C:H1' | 2.49 | 0.47 |
| 1:0:1086:A:C6 | 25:W:11:VAL:HG11 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 19:Q:32:GLU:HA | 19:Q:71:TYR:OH | 2.15 | 0.47 |
| 27:Y:102:LEU:HG | 37:Y:8888:HOH:O | 2.14 | 0.47 |
| 26:X:88:GLU:OE1 | 26:X:88:GLU:O | 2.32 | 0.47 |
| 4:B:57:GLU:O | 4:B:63:GLU:HB3 | 2.14 | 0.47 |
| 12:J:108:PRO:HG2 | 12:J:109:TYR:CD1 | 2.49 | 0.47 |
| 2:9:55:U:H4' | 2:9:56:A:H8 | 1.80 | 0.47 |
| 10:H:139:ALA:HB3 | 37:H:232:HOH:O | 2.15 | 0.47 |
| 1:0:306:A:P | 22:T:38:ARG:HH21 | 2.37 | 0.47 |
| 25:W:69:ARG:NH2 | 25:W:119:HIS:HB2 | 2.28 | 0.47 |
| 3:A:217:ARG:NH1 | 3:A:217:ARG:CG | 2.76 | 0.47 |
| 1:0:1909:A:N1 | 1:0:2128:G:H1' | 2.30 | 0.47 |
| 27:Y:189:ASN:HD22 | 27:Y:189:ASN:C | 2.17 | 0.47 |
| 4:B:279:THR:HG22 | 4:B:280:VAL:N | 2.29 | 0.47 |
| 1:0:711:G:C2 | 1:0:718:C:C2 | 3.02 | 0.47 |
| 7:E:137:ASP:O | 7:E:141:VAL:HG23 | 2.15 | 0.47 |
| 18:P:87:ARG:HA | 37:P:188:HOH:O | 2.13 | 0.47 |
| 1:0:512:G:O3' | 1:0:513:A:H8 | 1.96 | 0.47 |
| 1:0:255:A:H2' | 1:0:256:C:O4' | 2.14 | 0.47 |
| 11:I:98:ASP:C | 11:I:100:VAL:H | 2.17 | 0.47 |
| 14:L:68:GLU:O | 14:L:69:ILE:C | 2.53 | 0.47 |
| 17:O:47:ARG:HA | 17:O:50:ARG:NH1 | 2.29 | 0.47 |
| 4:B:277:GLU:N | 4:B:278:PRO:HD2 | 2.29 | 0.47 |
| 1:0:466:A:H2' | 1:0:467:G:O4' | 2.14 | 0.47 |
| 1:0:2717:C:O2' | 1:0:2718:C:H5'' | 2.15 | 0.47 |
| 1:0:1185:U:O2' | 1:0:1186:C:H5' | 2.15 | 0.47 |
| 1:0:1167:G:H2' | 1:0:1168:C:C6 | 2.49 | 0.47 |
| 16:N:110:THR:HB | 16:N:113:SER:OG | 2.15 | 0.47 |
| 25:W:73:LEU:HD12 | 25:W:73:LEU:HA | 1.70 | 0.47 |
| 1:0:1878:G:O2' | 1:0:1879:U:C6 | 2.64 | 0.47 |
| 1:0:2598:U:O2 | 1:0:2600:A:H8 | 1.97 | 0.47 |
| 1:0:656:G:H4' | 37:C:8561:HOH:O | 2.14 | 0.47 |
| 31:3:69:TYR:CZ | 31:3:80:ARG:HD2 | 2.50 | 0.47 |
| 3:A:206:ARG:HH12 | 3:A:208:HIS:CE1 | 2.33 | 0.47 |
| 11:I:102:GLN:HA | 11:I:105:GLU:OE2 | 2.15 | 0.47 |
| 6:D:12:GLU:HB3 | 37:D:3359:HOH:O | 2.14 | 0.47 |
| 11:I:94:ASP:O | 11:I:95:LEU:HG | 2.14 | 0.47 |
| 10:H:43:ALA:HB1 | 10:H:140:TYR:CE2 | 2.49 | 0.47 |
| 13:K:87:ARG:NE | 37:K:4854:HOH:O | 2.48 | 0.47 |
| 8:F:100:ASP:O | 8:F:101:ALA:O | 2.32 | 0.47 |
| 1:0:506:G:N2 | 1:0:509:A:H5' | 2.26 | 0.47 |
| 15:M:59:GLY:HA3 | 15:M:141:ILE:CD1 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:163:VAL:O | 6:D:167:GLU:HB2 | 2.15 | 0.47 |
| 27:Y:154:ARG:NH1 | 27:Y:155:ARG:HG3 | 2.30 | 0.47 |
| 6:D:58:VAL:HG12 | 6:D:60:GLU:HG2 | 1.97 | 0.47 |
| 27:Y:108:ASP:OD1 | 27:Y:108:ASP:N | 2.48 | 0.47 |
| 1:O:675:U:H2' | 1:O:676:C:H5' | 1.96 | 0.47 |
| 16:N:61:ALA:HB3 | 16:N:88:ALA:HB2 | 1.96 | 0.47 |
| 1:O:1388:U:H2' | 1:O:1389:G:O4' | 2.14 | 0.47 |
| 16:N:179:LEU:C | 16:N:181:ASP:H | 2.18 | 0.47 |
| 16:N:179:LEU:HD23 | 16:N:184:ILE:CD1 | 2.45 | 0.47 |
| 1:O:2381:C:H2' | 1:O:2382:A:H8 | 1.78 | 0.47 |
| 1:O:1189:A:H1' | 1:O:1209:C:H1' | 1.97 | 0.47 |
| 10:H:41:LYS:HD3 | 10:H:46:TYR:CZ | 2.50 | 0.47 |
| 12:J:107:ASN:C | 12:J:107:ASN:ND2 | 2.67 | 0.47 |
| 1:O:1798:C:C4' | 18:P:66:GLN:HG2 | 2.45 | 0.47 |
| 16:N:115:VAL:HG23 | 16:N:116:PHE:N | 2.30 | 0.47 |
| 11:I:69:PRO:HG2 | 11:I:72:GLU:HB2 | 1.97 | 0.47 |
| 20:R:39:THR:O | 20:R:40:ALA:C | 2.51 | 0.47 |
| 1:O:695:C:O2' | 1:O:696:C:H5' | 2.14 | 0.47 |
| 22:T:24:ARG:NH1 | 22:T:24:ARG:HG2 | 2.30 | 0.47 |
| 31:3:3:MET:O | 31:3:90:PHE:HA | 2.14 | 0.47 |
| 1:O:212:A:O4' | 1:O:214:U:C6 | 2.68 | 0.47 |
| 1:O:1486:A:C5 | 30:2:2:LYS:HG3 | 2.49 | 0.47 |
| 26:X:30:MET:CE | 26:X:58:ALA:HB3 | 2.44 | 0.47 |
| 1:O:682:A:H5'' | 37:O:3492:HOH:O | 2.15 | 0.47 |
| 1:O:2699:A:H2' | 1:O:2700:G:O4' | 2.15 | 0.47 |
| 1:O:1485:A:H4' | 37:O:3088:HOH:O | 2.14 | 0.47 |
| 5:C:55:ARG:HB2 | 37:C:8510:HOH:O | 2.14 | 0.47 |
| 5:C:104:ASP:O | 5:C:108:GLN:HG3 | 2.14 | 0.47 |
| 1:O:113:A:OP2 | 1:O:114:A:H2' | 2.15 | 0.47 |
| 1:O:2656:G:C2' | 1:O:2657:G:H5' | 2.45 | 0.47 |
| 15:M:99:ARG:HH11 | 15:M:99:ARG:HG2 | 1.80 | 0.47 |
| 4:B:62:ARG:NH2 | 4:B:66:GLU:O | 2.47 | 0.47 |
| 10:H:48:VAL:HA | 10:H:170:ARG:O | 2.15 | 0.47 |
| 12:J:39:VAL:HG11 | 12:J:107:ASN:HB2 | 1.97 | 0.47 |
| 14:L:89:PHE:CD1 | 14:L:89:PHE:N | 2.82 | 0.47 |
| 6:D:44:ILE:HG23 | 6:D:44:ILE:O | 2.15 | 0.47 |
| 4:B:41:PHE:HA | 4:B:79:MET:CE | 2.45 | 0.47 |
| 37:O:9363:HOH:O | 25:W:119:HIS:HE1 | 1.96 | 0.47 |
| 25:W:13:MET:CE | 25:W:17:ILE:HG22 | 2.44 | 0.47 |
| 17:O:14:LEU:HA | 17:O:102:ILE:HD11 | 1.96 | 0.47 |
| 6:D:23:VAL:CG2 | 6:D:73:VAL:HB | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2781:U:C2' | 1:0:2782:G:H5' | 2.44 | 0.47 |
| 21:S:52:VAL:CG2 | 21:S:66:VAL:HG13 | 2.44 | 0.47 |
| 20:R:111:ILE:HG23 | 20:R:145:LEU:HD11 | 1.95 | 0.47 |
| 18:P:18:LYS:O | 18:P:21:VAL:HG22 | 2.15 | 0.47 |
| 15:M:69:LYS:HG3 | 15:M:126:GLN:CA | 2.45 | 0.47 |
| 1:0:292:G:H2' | 1:0:358:G:N2 | 2.29 | 0.47 |
| 1:0:11:A:H5' | 1:0:12:U:OP2 | 2.15 | 0.47 |
| 22:T:70:ALA:O | 22:T:71:VAL:HG23 | 2.14 | 0.47 |
| 1:0:2003:U:H4' | 1:0:2004:U:H5 | 1.79 | 0.47 |
| 18:P:38:GLU:HA | 18:P:41:ARG:HH11 | 1.80 | 0.47 |
| 25:W:131:PRO:HG2 | 25:W:134:GLU:HB2 | 1.96 | 0.47 |
| 14:L:143:THR:CG2 | 14:L:144:ASP:N | 2.78 | 0.47 |
| 1:0:1685:A:H4' | 1:0:1686:C:OP2 | 2.15 | 0.47 |
| 1:0:2681:A:H4' | 1:0:2682:C:C5' | 2.45 | 0.47 |
| 1:0:1882:C:H2' | 1:0:1883:U:C6 | 2.49 | 0.47 |
| 4:B:27:ASN:N | 4:B:27:ASN:HD22 | 2.11 | 0.47 |
| 37:0:3490:HOH:O | 7:E:143:GLN:HG2 | 2.15 | 0.47 |
| 4:B:75:GLU:C | 4:B:77:PRO:HD3 | 2.35 | 0.47 |
| 1:0:2842:G:H5' | 20:R:68:HIS:O | 2.15 | 0.47 |
| 7:E:107:PHE:CE1 | 7:E:152:THR:HB | 2.50 | 0.47 |
| 1:0:183:A:O2' | 1:0:184:G:H5' | 2.15 | 0.47 |
| 4:B:258:GLY:H | 4:B:260:HIS:CE1 | 2.33 | 0.47 |
| 6:D:64:ARG:CD | 6:D:67:ASP:HB3 | 2.45 | 0.47 |
| 6:D:84:LEU:HA | 6:D:87:ALA:HB3 | 1.97 | 0.47 |
| 8:F:58:GLU:HG3 | 8:F:61:MET:HE1 | 1.97 | 0.47 |
| 1:0:2503:A:H2 | 1:0:2517:A:N7 | 2.13 | 0.47 |
| 1:0:157:G:H3' | 37:0:3755:HOH:O | 2.15 | 0.47 |
| 4:B:53:LEU:HD11 | 4:B:327:VAL:HG22 | 1.97 | 0.47 |
| 1:0:710:G:O2' | 1:0:711:G:H5' | 2.14 | 0.47 |
| 14:L:54:PRO:HG2 | 14:L:57:VAL:CG2 | 2.44 | 0.47 |
| 23:U:13:ILE:HG12 | 23:U:32:CYS:CB | 2.45 | 0.47 |
| 1:0:1930:A:H2' | 1:0:1931:A:C8 | 2.50 | 0.47 |
| 18:P:67:LYS:O | 18:P:68:LYS:C | 2.53 | 0.47 |
| 2:9:51:A:H5' | 16:N:160:SER:HB3 | 1.96 | 0.47 |
| 1:0:1186:C:H2' | 1:0:1187:U:O4' | 2.15 | 0.46 |
| 30:2:41:HIS:HB3 | 30:2:44:ARG:HB2 | 1.97 | 0.46 |
| 1:0:2436:U:H5' | 31:3:68:LYS:HE2 | 1.96 | 0.46 |
| 26:X:43:VAL:CG1 | 26:X:44:ASP:H | 2.25 | 0.46 |
| 1:0:1735:C:H5' | 4:B:235:ARG:HH21 | 1.79 | 0.46 |
| 1:0:2570:G:H8 | 37:0:4714:HOH:O | 1.98 | 0.46 |
| 20:R:33:ARG:HH11 | 20:R:60:LYS:HG3 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:694:A:C2' | 1:0:695:C:H5' | 2.45 | 0.46 |
| 1:0:1883:U:O2' | 1:0:1884:G:H5' | 2.15 | 0.46 |
| 17:O:26:TRP:N | 37:O:3062:HOH:O | 2.48 | 0.46 |
| 4:B:56:ASP:HB3 | 4:B:322:ARG:HE | 1.80 | 0.46 |
| 1:0:1477:C:C5' | 1:0:1868:G:H5'' | 2.45 | 0.46 |
| 23:U:6:CYS:SG | 23:U:8:TYR:HB3 | 2.55 | 0.46 |
| 11:I:98:ASP:HA | 11:I:101:LYS:HG3 | 1.97 | 0.46 |
| 6:D:59:GLY:O | 6:D:61:PHE:N | 2.49 | 0.46 |
| 7:E:158:ASP:OD1 | 7:E:160:ARG:N | 2.49 | 0.46 |
| 3:A:223:ARG:O | 3:A:223:ARG:HG2 | 2.14 | 0.46 |
| 25:W:26:ILE:CG1 | 25:W:26:ILE:O | 2.63 | 0.46 |
| 10:H:49:GLN:O | 10:H:169:GLU:HB2 | 2.15 | 0.46 |
| 30:2:36:ASN:HB3 | 30:2:39:ARG:HE | 1.80 | 0.46 |
| 4:B:243:ASN:HA | 4:B:244:PRO:C | 2.35 | 0.46 |
| 21:S:45:TYR:CE2 | 21:S:81:ILE:HD13 | 2.47 | 0.46 |
| 1:0:1587:U:H2' | 1:0:1588:G:O4' | 2.14 | 0.46 |
| 28:Z:60:CYS:SG | 28:Z:62:TYR:HB2 | 2.55 | 0.46 |
| 10:H:31:ILE:HA | 10:H:66:GLU:OE1 | 2.15 | 0.46 |
| 6:D:167:GLU:C | 6:D:169:THR:H | 2.19 | 0.46 |
| 1:0:2781:U:O2' | 1:0:2782:G:H5' | 2.15 | 0.46 |
| 10:H:98:LEU:O | 10:H:124:VAL:HG22 | 2.15 | 0.46 |
| 4:B:214:PRO:HD2 | 37:B:8820:HOH:O | 2.15 | 0.46 |
| 1:0:742:G:O2' | 1:0:743:G:H5' | 2.15 | 0.46 |
| 1:0:2067:A:H2' | 1:0:2068:G:O4' | 2.15 | 0.46 |
| 1:0:2730:G:O2' | 1:0:2731:G:H5' | 2.16 | 0.46 |
| 29:1:21:ARG:HD2 | 29:1:37:CYS:SG | 2.54 | 0.46 |
| 14:L:55:GLN:HA | 14:L:58:GLN:NE2 | 2.25 | 0.46 |
| 10:H:50:ILE:HB | 37:H:232:HOH:O | 2.14 | 0.46 |
| 22:T:49:GLU:HG3 | 22:T:97:ARG:HB3 | 1.98 | 0.46 |
| 14:L:73:VAL:HG11 | 14:L:118:LEU:HD21 | 1.97 | 0.46 |
| 1:0:1603:A:C5' | 1:0:1605:G:H5' | 2.45 | 0.46 |
| 8:F:38:LYS:HZ1 | 15:M:3:SER:HA | 1.79 | 0.46 |
| 1:0:776:A:OP1 | 29:1:28:HIS:HE1 | 1.98 | 0.46 |
| 8:F:22:VAL:CG2 | 8:F:104:ALA:HB2 | 2.45 | 0.46 |
| 14:L:17:SER:C | 14:L:19:LYS:N | 2.68 | 0.46 |
| 21:S:8:PRO:HD2 | 24:V:32:ALA:HA | 1.96 | 0.46 |
| 1:0:825:U:H5'' | 1:0:826:U:OP1 | 2.16 | 0.46 |
| 1:0:1070:A:O5' | 1:0:1070:A:H8 | 1.99 | 0.46 |
| 1:0:843:A:C2 | 1:0:846:A:C8 | 3.03 | 0.46 |
| 28:Z:13:ARG:NH1 | 28:Z:14:PHE:CZ | 2.83 | 0.46 |
| 13:K:115:ARG:HG3 | 13:K:116:GLU:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:444:C:H1' | 37:0:7106:HOH:O | 2.14 | 0.46 |
| 21:S:56:ASN:O | 30:2:8:LYS:NZ | 2.47 | 0.46 |
| 4:B:30:PRO:HG2 | 4:B:313:PRO:HD2 | 1.96 | 0.46 |
| 13:K:113:ILE:HD12 | 13:K:128:ALA:CB | 2.45 | 0.46 |
| 22:T:50:VAL:HG11 | 22:T:55:PHE:HB2 | 1.96 | 0.46 |
| 19:Q:11:ARG:HD2 | 37:Q:5620:HOH:O | 2.15 | 0.46 |
| 7:E:11:VAL:CG1 | 7:E:12:ASP:N | 2.77 | 0.46 |
| 1:0:952:G:H4' | 37:0:6512:HOH:O | 2.16 | 0.46 |
| 16:N:58:LEU:HD12 | 16:N:58:LEU:H | 1.80 | 0.46 |
| 13:K:41:LYS:O | 13:K:42:ASN:HB2 | 2.15 | 0.46 |
| 8:F:13:GLU:OE2 | 8:F:78:GLU:HG2 | 2.15 | 0.46 |
| 37:0:3833:HOH:O | 5:C:149:LYS:HE3 | 2.14 | 0.46 |
| 7:E:156:ASP:N | 7:E:156:ASP:OD1 | 2.47 | 0.46 |
| 24:V:12:THR:H | 24:V:15:GLU:HB2 | 1.81 | 0.46 |
| 3:A:171:LYS:HB3 | 28:Z:18:TYR:CE2 | 2.50 | 0.46 |
| 1:0:816:G:C6 | 1:0:817:G:N1 | 2.83 | 0.46 |
| 1:0:338:C:H4' | 5:C:174:ILE:HD11 | 1.96 | 0.46 |
| 7:E:9:GLU:HG3 | 7:E:10:ASP:N | 2.29 | 0.46 |
| 5:C:129:HIS:HD2 | 5:C:165:ASP:OD2 | 1.98 | 0.46 |
| 1:0:1613:C:H2' | 1:0:1614:G:O4' | 2.15 | 0.46 |
| 3:A:9:ARG:O | 3:A:11:ARG:N | 2.49 | 0.46 |
| 4:B:248:ARG:O | 4:B:251:VAL:CG1 | 2.64 | 0.46 |
| 1:0:2324:G:H4' | 1:0:2418:G:O2' | 2.15 | 0.46 |
| 1:0:407:A:H2' | 1:0:408:A:C8 | 2.51 | 0.46 |
| 14:L:35:ARG:HB2 | 14:L:43:HIS:CD2 | 2.51 | 0.46 |
| 1:0:348:C:H2' | 1:0:349:U:H6 | 1.80 | 0.46 |
| 6:D:92:GLU:HB2 | 37:D:3862:HOH:O | 2.16 | 0.46 |
| 25:W:4:LEU:HD23 | 25:W:54:PHE:CB | 2.41 | 0.46 |
| 16:N:98:GLU:O | 16:N:127:LEU:HD12 | 2.15 | 0.46 |
| 1:0:130:C:H5' | 37:0:5015:HOH:O | 2.15 | 0.46 |
| 2:9:8:G:O6 | 16:N:11:ARG:NH1 | 2.47 | 0.46 |
| 1:0:1561:U:C5' | 37:0:7201:HOH:O | 2.61 | 0.46 |
| 1:0:2668:G:H2' | 1:0:2669:U:C6 | 2.51 | 0.46 |
| 8:F:66:LEU:O | 8:F:69:GLU:HG2 | 2.15 | 0.46 |
| 16:N:42:HIS:HA | 16:N:75:THR:O | 2.16 | 0.46 |
| 3:A:1:GLY:N | 37:A:8900:HOH:O | 2.48 | 0.46 |
| 4:B:205:VAL:N | 37:B:8954:HOH:O | 2.49 | 0.46 |
| 28:Z:20:ARG:O | 28:Z:21:VAL:C | 2.54 | 0.46 |
| 1:0:2911:C:H2' | 1:0:2912:C:H6 | 1.81 | 0.46 |
| 25:W:26:ILE:HG13 | 25:W:26:ILE:O | 2.16 | 0.46 |
| 25:W:6:GLN:HG2 | 25:W:29:VAL:HA | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:Q:28:ARG:HD3 | 19:Q:92:ARG:NH1 | 2.30 | 0.46 |
| 1:0:1197:G:N2 | 1:0:1202:A:H62 | 2.12 | 0.46 |
| 1:0:2894:C:O2' | 1:0:2895:C:H5' | 2.15 | 0.46 |
| 12:J:131:THR:HB | 12:J:134:GLU:OE1 | 2.15 | 0.46 |
| 1:0:35:U:H5' | 5:C:47:GLY:O | 2.16 | 0.46 |
| 1:0:1268:C:H2' | 1:0:1269:G:C8 | 2.50 | 0.46 |
| 1:0:727:G:H3' | 1:0:728:C:H6 | 1.81 | 0.46 |
| 1:0:2787:C:H2' | 1:0:2788:A:O4' | 2.14 | 0.46 |
| 20:R:17:MET:HE1 | 20:R:19:ARG:NH2 | 2.31 | 0.46 |
| 1:0:612:U:H2' | 1:0:613:C:C6 | 2.51 | 0.46 |
| 1:0:1353:C:P | 37:0:4479:HOH:O | 2.74 | 0.46 |
| 6:D:103:ASN:ND2 | 6:D:134:LEU:H | 2.13 | 0.46 |
| 4:B:79:MET:O | 4:B:80:ARG:HG3 | 2.15 | 0.46 |
| 22:T:101:LEU:CD1 | 22:T:112:LEU:HD11 | 2.45 | 0.46 |
| 14:L:123:ASP:OD1 | 14:L:145:LEU:HB3 | 2.16 | 0.46 |
| 19:Q:25:PRO:HA | 19:Q:26:PRO:HD3 | 1.84 | 0.46 |
| 1:0:1878:G:O2' | 1:0:1879:U:P | 2.74 | 0.46 |
| 1:0:625:U:H5'' | 1:0:1044:C:N4 | 2.31 | 0.46 |
| 10:H:80:LEU:HD12 | 10:H:86:TYR:CD2 | 2.51 | 0.46 |
| 1:0:1072:G:P | 27:Y:154:ARG:NH2 | 2.88 | 0.46 |
| 6:D:10:PHE:CG | 6:D:11:HIS:N | 2.83 | 0.46 |
| 1:0:812:A:H1' | 37:0:3756:HOH:O | 2.16 | 0.46 |
| 1:0:1829:A:H2' | 1:0:1830:C:H5' | 1.98 | 0.46 |
| 1:0:2878:U:H2' | 1:0:2879:A:O4' | 2.15 | 0.46 |
| 1:0:858:U:H2' | 1:0:859:C:C6 | 2.50 | 0.46 |
| 1:0:1175:G:H4' | 37:0:6633:HOH:O | 2.16 | 0.46 |
| 9:G:20:VAL:O | 9:G:24:VAL:HG23 | 2.16 | 0.46 |
| 22:T:41:ARG:HG2 | 22:T:41:ARG:HH11 | 1.80 | 0.46 |
| 18:P:105:LEU:HD21 | 18:P:137:LEU:HD21 | 1.97 | 0.46 |
| 1:0:1334:C:H2' | 1:0:1335:C:C6 | 2.51 | 0.46 |
| 12:J:84:ARG:HB2 | 12:J:98:PHE:CE1 | 2.51 | 0.46 |
| 1:0:1245:C:O5' | 1:0:1245:C:H6 | 1.98 | 0.46 |
| 3:A:173:GLY:O | 3:A:176:HIS:HB3 | 2.16 | 0.46 |
| 25:W:80:ASP:HB2 | 37:W:3312:HOH:O | 2.16 | 0.46 |
| 4:B:313:PRO:O | 4:B:314:ALA:C | 2.54 | 0.46 |
| 18:P:59:ARG:NH2 | 18:P:66:GLN:NE2 | 2.57 | 0.46 |
| 12:J:126:ASN:O | 12:J:129:PHE:HE2 | 1.99 | 0.46 |
| 37:0:3554:HOH:O | 22:T:9:LYS:CD | 2.63 | 0.46 |
| 2:9:1:U:C4' | 2:9:3:A:OP1 | 2.64 | 0.46 |
| 4:B:280:VAL:CG1 | 4:B:281:ASP:N | 2.78 | 0.46 |
| 5:C:135:GLU:O | 5:C:136:VAL:HB | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:9:44:A:H1' | 6:D:76:ARG:NH2 | 2.31 | 0.46 |
| 1:0:945:U:O2' | 25:W:43:GLY:HA3 | 2.16 | 0.46 |
| 21:S:50:GLU:HG2 | 21:S:69:SER:HA | 1.99 | 0.46 |
| 1:0:29:C:O2' | 1:0:30:U:H5' | 2.16 | 0.46 |
| 4:B:115:VAL:HA | 4:B:116:PRO:HD3 | 1.87 | 0.46 |
| 1:0:1855:G:O6 | 3:A:142:SER:HB3 | 2.16 | 0.46 |
| 14:L:26:HIS:HB2 | 37:L:8812:HOH:O | 2.16 | 0.46 |
| 1:0:2442:G:H2' | 37:0:9007:HOH:O | 2.15 | 0.46 |
| 6:D:24:HIS:HB2 | 6:D:72:LYS:HB3 | 1.98 | 0.46 |
| 1:0:926:A:O2' | 14:L:41:HIS:CD2 | 2.68 | 0.46 |
| 1:0:247:A:H2' | 37:0:3722:HOH:O | 2.16 | 0.46 |
| 4:B:16:ARG:NH2 | 37:B:8854:HOH:O | 2.32 | 0.46 |
| 22:T:29:ALA:N | 37:T:5241:HOH:O | 2.48 | 0.46 |
| 15:M:47:ASP:CG | 15:M:48:LYS:N | 2.69 | 0.46 |
| 6:D:95:THR:OG1 | 6:D:174:VAL:HA | 2.16 | 0.45 |
| 8:F:58:GLU:HA | 8:F:61:MET:CE | 2.45 | 0.45 |
| 29:1:37:CYS:SG | 29:1:39:PHE:HB2 | 2.56 | 0.45 |
| 16:N:77:ASN:OD1 | 16:N:79:PRO:HD2 | 2.16 | 0.45 |
| 1:0:558:C:C2' | 1:0:559:U:H5'' | 2.45 | 0.45 |
| 1:0:2526:C:C2' | 1:0:2527:U:H5' | 2.46 | 0.45 |
| 16:N:73:ALA:N | 37:N:8863:HOH:O | 2.46 | 0.45 |
| 5:C:21:VAL:HG23 | 5:C:22:PHE:HD1 | 1.79 | 0.45 |
| 7:E:84:MET:HB2 | 7:E:131:LEU:HB2 | 1.98 | 0.45 |
| 1:0:2032:U:H2' | 1:0:2033:G:C5' | 2.46 | 0.45 |
| 1:0:2314:G:H2' | 1:0:2315:C:H5' | 1.97 | 0.45 |
| 5:C:149:LYS:HB2 | 5:C:152:GLU:HG3 | 1.98 | 0.45 |
| 1:0:611:U:H2' | 1:0:612:U:C6 | 2.51 | 0.45 |
| 1:0:1553:C:H2' | 1:0:1554:C:H6 | 1.81 | 0.45 |
| 1:0:1461:U:H2' | 1:0:1462:C:C6 | 2.51 | 0.45 |
| 1:0:2241:C:H2' | 1:0:2242:U:C6 | 2.51 | 0.45 |
| 24:V:58:THR:O | 24:V:62:GLU:HG3 | 2.16 | 0.45 |
| 1:0:652:G:H5'' | 37:0:9812:HOH:O | 2.16 | 0.45 |
| 1:0:97:G:N1 | 22:T:107:LYS:HG3 | 2.31 | 0.45 |
| 5:C:16:VAL:CG1 | 5:C:17:ASP:H | 2.27 | 0.45 |
| 1:0:1159:G:P | 37:0:4097:HOH:O | 2.74 | 0.45 |
| 1:0:317:A:OP1 | 22:T:52:ARG:O | 2.34 | 0.45 |
| 6:D:25:MET:CE | 6:D:37:ALA:HB1 | 2.40 | 0.45 |
| 22:T:9:LYS:CE | 22:T:13:ARG:NH1 | 2.79 | 0.45 |
| 16:N:5:ARG:HB2 | 37:N:8854:HOH:O | 2.15 | 0.45 |
| 4:B:148:PRO:HD2 | 37:B:8881:HOH:O | 2.16 | 0.45 |
| 11:I:108:HIS:H | 11:I:109:PRO:HD2 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:O:9753:HOH:O | 26:X:23:HIS:HD2 | 1.98 | 0.45 |
| 10:H:91:ARG:H | 10:H:91:ARG:HG2 | 1.64 | 0.45 |
| 1:O:470:U:O2' | 29:1:16:HIS:CD2 | 2.69 | 0.45 |
| 31:3:18:GLN:HG3 | 37:3:8861:HOH:O | 2.16 | 0.45 |
| 11:I:125:GLY:HA3 | 37:I:3512:HOH:O | 2.15 | 0.45 |
| 19:Q:72:LYS:HG2 | 19:Q:85:ILE:HD13 | 1.98 | 0.45 |
| 24:V:11:MET:HE1 | 24:V:15:GLU:O | 2.16 | 0.45 |
| 30:2:20:ARG:CG | 30:2:20:ARG:NH1 | 2.72 | 0.45 |
| 6:D:64:ARG:O | 6:D:67:ASP:OD1 | 2.34 | 0.45 |
| 11:I:95:LEU:HD22 | 11:I:99:GLN:CB | 2.35 | 0.45 |
| 22:T:50:VAL:HG11 | 37:T:6384:HOH:O | 2.16 | 0.45 |
| 6:D:40:ILE:HG23 | 37:D:5583:HOH:O | 2.15 | 0.45 |
| 25:W:76:ASP:O | 25:W:77:ALA:O | 2.35 | 0.45 |
| 4:B:5:ARG:HD2 | 4:B:8:LYS:HZ1 | 1.80 | 0.45 |
| 15:M:42:ARG:HA | 15:M:43:PRO:HD3 | 1.81 | 0.45 |
| 1:O:2053:G:H4' | 20:R:136:TRP:CD2 | 2.51 | 0.45 |
| 1:O:290:C:H2' | 1:O:291:C:O4' | 2.15 | 0.45 |
| 1:O:2326:C:H4' | 1:O:2412:G:H4' | 1.98 | 0.45 |
| 3:A:235:ARG:HD3 | 37:A:8833:HOH:O | 2.15 | 0.45 |
| 1:O:958:G:H2' | 1:O:959:C:C6 | 2.51 | 0.45 |
| 18:P:109:ARG:NH1 | 18:P:119:TYR:CE2 | 2.84 | 0.45 |
| 1:O:920:C:H5' | 1:O:921:G:C4 | 2.51 | 0.45 |
| 5:C:16:VAL:CG1 | 5:C:17:ASP:N | 2.80 | 0.45 |
| 1:O:1940:C:H4' | 37:O:7117:HOH:O | 2.14 | 0.45 |
| 8:F:58:GLU:OE2 | 15:M:20:LEU:HD13 | 2.17 | 0.45 |
| 8:F:63:ILE:HB | 8:F:64:PRO:CD | 2.42 | 0.45 |
| 22:T:9:LYS:NZ | 22:T:13:ARG:NH1 | 2.64 | 0.45 |
| 19:Q:25:PRO:HB2 | 37:Q:4350:HOH:O | 2.17 | 0.45 |
| 1:O:2246:U:N3 | 1:O:2256:G:C2 | 2.85 | 0.45 |
| 27:Y:97:LEU:CD2 | 27:Y:235:GLU:HG3 | 2.46 | 0.45 |
| 21:S:6:LYS:HB2 | 21:S:27:ALA:O | 2.14 | 0.45 |
| 1:O:1515:A:H2' | 1:O:1516:U:C6 | 2.51 | 0.45 |
| 7:E:14:GLU:HG2 | 7:E:15:GLN:N | 2.31 | 0.45 |
| 28:Z:25:ARG:O | 28:Z:29:ILE:HG13 | 2.17 | 0.45 |
| 1:O:1163:G:H5' | 11:I:110:ASP:O | 2.17 | 0.45 |
| 10:H:149:VAL:HG21 | 37:H:232:HOH:O | 2.16 | 0.45 |
| 1:O:903:U:O4 | 14:L:18:HIS:HB2 | 2.17 | 0.45 |
| 27:Y:99:ALA:HB2 | 27:Y:233:TYR:CE2 | 2.51 | 0.45 |
| 1:O:80:A:H5'' | 22:T:41:ARG:CZ | 2.47 | 0.45 |
| 16:N:175:LEU:HA | 16:N:175:LEU:HD12 | 1.81 | 0.45 |
| 1:O:23:G:H1' | 1:O:520:A:N6 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:1855:G:H4' | 1:0:1856:C:O5' | 2.16 | 0.45 |
| 7:E:23:GLU:HG2 | 7:E:28:SER:HB3 | 1.99 | 0.45 |
| 1:0:2541:U:H5' | 1:0:2611:G:O6 | 2.16 | 0.45 |
| 1:0:2437:A:H2' | 1:0:2438:G:C8 | 2.51 | 0.45 |
| 21:S:25:GLN:HG2 | 21:S:65:VAL:HG22 | 1.98 | 0.45 |
| 1:0:2543:G:H2' | 1:0:2544:G:O4' | 2.16 | 0.45 |
| 13:K:110:LYS:O | 13:K:111:GLY:O | 2.34 | 0.45 |
| 25:W:21:LEU:HD21 | 25:W:48:VAL:HG13 | 1.96 | 0.45 |
| 10:H:65:LEU:H | 10:H:65:LEU:HD22 | 1.82 | 0.45 |
| 1:0:2506:A:O2' | 1:0:2507:G:C8 | 2.56 | 0.45 |
| 11:I:86:GLU:O | 11:I:89:GLU:HB2 | 2.16 | 0.45 |
| 22:T:41:ARG:O | 22:T:42:VAL:C | 2.55 | 0.45 |
| 1:0:2904:U:H4' | 26:X:8:ARG:HH12 | 1.80 | 0.45 |
| 3:A:32:VAL:O | 3:A:33:GLU:C | 2.54 | 0.45 |
| 4:B:148:PRO:HB2 | 4:B:156:LYS:O | 2.16 | 0.45 |
| 1:0:1067:A:H5' | 37:0:4151:HOH:O | 2.15 | 0.45 |
| 6:D:10:PHE:HA | 37:D:7345:HOH:O | 2.17 | 0.45 |
| 8:F:4:VAL:HA | 8:F:76:PHE:CE1 | 2.51 | 0.45 |
| 15:M:74:LYS:HE2 | 37:M:8928:HOH:O | 2.16 | 0.45 |
| 3:A:30:ARG:HB3 | 3:A:30:ARG:HE | 1.55 | 0.45 |
| 1:0:395:A:H5'' | 37:0:3721:HOH:O | 2.17 | 0.45 |
| 1:0:1127:C:C5 | 1:0:1128:U:C4 | 3.05 | 0.45 |
| 11:I:87:PRO:HD3 | 37:I:6825:HOH:O | 2.16 | 0.45 |
| 1:0:2084:C:H2' | 1:0:2085:A:H8 | 1.82 | 0.45 |
| 1:0:1894:C:C2 | 1:0:1939:U:C4 | 3.04 | 0.45 |
| 25:W:132:VAL:HG23 | 25:W:138:LEU:O | 2.17 | 0.45 |
| 10:H:48:VAL:HG21 | 10:H:143:VAL:HA | 1.99 | 0.45 |
| 10:H:122:LYS:HE3 | 10:H:122:LYS:HB2 | 1.81 | 0.45 |
| 4:B:162:MET:CE | 4:B:310:ARG:HD3 | 2.47 | 0.45 |
| 1:0:2897:C:O2' | 1:0:2898:G:H5' | 2.17 | 0.45 |
| 6:D:49:PRO:HA | 6:D:73:VAL:HG22 | 1.99 | 0.45 |
| 13:K:23:ASN:HD21 | 13:K:107:THR:HB | 1.81 | 0.45 |
| 18:P:67:LYS:O | 18:P:70:ALA:N | 2.50 | 0.45 |
| 17:O:66:GLY:HA3 | 17:O:84:THR:HG22 | 1.97 | 0.45 |
| 27:Y:163:THR:HB | 37:Y:8908:HOH:O | 2.16 | 0.45 |
| 5:C:88:SER:O | 5:C:91:PRO:HD3 | 2.17 | 0.45 |
| 1:0:1173:A:H2 | 37:0:6065:HOH:O | 2.00 | 0.45 |
| 1:0:1500:U:OP2 | 18:P:41:ARG:NH2 | 2.49 | 0.45 |
| 1:0:1735:C:H5' | 4:B:235:ARG:NH2 | 2.32 | 0.45 |
| 1:0:1181:A:H2' | 1:0:1182:C:C5' | 2.43 | 0.45 |
| 11:I:72:GLU:C | 11:I:74:ILE:N | 2.69 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:338:C:H4' | 5:C:174:ILE:HD12 | 1.99 | 0.45 |
| 2:9:39:U:HO2' | 2:9:42:C:H5 | 1.65 | 0.45 |
| 12:J:99:GLU:HA | 37:J:8876:HOH:O | 2.15 | 0.45 |
| 1:0:344:C:H2' | 1:0:345:G:O4' | 2.17 | 0.45 |
| 25:W:5:VAL:HG11 | 25:W:153:MET:CE | 2.47 | 0.45 |
| 1:0:2239:C:H6 | 37:0:6451:HOH:O | 1.99 | 0.45 |
| 37:0:3035:HOH:O | 14:L:22:ARG:HG2 | 2.16 | 0.45 |
| 37:0:3324:HOH:O | 21:S:13:LYS:HE2 | 2.16 | 0.45 |
| 1:0:1517:C:H2' | 1:0:1518:A:C8 | 2.51 | 0.45 |
| 1:0:1539:U:O2' | 1:0:1540:G:H5' | 2.17 | 0.45 |
| 1:0:1942:A:O3' | 3:A:213:LYS:HE2 | 2.16 | 0.45 |
| 16:N:115:VAL:O | 16:N:118:ILE:HB | 2.16 | 0.45 |
| 17:O:32:ARG:HG2 | 17:O:32:ARG:NH1 | 2.32 | 0.45 |
| 1:0:745:G:H5'' | 1:0:746:A:OP1 | 2.16 | 0.45 |
| 1:0:2488:A:H2 | 37:0:7044:HOH:O | 2.00 | 0.45 |
| 11:I:124:VAL:O | 11:I:124:VAL:HG12 | 2.17 | 0.45 |
| 16:N:139:TRP:CZ2 | 16:N:176:ARG:NH1 | 2.85 | 0.45 |
| 4:B:141:ARG:HB3 | 4:B:164:THR:O | 2.16 | 0.45 |
| 21:S:16:ASN:O | 21:S:20:PHE:N | 2.50 | 0.45 |
| 5:C:139:VAL:CG1 | 37:C:8657:HOH:O | 2.63 | 0.45 |
| 13:K:75:ARG:HH21 | 13:K:94:ALA:HB2 | 1.82 | 0.45 |
| 1:0:2587:OMU:H2' | 1:0:2589:U:H5'' | 1.98 | 0.45 |
| 13:K:132:VAL:HG21 | 23:U:22:VAL:HG11 | 1.98 | 0.45 |
| 1:0:2787:C:H5 | 37:0:4434:HOH:O | 1.99 | 0.45 |
| 2:9:95:C:O2' | 2:9:96:C:H5' | 2.17 | 0.45 |
| 37:0:9331:HOH:O | 20:R:139:PRO:HD3 | 2.15 | 0.45 |
| 5:C:180:SER:N | 37:C:8579:HOH:O | 2.47 | 0.45 |
| 17:O:107:GLU:O | 17:O:108:GLY:C | 2.55 | 0.45 |
| 3:A:145:MET:HG2 | 37:A:8828:HOH:O | 2.15 | 0.45 |
| 25:W:106:THR:OG1 | 25:W:109:GLU:HG3 | 2.17 | 0.45 |
| 1:0:603:A:H4' | 1:0:604:G:O5' | 2.16 | 0.45 |
| 6:D:128:LEU:O | 6:D:128:LEU:HD23 | 2.17 | 0.45 |
| 19:Q:75:ILE:CD1 | 19:Q:84:ILE:HD11 | 2.47 | 0.45 |
| 1:0:10:U:O4 | 1:0:532:A:OP2 | 2.33 | 0.45 |
| 1:0:1942:A:H3' | 37:0:7117:HOH:O | 2.17 | 0.45 |
| 3:A:36:ASP:HB2 | 3:A:84:VAL:H | 1.81 | 0.45 |
| 23:U:52:THR:CG2 | 23:U:54:THR:HB | 2.47 | 0.45 |
| 20:R:125:ARG:HB3 | 20:R:125:ARG:NH1 | 2.32 | 0.45 |
| 22:T:9:LYS:HE3 | 22:T:13:ARG:NH1 | 2.31 | 0.45 |
| 1:0:746:A:H5' | 37:0:5310:HOH:O | 2.17 | 0.45 |
| 16:N:67:ALA:O | 16:N:69:TYR:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:32:VAL:O | 3:A:34:ASP:N | 2.49 | 0.45 |
| 6:D:164:ALA:O | 6:D:165:PHE:C | 2.56 | 0.45 |
| 1:0:1643:C:O2' | 1:0:1644:C:H5' | 2.16 | 0.45 |
| 1:0:2651:C:H2' | 1:0:2652:U:O4' | 2.17 | 0.45 |
| 1:0:1072:G:P | 27:Y:154:ARG:HH22 | 2.39 | 0.45 |
| 1:0:1071:G:H4' | 27:Y:154:ARG:NH2 | 2.32 | 0.45 |
| 1:0:612:U:H2' | 1:0:613:C:H6 | 1.81 | 0.45 |
| 1:0:2318:C:H1' | 37:0:3939:HOH:O | 2.17 | 0.45 |
| 1:0:2057:U:O5' | 1:0:2057:U:H6 | 1.99 | 0.45 |
| 19:Q:93:ARG:HG3 | 19:Q:93:ARG:HH11 | 1.81 | 0.45 |
| 1:0:941:G:C5 | 1:0:942:U:C4 | 3.05 | 0.45 |
| 1:0:586:C:H5'' | 37:0:7055:HOH:O | 2.17 | 0.45 |
| 1:0:1682:A:H5'' | 37:0:9263:HOH:O | 2.17 | 0.45 |
| 1:0:645:U:OP2 | 14:L:4:LYS:HE2 | 2.17 | 0.45 |
| 28:Z:38:ALA:N | 37:Z:8725:HOH:O | 2.50 | 0.45 |
| 5:C:194:PHE:HA | 5:C:234:VAL:HG13 | 1.98 | 0.44 |
| 30:2:41:HIS:H | 30:2:45:ASN:ND2 | 2.09 | 0.44 |
| 29:1:8:GLN:NE2 | 29:1:11:LYS:NZ | 2.60 | 0.44 |
| 37:0:7197:HOH:O | 22:T:9:LYS:HD2 | 2.16 | 0.44 |
| 5:C:20:ASP:O | 5:C:23:GLU:N | 2.47 | 0.44 |
| 1:0:1755:A:H2' | 1:0:1756:G:O4' | 2.17 | 0.44 |
| 6:D:81:GLU:C | 6:D:83:PHE:N | 2.70 | 0.44 |
| 16:N:184:ILE:HG23 | 16:N:184:ILE:O | 2.18 | 0.44 |
| 5:C:200:PRO:HB3 | 5:C:212:VAL:HG23 | 1.99 | 0.44 |
| 5:C:126:ASP:C | 5:C:128:GLY:N | 2.69 | 0.44 |
| 1:0:241:A:C2 | 1:0:378:A:H4' | 2.51 | 0.44 |
| 2:9:110:G:C2' | 2:9:111:U:H5' | 2.47 | 0.44 |
| 6:D:28:GLY:O | 6:D:29:HIS:HB3 | 2.17 | 0.44 |
| 26:X:74:ALA:CB | 26:X:85:VAL:HG22 | 2.48 | 0.44 |
| 10:H:41:LYS:HD3 | 10:H:46:TYR:CE1 | 2.52 | 0.44 |
| 1:0:2720:C:O2 | 13:K:87:ARG:NH2 | 2.49 | 0.44 |
| 10:H:50:ILE:HD12 | 10:H:149:VAL:CG1 | 2.48 | 0.44 |
| 4:B:304:PRO:CG | 4:B:307:ARG:NH1 | 2.80 | 0.44 |
| 1:0:1496:A:N6 | 37:0:6898:HOH:O | 2.49 | 0.44 |
| 1:0:506:G:N2 | 1:0:508:A:H3' | 2.32 | 0.44 |
| 23:U:17:THR:HG22 | 23:U:18:GLY:H | 1.81 | 0.44 |
| 1:0:1151:G:OP1 | 9:G:63:ARG:NH1 | 2.50 | 0.44 |
| 1:0:2633:A:H2' | 1:0:2634:G:H5' | 1.99 | 0.44 |
| 1:0:2831:C:C2' | 1:0:2832:C:H5' | 2.48 | 0.44 |
| 16:N:114:LYS:O | 16:N:117:ALA:HB3 | 2.17 | 0.44 |
| 1:0:106:A:H2' | 1:0:107:U:O4' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:139:ASP:HB2 | 4:B:165:ARG:HE | 1.81 | 0.44 |
| 1:0:1154:A:H2' | 1:0:1155:G:C8 | 2.52 | 0.44 |
| 7:E:101:GLU:HG3 | 7:E:101:GLU:O | 2.16 | 0.44 |
| 31:3:15:ASN:HB2 | 37:3:8846:HOH:O | 2.17 | 0.44 |
| 1:0:1020:A:H1' | 37:Q:6976:HOH:O | 2.16 | 0.44 |
| 1:0:2453:G:H3' | 37:0:5707:HOH:O | 2.16 | 0.44 |
| 4:B:240:GLY:HA3 | 37:B:8829:HOH:O | 2.17 | 0.44 |
| 3:A:94:LEU:CG | 3:A:99:ILE:HD11 | 2.40 | 0.44 |
| 18:P:13:VAL:HG11 | 18:P:40:VAL:CG1 | 2.47 | 0.44 |
| 10:H:6:ALA:HA | 10:H:61:ARG:NH1 | 2.32 | 0.44 |
| 1:0:2850:C:C6 | 1:0:2850:C:H5' | 2.44 | 0.44 |
| 22:T:48:VAL:HG12 | 22:T:96:VAL:HG22 | 2.00 | 0.44 |
| 2:9:3:A:N6 | 2:9:22:G:H1' | 2.33 | 0.44 |
| 1:0:2831:C:H2' | 1:0:2832:C:C5' | 2.46 | 0.44 |
| 1:0:1044:C:H5'' | 37:0:8844:HOH:O | 2.17 | 0.44 |
| 1:0:485:A:HO2' | 1:0:487:G:H8 | 1.65 | 0.44 |
| 1:0:1822:A:O2' | 1:0:1823:G:H5' | 2.17 | 0.44 |
| 30:2:22:PRO:HG2 | 30:2:25:VAL:CG2 | 2.47 | 0.44 |
| 17:O:7:LEU:HD22 | 37:O:5650:HOH:O | 2.16 | 0.44 |
| 7:E:32:ARG:O | 7:E:33:LEU:HD23 | 2.17 | 0.44 |
| 1:0:222:A:H2' | 1:0:223:G:O4' | 2.17 | 0.44 |
| 4:B:38:VAL:HA | 4:B:166:VAL:HG22 | 2.00 | 0.44 |
| 24:V:12:THR:O | 24:V:15:GLU:N | 2.48 | 0.44 |
| 25:W:132:VAL:HG21 | 25:W:141:HIS:CD2 | 2.52 | 0.44 |
| 11:I:127:CYS:N | 37:I:5371:HOH:O | 2.45 | 0.44 |
| 25:W:96:LEU:O | 25:W:99:ALA:N | 2.51 | 0.44 |
| 6:D:164:ALA:O | 6:D:167:GLU:N | 2.50 | 0.44 |
| 7:E:170:ARG:NH2 | 37:E:4761:HOH:O | 2.49 | 0.44 |
| 1:0:2265:U:H2' | 1:0:2266:A:H8 | 1.81 | 0.44 |
| 23:U:25:ASP:OD2 | 23:U:27:ALA:HB2 | 2.17 | 0.44 |
| 37:0:3634:HOH:O | 15:M:48:LYS:NZ | 2.44 | 0.44 |
| 27:Y:122:ARG:NH2 | 37:Y:8835:HOH:O | 2.50 | 0.44 |
| 10:H:151:GLU:OE1 | 10:H:151:GLU:HA | 2.17 | 0.44 |
| 1:0:2508:C:H2' | 37:0:6533:HOH:O | 2.17 | 0.44 |
| 1:0:1947:G:N2 | 1:0:1966:U:C2 | 2.85 | 0.44 |
| 5:C:214:THR:HG23 | 5:C:216:SER:H | 1.82 | 0.44 |
| 1:0:1872:C:H5 | 3:A:20:SER:HB3 | 1.82 | 0.44 |
| 11:I:84:SER:N | 37:I:7210:HOH:O | 2.50 | 0.44 |
| 17:O:10:LEU:HD13 | 17:O:99:GLU:HG3 | 1.98 | 0.44 |
| 12:J:47:THR:O | 12:J:53:ILE:HD11 | 2.18 | 0.44 |
| 2:9:13:A:OP1 | 2:9:113:C:H5' | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:27:ARG:HG3 | 5:C:27:ARG:HH11 | 1.82 | 0.44 |
| 15:M:49:ALA:HB1 | 15:M:54:TYR:HB2 | 1.99 | 0.44 |
| 1:0:820:G:O2' | 1:0:856:G:H4' | 2.17 | 0.44 |
| 5:C:133:ARG:HD2 | 37:C:8615:HOH:O | 2.17 | 0.44 |
| 22:T:48:VAL:HG22 | 22:T:98:VAL:HA | 1.99 | 0.44 |
| 1:0:1174:A:H5' | 37:0:4217:HOH:O | 2.17 | 0.44 |
| 10:H:131:GLN:O | 10:H:134:GLU:HG3 | 2.18 | 0.44 |
| 14:L:145:LEU:O | 14:L:148:GLU:HG3 | 2.18 | 0.44 |
| 1:0:1845:A:O3' | 3:A:187:PRO:HB2 | 2.16 | 0.44 |
| 12:J:131:THR:HG22 | 12:J:133:GLY:N | 2.33 | 0.44 |
| 3:A:51:ARG:NH2 | 37:A:8843:HOH:O | 2.49 | 0.44 |
| 10:H:79:GLU:O | 10:H:80:LEU:HD23 | 2.17 | 0.44 |
| 22:T:73:HIS:HD2 | 22:T:88:PRO:HG3 | 1.82 | 0.44 |
| 6:D:60:GLU:O | 6:D:61:PHE:C | 2.55 | 0.44 |
| 10:H:4:LYS:HB3 | 10:H:5:PRO:CD | 2.48 | 0.44 |
| 16:N:108:SER:HA | 16:N:109:PRO:HD3 | 1.83 | 0.44 |
| 14:L:101:ASP:N | 14:L:101:ASP:OD1 | 2.51 | 0.44 |
| 30:2:26:MET:O | 30:2:31:ARG:N | 2.43 | 0.44 |
| 1:0:1314:U:H5'' | 1:0:1316:G:O4' | 2.17 | 0.44 |
| 26:X:26:ALA:HB2 | 26:X:63:ARG:HA | 1.99 | 0.44 |
| 22:T:71:VAL:HG11 | 22:T:90:PRO:CB | 2.37 | 0.44 |
| 25:W:48:VAL:O | 25:W:48:VAL:CG1 | 2.66 | 0.44 |
| 16:N:144:GLY:O | 16:N:147:ILE:CG2 | 2.65 | 0.44 |
| 10:H:36:MET:HB3 | 10:H:73:ASN:ND2 | 2.32 | 0.44 |
| 26:X:43:VAL:CG1 | 26:X:44:ASP:N | 2.79 | 0.44 |
| 1:0:1450:C:C4' | 1:0:1451:C:OP2 | 2.61 | 0.44 |
| 1:0:820:G:H5' | 1:0:821:U:H5' | 1.98 | 0.44 |
| 24:V:33:VAL:CG1 | 24:V:38:GLY:HA3 | 2.44 | 0.44 |
| 1:0:1506:U:H5' | 1:0:1506:U:C6 | 2.50 | 0.44 |
| 10:H:91:ARG:HD3 | 10:H:135:GLN:HB2 | 1.99 | 0.44 |
| 1:0:1149:U:C5 | 1:0:1215:A:C5 | 3.06 | 0.44 |
| 18:P:109:ARG:C | 18:P:111:GLU:H | 2.20 | 0.44 |
| 1:0:1864:C:C5 | 15:M:75:ARG:HD2 | 2.53 | 0.44 |
| 1:0:2860:G:H1' | 37:0:6361:HOH:O | 2.18 | 0.44 |
| 1:0:1484:G:H2' | 37:0:8922:HOH:O | 2.17 | 0.44 |
| 11:I:71:ALA:O | 11:I:75:LYS:HG3 | 2.16 | 0.44 |
| 1:0:1471:A:H2' | 1:0:1472:C:C6 | 2.53 | 0.44 |
| 2:9:80:A:C2 | 2:9:103:A:C4 | 3.06 | 0.44 |
| 20:R:113:HIS:HE1 | 20:R:144:GLU:CD | 2.21 | 0.44 |
| 1:0:2379:G:H4' | 1:0:2380:A:H5'' | 1.98 | 0.44 |
| 11:I:127:CYS:O | 11:I:130:LEU:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:104:PHE:N | 6:D:104:PHE:CD2 | 2.86 | 0.44 |
| 6:D:94:ALA:HA | 6:D:174:VAL:O | 2.17 | 0.44 |
| 3:A:35:GLY:O | 3:A:36:ASP:CB | 2.53 | 0.44 |
| 1:0:777:U:O2' | 29:1:11:LYS:HG2 | 2.17 | 0.44 |
| 16:N:67:ALA:C | 16:N:69:TYR:N | 2.69 | 0.44 |
| 1:0:2281:C:H2' | 1:0:2282:U:H5' | 2.00 | 0.44 |
| 1:0:793:A:C5' | 18:P:83:LYS:HG2 | 2.48 | 0.44 |
| 1:0:2764:C:H2' | 1:0:2765:C:C6 | 2.53 | 0.44 |
| 6:D:10:PHE:CD2 | 6:D:11:HIS:N | 2.85 | 0.44 |
| 28:Z:28:GLU:O | 28:Z:31:SER:N | 2.51 | 0.44 |
| 4:B:189:ALA:O | 4:B:192:ASP:HB2 | 2.18 | 0.44 |
| 25:W:142:ASP:HB2 | 37:W:2729:HOH:O | 2.18 | 0.44 |
| 1:0:1001:U:H1' | 37:H:219:HOH:O | 2.17 | 0.44 |
| 2:9:31:C:H2' | 2:9:32:G:O4' | 2.18 | 0.44 |
| 22:T:14:ALA:HA | 22:T:15:PRO:HD3 | 1.88 | 0.44 |
| 8:F:1:PRO:HB2 | 37:F:5897:HOH:O | 2.18 | 0.44 |
| 14:L:65:ASP:CG | 14:L:111:ALA:HB3 | 2.37 | 0.44 |
| 16:N:144:GLY:O | 16:N:147:ILE:HG22 | 2.18 | 0.44 |
| 22:T:16:LEU:HA | 22:T:19:ARG:HG3 | 2.00 | 0.44 |
| 5:C:115:LEU:HD13 | 5:C:115:LEU:HA | 1.85 | 0.44 |
| 1:0:945:U:H2' | 1:0:946:C:H6 | 1.81 | 0.44 |
| 22:T:20:HIS:O | 22:T:23:VAL:HG23 | 2.18 | 0.44 |
| 3:A:206:ARG:NH1 | 3:A:208:HIS:NE2 | 2.66 | 0.44 |
| 1:0:1086:A:N6 | 25:W:11:VAL:HG11 | 2.33 | 0.44 |
| 18:P:82:GLY:HA2 | 37:P:174:HOH:O | 2.17 | 0.44 |
| 7:E:23:GLU:HG2 | 7:E:28:SER:CB | 2.47 | 0.44 |
| 1:0:2438:G:H5' | 37:0:5953:HOH:O | 2.18 | 0.44 |
| 1:0:2107:U:O2' | 1:0:2108:A:H5' | 2.18 | 0.44 |
| 23:U:35:LYS:HB2 | 37:U:774:HOH:O | 2.17 | 0.44 |
| 1:0:1743:G:O4' | 13:K:78:LYS:HD3 | 2.17 | 0.44 |
| 1:0:1056:U:H2' | 1:0:1057:A:O4' | 2.18 | 0.44 |
| 22:T:37:GLN:HB3 | 37:T:6711:HOH:O | 2.16 | 0.44 |
| 1:0:533:U:H3' | 37:0:3547:HOH:O | 2.16 | 0.44 |
| 1:0:249:G:H2' | 1:0:250:C:C6 | 2.53 | 0.44 |
| 1:0:1160:G:O2' | 1:0:1190:G:H1' | 2.17 | 0.44 |
| 1:0:1943:C:O4' | 3:A:212:PRO:HA | 2.18 | 0.44 |
| 1:0:2846:C:H4' | 4:B:156:LYS:HB3 | 2.00 | 0.44 |
| 7:E:84:MET:HE1 | 7:E:133:VAL:CG2 | 2.48 | 0.44 |
| 1:0:2064:U:H5' | 1:0:2652:U:H4' | 2.00 | 0.44 |
| 11:I:97:VAL:HG12 | 11:I:101:LYS:HE3 | 1.99 | 0.44 |
| 1:0:1782:G:O2' | 1:0:1783:A:H5' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:363:C:H2' | 1:0:364:U:H6 | 1.82 | 0.44 |
| 1:0:812:A:H2' | 1:0:813:C:O4' | 2.18 | 0.44 |
| 1:0:1462:C:O2' | 1:0:1463:U:H5' | 2.18 | 0.44 |
| 4:B:224:LYS:HA | 4:B:224:LYS:HD3 | 1.79 | 0.44 |
| 4:B:215:VAL:O | 4:B:219:GLY:HA2 | 2.18 | 0.44 |
| 16:N:37:ARG:NH2 | 16:N:105:GLY:CA | 2.81 | 0.43 |
| 16:N:93:GLN:HG3 | 16:N:125:ALA:O | 2.18 | 0.43 |
| 37:0:9600:HOH:O | 13:K:39:GLY:HA3 | 2.18 | 0.43 |
| 2:9:49:G:O2' | 2:9:50:G:H5' | 2.17 | 0.43 |
| 1:0:969:G:H2' | 1:0:970:U:C6 | 2.52 | 0.43 |
| 1:0:2281:C:C2' | 1:0:2282:U:H5' | 2.48 | 0.43 |
| 1:0:74:G:H2' | 1:0:75:U:C6 | 2.52 | 0.43 |
| 15:M:158:ARG:HB2 | 15:M:163:LEU:HB2 | 1.99 | 0.43 |
| 1:0:321:A:C2' | 1:0:322:G:H5' | 2.48 | 0.43 |
| 14:L:35:ARG:O | 14:L:40:PHE:HA | 2.18 | 0.43 |
| 1:0:1723:G:H2' | 37:0:9433:HOH:O | 2.18 | 0.43 |
| 1:0:1555:G:O2' | 1:0:1556:G:H5' | 2.18 | 0.43 |
| 8:F:32:GLY:N | 37:F:3111:HOH:O | 2.51 | 0.43 |
| 22:T:55:PHE:N | 22:T:55:PHE:CD1 | 2.86 | 0.43 |
| 10:H:73:ASN:HB2 | 10:H:88:MET:HE1 | 1.98 | 0.43 |
| 16:N:115:VAL:HG23 | 37:N:8856:HOH:O | 2.18 | 0.43 |
| 20:R:22:GLN:HG2 | 20:R:140:GLN:HE21 | 1.83 | 0.43 |
| 23:U:17:THR:CG2 | 23:U:18:GLY:H | 2.30 | 0.43 |
| 24:V:42:ASN:O | 24:V:44:GLY:N | 2.52 | 0.43 |
| 17:O:35:LYS:HB3 | 17:O:36:PRO:HD2 | 1.99 | 0.43 |
| 3:A:93:THR:HG23 | 3:A:154:ALA:O | 2.18 | 0.43 |
| 5:C:21:VAL:HG23 | 5:C:22:PHE:N | 2.34 | 0.43 |
| 27:Y:126:PRO:HG2 | 27:Y:128:PHE:CZ | 2.53 | 0.43 |
| 21:S:52:VAL:HG22 | 21:S:66:VAL:HG13 | 2.00 | 0.43 |
| 1:0:1644:C:H2' | 1:0:1645:U:H6 | 1.84 | 0.43 |
| 5:C:84:VAL:O | 5:C:85:LYS:CB | 2.66 | 0.43 |
| 1:0:371:U:H2' | 1:0:372:A:C8 | 2.52 | 0.43 |
| 16:N:179:LEU:HA | 16:N:184:ILE:CD1 | 2.48 | 0.43 |
| 13:K:115:ARG:CG | 13:K:116:GLU:N | 2.81 | 0.43 |
| 1:0:958:G:O2' | 1:0:959:C:H5' | 2.18 | 0.43 |
| 1:0:920:C:H4' | 1:0:921:G:C2 | 2.52 | 0.43 |
| 1:0:1556:G:O2' | 1:0:1557:G:H5' | 2.17 | 0.43 |
| 23:U:34:SER:HA | 23:U:37:GLU:OE1 | 2.17 | 0.43 |
| 17:O:39:THR:O | 17:O:115:ARG:NH2 | 2.51 | 0.43 |
| 5:C:13:ASP:OD1 | 5:C:13:ASP:O | 2.36 | 0.43 |
| 1:0:1659:A:H2' | 1:0:1660:G:O4' | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1023:C:H2' | 1:0:1024:G:O4' | 2.18 | 0.43 |
| 1:0:1414:A:H2' | 1:0:1415:G:O4' | 2.19 | 0.43 |
| 1:0:169:A:H1' | 31:3:48:ASN:ND2 | 2.33 | 0.43 |
| 7:E:120:GLY:C | 7:E:122:THR:H | 2.21 | 0.43 |
| 13:K:11:GLY:O | 13:K:12:LEU:HD23 | 2.18 | 0.43 |
| 11:I:127:CYS:O | 11:I:129:SER:N | 2.51 | 0.43 |
| 20:R:91:LEU:CD2 | 20:R:143:VAL:HG22 | 2.49 | 0.43 |
| 22:T:35:TYR:CG | 22:T:112:LEU:HD22 | 2.53 | 0.43 |
| 1:0:1181:A:C2 | 1:0:1192:A:C8 | 3.06 | 0.43 |
| 31:3:22:VAL:HG11 | 31:3:67:LEU:HD13 | 1.99 | 0.43 |
| 3:A:82:VAL:HG13 | 3:A:93:THR:HB | 2.00 | 0.43 |
| 12:J:70:PHE:N | 37:J:8869:HOH:O | 2.51 | 0.43 |
| 14:L:17:SER:O | 14:L:19:LYS:N | 2.51 | 0.43 |
| 18:P:138:GLU:O | 18:P:140:TYR:N | 2.51 | 0.43 |
| 20:R:19:ARG:HA | 20:R:142:ASP:OD1 | 2.17 | 0.43 |
| 10:H:4:LYS:N | 37:H:221:HOH:O | 2.52 | 0.43 |
| 3:A:132:ASP:OD1 | 3:A:133:ARG:N | 2.48 | 0.43 |
| 1:0:92:G:O2' | 1:0:93:C:H5' | 2.18 | 0.43 |
| 1:0:1426:C:H4' | 1:0:1427:A:C8 | 2.52 | 0.43 |
| 1:0:2820:A:H2' | 1:0:2821:C:O4' | 2.18 | 0.43 |
| 14:L:112:GLY:O | 14:L:132:LYS:NZ | 2.36 | 0.43 |
| 1:0:541:C:O2' | 1:0:542:A:H5'' | 2.17 | 0.43 |
| 30:2:41:HIS:N | 30:2:45:ASN:HD22 | 2.09 | 0.43 |
| 1:0:259:G:H21 | 15:M:58:GLN:NE2 | 2.15 | 0.43 |
| 1:0:31:C:H2' | 37:0:7457:HOH:O | 2.17 | 0.43 |
| 22:T:48:VAL:CG1 | 22:T:96:VAL:HG13 | 2.45 | 0.43 |
| 2:9:73:A:H2' | 2:9:74:G:C8 | 2.54 | 0.43 |
| 22:T:103:LEU:C | 22:T:105:ASP:H | 2.21 | 0.43 |
| 25:W:60:GLU:O | 25:W:63:GLU:HB2 | 2.18 | 0.43 |
| 3:A:194:MET:HE2 | 3:A:199:HIS:CB | 2.49 | 0.43 |
| 1:0:2793:A:H2' | 1:0:2794:G:H5' | 1.99 | 0.43 |
| 3:A:48:ASP:HB3 | 37:A:8898:HOH:O | 2.16 | 0.43 |
| 37:0:9572:HOH:O | 14:L:41:HIS:HE1 | 2.01 | 0.43 |
| 1:0:2121:G:H3' | 37:0:6357:HOH:O | 2.19 | 0.43 |
| 8:F:119:ARG:HD3 | 8:F:119:ARG:C | 2.37 | 0.43 |
| 15:M:87:GLY:O | 15:M:91:ILE:HD11 | 2.19 | 0.43 |
| 1:0:2432:C:H1' | 37:0:6075:HOH:O | 2.17 | 0.43 |
| 17:O:15:LYS:O | 17:O:16:SER:C | 2.56 | 0.43 |
| 6:D:104:PHE:N | 6:D:104:PHE:HD2 | 2.17 | 0.43 |
| 25:W:21:LEU:HB3 | 25:W:26:ILE:CG1 | 2.49 | 0.43 |
| 12:J:11:ILE:HD11 | 12:J:109:TYR:CD2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1798:C:H4' | 18:P:66:GLN:HG2 | 1.99 | 0.43 |
| 6:D:136:ARG:O | 6:D:138:GLY:N | 2.50 | 0.43 |
| 4:B:79:MET:HG2 | 4:B:146:THR:HG22 | 2.01 | 0.43 |
| 1:0:1688:G:H2' | 1:0:1692:C:H42 | 1.83 | 0.43 |
| 1:0:368:C:H2' | 1:0:369:G:H5' | 2.00 | 0.43 |
| 1:0:1181:A:C2' | 1:0:1182:C:H5' | 2.47 | 0.43 |
| 1:0:1182:C:H6 | 1:0:1182:C:O5' | 2.01 | 0.43 |
| 10:H:27:PRO:HD3 | 10:H:123:ILE:HG22 | 1.98 | 0.43 |
| 15:M:133:LEU:O | 15:M:134:ILE:HD13 | 2.18 | 0.43 |
| 4:B:280:VAL:HG13 | 4:B:334:SER:HA | 2.00 | 0.43 |
| 27:Y:125:LYS:HB2 | 27:Y:126:PRO:HD2 | 2.00 | 0.43 |
| 1:0:2266:A:H2' | 1:0:2267:G:C8 | 2.53 | 0.43 |
| 1:0:2434:A:H2' | 1:0:2435:U:O4' | 2.18 | 0.43 |
| 4:B:77:PRO:HG2 | 4:B:151:VAL:HG22 | 2.00 | 0.43 |
| 7:E:103:VAL:HG21 | 7:E:115:ARG:NH2 | 2.33 | 0.43 |
| 1:0:818:A:O2' | 28:Z:13:ARG:HD3 | 2.19 | 0.43 |
| 1:0:1557:G:O2' | 1:0:1558:C:H5' | 2.18 | 0.43 |
| 22:T:62:VAL:N | 37:T:3851:HOH:O | 2.51 | 0.43 |
| 22:T:85:GLU:HG2 | 22:T:86:GLU:H | 1.83 | 0.43 |
| 5:C:98:ARG:NH1 | 37:C:8559:HOH:O | 2.51 | 0.43 |
| 22:T:65:VAL:HG22 | 22:T:72:ILE:HG22 | 2.01 | 0.43 |
| 11:I:107:LYS:CD | 11:I:110:ASP:HB2 | 2.36 | 0.43 |
| 30:2:41:HIS:O | 30:2:45:ASN:HB2 | 2.18 | 0.43 |
| 12:J:127:ILE:HG12 | 12:J:127:ILE:O | 2.19 | 0.43 |
| 22:T:48:VAL:HG11 | 22:T:96:VAL:HG22 | 2.01 | 0.43 |
| 1:0:88:G:C8 | 1:0:88:G:H5' | 2.43 | 0.43 |
| 2:9:63:C:O2' | 2:9:64:C:H5' | 2.19 | 0.43 |
| 25:W:90:TYR:CD1 | 25:W:90:TYR:N | 2.86 | 0.43 |
| 25:W:125:HIS:HE1 | 37:W:3071:HOH:O | 2.01 | 0.43 |
| 1:0:263:U:O4' | 8:F:59:ILE:HD13 | 2.17 | 0.43 |
| 1:0:638:C:H2' | 1:0:639:A:H8 | 1.83 | 0.43 |
| 26:X:12:ILE:O | 26:X:69:LYS:HA | 2.17 | 0.43 |
| 3:A:164:ARG:HE | 3:A:164:ARG:HB3 | 1.60 | 0.43 |
| 19:Q:93:ARG:NH1 | 19:Q:93:ARG:HG3 | 2.34 | 0.43 |
| 1:0:1091:U:O2' | 1:0:1092:A:H5' | 2.19 | 0.43 |
| 1:0:185:G:H4' | 1:0:186:A:H4' | 2.01 | 0.43 |
| 1:0:275:G:C2 | 1:0:376:C:N3 | 2.87 | 0.43 |
| 23:U:48:ASN:ND2 | 37:U:3104:HOH:O | 2.50 | 0.43 |
| 1:0:2311:A:H5' | 10:H:120:PHE:CD1 | 2.53 | 0.43 |
| 1:0:2834:G:OP1 | 26:X:39:LYS:HE2 | 2.18 | 0.43 |
| 1:0:1145:G:H1 | 1:0:1218:U:H3 | 1.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:M:184:ARG:HG3 | 15:M:185:PRO:HA | 2.00 | 0.43 |
| 1:0:1157:C:H2' | 1:0:1158:G:H8 | 1.82 | 0.43 |
| 1:0:1942:A:O2' | 1:0:1943:C:H5' | 2.19 | 0.43 |
| 16:N:34:LEU:HD13 | 16:N:47:LEU:HD23 | 1.99 | 0.43 |
| 1:0:1840:A:H4' | 1:0:1841:C:O5' | 2.18 | 0.43 |
| 13:K:55:VAL:CG1 | 13:K:56:SER:N | 2.81 | 0.43 |
| 4:B:62:ARG:CA | 4:B:65:MET:HE3 | 2.47 | 0.43 |
| 15:M:55:LYS:O | 15:M:57:LYS:N | 2.52 | 0.43 |
| 10:H:36:MET:SD | 10:H:88:MET:HE2 | 2.59 | 0.43 |
| 1:0:100:C:H2' | 1:0:101:C:H6 | 1.84 | 0.43 |
| 18:P:10:ALA:HA | 18:P:13:VAL:HG12 | 2.01 | 0.43 |
| 16:N:171:HIS:CE1 | 37:N:8863:HOH:O | 2.71 | 0.43 |
| 1:0:1588:G:C6 | 1:0:1589:G:N1 | 2.86 | 0.43 |
| 20:R:39:THR:HB | 20:R:42:GLU:CD | 2.39 | 0.43 |
| 19:Q:28:ARG:CD | 19:Q:92:ARG:NH1 | 2.81 | 0.43 |
| 15:M:61:ILE:HG22 | 15:M:62:VAL:N | 2.33 | 0.43 |
| 5:C:168:ARG:NH2 | 5:C:190:ALA:O | 2.51 | 0.43 |
| 1:0:153:C:P | 37:0:6629:HOH:O | 2.76 | 0.43 |
| 1:0:1544:U:H2' | 1:0:1545:C:H6 | 1.84 | 0.43 |
| 18:P:94:TRP:CH2 | 18:P:98:ILE:HG13 | 2.54 | 0.43 |
| 1:0:2381:C:H2' | 1:0:2382:A:C8 | 2.53 | 0.43 |
| 1:0:250:C:H6 | 1:0:250:C:O5' | 2.01 | 0.43 |
| 3:A:60:PHE:HD1 | 3:A:64:ASP:O | 2.02 | 0.43 |
| 37:0:6069:HOH:O | 27:Y:158:LYS:HD3 | 2.17 | 0.43 |
| 3:A:165:THR:HG22 | 3:A:165:THR:O | 2.19 | 0.43 |
| 7:E:112:ALA:HA | 7:E:113:PRO:HD3 | 1.83 | 0.43 |
| 3:A:215:ILE:HG13 | 3:A:216:SER:N | 2.32 | 0.43 |
| 1:0:350:G:O2' | 1:0:351:A:H5' | 2.18 | 0.43 |
| 6:D:94:ALA:HB3 | 6:D:97:GLN:HG3 | 1.99 | 0.43 |
| 8:F:45:ALA:HA | 37:F:3461:HOH:O | 2.18 | 0.43 |
| 5:C:188:ARG:HD2 | 37:C:8677:HOH:O | 2.19 | 0.43 |
| 1:0:795:G:H1' | 1:0:817:G:N2 | 2.33 | 0.43 |
| 18:P:16:VAL:HG13 | 18:P:20:ARG:CZ | 2.49 | 0.43 |
| 1:0:1014:A:H2' | 1:0:1015:C:H5' | 1.99 | 0.43 |
| 3:A:232:ARG:NH2 | 3:A:236:GLY:O | 2.51 | 0.43 |
| 4:B:76:THR:N | 4:B:77:PRO:HD3 | 2.34 | 0.43 |
| 1:0:1811:A:C2 | 1:0:2752:C:H1' | 2.54 | 0.43 |
| 1:0:835:U:OP1 | 4:B:230:GLN:NE2 | 2.48 | 0.43 |
| 37:0:3038:HOH:O | 11:I:87:PRO:HG2 | 2.19 | 0.43 |
| 23:U:36:CYS:O | 23:U:37:GLU:C | 2.56 | 0.43 |
| 27:Y:110:SER:O | 27:Y:111:ASP:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:911:G:H5' | 1:0:932:U:OP1 | 2.19 | 0.43 |
| 27:Y:149:GLN:NE2 | 37:Y:8910:HOH:O | 2.50 | 0.43 |
| 1:0:2830:U:H4' | 37:0:9892:HOH:O | 2.19 | 0.43 |
| 1:0:1808:C:O2' | 1:0:1809:G:H5' | 2.19 | 0.43 |
| 5:C:5:ILE:CG2 | 5:C:6:TYR:N | 2.82 | 0.43 |
| 13:K:10:GLN:N | 13:K:10:GLN:NE2 | 2.42 | 0.43 |
| 1:0:1163:G:N2 | 37:0:5830:HOH:O | 2.51 | 0.43 |
| 15:M:33:ASN:HB2 | 37:M:8866:HOH:O | 2.19 | 0.43 |
| 1:0:902:G:N7 | 14:L:18:HIS:CD2 | 2.79 | 0.43 |
| 1:0:951:A:C2' | 1:0:952:G:H5' | 2.49 | 0.43 |
| 2:9:61:C:H2' | 2:9:62:A:C8 | 2.53 | 0.43 |
| 3:A:55:VAL:CG1 | 3:A:67:LEU:HB3 | 2.48 | 0.43 |
| 2:9:51:A:C5 | 16:N:41:LYS:HE2 | 2.54 | 0.43 |
| 1:0:1379:A:H1' | 37:0:9503:HOH:O | 2.19 | 0.43 |
| 1:0:644:G:N3 | 1:0:644:G:H5' | 2.34 | 0.43 |
| 5:C:35:VAL:HG21 | 5:C:227:GLY:HA2 | 2.00 | 0.43 |
| 1:0:622:G:P | 27:Y:148:GLY:HA3 | 2.58 | 0.43 |
| 1:0:1350:U:H1' | 37:0:9473:HOH:O | 2.19 | 0.43 |
| 25:W:108:ARG:C | 25:W:110:GLN:N | 2.72 | 0.43 |
| 2:9:56:A:O2' | 6:D:14:ARG:HD3 | 2.19 | 0.43 |
| 14:L:147:GLU:C | 37:L:8856:HOH:O | 2.57 | 0.43 |
| 17:O:14:LEU:CG | 17:O:102:ILE:HD11 | 2.49 | 0.43 |
| 27:Y:189:ASN:HD22 | 27:Y:191:ASP:N | 2.17 | 0.43 |
| 26:X:8:ARG:NH1 | 37:X:2479:HOH:O | 2.52 | 0.43 |
| 2:9:22:G:H5' | 37:9:8723:HOH:O | 2.19 | 0.43 |
| 17:O:26:TRP:CE3 | 17:O:26:TRP:HA | 2.53 | 0.43 |
| 4:B:182:VAL:O | 4:B:184:ASP:N | 2.52 | 0.43 |
| 25:W:1:MET:N | 25:W:103:GLU:OE2 | 2.52 | 0.43 |
| 8:F:67:ALA:C | 8:F:69:GLU:H | 2.22 | 0.43 |
| 37:0:4471:HOH:O | 15:M:4:ALA:HB3 | 2.19 | 0.43 |
| 1:0:2870:C:O2' | 1:0:2871:G:H5' | 2.18 | 0.43 |
| 1:0:1827:G:H2' | 1:0:1828:G:C8 | 2.54 | 0.43 |
| 1:0:1828:G:H5' | 37:0:3780:HOH:O | 2.18 | 0.43 |
| 22:T:63:ILE:HD11 | 22:T:75:GLU:OE1 | 2.19 | 0.43 |
| 1:0:204:A:H2' | 1:0:205:U:H5' | 2.00 | 0.43 |
| 8:F:37:THR:O | 8:F:41:GLU:HG3 | 2.18 | 0.43 |
| 1:0:166:A:N7 | 14:L:25:GLY:HA2 | 2.34 | 0.43 |
| 6:D:89:PRO:O | 6:D:91:ALA:N | 2.52 | 0.42 |
| 6:D:91:ALA:HB1 | 37:D:5198:HOH:O | 2.18 | 0.42 |
| 4:B:55:ASN:CB | 4:B:63:GLU:HA | 2.40 | 0.42 |
| 6:D:138:GLY:O | 6:D:141:VAL:HG23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:153:THR:C | 6:D:155:HIS:H | 2.22 | 0.42 |
| 21:S:39:ASP:O | 21:S:40:ALA:C | 2.57 | 0.42 |
| 20:R:125:ARG:O | 20:R:126:LYS:CB | 2.62 | 0.42 |
| 22:T:48:VAL:CG1 | 22:T:49:GLU:N | 2.81 | 0.42 |
| 1:0:795:G:N3 | 1:0:817:G:C2 | 2.87 | 0.42 |
| 1:0:319:A:H4' | 1:0:338:C:C4 | 2.53 | 0.42 |
| 1:0:2673:U:C2' | 1:0:2674:G:H5' | 2.48 | 0.42 |
| 3:A:191:GLY:O | 3:A:194:MET:HG3 | 2.19 | 0.42 |
| 1:0:2669:U:H2' | 1:0:2670:G:C8 | 2.53 | 0.42 |
| 1:0:2781:U:H2' | 1:0:2782:G:H5' | 2.01 | 0.42 |
| 1:0:764:C:H2' | 1:0:765:G:O4' | 2.19 | 0.42 |
| 4:B:277:GLU:N | 4:B:278:PRO:CD | 2.81 | 0.42 |
| 1:0:275:G:N2 | 1:0:376:C:C2 | 2.87 | 0.42 |
| 26:X:27:ASP:OD2 | 26:X:27:ASP:N | 2.48 | 0.42 |
| 1:0:240:C:H2' | 1:0:240:C:O2 | 2.19 | 0.42 |
| 1:0:1759:A:N3 | 1:0:1818:C:H2' | 2.34 | 0.42 |
| 5:C:51:TYR:CE2 | 29:1:53:LYS:HB3 | 2.54 | 0.42 |
| 1:0:2518:C:H2' | 1:0:2519:C:O4' | 2.19 | 0.42 |
| 3:A:74:VAL:O | 28:Z:65:THR:HG23 | 2.19 | 0.42 |
| 1:0:1876:C:C4 | 3:A:123:GLY:HA3 | 2.54 | 0.42 |
| 1:0:2385:G:H2' | 1:0:2386:U:C6 | 2.54 | 0.42 |
| 4:B:57:GLU:OE1 | 4:B:60:SER:HB2 | 2.19 | 0.42 |
| 1:0:2506:A:O2' | 1:0:2507:G:O5' | 2.38 | 0.42 |
| 13:K:98:VAL:HG12 | 13:K:99:ASP:N | 2.34 | 0.42 |
| 6:D:35:ALA:N | 37:D:5576:HOH:O | 2.52 | 0.42 |
| 1:0:2001:G:O2' | 1:0:2002:C:H5' | 2.19 | 0.42 |
| 22:T:28:SER:HB2 | 37:T:4606:HOH:O | 2.19 | 0.42 |
| 16:N:119:GLN:HG2 | 16:N:123:ILE:HD11 | 2.01 | 0.42 |
| 15:M:43:PRO:HD2 | 37:M:8919:HOH:O | 2.19 | 0.42 |
| 18:P:16:VAL:HG12 | 18:P:17:GLY:H | 1.83 | 0.42 |
| 8:F:48:VAL:HG23 | 8:F:74:PHE:HB2 | 2.00 | 0.42 |
| 5:C:15:GLU:O | 5:C:15:GLU:HG3 | 2.19 | 0.42 |
| 1:0:695:C:H2' | 1:0:696:C:H6 | 1.84 | 0.42 |
| 10:H:68:SER:O | 10:H:69:ARG:C | 2.57 | 0.42 |
| 6:D:169:THR:HG22 | 6:D:169:THR:O | 2.19 | 0.42 |
| 21:S:77:VAL:O | 21:S:80:ARG:HG2 | 2.20 | 0.42 |
| 26:X:25:ARG:HD3 | 26:X:64:ALA:O | 2.19 | 0.42 |
| 19:Q:40:HIS:CE1 | 19:Q:94:GLN:HA | 2.54 | 0.42 |
| 1:0:64:G:H2' | 1:0:65:C:O4' | 2.19 | 0.42 |
| 2:9:28:U:H2' | 2:9:29:C:C6 | 2.54 | 0.42 |
| 1:0:2064:U:H5' | 1:0:2652:U:O3' | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:1353:C:H6 | 37:0:4479:HOH:O | 2.01 | 0.42 |
| 28:Z:28:GLU:O | 28:Z:29:ILE:C | 2.58 | 0.42 |
| 37:0:4423:HOH:O | 3:A:6:GLY:HA3 | 2.19 | 0.42 |
| 1:0:488:U:H2' | 37:0:3801:HOH:O | 2.19 | 0.42 |
| 1:0:2607:U:H4' | 37:0:9249:HOH:O | 2.18 | 0.42 |
| 1:0:2687:G:O2' | 1:0:2688:U:H5' | 2.18 | 0.42 |
| 21:S:29:ASP:OD1 | 21:S:31:ARG:NH1 | 2.53 | 0.42 |
| 22:T:71:VAL:CG1 | 22:T:72:ILE:N | 2.81 | 0.42 |
| 25:W:110:GLN:HE21 | 25:W:110:GLN:CA | 2.27 | 0.42 |
| 12:J:39:VAL:CG1 | 12:J:107:ASN:HB2 | 2.49 | 0.42 |
| 4:B:41:PHE:CD1 | 4:B:79:MET:HE2 | 2.55 | 0.42 |
| 5:C:27:ARG:NH1 | 5:C:29:ASP:OD2 | 2.52 | 0.42 |
| 1:0:1496:A:H2' | 1:0:1497:G:C8 | 2.54 | 0.42 |
| 10:H:12:ILE:HD12 | 10:H:57:THR:CG2 | 2.46 | 0.42 |
| 7:E:93:MET:HG2 | 7:E:94:GLN:H | 1.84 | 0.42 |
| 13:K:34:VAL:HG22 | 13:K:47:ALA:HB2 | 2.01 | 0.42 |
| 12:J:88:PRO:HA | 35:J:8802:CL:CL | 2.57 | 0.42 |
| 5:C:19:PRO:HD2 | 5:C:240:LEU:HD21 | 2.02 | 0.42 |
| 26:X:12:ILE:HB | 26:X:70:ILE:CG2 | 2.49 | 0.42 |
| 1:0:1215:A:O3' | 1:0:1216:G:C4' | 2.67 | 0.42 |
| 15:M:69:LYS:HG3 | 15:M:126:GLN:HA | 2.00 | 0.42 |
| 1:0:39:G:N2 | 1:0:444:C:C2 | 2.87 | 0.42 |
| 1:0:823:U:H2' | 1:0:824:G:O4' | 2.19 | 0.42 |
| 1:0:1933:G:O2' | 1:0:1934:A:H5' | 2.18 | 0.42 |
| 1:0:480:C:H4' | 37:0:7494:HOH:O | 2.18 | 0.42 |
| 15:M:139:PRO:HA | 15:M:142:GLN:HB2 | 2.01 | 0.42 |
| 4:B:122:ASP:O | 4:B:123:ALA:C | 2.57 | 0.42 |
| 1:0:1055:G:OP2 | 10:H:99:ARG:NH1 | 2.52 | 0.42 |
| 4:B:241:PRO:HD2 | 37:B:8956:HOH:O | 2.19 | 0.42 |
| 1:0:659:A:N1 | 17:O:42:GLU:OE2 | 2.52 | 0.42 |
| 7:E:81:GLU:HA | 7:E:133:VAL:O | 2.20 | 0.42 |
| 5:C:19:PRO:HD2 | 5:C:240:LEU:CD2 | 2.49 | 0.42 |
| 1:0:2248:C:C2 | 1:0:2254:G:C2 | 3.07 | 0.42 |
| 1:0:345:G:N2 | 1:0:346:U:H1' | 2.34 | 0.42 |
| 1:0:445:U:H2' | 1:0:446:G:C8 | 2.53 | 0.42 |
| 7:E:101:GLU:CB | 7:E:117:THR:HA | 2.50 | 0.42 |
| 28:Z:42:CYS:SG | 28:Z:43:GLY:N | 2.92 | 0.42 |
| 1:0:2011:A:H5' | 1:0:2013:G:H1' | 2.01 | 0.42 |
| 27:Y:144:ARG:CZ | 37:Y:8921:HOH:O | 2.66 | 0.42 |
| 14:L:98:GLU:C | 14:L:99:GLU:HG3 | 2.39 | 0.42 |
| 16:N:23:ARG:NH1 | 37:N:8842:HOH:O | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:G:12:ILE:HG22 | 9:G:12:ILE:O | 2.19 | 0.42 |
| 16:N:116:PHE:O | 16:N:119:GLN:HB3 | 2.19 | 0.42 |
| 16:N:132:ASN:N | 37:N:8851:HOH:O | 2.52 | 0.42 |
| 5:C:246:ARG:CZ | 37:C:8633:HOH:O | 2.67 | 0.42 |
| 24:V:42:ASN:N | 24:V:43:PRO:HD3 | 2.34 | 0.42 |
| 1:O:1853:C:O2' | 3:A:217:ARG:NH2 | 2.53 | 0.42 |
| 22:T:103:LEU:O | 22:T:105:ASP:N | 2.53 | 0.42 |
| 14:L:73:VAL:HG23 | 14:L:74:THR:N | 2.35 | 0.42 |
| 17:O:14:LEU:HA | 17:O:102:ILE:CD1 | 2.49 | 0.42 |
| 1:O:2673:U:H2' | 1:O:2674:G:H5' | 2.01 | 0.42 |
| 1:O:1221:G:C8 | 37:O:5773:HOH:O | 2.57 | 0.42 |
| 1:O:1878:G:C1' | 37:O:5905:HOH:O | 2.65 | 0.42 |
| 1:O:733:U:H5'' | 37:O:9658:HOH:O | 2.18 | 0.42 |
| 6:D:170:TYR:CD1 | 6:D:170:TYR:N | 2.87 | 0.42 |
| 8:F:77:VAL:HG21 | 8:F:83:LEU:HD13 | 2.01 | 0.42 |
| 2:9:110:G:H2' | 2:9:111:U:H5' | 2.01 | 0.42 |
| 1:O:2408:A:H4' | 31:3:15:ASN:O | 2.20 | 0.42 |
| 1:O:1916:C:H2' | 1:O:1917:G:O4' | 2.20 | 0.42 |
| 27:Y:98:GLN:HA | 37:Y:8839:HOH:O | 2.19 | 0.42 |
| 10:H:34:HIS:HD2 | 10:H:90:LEU:O | 2.03 | 0.42 |
| 13:K:63:GLU:HG2 | 37:K:6344:HOH:O | 2.19 | 0.42 |
| 5:C:144:PHE:HE1 | 5:C:153:VAL:HG13 | 1.84 | 0.42 |
| 22:T:30:ASP:O | 22:T:33:GLU:HB3 | 2.20 | 0.42 |
| 30:2:48:ASP:O | 30:2:49:GLU:CB | 2.66 | 0.42 |
| 2:9:56:A:H1' | 6:D:14:ARG:HG2 | 2.02 | 0.42 |
| 1:O:2909:G:H2' | 1:O:2910:A:H8 | 1.84 | 0.42 |
| 4:B:79:MET:C | 4:B:80:ARG:HG3 | 2.40 | 0.42 |
| 1:O:282:C:H1' | 1:O:368:C:H41 | 1.79 | 0.42 |
| 2:9:72:C:O2' | 2:9:73:A:H5' | 2.20 | 0.42 |
| 1:O:2291:A:N9 | 1:O:2309:C:H5' | 2.35 | 0.42 |
| 22:T:103:LEU:HD22 | 22:T:112:LEU:CD1 | 2.49 | 0.42 |
| 1:O:1473:U:C1' | 29:1:42:SER:HB3 | 2.50 | 0.42 |
| 1:O:1166:A:H1' | 1:O:1192:A:C2 | 2.55 | 0.42 |
| 37:O:9010:HOH:O | 5:C:107:ARG:NH1 | 2.53 | 0.42 |
| 11:I:115:ASP:C | 11:I:117:THR:N | 2.69 | 0.42 |
| 2:9:47:A:C2 | 2:9:48:C:C2 | 3.08 | 0.42 |
| 1:O:1213:C:C2' | 1:O:1214:G:H5' | 2.50 | 0.42 |
| 1:O:949:U:O2' | 19:Q:40:HIS:HE1 | 2.03 | 0.42 |
| 15:M:66:SER:HB3 | 15:M:128:TRP:NE1 | 2.34 | 0.42 |
| 5:C:40:ALA:O | 5:C:43:LYS:HB2 | 2.20 | 0.42 |
| 1:O:2453:G:H4' | 14:L:50:GLY:C | 2.39 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:214:THR:CG2 | 5:C:216:SER:H | 2.32 | 0.42 |
| 10:H:92:LYS:HD3 | 10:H:92:LYS:HA | 1.88 | 0.42 |
| 1:0:1396:C:H1' | 18:P:1:THR:O | 2.20 | 0.42 |
| 15:M:146:ASP:O | 15:M:147:LEU:HG | 2.18 | 0.42 |
| 37:0:5502:HOH:O | 7:E:57:LYS:HE2 | 2.19 | 0.42 |
| 1:0:567:U:H5'' | 37:0:6184:HOH:O | 2.20 | 0.42 |
| 2:9:4:G:H1' | 37:9:8716:HOH:O | 2.20 | 0.42 |
| 3:A:180:LYS:HB2 | 37:A:8916:HOH:O | 2.20 | 0.42 |
| 1:0:2717:C:OP1 | 4:B:207:LYS:HG3 | 2.19 | 0.42 |
| 24:V:1:THR:C | 24:V:3:LEU:H | 2.23 | 0.42 |
| 15:M:24:GLN:O | 15:M:28:GLN:HG3 | 2.19 | 0.42 |
| 6:D:166:ILE:HG13 | 6:D:166:ILE:H | 1.68 | 0.42 |
| 4:B:178:ALA:O | 4:B:179:LEU:C | 2.57 | 0.42 |
| 20:R:66:VAL:HG13 | 20:R:79:ARG:HE | 1.85 | 0.42 |
| 1:0:2689:A:H2' | 1:0:2690:U:H5' | 2.02 | 0.42 |
| 16:N:176:ARG:O | 16:N:180:LEU:HD13 | 2.19 | 0.42 |
| 1:0:2694:A:C4' | 7:E:91:PHE:HE1 | 2.31 | 0.42 |
| 6:D:23:VAL:HG22 | 6:D:73:VAL:HB | 2.02 | 0.42 |
| 13:K:23:ASN:HA | 37:K:7075:HOH:O | 2.19 | 0.42 |
| 1:0:2132:C:H2' | 37:0:7327:HOH:O | 2.20 | 0.42 |
| 20:R:141:VAL:HG12 | 20:R:142:ASP:N | 2.34 | 0.42 |
| 4:B:71:VAL:HG11 | 4:B:296:LEU:HB3 | 2.02 | 0.42 |
| 3:A:70:ALA:HA | 3:A:71:PRO:HD3 | 1.84 | 0.42 |
| 18:P:58:SER:HB3 | 37:P:184:HOH:O | 2.20 | 0.42 |
| 1:0:417:G:P | 37:0:7190:HOH:O | 2.77 | 0.42 |
| 1:0:1235:G:N2 | 37:0:4680:HOH:O | 2.51 | 0.42 |
| 1:0:328:U:O4' | 5:C:202:THR:HG22 | 2.20 | 0.42 |
| 15:M:18:GLY:O | 15:M:21:ALA:HB3 | 2.19 | 0.42 |
| 7:E:100:ASP:HB2 | 37:E:2789:HOH:O | 2.18 | 0.42 |
| 22:T:71:VAL:HG13 | 22:T:91:LEU:H | 1.85 | 0.42 |
| 25:W:108:ARG:C | 25:W:110:GLN:H | 2.23 | 0.42 |
| 3:A:36:ASP:O | 3:A:37:VAL:C | 2.58 | 0.42 |
| 1:0:1684:A:H1' | 30:2:43:ARG:NH2 | 2.28 | 0.42 |
| 14:L:105:TYR:N | 37:L:8868:HOH:O | 2.53 | 0.42 |
| 1:0:2000:G:O2' | 1:0:2001:G:H5' | 2.20 | 0.42 |
| 1:0:2002:C:C2' | 1:0:2003:U:H5' | 2.49 | 0.42 |
| 1:0:1335:C:OP2 | 27:Y:207:SER:CB | 2.67 | 0.42 |
| 10:H:86:TYR:C | 10:H:86:TYR:CD1 | 2.93 | 0.42 |
| 37:0:5206:HOH:O | 3:A:164:ARG:CZ | 2.67 | 0.42 |
| 6:D:11:HIS:CG | 6:D:12:GLU:N | 2.88 | 0.42 |
| 15:M:47:ASP:CG | 15:M:48:LYS:H | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:O:6661:HOH:O | 3:A:165:THR:HG23 | 2.18 | 0.42 |
| 31:3:87:ARG:HG2 | 37:3:8869:HOH:O | 2.19 | 0.42 |
| 14:L:82:ALA:O | 14:L:83:GLU:C | 2.58 | 0.42 |
| 1:O:414:C:H5' | 37:O:5897:HOH:O | 2.20 | 0.42 |
| 26:X:45:GLU:HG3 | 37:X:6178:HOH:O | 2.19 | 0.42 |
| 8:F:60:VAL:O | 8:F:62:HIS:N | 2.53 | 0.42 |
| 1:O:281:U:H2' | 1:O:282:C:O4' | 2.19 | 0.42 |
| 12:J:121:LEU:HD21 | 12:J:129:PHE:CD2 | 2.55 | 0.42 |
| 10:H:57:THR:N | 10:H:132:ALA:HB2 | 2.34 | 0.42 |
| 1:O:319:A:H4' | 1:O:338:C:C5 | 2.54 | 0.42 |
| 1:O:1008:C:OP1 | 10:H:19:ARG:NH2 | 2.51 | 0.42 |
| 27:Y:234:VAL:CG1 | 27:Y:235:GLU:N | 2.82 | 0.42 |
| 12:J:42:GLU:HG2 | 12:J:43:ARG:HG3 | 2.01 | 0.42 |
| 1:O:1311:G:C2 | 1:O:1312:G:C8 | 3.08 | 0.42 |
| 4:B:279:THR:CG2 | 4:B:280:VAL:N | 2.83 | 0.42 |
| 4:B:88:GLU:HB3 | 4:B:97:LEU:HG | 2.01 | 0.42 |
| 1:O:1276:U:H3' | 17:O:19:ARG:HH11 | 1.85 | 0.42 |
| 13:K:41:LYS:HE3 | 37:K:7871:HOH:O | 2.18 | 0.42 |
| 1:O:2134:G:N2 | 1:O:2242:U:C2 | 2.88 | 0.42 |
| 13:K:78:LYS:HA | 13:K:79:PRO:HD3 | 1.86 | 0.42 |
| 15:M:139:PRO:O | 15:M:143:ASN:ND2 | 2.53 | 0.42 |
| 14:L:67:ARG:O | 14:L:71:GLU:HG3 | 2.20 | 0.42 |
| 13:K:72:VAL:O | 13:K:95:ALA:HA | 2.19 | 0.42 |
| 1:O:366:U:H2' | 1:O:367:G:O4' | 2.20 | 0.42 |
| 27:Y:103:THR:O | 27:Y:103:THR:HG22 | 2.20 | 0.42 |
| 1:O:1449:G:H2' | 1:O:1493:A:C2 | 2.55 | 0.42 |
| 8:F:11:ASP:HA | 8:F:14:ASP:OD2 | 2.19 | 0.42 |
| 1:O:598:C:H2' | 1:O:599:G:H8 | 1.82 | 0.42 |
| 11:I:91:PHE:CD2 | 11:I:131:GLY:HA2 | 2.55 | 0.42 |
| 1:O:426:G:H2' | 1:O:427:C:O4' | 2.20 | 0.42 |
| 1:O:432:G:N2 | 1:O:433:C:C2 | 2.87 | 0.42 |
| 1:O:52:A:H2' | 1:O:53:C:O4' | 2.20 | 0.42 |
| 1:O:57:C:H2' | 1:O:58:C:O4' | 2.20 | 0.42 |
| 4:B:7:ARG:HB2 | 4:B:7:ARG:CZ | 2.50 | 0.42 |
| 16:N:43:VAL:O | 16:N:43:VAL:HG12 | 2.20 | 0.42 |
| 1:O:907:A:H4' | 1:O:1328:A:C2 | 2.55 | 0.42 |
| 4:B:24:PRO:C | 4:B:25:ARG:HD3 | 2.39 | 0.42 |
| 26:X:22:ASN:O | 26:X:25:ARG:HG3 | 2.20 | 0.42 |
| 1:O:2825:C:H4' | 1:O:2826:G:O5' | 2.20 | 0.42 |
| 16:N:62:HIS:O | 16:N:65:ASP:OD1 | 2.38 | 0.42 |
| 5:C:93:LYS:HB3 | 5:C:95:GLU:OE1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 21:S:7:HIS:HB2 | 21:S:8:PRO:CD | 2.50 | 0.42 |
| 3:A:206:ARG:HH11 | 3:A:208:HIS:CD2 | 2.38 | 0.42 |
| 1:0:2764:C:O2' | 1:0:2765:C:H5' | 2.20 | 0.42 |
| 1:0:383:A:H4' | 37:0:5126:HOH:O | 2.19 | 0.42 |
| 18:P:138:GLU:C | 18:P:140:TYR:N | 2.73 | 0.42 |
| 1:0:613:C:H2' | 1:0:614:U:H6 | 1.85 | 0.42 |
| 1:0:1758:U:H2' | 1:0:1759:A:O4' | 2.20 | 0.42 |
| 22:T:3:GLN:HA | 22:T:4:PRO:HD3 | 1.97 | 0.42 |
| 12:J:51:GLU:O | 12:J:55:GLU:HG3 | 2.19 | 0.42 |
| 1:0:1860:U:H2' | 1:0:1861:C:O4' | 2.19 | 0.42 |
| 1:0:1846:U:O2' | 3:A:172:ALA:HB2 | 2.19 | 0.42 |
| 1:0:2511:A:H2' | 1:0:2512:U:O4' | 2.19 | 0.41 |
| 6:D:35:ALA:C | 6:D:37:ALA:H | 2.22 | 0.41 |
| 1:0:2896:A:P | 26:X:15:ARG:NH1 | 2.93 | 0.41 |
| 9:G:24:VAL:HA | 9:G:27:ILE:HD12 | 2.02 | 0.41 |
| 8:F:99:THR:HG23 | 8:F:99:THR:O | 2.20 | 0.41 |
| 21:S:39:ASP:HB3 | 21:S:43:GLU:OE2 | 2.20 | 0.41 |
| 17:O:32:ARG:HG2 | 17:O:32:ARG:HH11 | 1.85 | 0.41 |
| 1:0:2392:C:O5' | 1:0:2392:C:H6 | 2.03 | 0.41 |
| 2:9:3:A:O5' | 2:9:3:A:C8 | 2.74 | 0.41 |
| 1:0:1504:A:O2' | 1:0:1506:U:OP2 | 2.31 | 0.41 |
| 17:O:96:VAL:HG12 | 17:O:97:SER:N | 2.35 | 0.41 |
| 17:O:77:ALA:HB1 | 17:O:98:LEU:HD12 | 2.02 | 0.41 |
| 1:0:1044:C:C5' | 37:0:8844:HOH:O | 2.67 | 0.41 |
| 23:U:6:CYS:C | 23:U:8:TYR:N | 2.74 | 0.41 |
| 1:0:1703:G:N2 | 18:P:57:ASN:HD21 | 2.18 | 0.41 |
| 1:0:2248:C:H2' | 1:0:2249:G:H8 | 1.85 | 0.41 |
| 1:0:858:U:H2' | 1:0:859:C:H6 | 1.85 | 0.41 |
| 2:9:9:C:H2' | 2:9:10:C:H5' | 2.02 | 0.41 |
| 1:0:790:A:H2' | 1:0:791:A:O4' | 2.20 | 0.41 |
| 1:0:1601:G:H1' | 37:0:9701:HOH:O | 2.18 | 0.41 |
| 8:F:49:PHE:N | 8:F:49:PHE:CD1 | 2.87 | 0.41 |
| 1:0:1996:U:O2' | 1:0:1997:A:H5' | 2.20 | 0.41 |
| 5:C:141:SER:C | 5:C:143:ASP:H | 2.23 | 0.41 |
| 25:W:140:LYS:C | 25:W:141:HIS:HD2 | 2.23 | 0.41 |
| 10:H:46:TYR:HE2 | 10:H:85:ASP:O | 2.03 | 0.41 |
| 1:0:2506:A:H1' | 37:0:3545:HOH:O | 2.20 | 0.41 |
| 14:L:117:GLU:HG3 | 14:L:117:GLU:O | 2.21 | 0.41 |
| 6:D:140:ARG:HG3 | 6:D:140:ARG:HH11 | 1.84 | 0.41 |
| 1:0:794:U:H3 | 1:0:819:A:N6 | 2.11 | 0.41 |
| 28:Z:17:ARG:HB2 | 28:Z:18:TYR:CE1 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:R:125:ARG:NH1 | 20:R:134:SER:HB2 | 2.33 | 0.41 |
| 22:T:49:GLU:CG | 22:T:97:ARG:HB3 | 2.50 | 0.41 |
| 2:9:73:A:N1 | 2:9:108:C:N3 | 2.68 | 0.41 |
| 16:N:67:ALA:HA | 16:N:71:TRP:CB | 2.48 | 0.41 |
| 16:N:70:GLY:O | 16:N:71:TRP:C | 2.57 | 0.41 |
| 1:0:1503:U:H2' | 1:0:1504:A:O4' | 2.20 | 0.41 |
| 1:0:2420:G:H2' | 1:0:2421:G:C8 | 2.55 | 0.41 |
| 2:9:41:C:O4' | 6:D:50:VAL:HG22 | 2.21 | 0.41 |
| 7:E:2:ARG:HA | 7:E:49:ILE:O | 2.20 | 0.41 |
| 1:0:253:U:H1' | 1:0:256:C:H41 | 1.86 | 0.41 |
| 1:0:1771:U:H4' | 1:0:1772:C:OP2 | 2.19 | 0.41 |
| 25:W:36:PRO:HD2 | 25:W:41:TYR:CD1 | 2.55 | 0.41 |
| 1:0:372:A:H2' | 1:0:373:G:H8 | 1.86 | 0.41 |
| 5:C:150:THR:C | 5:C:152:GLU:N | 2.74 | 0.41 |
| 16:N:178:THR:O | 16:N:181:ASP:HB3 | 2.20 | 0.41 |
| 1:0:2729:C:H2' | 1:0:2730:G:H8 | 1.85 | 0.41 |
| 20:R:6:VAL:HG21 | 20:R:113:HIS:CD2 | 2.54 | 0.41 |
| 1:0:2135:A:O2' | 1:0:2136:G:H5' | 2.19 | 0.41 |
| 1:0:1194:A:O5' | 1:0:1194:A:H8 | 2.02 | 0.41 |
| 12:J:21:ARG:HG2 | 12:J:21:ARG:HH11 | 1.85 | 0.41 |
| 1:0:2096:A:H3' | 1:0:2096:A:N3 | 2.35 | 0.41 |
| 1:0:844:A:H2' | 37:0:9368:HOH:O | 2.19 | 0.41 |
| 1:0:847:C:H5 | 37:0:9056:HOH:O | 2.02 | 0.41 |
| 1:0:2365:G:H4' | 19:Q:45:PRO:O | 2.20 | 0.41 |
| 37:0:3151:HOH:O | 19:Q:16:ASN:HB2 | 2.19 | 0.41 |
| 5:C:2:GLN:HB3 | 37:C:8537:HOH:O | 2.20 | 0.41 |
| 4:B:57:GLU:HA | 4:B:58:PRO:HD2 | 1.90 | 0.41 |
| 1:0:1439:C:H4' | 20:R:132:ARG:NH1 | 2.34 | 0.41 |
| 3:A:94:LEU:N | 3:A:94:LEU:CD2 | 2.81 | 0.41 |
| 1:0:447:A:O2' | 1:0:448:G:H5' | 2.20 | 0.41 |
| 22:T:9:LYS:HE3 | 22:T:13:ARG:HD2 | 2.01 | 0.41 |
| 25:W:68:THR:HG23 | 25:W:69:ARG:N | 2.36 | 0.41 |
| 26:X:21:PRO:HG2 | 26:X:24:LYS:HD3 | 2.01 | 0.41 |
| 1:0:1773:G:H2' | 1:0:1774:G:H5' | 2.02 | 0.41 |
| 1:0:1773:G:C2' | 1:0:1774:G:H5' | 2.50 | 0.41 |
| 3:A:206:ARG:NH1 | 3:A:208:HIS:CD2 | 2.88 | 0.41 |
| 1:0:2766:A:O2' | 1:0:2767:C:H5' | 2.20 | 0.41 |
| 17:O:47:ARG:HA | 17:O:50:ARG:HH12 | 1.85 | 0.41 |
| 10:H:37:GLY:HA3 | 10:H:87:LYS:HA | 2.01 | 0.41 |
| 1:0:1353:C:N3 | 14:L:5:LYS:NZ | 2.68 | 0.41 |
| 1:0:1856:C:H5' | 1:0:1858:A:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:128:LEU:N | 37:D:6007:HOH:O | 2.52 | 0.41 |
| 30:2:21:VAL:O | 30:2:22:PRO:C | 2.58 | 0.41 |
| 1:0:566:A:H2' | 1:0:567:U:O4' | 2.20 | 0.41 |
| 25:W:93:ILE:HB | 37:W:4301:HOH:O | 2.19 | 0.41 |
| 3:A:54:PRO:HG2 | 3:A:160:ALA:HB3 | 2.02 | 0.41 |
| 1:0:1548:U:O2' | 1:0:1549:C:H5' | 2.20 | 0.41 |
| 4:B:112:THR:OG1 | 4:B:158:LYS:HG3 | 2.21 | 0.41 |
| 1:0:1576:G:H2' | 1:0:1577:U:O4' | 2.21 | 0.41 |
| 1:0:2039:A:H4' | 1:0:2760:C:O2' | 2.21 | 0.41 |
| 1:0:2416:G:H2' | 1:0:2417:C:C6 | 2.55 | 0.41 |
| 1:0:890:C:O2' | 29:1:50:TRP:O | 2.35 | 0.41 |
| 2:9:27:C:N3 | 37:9:8644:HOH:O | 2.37 | 0.41 |
| 1:0:329:A:OP2 | 5:C:206:ASN:HB2 | 2.19 | 0.41 |
| 1:0:474:C:O3' | 5:C:73:LEU:CD2 | 2.68 | 0.41 |
| 1:0:2079:G:H2' | 1:0:2080:G:O4' | 2.20 | 0.41 |
| 1:0:1246:A:H8 | 1:0:1246:A:H5' | 1.85 | 0.41 |
| 1:0:182:G:O3' | 15:M:157:ASP:OD2 | 2.38 | 0.41 |
| 15:M:31:TRP:C | 15:M:33:ASN:H | 2.24 | 0.41 |
| 10:H:50:ILE:HD12 | 10:H:149:VAL:HG11 | 2.03 | 0.41 |
| 15:M:134:ILE:O | 15:M:136:PRO:CD | 2.67 | 0.41 |
| 1:0:318:U:O2' | 1:0:319:A:OP1 | 2.35 | 0.41 |
| 18:P:135:ALA:O | 18:P:139:ARG:HG3 | 2.20 | 0.41 |
| 17:O:26:TRP:HA | 17:O:26:TRP:HE3 | 1.84 | 0.41 |
| 1:0:1266:U:O2' | 1:0:1267:C:H5' | 2.20 | 0.41 |
| 1:0:1711:A:C2' | 1:0:1712:A:H5' | 2.50 | 0.41 |
| 21:S:7:HIS:HD2 | 21:S:27:ALA:HB3 | 1.83 | 0.41 |
| 13:K:76:GLN:HA | 13:K:93:ASN:HA | 2.01 | 0.41 |
| 1:0:2090:G:H2' | 1:0:2091:G:C8 | 2.55 | 0.41 |
| 6:D:81:GLU:O | 6:D:83:PHE:N | 2.53 | 0.41 |
| 1:0:1194:A:O2' | 1:0:1195:G:H5' | 2.21 | 0.41 |
| 6:D:19:GLU:HG3 | 37:D:6165:HOH:O | 2.20 | 0.41 |
| 2:9:19:G:O2' | 2:9:20:G:H5' | 2.21 | 0.41 |
| 1:0:2613:G:O2' | 1:0:2614:C:H5' | 2.20 | 0.41 |
| 37:0:5207:HOH:O | 14:L:34:GLY:HA2 | 2.19 | 0.41 |
| 31:3:43:ASN:ND2 | 37:3:8806:HOH:O | 2.54 | 0.41 |
| 12:J:24:SER:HA | 12:J:86:MET:SD | 2.61 | 0.41 |
| 1:0:201:G:N2 | 35:0:8805:CL:CL | 2.91 | 0.41 |
| 1:0:178:U:H2' | 1:0:179:C:H6 | 1.84 | 0.41 |
| 25:W:52:VAL:CG2 | 25:W:53:ALA:N | 2.82 | 0.41 |
| 14:L:90:ARG:NH2 | 14:L:121:ILE:HD11 | 2.36 | 0.41 |
| 26:X:43:VAL:HG22 | 26:X:76:ARG:HH12 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:X:43:VAL:CG1 | 26:X:47:ALA:HB3 | 2.50 | 0.41 |
| 37:O:6465:HOH:O | 22:T:38:ARG:NH1 | 2.54 | 0.41 |
| 4:B:36:PRO:CG | 4:B:169:GLY:H | 2.27 | 0.41 |
| 25:W:90:TYR:CE2 | 25:W:99:ALA:HB2 | 2.56 | 0.41 |
| 7:E:84:MET:HA | 7:E:167:TYR:O | 2.20 | 0.41 |
| 17:O:78:ALA:C | 17:O:98:LEU:HD13 | 2.41 | 0.41 |
| 26:X:25:ARG:HB3 | 26:X:66:THR:HG22 | 2.03 | 0.41 |
| 5:C:94:THR:HG22 | 37:C:8684:HOH:O | 2.21 | 0.41 |
| 3:A:48:ASP:HA | 3:A:49:PRO:HD3 | 1.93 | 0.41 |
| 1:O:721:A:H5'' | 17:O:51:TYR:CE2 | 2.55 | 0.41 |
| 1:O:622:G:O2' | 1:O:623:U:H5' | 2.19 | 0.41 |
| 20:R:59:PHE:HZ | 20:R:81:PRO:HG3 | 1.85 | 0.41 |
| 1:O:963:C:O5' | 1:O:963:C:H6 | 2.03 | 0.41 |
| 20:R:89:LEU:HA | 20:R:89:LEU:HD23 | 1.85 | 0.41 |
| 1:O:569:A:H5'' | 1:O:587:A:N1 | 2.35 | 0.41 |
| 1:O:1746:A:O4' | 1:O:1747:A:C2 | 2.73 | 0.41 |
| 1:O:1051:C:H2' | 1:O:1052:G:O4' | 2.21 | 0.41 |
| 5:C:5:ILE:HD11 | 5:C:16:VAL:HG23 | 2.03 | 0.41 |
| 5:C:233:THR:CG2 | 5:C:234:VAL:N | 2.80 | 0.41 |
| 16:N:155:GLU:HG2 | 16:N:156:GLU:HG3 | 2.03 | 0.41 |
| 1:O:251:C:C2 | 1:O:259:G:C2 | 3.09 | 0.41 |
| 1:O:2839:C:H2' | 1:O:2840:A:H5'' | 2.02 | 0.41 |
| 1:O:1634:G:H2' | 1:O:1635:U:C6 | 2.54 | 0.41 |
| 16:N:113:SER:N | 37:N:8848:HOH:O | 2.53 | 0.41 |
| 16:N:74:PRO:HG2 | 16:N:159:TYR:CZ | 2.56 | 0.41 |
| 1:O:1667:A:H2' | 1:O:1668:U:C6 | 2.55 | 0.41 |
| 25:W:73:LEU:HD12 | 25:W:113:SER:HA | 2.03 | 0.41 |
| 1:O:243:A:H61 | 1:O:269:G:C1' | 2.33 | 0.41 |
| 37:9:8645:HOH:O | 16:N:41:LYS:HD2 | 2.20 | 0.41 |
| 1:O:2911:C:H2' | 1:O:2912:C:C6 | 2.56 | 0.41 |
| 24:V:51:LYS:O | 24:V:54:ALA:HB3 | 2.21 | 0.41 |
| 31:3:8:ASN:O | 31:3:9:THR:HB | 2.20 | 0.41 |
| 16:N:37:ARG:HA | 16:N:37:ARG:HD3 | 1.94 | 0.41 |
| 16:N:90:LEU:HD23 | 16:N:125:ALA:HB1 | 2.03 | 0.41 |
| 25:W:24:LEU:O | 25:W:26:ILE:HG23 | 2.21 | 0.41 |
| 4:B:314:ALA:CB | 4:B:317:PRO:HG3 | 2.50 | 0.41 |
| 8:F:46:GLU:N | 37:F:3461:HOH:O | 2.53 | 0.41 |
| 2:9:106:U:O2' | 2:9:107:C:H5' | 2.21 | 0.41 |
| 11:I:72:GLU:C | 11:I:74:ILE:H | 2.24 | 0.41 |
| 10:H:123:ILE:CD1 | 10:H:123:ILE:N | 2.84 | 0.41 |
| 1:O:338:C:H5'' | 37:O:5626:HOH:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1789:G:H2' | 1:0:1790:C:O5' | 2.21 | 0.41 |
| 1:0:2898:G:H4' | 4:B:288:GLY:HA2 | 2.02 | 0.41 |
| 17:O:77:ALA:HA | 17:O:96:VAL:O | 2.21 | 0.41 |
| 1:0:440:C:H2' | 1:0:441:A:C8 | 2.56 | 0.41 |
| 3:A:9:ARG:O | 3:A:10:GLY:C | 2.59 | 0.41 |
| 1:0:1761:U:H4' | 18:P:82:GLY:O | 2.20 | 0.41 |
| 1:0:183:A:H1' | 15:M:161:ARG:NH1 | 2.36 | 0.41 |
| 1:0:1552:G:C6 | 1:0:1553:C:C4 | 3.08 | 0.41 |
| 1:0:1849:G:H1' | 1:0:2011:A:N1 | 2.35 | 0.41 |
| 2:9:4:G:O2' | 16:N:44:ARG:NH2 | 2.54 | 0.41 |
| 1:0:431:G:O2' | 1:0:432:G:H5' | 2.21 | 0.41 |
| 17:O:33:LEU:HA | 17:O:40:HIS:NE2 | 2.36 | 0.41 |
| 31:3:7:PHE:C | 31:3:7:PHE:CD1 | 2.93 | 0.41 |
| 1:0:302:A:H5'' | 37:0:7219:HOH:O | 2.21 | 0.41 |
| 37:0:9502:HOH:O | 15:M:182:LYS:HE3 | 2.20 | 0.41 |
| 1:0:151:A:C2 | 1:0:442:A:C8 | 3.09 | 0.41 |
| 7:E:68:HIS:O | 7:E:72:MET:HG3 | 2.21 | 0.41 |
| 12:J:142:ASN:O | 12:J:144:THR:HG23 | 2.21 | 0.41 |
| 3:A:211:LYS:CB | 37:A:8914:HOH:O | 2.64 | 0.41 |
| 1:0:2506:A:N6 | 1:0:2511:A:O2' | 2.52 | 0.41 |
| 24:V:39:ALA:H | 24:V:40:PRO:CD | 2.25 | 0.41 |
| 6:D:35:ALA:HB3 | 37:D:6716:HOH:O | 2.20 | 0.41 |
| 25:W:131:PRO:O | 25:W:136:GLY:N | 2.48 | 0.41 |
| 17:O:14:LEU:HG | 17:O:102:ILE:HD11 | 2.03 | 0.41 |
| 25:W:62:LEU:HD23 | 25:W:97:ALA:HB1 | 2.02 | 0.41 |
| 1:0:68:U:O2' | 1:0:69:A:H5'' | 2.21 | 0.41 |
| 10:H:32:ALA:N | 10:H:66:GLU:OE1 | 2.44 | 0.41 |
| 1:0:290:C:O2' | 1:0:291:C:H5' | 2.19 | 0.41 |
| 26:X:18:ARG:NH1 | 37:X:2351:HOH:O | 2.53 | 0.41 |
| 1:0:2598:U:O2 | 1:0:2600:A:C8 | 2.73 | 0.41 |
| 1:0:485:A:O2' | 1:0:487:G:H5' | 2.21 | 0.41 |
| 1:0:12:U:H2' | 1:0:13:G:H5' | 2.01 | 0.41 |
| 1:0:1904:A:H2' | 1:0:1905:U:O4' | 2.21 | 0.41 |
| 16:N:35:VAL:HB | 16:N:46:GLN:HB2 | 2.03 | 0.41 |
| 6:D:15:GLU:O | 6:D:16:PRO:O | 2.39 | 0.41 |
| 22:T:89:ARG:HD2 | 22:T:89:ARG:C | 2.41 | 0.41 |
| 3:A:87:GLU:HB2 | 37:A:8918:HOH:O | 2.20 | 0.41 |
| 1:0:218:C:C5 | 1:0:220:C:C4 | 3.08 | 0.41 |
| 13:K:28:GLU:HG2 | 13:K:58:THR:HB | 2.03 | 0.41 |
| 7:E:38:ILE:HA | 7:E:51:SER:HB2 | 2.02 | 0.41 |
| 1:0:2900:G:H2' | 1:0:2901:C:O4' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:244:C:OP1 | 8:F:42:ARG:NH2 | 2.51 | 0.41 |
| 1:0:1838:U:O2' | 1:0:2644:C:H5' | 2.21 | 0.41 |
| 18:P:97:ARG:HD2 | 37:P:162:HOH:O | 2.21 | 0.41 |
| 1:0:1079:A:H4' | 1:0:2078:U:H5' | 2.03 | 0.41 |
| 1:0:2296:C:H2' | 1:0:2297:U:H6 | 1.86 | 0.41 |
| 1:0:356:C:H3' | 1:0:357:A:H2' | 2.02 | 0.41 |
| 29:1:25:LYS:NZ | 37:1:3076:HOH:O | 2.52 | 0.41 |
| 1:0:1120:U:H2' | 1:0:1121:G:H5' | 2.02 | 0.41 |
| 25:W:3:ALA:O | 25:W:54:PHE:HA | 2.21 | 0.41 |
| 6:D:95:THR:O | 6:D:97:GLN:N | 2.54 | 0.41 |
| 3:A:36:ASP:CG | 3:A:85:SER:H | 2.25 | 0.41 |
| 10:H:140:TYR:N | 10:H:140:TYR:CD1 | 2.89 | 0.41 |
| 15:M:34:GLU:HB3 | 15:M:38:GLU:HG3 | 2.02 | 0.41 |
| 18:P:63:ARG:HA | 18:P:66:GLN:HB2 | 2.02 | 0.41 |
| 14:L:89:PHE:O | 14:L:119:THR:N | 2.50 | 0.41 |
| 6:D:25:MET:HE1 | 6:D:37:ALA:O | 2.20 | 0.41 |
| 4:B:162:MET:HG3 | 4:B:310:ARG:NE | 2.35 | 0.41 |
| 1:0:154:C:C2 | 1:0:155:C:C5 | 3.09 | 0.41 |
| 18:P:13:VAL:HG11 | 18:P:40:VAL:HG12 | 2.02 | 0.41 |
| 12:J:130:VAL:HG11 | 12:J:135:ILE:CG1 | 2.51 | 0.41 |
| 22:T:103:LEU:HD23 | 22:T:103:LEU:N | 2.35 | 0.41 |
| 15:M:46:LEU:HD22 | 15:M:50:ARG:CD | 2.51 | 0.41 |
| 1:0:1473:U:O4' | 29:1:42:SER:HB3 | 2.20 | 0.41 |
| 1:0:1191:A:H3' | 1:0:1192:A:H5'' | 2.02 | 0.41 |
| 17:O:25:VAL:HG23 | 17:O:26:TRP:N | 2.36 | 0.41 |
| 1:0:2676:C:H4' | 12:J:70:PHE:CD1 | 2.56 | 0.41 |
| 2:9:39:U:H3' | 37:9:8707:HOH:O | 2.20 | 0.41 |
| 2:9:38:A:H2 | 2:9:43:G:H5'' | 1.85 | 0.41 |
| 1:0:2032:U:H1' | 37:0:6047:HOH:O | 2.21 | 0.41 |
| 1:0:2028:U:H2' | 1:0:2029:C:H6 | 1.86 | 0.41 |
| 1:0:2445:U:H2' | 1:0:2446:G:H8 | 1.86 | 0.41 |
| 1:0:2765:C:H2' | 1:0:2766:A:C8 | 2.56 | 0.41 |
| 1:0:1767:A:O2' | 1:0:1768:C:H5' | 2.21 | 0.41 |
| 1:0:764:C:OP1 | 5:C:87:ARG:NH1 | 2.54 | 0.41 |
| 1:0:2731:G:H2' | 1:0:2732:U:O4' | 2.20 | 0.41 |
| 1:0:1553:C:H2' | 1:0:1554:C:C6 | 2.56 | 0.41 |
| 1:0:249:G:H1' | 1:0:265:U:O2 | 2.21 | 0.41 |
| 5:C:57:PRO:HD2 | 5:C:73:LEU:HD22 | 2.01 | 0.41 |
| 4:B:33:ASP:O | 4:B:34:GLY:O | 2.38 | 0.41 |
| 1:0:196:G:H1' | 1:0:198:A:N7 | 2.35 | 0.41 |
| 1:0:772:G:H2' | 1:0:773:A:O4' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1064:U:H2' | 1:0:1065:G:C8 | 2.56 | 0.41 |
| 1:0:1794:G:P | 18:P:133:SER:HB2 | 2.60 | 0.41 |
| 11:I:114:TYR:CD1 | 11:I:114:TYR:N | 2.88 | 0.41 |
| 30:2:13:LYS:O | 30:2:17:GLN:HG3 | 2.20 | 0.41 |
| 16:N:76:GLY:N | 37:N:8840:HOH:O | 2.50 | 0.41 |
| 11:I:126:THR:C | 37:I:7439:HOH:O | 2.59 | 0.41 |
| 37:0:9389:HOH:O | 15:M:186:SER:HB3 | 2.21 | 0.41 |
| 19:Q:77:ASP:N | 19:Q:80:LYS:O | 2.53 | 0.41 |
| 22:T:61:GLU:N | 37:T:4772:HOH:O | 2.53 | 0.41 |
| 5:C:236:THR:HG23 | 5:C:238:SER:H | 1.86 | 0.41 |
| 24:V:12:THR:HG23 | 24:V:14:ALA:N | 2.31 | 0.41 |
| 6:D:67:ASP:O | 6:D:69:ILE:HG13 | 2.20 | 0.41 |
| 12:J:77:GLY:O | 12:J:78:ILE:C | 2.59 | 0.41 |
| 16:N:47:LEU:HA | 16:N:47:LEU:HD22 | 1.79 | 0.41 |
| 25:W:108:ARG:O | 25:W:110:GLN:N | 2.54 | 0.41 |
| 14:L:89:PHE:N | 14:L:117:GLU:O | 2.54 | 0.41 |
| 6:D:17:ARG:HG3 | 6:D:18:ILE:N | 2.35 | 0.41 |
| 1:0:2909:G:H2' | 1:0:2910:A:C8 | 2.56 | 0.41 |
| 28:Z:47:VAL:HA | 28:Z:56:GLN:O | 2.20 | 0.41 |
| 37:0:9900:HOH:O | 27:Y:212:ARG:HB3 | 2.20 | 0.41 |
| 21:S:23:LYS:HE2 | 37:S:8522:HOH:O | 2.21 | 0.41 |
| 1:0:696:C:H4' | 37:0:7047:HOH:O | 2.21 | 0.41 |
| 3:A:199:HIS:CD2 | 3:A:201:PHE:HB2 | 2.56 | 0.41 |
| 5:C:21:VAL:C | 5:C:23:GLU:N | 2.73 | 0.41 |
| 3:A:66:ARG:HG2 | 37:A:8907:HOH:O | 2.21 | 0.41 |
| 1:0:2134:G:C6 | 1:0:2258:A:C8 | 3.09 | 0.41 |
| 1:0:735:C:N4 | 31:3:15:ASN:HD21 | 2.19 | 0.41 |
| 1:0:1821:A:O2' | 1:0:1822:A:H5' | 2.20 | 0.41 |
| 5:C:57:PRO:HG2 | 5:C:73:LEU:HD13 | 2.03 | 0.41 |
| 1:0:1304:U:H2' | 1:0:1305:C:C6 | 2.56 | 0.41 |
| 5:C:169:ALA:HB3 | 5:C:208:ALA:O | 2.21 | 0.41 |
| 3:A:77:GLY:O | 3:A:78:ASP:C | 2.60 | 0.41 |
| 1:0:135:G:OP1 | 15:M:39:ARG:NH1 | 2.53 | 0.41 |
| 25:W:56:GLU:O | 25:W:143:THR:HG23 | 2.20 | 0.41 |
| 6:D:75:LEU:HD22 | 6:D:79:MET:HB3 | 2.02 | 0.41 |
| 19:Q:86:VAL:HG22 | 19:Q:87:THR:N | 2.35 | 0.41 |
| 5:C:157:LEU:HD22 | 5:C:162:VAL:CG1 | 2.51 | 0.41 |
| 6:D:85:GLN:O | 6:D:86:THR:HG23 | 2.21 | 0.40 |
| 4:B:321:PRO:HA | 37:B:8958:HOH:O | 2.19 | 0.40 |
| 10:H:49:GLN:NE2 | 10:H:140:TYR:CE2 | 2.83 | 0.40 |
| 12:J:6:PHE:O | 12:J:8:ALA:N | 2.45 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:9:49:G:OP1 | 16:N:78:MET:HG2 | 2.21 | 0.40 |
| 2:9:34:A:H1' | 16:N:153:GLN:HE22 | 1.85 | 0.40 |
| 1:0:1097:A:H5'' | 25:W:125:HIS:CE1 | 2.56 | 0.40 |
| 4:B:109:LEU:CD1 | 4:B:113:LEU:HD12 | 2.50 | 0.40 |
| 5:C:93:LYS:HA | 37:C:8555:HOH:O | 2.21 | 0.40 |
| 1:0:2600:A:H2' | 1:0:2601:A:O4' | 2.21 | 0.40 |
| 20:R:100:ASP:C | 20:R:102:GLN:N | 2.74 | 0.40 |
| 1:0:727:G:H3' | 1:0:728:C:C6 | 2.56 | 0.40 |
| 8:F:4:VAL:HA | 8:F:76:PHE:CZ | 2.56 | 0.40 |
| 1:0:204:A:C2' | 1:0:205:U:H5' | 2.51 | 0.40 |
| 1:0:2296:C:H2' | 1:0:2297:U:C6 | 2.57 | 0.40 |
| 25:W:146:ILE:O | 25:W:150:LEU:HG | 2.21 | 0.40 |
| 25:W:118:LEU:N | 25:W:118:LEU:HD23 | 2.36 | 0.40 |
| 1:0:2649:A:H8 | 1:0:2649:A:H5' | 1.86 | 0.40 |
| 17:O:113:VAL:O | 17:O:114:ILE:HD13 | 2.21 | 0.40 |
| 16:N:94:GLU:HG3 | 16:N:186:LEU:HD12 | 2.03 | 0.40 |
| 1:0:2708:G:N2 | 13:K:1:MET:O | 2.54 | 0.40 |
| 1:0:2071:C:H5' | 37:O:9338:HOH:O | 2.21 | 0.40 |
| 13:K:69:LEU:HD12 | 13:K:97:ILE:HD13 | 2.03 | 0.40 |
| 1:0:706:G:N2 | 1:0:707:C:H41 | 2.18 | 0.40 |
| 1:0:268:U:H1' | 37:O:3602:HOH:O | 2.20 | 0.40 |
| 6:D:28:GLY:CA | 6:D:69:ILE:HG23 | 2.43 | 0.40 |
| 6:D:105:SER:HB2 | 6:D:131:THR:HG23 | 2.03 | 0.40 |
| 26:X:41:PHE:CZ | 26:X:74:ALA:HB3 | 2.56 | 0.40 |
| 22:T:71:VAL:CG1 | 22:T:90:PRO:HB3 | 2.37 | 0.40 |
| 22:T:52:ARG:C | 22:T:56:ALA:HB2 | 2.42 | 0.40 |
| 8:F:46:GLU:OE1 | 8:F:100:ASP:HA | 2.20 | 0.40 |
| 1:0:1494:A:C4 | 1:0:1495:C:C5 | 3.09 | 0.40 |
| 16:N:31:LYS:HB2 | 16:N:101:VAL:HG23 | 2.04 | 0.40 |
| 1:0:2779:G:H21 | 7:E:143:GLN:NE2 | 2.18 | 0.40 |
| 5:C:124:VAL:HA | 5:C:230:GLY:O | 2.20 | 0.40 |
| 29:1:53:LYS:HD3 | 29:1:53:LYS:HA | 1.93 | 0.40 |
| 19:Q:86:VAL:CG2 | 19:Q:87:THR:N | 2.84 | 0.40 |
| 2:9:37:C:H4' | 16:N:111:PRO:HD2 | 2.02 | 0.40 |
| 1:0:939:A:C2 | 1:0:1027:G:N3 | 2.90 | 0.40 |
| 5:C:1:MET:HG2 | 5:C:2:GLN:HE21 | 1.86 | 0.40 |
| 6:D:64:ARG:CG | 6:D:67:ASP:HB3 | 2.49 | 0.40 |
| 10:H:46:TYR:HA | 10:H:47:PRO:HD3 | 1.77 | 0.40 |
| 15:M:19:GLN:N | 37:M:8864:HOH:O | 2.54 | 0.40 |
| 9:G:64:ASN:O | 9:G:68:GLU:HG3 | 2.20 | 0.40 |
| 5:C:175:LYS:HD3 | 5:C:184:ARG:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:W:96:LEU:O | 25:W:97:ALA:C | 2.59 | 0.40 |
| 1:0:69:A:C2' | 1:0:70:A:OP2 | 2.70 | 0.40 |
| 1:0:695:C:H2' | 1:0:696:C:C6 | 2.57 | 0.40 |
| 3:A:76:VAL:HG23 | 28:Z:63:LYS:HB3 | 2.02 | 0.40 |
| 1:0:1845:A:P | 3:A:190:ARG:HH11 | 2.45 | 0.40 |
| 1:0:66:G:H2' | 37:0:9911:HOH:O | 2.20 | 0.40 |
| 16:N:62:HIS:O | 16:N:64:SER:N | 2.55 | 0.40 |
| 17:O:53:GLN:NE2 | 17:O:112:ARG:HH21 | 2.19 | 0.40 |
| 1:0:1771:U:O2 | 28:Z:19:GLY:HA2 | 2.21 | 0.40 |
| 18:P:103:THR:HB | 37:P:180:HOH:O | 2.21 | 0.40 |
| 27:Y:143:TRP:C | 37:Y:8921:HOH:O | 2.59 | 0.40 |
| 1:0:201:G:N2 | 1:0:202:U:C2 | 2.90 | 0.40 |
| 1:0:1456:C:H2' | 1:0:1457:U:C6 | 2.56 | 0.40 |
| 9:G:69:ARG:NH1 | 37:G:3513:HOH:O | 2.54 | 0.40 |
| 1:0:1370:G:H5'' | 37:R:8838:HOH:O | 2.21 | 0.40 |
| 7:E:162:PHE:CD1 | 7:E:162:PHE:N | 2.89 | 0.40 |
| 20:R:119:VAL:O | 20:R:119:VAL:HG12 | 2.21 | 0.40 |
| 1:0:2493:C:O2 | 1:0:2493:C:H2' | 2.22 | 0.40 |
| 1:0:394:G:H1 | 15:M:181:GLU:CD | 2.24 | 0.40 |
| 1:0:294:C:H2' | 1:0:295:C:O4' | 2.22 | 0.40 |
| 25:W:137:GLN:HE21 | 25:W:141:HIS:CE1 | 2.35 | 0.40 |
| 6:D:80:ALA:O | 6:D:84:LEU:HG | 2.20 | 0.40 |
| 4:B:79:MET:HB2 | 4:B:188:HIS:CE1 | 2.57 | 0.40 |
| 4:B:42:ALA:HB1 | 4:B:308:LEU:HD11 | 2.04 | 0.40 |
| 1:0:2768:A:H3' | 37:0:4229:HOH:O | 2.21 | 0.40 |
| 11:I:85:GLY:C | 11:I:86:GLU:HG3 | 2.41 | 0.40 |
| 1:0:2419:U:H5'' | 1:0:2420:G:H5' | 2.03 | 0.40 |
| 1:0:1851:G:O2' | 1:0:1852:A:H5' | 2.20 | 0.40 |
| 3:A:150:PRO:HD3 | 37:A:8886:HOH:O | 2.21 | 0.40 |
| 1:0:2479:A:H5'' | 37:0:4453:HOH:O | 2.21 | 0.40 |
| 27:Y:177:LYS:HG3 | 27:Y:183:GLU:OE2 | 2.21 | 0.40 |
| 13:K:120:ARG:HB3 | 13:K:121:PHE:CE1 | 2.55 | 0.40 |
| 1:0:1127:C:H2' | 1:0:1128:U:H5' | 2.03 | 0.40 |
| 15:M:5:TYR:O | 15:M:7:TYR:N | 2.55 | 0.40 |
| 4:B:153:SER:HB2 | 4:B:287:TYR:CZ | 2.57 | 0.40 |
| 29:1:22:CYS:HA | 37:1:2086:HOH:O | 2.20 | 0.40 |
| 20:R:63:ASN:N | 20:R:63:ASN:OD1 | 2.54 | 0.40 |
| 4:B:127:GLN:HG3 | 37:B:8943:HOH:O | 2.21 | 0.40 |
| 1:0:1839:A:H5' | 1:0:2643:G:H4' | 2.02 | 0.40 |
| 1:0:145:A:N3 | 15:M:111:ASN:HB3 | 2.37 | 0.40 |
| 18:P:124:ASP:HA | 37:P:167:HOH:O | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 12:J:143:LYS:HA | 12:J:145:TRP:CZ3 | 2.56 | 0.40 |
| 30:2:20:ARG:HG3 | 30:2:20:ARG:NH1 | 2.11 | 0.40 |
| 1:0:2769:C:H2' | 1:0:2770:G:C5' | 2.51 | 0.40 |
| 11:I:72:GLU:O | 11:I:74:ILE:N | 2.54 | 0.40 |
| 24:V:27:LEU:O | 24:V:30:ALA:HB3 | 2.21 | 0.40 |
| 1:0:694:A:H2' | 1:0:695:C:C5' | 2.51 | 0.40 |
| 6:D:162:ALA:C | 6:D:164:ALA:N | 2.73 | 0.40 |
| 1:0:2419:U:H5'' | 1:0:2420:G:C5' | 2.51 | 0.40 |
| 3:A:186:TRP:CG | 3:A:187:PRO:HA | 2.57 | 0.40 |
| 1:0:2880:A:C2' | 1:0:2881:C:H5' | 2.48 | 0.40 |
| 1:0:1641:A:C2' | 1:0:1642:A:H5' | 2.51 | 0.40 |
| 16:N:22:GLN:HA | 16:N:25:ARG:CZ | 2.52 | 0.40 |
| 16:N:42:HIS:CG | 16:N:62:HIS:HE1 | 2.40 | 0.40 |
| 1:0:47:G:N3 | 1:0:114:A:C2 | 2.90 | 0.40 |
| 1:0:95:A:H5'' | 1:0:97:G:O4' | 2.21 | 0.40 |
| 1:0:645:U:OP2 | 14:L:4:LYS:CE | 2.69 | 0.40 |
| 1:0:1483:C:O2' | 1:0:1484:G:H5' | 2.21 | 0.40 |
| 8:F:49:PHE:O | 8:F:95:ALA:HB1 | 2.21 | 0.40 |
| 1:0:1012:A:H8 | 1:0:1012:A:O5' | 2.05 | 0.40 |
| 1:0:2450:C:H6 | 1:0:2450:C:O5' | 2.04 | 0.40 |
| 1:0:2375:A:H2' | 1:0:2376:C:C6 | 2.57 | 0.40 |
| 28:Z:32:GLU:HA | 28:Z:35:GLU:HG3 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3 | A | 235/240 (98%) | 191 (81%) | 31 (13%) | 13 (6%) | 2 | 6 |
| 4 | B | 335/338 (99%) | 291 (87%) | 35 (10%) | 9 (3%) | 6 | 21 |
| 5 | C | 244/246 (99%) | 201 (82%) | 32 (13%) | 11 (4%) | 3 | 10 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 6 | D | 134/177 (76%) | 85 (63%) | 31 (23%) | 18 (13%) | 0 | 1 |
| 7 | E | 170/178 (96%) | 150 (88%) | 15 (9%) | 5 (3%) | 6 | 19 |
| 8 | F | 117/120 (98%) | 93 (80%) | 17 (14%) | 7 (6%) | 2 | 5 |
| 9 | G | 25/348 (7%) | 23 (92%) | 2 (8%) | 0 | 100 | 100 |
| 10 | H | 156/177 (88%) | 134 (86%) | 17 (11%) | 5 (3%) | 5 | 17 |
| 11 | I | 68/162 (42%) | 49 (72%) | 14 (21%) | 5 (7%) | 1 | 3 |
| 12 | J | 140/145 (97%) | 121 (86%) | 14 (10%) | 5 (4%) | 4 | 14 |
| 13 | K | 130/132 (98%) | 111 (85%) | 17 (13%) | 2 (2%) | 13 | 40 |
| 14 | L | 141/165 (86%) | 114 (81%) | 25 (18%) | 2 (1%) | 14 | 42 |
| 15 | M | 192/195 (98%) | 169 (88%) | 20 (10%) | 3 (2%) | 12 | 38 |
| 16 | N | 184/187 (98%) | 149 (81%) | 23 (12%) | 12 (6%) | 1 | 4 |
| 17 | O | 113/116 (97%) | 102 (90%) | 8 (7%) | 3 (3%) | 6 | 21 |
| 18 | P | 141/149 (95%) | 125 (89%) | 12 (8%) | 4 (3%) | 6 | 21 |
| 19 | Q | 93/96 (97%) | 86 (92%) | 5 (5%) | 2 (2%) | 8 | 28 |
| 20 | R | 145/152 (95%) | 122 (84%) | 18 (12%) | 5 (3%) | 5 | 16 |
| 21 | S | 79/85 (93%) | 69 (87%) | 9 (11%) | 1 (1%) | 15 | 44 |
| 22 | T | 117/120 (98%) | 92 (79%) | 19 (16%) | 6 (5%) | 2 | 8 |
| 23 | U | 51/66 (77%) | 43 (84%) | 7 (14%) | 1 (2%) | 9 | 30 |
| 24 | V | 63/71 (89%) | 50 (79%) | 9 (14%) | 4 (6%) | 2 | 4 |
| 25 | W | 152/154 (99%) | 136 (90%) | 14 (9%) | 2 (1%) | 15 | 44 |
| 26 | X | 80/92 (87%) | 69 (86%) | 8 (10%) | 3 (4%) | 4 | 13 |
| 27 | Y | 140/241 (58%) | 138 (99%) | 2 (1%) | 0 | 100 | 100 |
| 28 | Z | 71/83 (86%) | 56 (79%) | 10 (14%) | 5 (7%) | 1 | 3 |
| 29 | 1 | 54/57 (95%) | 51 (94%) | 3 (6%) | 0 | 100 | 100 |
| 30 | 2 | 47/50 (94%) | 44 (94%) | 1 (2%) | 2 (4%) | 3 | 10 |
| 31 | 3 | 90/92 (98%) | 84 (93%) | 6 (7%) | 0 | 100 | 100 |
| All | All | 3707/4434 (84%) | 3148 (85%) | 424 (11%) | 135 (4%) | 4 | 14 |

All (135) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 34 | ASP |
| 4 | B | 34 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 139 | ASP |
| 4 | B | 206 | THR |
| 5 | C | 8 | LEU |
| 6 | D | 16 | PRO |
| 6 | D | 56 | ARG |
| 6 | D | 139 | TYR |
| 6 | D | 165 | PHE |
| 6 | D | 173 | GLU |
| 8 | F | 101 | ALA |
| 14 | L | 105 | TYR |
| 16 | N | 154 | LEU |
| 16 | N | 164 | ASP |
| 16 | N | 184 | ILE |
| 18 | P | 116 | SER |
| 20 | R | 121 | GLU |
| 20 | R | 135 | ALA |
| 22 | T | 100 | ASP |
| 24 | V | 43 | PRO |
| 25 | W | 77 | ALA |
| 26 | X | 70 | ILE |
| 26 | X | 87 | ALA |
| 28 | Z | 20 | ARG |
| 28 | Z | 81 | ARG |
| 3 | A | 10 | GLY |
| 3 | A | 33 | GLU |
| 3 | A | 37 | VAL |
| 3 | A | 38 | ILE |
| 3 | A | 87 | GLU |
| 3 | A | 119 | ALA |
| 4 | B | 184 | ASP |
| 5 | C | 13 | ASP |
| 5 | C | 15 | GLU |
| 5 | C | 58 | ALA |
| 5 | C | 151 | GLN |
| 5 | C | 234 | VAL |
| 6 | D | 60 | GLU |
| 6 | D | 61 | PHE |
| 6 | D | 90 | LEU |
| 6 | D | 99 | ASP |
| 6 | D | 137 | PRO |
| 6 | D | 171 | ASP |
| 7 | E | 110 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | F | 44 | SER |
| 8 | F | 61 | MET |
| 8 | F | 68 | ASP |
| 10 | H | 143 | VAL |
| 12 | J | 34 | GLU |
| 12 | J | 89 | HIS |
| 13 | K | 111 | GLY |
| 15 | M | 6 | SER |
| 16 | N | 113 | SER |
| 16 | N | 134 | ASP |
| 16 | N | 183 | ASP |
| 17 | O | 20 | SER |
| 17 | O | 21 | SER |
| 20 | R | 20 | GLU |
| 22 | T | 104 | GLU |
| 28 | Z | 21 | VAL |
| 30 | 2 | 37 | HIS |
| 3 | A | 122 | SER |
| 4 | B | 183 | GLU |
| 5 | C | 178 | GLN |
| 5 | C | 244 | ALA |
| 6 | D | 96 | SER |
| 8 | F | 64 | PRO |
| 11 | I | 113 | SER |
| 11 | I | 128 | THR |
| 12 | J | 5 | GLU |
| 12 | J | 65 | ASN |
| 16 | N | 63 | SER |
| 16 | N | 65 | ASP |
| 16 | N | 133 | ASP |
| 18 | P | 139 | ARG |
| 20 | R | 126 | LYS |
| 23 | U | 7 | ASP |
| 30 | 2 | 22 | PRO |
| 3 | A | 101 | GLU |
| 4 | B | 107 | SER |
| 5 | C | 85 | LYS |
| 5 | C | 232 | LEU |
| 6 | D | 82 | GLU |
| 6 | D | 86 | THR |
| 7 | E | 121 | ASP |
| 10 | H | 19 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | H | 70 | LEU |
| 10 | H | 115 | GLY |
| 13 | K | 24 | THR |
| 16 | N | 68 | GLU |
| 17 | O | 108 | GLY |
| 18 | P | 68 | LYS |
| 20 | R | 130 | MET |
| 26 | X | 82 | GLU |
| 28 | Z | 28 | GLU |
| 3 | A | 35 | GLY |
| 3 | A | 236 | GLY |
| 4 | B | 2 | GLN |
| 6 | D | 44 | ILE |
| 7 | E | 17 | HIS |
| 7 | E | 98 | GLU |
| 10 | H | 82 | GLU |
| 12 | J | 7 | ASP |
| 16 | N | 165 | ALA |
| 19 | Q | 89 | ALA |
| 24 | V | 39 | ALA |
| 25 | W | 49 | ASN |
| 28 | Z | 67 | GLY |
| 5 | C | 142 | ASP |
| 6 | D | 45 | THR |
| 6 | D | 164 | ALA |
| 11 | I | 100 | VAL |
| 15 | M | 146 | ASP |
| 15 | M | 147 | LEU |
| 16 | N | 139 | TRP |
| 18 | P | 117 | SER |
| 24 | V | 20 | LEU |
| 3 | A | 102 | GLY |
| 11 | I | 109 | PRO |
| 24 | V | 2 | VAL |
| 3 | A | 192 | VAL |
| 7 | E | 136 | PRO |
| 8 | F | 43 | GLY |
| 11 | I | 92 | VAL |
| 14 | L | 69 | ILE |
| 21 | S | 47 | VAL |
| 22 | T | 53 | GLY |
| 4 | B | 181 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | D | 27 | ILE |
| 4 | B | 82 | VAL |
| 8 | F | 59 | ILE |
| 22 | T | 42 | VAL |
| 22 | T | 62 | VAL |
| 22 | T | 90 | PRO |
| 19 | Q | 18 | 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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | A | 179/182 (98%) | 171 (96%) | 8 (4%) | 34 | 68 |
| 4 | B | 282/283 (100%) | 258 (92%) | 24 (8%) | 13 | 36 |
| 5 | C | 193/193 (100%) | 182 (94%) | 11 (6%) | 25 | 58 |
| 6 | D | 117/148 (79%) | 109 (93%) | 8 (7%) | 20 | 49 |
| 7 | E | 152/156 (97%) | 147 (97%) | 5 (3%) | 45 | 79 |
| 8 | F | 93/94 (99%) | 90 (97%) | 3 (3%) | 46 | 80 |
| 9 | G | 27/283 (10%) | 26 (96%) | 1 (4%) | 41 | 76 |
| 10 | H | 134/145 (92%) | 125 (93%) | 9 (7%) | 20 | 50 |
| 11 | I | 58/130 (45%) | 55 (95%) | 3 (5%) | 29 | 62 |
| 12 | J | 118/121 (98%) | 111 (94%) | 7 (6%) | 24 | 57 |
| 13 | K | 106/106 (100%) | 104 (98%) | 2 (2%) | 65 | 91 |
| 14 | L | 113/127 (89%) | 108 (96%) | 5 (4%) | 35 | 69 |
| 15 | M | 158/159 (99%) | 151 (96%) | 7 (4%) | 35 | 69 |
| 16 | N | 149/150 (99%) | 143 (96%) | 6 (4%) | 38 | 73 |
| 17 | O | 93/94 (99%) | 88 (95%) | 5 (5%) | 27 | 60 |
| 18 | P | 113/117 (97%) | 107 (95%) | 6 (5%) | 28 | 61 |
| 19 | Q | 79/80 (99%) | 77 (98%) | 2 (2%) | 55 | 86 |
| 20 | R | 114/120 (95%) | 109 (96%) | 5 (4%) | 35 | 69 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 21 | S | 71/74 (96%) | 66 (93%) | 5 (7%) | 19 | 47 |
| 22 | T | 105/106 (99%) | 99 (94%) | 6 (6%) | 25 | 58 |
| 23 | U | 44/52 (85%) | 41 (93%) | 3 (7%) | 20 | 49 |
| 24 | V | 51/57 (90%) | 48 (94%) | 3 (6%) | 24 | 57 |
| 25 | W | 130/130 (100%) | 125 (96%) | 5 (4%) | 40 | 74 |
| 26 | X | 66/74 (89%) | 60 (91%) | 6 (9%) | 12 | 33 |
| 27 | Y | 120/196 (61%) | 114 (95%) | 6 (5%) | 30 | 64 |
| 28 | Z | 60/68 (88%) | 58 (97%) | 2 (3%) | 45 | 79 |
| 29 | 1 | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 30 | 2 | 45/46 (98%) | 42 (93%) | 3 (7%) | 20 | 50 |
| 31 | 3 | 79/79 (100%) | 75 (95%) | 4 (5%) | 29 | 63 |
| All | All | 3095/3617 (86%) | 2935 (95%) | 160 (5%) | 29 | 62 |

All (160) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 3 | ARG |
| 3 | A | 8 | ARG |
| 3 | A | 33 | GLU |
| 3 | A | 36 | ASP |
| 3 | A | 69 | LEU |
| 3 | A | 94 | LEU |
| 3 | A | 179 | MET |
| 3 | A | 217 | ARG |
| 4 | B | 7 | ARG |
| 4 | B | 11 | LEU |
| 4 | B | 27 | ASN |
| 4 | B | 49 | THR |
| 4 | B | 53 | LEU |
| 4 | B | 68 | THR |
| 4 | B | 97 | LEU |
| 4 | B | 103 | ASP |
| 4 | B | 110 | ASP |
| 4 | B | 140 | LEU |
| 4 | B | 149 | ASP |
| 4 | B | 162 | MET |
| 4 | B | 175 | LEU |
| 4 | B | 190 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 192 | ASP |
| 4 | B | 234 | ARG |
| 4 | B | 245 | SER |
| 4 | B | 251 | VAL |
| 4 | B | 254 | GLN |
| 4 | B | 256 | GLN |
| 4 | B | 265 | LEU |
| 4 | B | 274 | GLU |
| 4 | B | 277 | GLU |
| 4 | B | 307 | ARG |
| 5 | C | 2 | GLN |
| 5 | C | 42 | ARG |
| 5 | C | 76 | ARG |
| 5 | C | 78 | ARG |
| 5 | C | 87 | ARG |
| 5 | C | 91 | PRO |
| 5 | C | 115 | LEU |
| 5 | C | 187 | ARG |
| 5 | C | 214 | THR |
| 5 | C | 222 | ASP |
| 5 | C | 236 | THR |
| 6 | D | 24 | HIS |
| 6 | D | 61 | PHE |
| 6 | D | 86 | THR |
| 6 | D | 104 | PHE |
| 6 | D | 133 | ASN |
| 6 | D | 136 | ARG |
| 6 | D | 139 | TYR |
| 6 | D | 153 | THR |
| 7 | E | 7 | ILE |
| 7 | E | 100 | ASP |
| 7 | E | 126 | ILE |
| 7 | E | 156 | ASP |
| 7 | E | 164 | ASP |
| 8 | F | 46 | GLU |
| 8 | F | 65 | GLU |
| 8 | F | 78 | GLU |
| 9 | G | 64 | ASN |
| 10 | H | 21 | GLU |
| 10 | H | 44 | ASP |
| 10 | H | 61 | ARG |
| 10 | H | 62 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | H | 71 | SER |
| 10 | H | 87 | LYS |
| 10 | H | 114 | ASP |
| 10 | H | 157 | TYR |
| 10 | H | 170 | ARG |
| 11 | I | 81 | GLU |
| 11 | I | 108 | HIS |
| 11 | I | 114 | TYR |
| 12 | J | 46 | ILE |
| 12 | J | 52 | GLN |
| 12 | J | 74 | ARG |
| 12 | J | 79 | PHE |
| 12 | J | 92 | GLN |
| 12 | J | 99 | GLU |
| 12 | J | 107 | ASN |
| 13 | K | 7 | ASP |
| 13 | K | 10 | GLN |
| 14 | L | 18 | HIS |
| 14 | L | 30 | ARG |
| 14 | L | 35 | ARG |
| 14 | L | 99 | GLU |
| 14 | L | 144 | ASP |
| 15 | M | 23 | LEU |
| 15 | M | 46 | LEU |
| 15 | M | 68 | ARG |
| 15 | M | 93 | ARG |
| 15 | M | 116 | ASN |
| 15 | M | 130 | GLU |
| 15 | M | 186 | SER |
| 16 | N | 26 | LEU |
| 16 | N | 47 | LEU |
| 16 | N | 53 | ASN |
| 16 | N | 93 | GLN |
| 16 | N | 139 | TRP |
| 16 | N | 164 | ASP |
| 17 | O | 32 | ARG |
| 17 | O | 34 | GLU |
| 17 | O | 38 | ARG |
| 17 | O | 81 | PHE |
| 17 | O | 100 | GLN |
| 18 | P | 52 | LYS |
| 18 | P | 66 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | P | 91 | LYS |
| 18 | P | 94 | TRP |
| 18 | P | 98 | ILE |
| 18 | P | 110 | ASP |
| 19 | Q | 57 | ASP |
| 19 | Q | 95 | GLU |
| 20 | R | 39 | THR |
| 20 | R | 82 | GLU |
| 20 | R | 109 | MET |
| 20 | R | 142 | ASP |
| 20 | R | 143 | VAL |
| 21 | S | 7 | HIS |
| 21 | S | 30 | ASP |
| 21 | S | 71 | ASP |
| 21 | S | 72 | ASP |
| 21 | S | 80 | ARG |
| 22 | T | 5 | ASP |
| 22 | T | 23 | VAL |
| 22 | T | 39 | ASN |
| 22 | T | 96 | VAL |
| 22 | T | 112 | LEU |
| 22 | T | 115 | GLU |
| 23 | U | 11 | THR |
| 23 | U | 48 | ASN |
| 23 | U | 53 | ASP |
| 24 | V | 13 | PRO |
| 24 | V | 43 | PRO |
| 24 | V | 65 | ASP |
| 25 | W | 1 | MET |
| 25 | W | 26 | ILE |
| 25 | W | 144 | GLU |
| 25 | W | 146 | ILE |
| 25 | W | 154 | ARG |
| 26 | X | 27 | ASP |
| 26 | X | 49 | ARG |
| 26 | X | 72 | VAL |
| 26 | X | 80 | GLU |
| 26 | X | 82 | GLU |
| 26 | X | 88 | GLU |
| 27 | Y | 154 | ARG |
| 27 | Y | 163 | THR |
| 27 | Y | 187 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | Y | 189 | ASN |
| 27 | Y | 191 | ASP |
| 27 | Y | 201 | GLU |
| 28 | Z | 36 | ASP |
| 28 | Z | 41 | ASN |
| 30 | 2 | 16 | ASN |
| 30 | 2 | 18 | ASN |
| 30 | 2 | 20 | ARG |
| 31 | 3 | 11 | CYS |
| 31 | 3 | 70 | ARG |
| 31 | 3 | 87 | ARG |
| 31 | 3 | 89 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 29 | HIS |
| 3 | A | 47 | HIS |
| 3 | A | 125 | ASN |
| 3 | A | 127 | GLN |
| 3 | A | 199 | HIS |
| 4 | B | 2 | GLN |
| 4 | B | 27 | ASN |
| 4 | B | 145 | HIS |
| 4 | B | 221 | GLN |
| 4 | B | 238 | ASN |
| 4 | B | 256 | GLN |
| 4 | B | 260 | HIS |
| 4 | B | 320 | GLN |
| 4 | B | 332 | ASN |
| 5 | C | 2 | GLN |
| 5 | C | 39 | GLN |
| 5 | C | 129 | HIS |
| 6 | D | 47 | GLN |
| 6 | D | 97 | GLN |
| 6 | D | 103 | ASN |
| 6 | D | 133 | ASN |
| 7 | E | 143 | GLN |
| 9 | G | 17 | GLN |
| 9 | G | 64 | ASN |
| 10 | H | 34 | HIS |
| 10 | H | 59 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | H | 62 | HIS |
| 10 | H | 73 | ASN |
| 10 | H | 148 | HIS |
| 11 | I | 88 | GLN |
| 12 | J | 52 | GLN |
| 12 | J | 92 | GLN |
| 12 | J | 107 | ASN |
| 13 | K | 10 | GLN |
| 14 | L | 7 | GLN |
| 14 | L | 18 | HIS |
| 14 | L | 41 | HIS |
| 14 | L | 42 | ASN |
| 14 | L | 43 | HIS |
| 14 | L | 58 | GLN |
| 15 | M | 24 | GLN |
| 15 | M | 58 | GLN |
| 15 | M | 137 | ASN |
| 15 | M | 190 | ASN |
| 16 | N | 40 | ASN |
| 16 | N | 107 | ASN |
| 16 | N | 153 | GLN |
| 17 | O | 53 | GLN |
| 18 | P | 50 | GLN |
| 18 | P | 57 | ASN |
| 18 | P | 66 | GLN |
| 18 | P | 118 | GLN |
| 19 | Q | 16 | ASN |
| 19 | Q | 40 | HIS |
| 19 | Q | 59 | GLN |
| 20 | R | 61 | GLN |
| 20 | R | 94 | ASN |
| 20 | R | 98 | ASN |
| 20 | R | 113 | HIS |
| 20 | R | 117 | HIS |
| 20 | R | 140 | GLN |
| 21 | S | 51 | GLN |
| 22 | T | 11 | GLN |
| 22 | T | 39 | ASN |
| 22 | T | 43 | ASN |
| 22 | T | 64 | ASN |
| 22 | T | 73 | HIS |
| 23 | U | 39 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | V | 60 | GLN |
| 25 | W | 28 | HIS |
| 25 | W | 59 | GLN |
| 25 | W | 87 | HIS |
| 25 | W | 110 | GLN |
| 25 | W | 119 | HIS |
| 25 | W | 125 | HIS |
| 25 | W | 141 | HIS |
| 26 | X | 23 | HIS |
| 26 | X | 36 | HIS |
| 27 | Y | 149 | GLN |
| 27 | Y | 189 | ASN |
| 29 | 1 | 8 | GLN |
| 29 | 1 | 16 | HIS |
| 29 | 1 | 28 | HIS |
| 30 | 2 | 16 | ASN |
| 30 | 2 | 18 | ASN |
| 30 | 2 | 41 | HIS |
| 30 | 2 | 45 | ASN |
| 31 | 3 | 15 | ASN |
| 31 | 3 | 30 | GLN |
| 31 | 3 | 48 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 0 | 2744/2922 (93%) | 247 (9%) | 26 (0%) |
| 2 | 9 | 121/122 (99%) | 17 (14%) | 1 (0%) |
| All | All | 2865/3044 (94%) | 264 (9%) | 27 (0%) |

All (264) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 31 | C |
| 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 |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 115 | U |
| 1 | 0 | 120 | A |
| 1 | 0 | 130 | C |
| 1 | 0 | 138 | U |
| 1 | 0 | 141 | C |
| 1 | 0 | 151 | A |
| 1 | 0 | 166 | A |
| 1 | 0 | 186 | A |
| 1 | 0 | 191 | A |
| 1 | 0 | 192 | A |
| 1 | 0 | 200 | C |
| 1 | 0 | 219 | G |
| 1 | 0 | 236 | A |
| 1 | 0 | 237 | G |
| 1 | 0 | 271 | C |
| 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 | 319 | A |
| 1 | 0 | 331 | 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 | 473 | A |
| 1 | 0 | 486 | A |
| 1 | 0 | 487 | G |
| 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 |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 545 | G |
| 1 | 0 | 553 | G |
| 1 | 0 | 559 | U |
| 1 | 0 | 588 | G |
| 1 | 0 | 604 | G |
| 1 | 0 | 620 | A |
| 1 | 0 | 632 | A |
| 1 | 0 | 644 | G |
| 1 | 0 | 660 | A |
| 1 | 0 | 674 | A |
| 1 | 0 | 688 | A |
| 1 | 0 | 701 | U |
| 1 | 0 | 759 | C |
| 1 | 0 | 777 | U |
| 1 | 0 | 809 | G |
| 1 | 0 | 821 | U |
| 1 | 0 | 835 | U |
| 1 | 0 | 841 | A |
| 1 | 0 | 857 | A |
| 1 | 0 | 858 | 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 | 884 | C |
| 1 | 0 | 885 | G |
| 1 | 0 | 898 | G |
| 1 | 0 | 905 | C |
| 1 | 0 | 920 | C |
| 1 | 0 | 921 | G |
| 1 | 0 | 923 | A |
| 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 |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 1120 | U |
| 1 | 0 | 1127 | C |
| 1 | 0 | 1130 | U |
| 1 | 0 | 1137 | G |
| 1 | 0 | 1151 | G |
| 1 | 0 | 1164 | U |
| 1 | 0 | 1166 | A |
| 1 | 0 | 1174 | A |
| 1 | 0 | 1175 | G |
| 1 | 0 | 1185 | U |
| 1 | 0 | 1193 | A |
| 1 | 0 | 1206 | U |
| 1 | 0 | 1208 | C |
| 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 | G |
| 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 | 1457 | U |
| 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 | 1528 | A |
| 1 | 0 | 1562 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 1580 | A |
| 1 | 0 | 1592 | G |
| 1 | 0 | 1617 | C |
| 1 | 0 | 1625 | U |
| 1 | 0 | 1626 | A |
| 1 | 0 | 1634 | G |
| 1 | 0 | 1656 | 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 |
| 1 | 0 | 1723 | G |
| 1 | 0 | 1725 | C |
| 1 | 0 | 1730 | G |
| 1 | 0 | 1731 | C |
| 1 | 0 | 1752 | G |
| 1 | 0 | 1778 | A |
| 1 | 0 | 1779 | A |
| 1 | 0 | 1798 | C |
| 1 | 0 | 1819 | G |
| 1 | 0 | 1820 | G |
| 1 | 0 | 1829 | A |
| 1 | 0 | 1856 | C |
| 1 | 0 | 1873 | G |
| 1 | 0 | 1879 | U |
| 1 | 0 | 1919 | A |
| 1 | 0 | 1942 | A |
| 1 | 0 | 1968 | 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 | 2004 | U |
| 1 | 0 | 2006 | C |
| 1 | 0 | 2008 | U |
| 1 | 0 | 2011 | A |
| 1 | 0 | 2012 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 2133 | U |
| 1 | 0 | 2238 | A |
| 1 | 0 | 2243 | C |
| 1 | 0 | 2258 | A |
| 1 | 0 | 2271 | G |
| 1 | 0 | 2272 | G |
| 1 | 0 | 2291 | A |
| 1 | 0 | 2317 | C |
| 1 | 0 | 2321 | A |
| 1 | 0 | 2346 | C |
| 1 | 0 | 2354 | A |
| 1 | 0 | 2369 | A |
| 1 | 0 | 2422 | U |
| 1 | 0 | 2462 | G |
| 1 | 0 | 2465 | A |
| 1 | 0 | 2467 | A |
| 1 | 0 | 2469 | 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 | 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 |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 2613 | G |
| 1 | 0 | 2638 | G |
| 1 | 0 | 2648 | U |
| 1 | 0 | 2649 | A |
| 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 | 2762 | C |
| 1 | 0 | 2768 | A |
| 1 | 0 | 2786 | G |
| 1 | 0 | 2792 | A |
| 1 | 0 | 2800 | A |
| 1 | 0 | 2811 | A |
| 1 | 0 | 2812 | A |
| 1 | 0 | 2825 | C |
| 1 | 0 | 2836 | G |
| 1 | 0 | 2840 | A |
| 1 | 0 | 2850 | C |
| 1 | 0 | 2867 | G |
| 1 | 0 | 2876 | G |
| 1 | 0 | 2890 | A |
| 1 | 0 | 2896 | A |
| 1 | 0 | 2903 | C |
| 1 | 0 | 2914 | A |
| 2 | 9 | 2 | U |
| 2 | 9 | 7 | G |
| 2 | 9 | 14 | G |
| 2 | 9 | 22 | G |
| 2 | 9 | 23 | U |
| 2 | 9 | 24 | U |
| 2 | 9 | 25 | G |
| 2 | 9 | 34 | A |
| 2 | 9 | 40 | C |
| 2 | 9 | 41 | C |
| 2 | 9 | 43 | G |
| 2 | 9 | 52 | A |
| 2 | 9 | 57 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 9 | 66 | G |
| 2 | 9 | 77 | A |
| 2 | 9 | 114 | G |
| 2 | 9 | 122 | C |

All (27) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 69 | A |
| 1 | 0 | 129 | A |
| 1 | 0 | 318 | U |
| 1 | 0 | 644 | G |
| 1 | 0 | 857 | A |
| 1 | 0 | 871 | G |
| 1 | 0 | 877 | G |
| 1 | 0 | 898 | G |
| 1 | 0 | 1080 | C |
| 1 | 0 | 1120 | U |
| 1 | 0 | 1237 | U |
| 1 | 0 | 1246 | A |
| 1 | 0 | 1352 | A |
| 1 | 0 | 1377 | C |
| 1 | 0 | 1450 | C |
| 1 | 0 | 1506 | U |
| 1 | 0 | 1942 | A |
| 1 | 0 | 1979 | G |
| 1 | 0 | 2011 | A |
| 1 | 0 | 2313 | C |
| 1 | 0 | 2467 | A |
| 1 | 0 | 2526 | C |
| 1 | 0 | 2536 | C |
| 1 | 0 | 2649 | A |
| 1 | 0 | 2718 | C |
| 1 | 0 | 2791 | U |
| 2 | 9 | 65 | A |

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

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | OMU | 0 | 2587 | 1 | 12,22,23 | 0.96 | 1 (8%) | 19,31,34 | 3.16 | 2 (10%) |
| 1 | OMG | 0 | 2588 | 1 | 17,26,27 | 1.05 | 1 (5%) | 21,38,41 | 2.55 | 3 (14%) |
| 1 | UR3 | 0 | 2619 | 1 | 12,22,23 | 0.80 | 0 | 16,32,35 | 0.75 | 0 |
| 1 | PSU | 0 | 2621 | 1 | 13,21,22 | 1.45 | 2 (15%) | 18,30,33 | 6.12 | 3 (16%) |
| 1 | 1MA | 0 | 628 | 1 | 14,25,26 | 1.02 | 1 (7%) | 15,37,40 | 1.12 | 1 (6%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | OMU | 0 | 2587 | 1 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | OMG | 0 | 2588 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | UR3 | 0 | 2619 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | PSU | 0 | 2621 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 1MA | 0 | 628 | 1 | - | 0/3/25/26 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1 | 0 | 2621 | PSU | C5-C1' | -4.25 | 1.48 | 1.52 |
| 1 | 0 | 2587 | OMU | C4-N3 | 2.13 | 1.37 | 1.33 |
| 1 | 0 | 2621 | PSU | C4-N3 | 2.53 | 1.37 | 1.33 |
| 1 | 0 | 628 | 1MA | C6-N6 | 2.76 | 1.34 | 1.29 |
| 1 | 0 | 2588 | OMG | C6-N1 | 3.22 | 1.39 | 1.33 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 0 | 2621 | PSU | N1-C2-N3 | -21.54 | 114.59 | 128.33 |
| 1 | 0 | 2588 | OMG | C5-C6-N1 | -8.69 | 111.71 | 123.59 |
| 1 | 0 | 628 | 1MA | C2-N3-C4 | -3.60 | 110.82 | 116.40 |
| 1 | 0 | 2587 | OMU | C5-C4-N3 | -3.27 | 114.73 | 123.12 |
| 1 | 0 | 2588 | OMG | N3-C2-N1 | -2.35 | 123.87 | 127.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 0 | 2621 | PSU | C6-N1-C2 | 2.84 | 120.04 | 115.47 |
| 1 | 0 | 2588 | OMG | C6-N1-C2 | 6.63 | 125.14 | 115.94 |
| 1 | 0 | 2587 | OMU | C4-N3-C2 | 13.15 | 127.16 | 114.14 |
| 1 | 0 | 2621 | PSU | C4-N3-C2 | 13.74 | 127.13 | 115.25 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | 0 | 2587 | OMU | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 | 2749/2922 (94%) | -0.21 | 10 (0%) 93 90 | 29, 55, 100, 157 | 0 |
| 2 | 9 | 122/122 (100%) | -0.20 | 2 (1%) 74 66 | 44, 68, 95, 159 | 0 |
| 3 | A | 237/240 (98%) | 0.13 | 10 (4%) 40 28 | 34, 62, 95, 116 | 0 |
| 4 | B | 337/338 (99%) | -0.05 | 5 (1%) 76 68 | 32, 64, 90, 97 | 0 |
| 5 | C | 246/246 (100%) | -0.19 | 1 (0%) 93 90 | 29, 58, 81, 90 | 0 |
| 6 | D | 140/177 (79%) | 1.30 | 43 (30%) 1 0 | 62, 107, 129, 138 | 0 |
| 7 | E | 172/178 (96%) | 0.60 | 12 (6%) 19 11 | 52, 75, 97, 101 | 0 |
| 8 | F | 119/120 (99%) | 0.66 | 14 (11%) 6 3 | 65, 84, 105, 117 | 0 |
| 9 | G | 29/348 (8%) | 1.83 | 10 (34%) 0 0 | 76, 98, 106, 107 | 0 |
| 10 | H | 160/177 (90%) | -0.01 | 1 (0%) 90 86 | 40, 61, 96, 107 | 0 |
| 11 | I | 70/162 (43%) | 2.77 | 44 (62%) 0 0 | 112, 126, 144, 147 | 0 |
| 12 | J | 142/145 (97%) | -0.19 | 1 (0%) 89 84 | 43, 58, 82, 95 | 0 |
| 13 | K | 132/132 (100%) | -0.04 | 0 100 100 | 40, 61, 84, 89 | 0 |
| 14 | L | 145/165 (87%) | 0.30 | 12 (8%) 14 7 | 29, 75, 115, 126 | 0 |
| 15 | M | 194/195 (99%) | -0.23 | 0 100 100 | 40, 55, 69, 79 | 0 |
| 16 | N | 186/187 (99%) | 0.26 | 11 (5%) 26 16 | 46, 71, 115, 125 | 0 |
| 17 | O | 115/116 (99%) | -0.04 | 0 100 100 | 47, 65, 81, 83 | 0 |
| 18 | P | 143/149 (95%) | 0.21 | 1 (0%) 89 84 | 44, 66, 80, 86 | 0 |
| 19 | Q | 95/96 (98%) | -0.11 | 0 100 100 | 39, 51, 64, 79 | 0 |
| 20 | R | 147/152 (96%) | 0.25 | 10 (6%) 20 12 | 41, 56, 114, 128 | 0 |
| 21 | S | 81/85 (95%) | 0.23 | 4 (4%) 33 22 | 52, 72, 88, 95 | 0 |
| 22 | T | 119/120 (99%) | 0.53 | 6 (5%) 32 21 | 51, 69, 94, 111 | 0 |
| 23 | U | 53/66 (80%) | 0.15 | 3 (5%) 27 17 | 51, 64, 79, 85 | 0 |
| 24 | V | 65/71 (91%) | 1.02 | 13 (20%) 1 1 | 63, 85, 118, 122 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | W | 154/154 (100%) | -0.19 | 0 100 100 | 41, 56, 76, 85 | 0 |
| 26 | X | 82/92 (89%) | 0.39 | 6 (7%) 18 10 | 49, 66, 87, 101 | 0 |
| 27 | Y | 142/241 (58%) | 0.06 | 6 (4%) 40 28 | 31, 53, 79, 95 | 0 |
| 28 | Z | 73/83 (87%) | -0.10 | 0 100 100 | 53, 69, 86, 102 | 0 |
| 29 | 1 | 56/57 (98%) | -0.41 | 0 100 100 | 35, 43, 49, 58 | 0 |
| 30 | 2 | 49/50 (98%) | 0.22 | 3 (6%) 25 15 | 40, 66, 94, 104 | 0 |
| 31 | 3 | 92/92 (100%) | 0.09 | 1 (1%) 82 74 | 42, 63, 76, 91 | 0 |
| All | All | 6646/7478 (88%) | 0.03 | 229 (3%) 49 36 | 29, 61, 106, 159 | 0 |

All (229) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 24 | V | 1 | THR | 9.8 |
| 20 | R | 131 | GLY | 7.4 |
| 22 | T | 119 | ALA | 6.8 |
| 6 | D | 69 | ILE | 6.5 |
| 20 | R | 134 | SER | 6.1 |
| 11 | I | 97 | VAL | 6.0 |
| 11 | I | 104 | ALA | 6.0 |
| 20 | R | 130 | MET | 5.9 |
| 11 | I | 92 | VAL | 5.8 |
| 9 | G | 27 | ILE | 5.8 |
| 20 | R | 129 | ALA | 5.7 |
| 11 | I | 83 | GLY | 5.3 |
| 6 | D | 64 | ARG | 5.2 |
| 6 | D | 63 | ILE | 5.1 |
| 11 | I | 112 | LEU | 5.1 |
| 11 | I | 80 | PHE | 5.1 |
| 11 | I | 71 | ALA | 5.0 |
| 11 | I | 74 | ILE | 4.9 |
| 24 | V | 8 | ILE | 4.9 |
| 24 | V | 43 | PRO | 4.9 |
| 9 | G | 23 | ILE | 4.8 |
| 24 | V | 40 | PRO | 4.8 |
| 6 | D | 56 | ARG | 4.5 |
| 6 | D | 66 | GLY | 4.5 |
| 11 | I | 113 | SER | 4.5 |
| 6 | D | 65 | GLU | 4.5 |
| 11 | I | 128 | THR | 4.5 |
| 11 | I | 91 | PHE | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20 | R | 132 | ARG | 4.3 |
| 6 | D | 57 | THR | 4.2 |
| 11 | I | 72 | GLU | 4.2 |
| 6 | D | 10 | PHE | 4.2 |
| 22 | T | 112 | LEU | 4.1 |
| 11 | I | 98 | ASP | 4.1 |
| 6 | D | 88 | LEU | 4.1 |
| 11 | I | 93 | ALA | 4.1 |
| 6 | D | 27 | ILE | 4.1 |
| 11 | I | 108 | HIS | 4.1 |
| 20 | R | 127 | PRO | 4.0 |
| 6 | D | 61 | PHE | 4.0 |
| 20 | R | 128 | ARG | 4.0 |
| 11 | I | 78 | ALA | 3.9 |
| 14 | L | 60 | GLU | 3.9 |
| 2 | 9 | 1 | U | 3.9 |
| 6 | D | 18 | ILE | 3.8 |
| 11 | I | 109 | PRO | 3.8 |
| 11 | I | 86 | GLU | 3.8 |
| 6 | D | 58 | VAL | 3.8 |
| 7 | E | 45 | ASP | 3.8 |
| 31 | 3 | 92 | GLU | 3.7 |
| 22 | T | 117 | ASP | 3.6 |
| 6 | D | 85 | GLN | 3.6 |
| 22 | T | 118 | SER | 3.6 |
| 11 | I | 111 | LEU | 3.6 |
| 11 | I | 76 | ASP | 3.6 |
| 20 | R | 135 | ALA | 3.6 |
| 7 | E | 44 | GLY | 3.6 |
| 14 | L | 105 | TYR | 3.5 |
| 8 | F | 17 | LEU | 3.5 |
| 16 | N | 166 | ALA | 3.4 |
| 11 | I | 82 | THR | 3.4 |
| 11 | I | 123 | VAL | 3.4 |
| 14 | L | 106 | VAL | 3.4 |
| 3 | A | 35 | GLY | 3.4 |
| 18 | P | 1 | THR | 3.3 |
| 11 | I | 106 | GLN | 3.3 |
| 14 | L | 80 | ASP | 3.3 |
| 11 | I | 132 | VAL | 3.3 |
| 16 | N | 159 | TYR | 3.3 |
| 3 | A | 237 | GLY | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | I | 116 | LEU | 3.3 |
| 11 | I | 67 | VAL | 3.2 |
| 11 | I | 118 | ASN | 3.2 |
| 9 | G | 21 | ASP | 3.2 |
| 27 | Y | 95 | THR | 3.2 |
| 11 | I | 68 | PRO | 3.2 |
| 8 | F | 19 | ALA | 3.2 |
| 6 | D | 62 | ASP | 3.2 |
| 6 | D | 44 | ILE | 3.1 |
| 11 | I | 70 | THR | 3.1 |
| 27 | Y | 97 | LEU | 3.1 |
| 1 | 0 | 284 | C | 3.1 |
| 23 | U | 51 | TRP | 3.1 |
| 8 | F | 16 | ALA | 3.1 |
| 6 | D | 25 | MET | 3.0 |
| 1 | 0 | 282 | C | 3.0 |
| 8 | F | 106 | ALA | 3.0 |
| 11 | I | 114 | TYR | 3.0 |
| 9 | G | 24 | VAL | 3.0 |
| 24 | V | 39 | ALA | 3.0 |
| 3 | A | 82 | VAL | 3.0 |
| 6 | D | 170 | TYR | 3.0 |
| 16 | N | 158 | LEU | 3.0 |
| 30 | 2 | 49 | GLU | 2.9 |
| 6 | D | 41 | LEU | 2.9 |
| 8 | F | 6 | PHE | 2.9 |
| 9 | G | 71 | LEU | 2.9 |
| 20 | R | 126 | LYS | 2.9 |
| 11 | I | 88 | GLN | 2.9 |
| 8 | F | 47 | LEU | 2.9 |
| 6 | D | 23 | VAL | 2.9 |
| 6 | D | 43 | GLU | 2.9 |
| 6 | D | 90 | LEU | 2.8 |
| 11 | I | 117 | THR | 2.8 |
| 3 | A | 36 | ASP | 2.8 |
| 11 | I | 81 | GLU | 2.8 |
| 11 | I | 100 | VAL | 2.8 |
| 1 | 0 | 1172 | G | 2.8 |
| 1 | 0 | 2237 | G | 2.8 |
| 22 | T | 116 | ASP | 2.8 |
| 1 | 0 | 1199 | A | 2.8 |
| 4 | B | 104 | GLU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 24 | V | 3 | LEU | 2.7 |
| 11 | I | 121 | LYS | 2.7 |
| 16 | N | 149 | GLU | 2.7 |
| 3 | A | 38 | ILE | 2.7 |
| 6 | D | 134 | LEU | 2.7 |
| 14 | L | 123 | ASP | 2.7 |
| 8 | F | 107 | ASP | 2.7 |
| 21 | S | 81 | ILE | 2.7 |
| 6 | D | 166 | ILE | 2.7 |
| 7 | E | 43 | ASP | 2.7 |
| 11 | I | 90 | ASP | 2.7 |
| 26 | X | 88 | GLU | 2.7 |
| 6 | D | 106 | PHE | 2.7 |
| 8 | F | 75 | ILE | 2.7 |
| 14 | L | 140 | VAL | 2.7 |
| 1 | 0 | 1951 | G | 2.6 |
| 6 | D | 28 | GLY | 2.6 |
| 7 | E | 11 | VAL | 2.6 |
| 20 | R | 125 | ARG | 2.6 |
| 7 | E | 10 | ASP | 2.6 |
| 10 | H | 76 | LEU | 2.6 |
| 11 | I | 134 | ILE | 2.6 |
| 24 | V | 38 | GLY | 2.6 |
| 6 | D | 68 | PRO | 2.6 |
| 11 | I | 110 | ASP | 2.5 |
| 9 | G | 65 | THR | 2.5 |
| 24 | V | 37 | GLY | 2.5 |
| 16 | N | 183 | ASP | 2.5 |
| 7 | E | 95 | VAL | 2.5 |
| 11 | I | 105 | GLU | 2.5 |
| 11 | I | 79 | GLY | 2.5 |
| 8 | F | 98 | VAL | 2.5 |
| 30 | 2 | 35 | ARG | 2.5 |
| 1 | 0 | 735 | C | 2.5 |
| 26 | X | 41 | PHE | 2.5 |
| 6 | D | 70 | GLY | 2.5 |
| 9 | G | 28 | GLU | 2.4 |
| 24 | V | 49 | LEU | 2.4 |
| 27 | Y | 235 | GLU | 2.4 |
| 6 | D | 67 | ASP | 2.4 |
| 26 | X | 72 | VAL | 2.4 |
| 30 | 2 | 39 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | E | 131 | LEU | 2.4 |
| 6 | D | 104 | PHE | 2.4 |
| 6 | D | 17 | ARG | 2.3 |
| 3 | A | 37 | VAL | 2.3 |
| 6 | D | 128 | LEU | 2.3 |
| 14 | L | 120 | LEU | 2.3 |
| 26 | X | 10 | VAL | 2.3 |
| 11 | I | 73 | LEU | 2.3 |
| 24 | V | 9 | ARG | 2.3 |
| 16 | N | 186 | LEU | 2.3 |
| 2 | 9 | 23 | U | 2.3 |
| 21 | S | 68 | LEU | 2.3 |
| 1 | 0 | 960 | G | 2.3 |
| 24 | V | 63 | GLU | 2.3 |
| 1 | 0 | 1950 | G | 2.2 |
| 7 | E | 100 | ASP | 2.2 |
| 26 | X | 85 | VAL | 2.2 |
| 4 | B | 115 | VAL | 2.2 |
| 8 | F | 108 | VAL | 2.2 |
| 6 | D | 47 | GLN | 2.2 |
| 11 | I | 99 | GLN | 2.2 |
| 4 | B | 105 | PHE | 2.2 |
| 14 | L | 59 | GLU | 2.2 |
| 14 | L | 81 | VAL | 2.2 |
| 6 | D | 55 | LYS | 2.2 |
| 27 | Y | 96 | GLU | 2.2 |
| 7 | E | 47 | VAL | 2.2 |
| 16 | N | 150 | TYR | 2.2 |
| 6 | D | 51 | ARG | 2.2 |
| 26 | X | 74 | ALA | 2.2 |
| 16 | N | 172 | PHE | 2.2 |
| 23 | U | 52 | THR | 2.2 |
| 9 | G | 26 | MET | 2.2 |
| 3 | A | 96 | LEU | 2.2 |
| 6 | D | 29 | HIS | 2.2 |
| 3 | A | 64 | ASP | 2.1 |
| 24 | V | 41 | GLU | 2.1 |
| 22 | T | 63 | ILE | 2.1 |
| 11 | I | 84 | SER | 2.1 |
| 27 | Y | 108 | ASP | 2.1 |
| 4 | B | 128 | ILE | 2.1 |
| 24 | V | 59 | ILE | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | E | 93 | MET | 2.1 |
| 21 | S | 48 | THR | 2.1 |
| 7 | E | 108 | LEU | 2.1 |
| 23 | U | 54 | THR | 2.1 |
| 6 | D | 171 | ASP | 2.1 |
| 9 | G | 15 | TRP | 2.1 |
| 9 | G | 67 | LEU | 2.1 |
| 12 | J | 105 | LEU | 2.1 |
| 5 | C | 244 | ALA | 2.1 |
| 6 | D | 83 | PHE | 2.1 |
| 16 | N | 75 | THR | 2.1 |
| 14 | L | 90 | ARG | 2.1 |
| 3 | A | 98 | GLU | 2.1 |
| 7 | E | 42 | VAL | 2.1 |
| 4 | B | 119 | HIS | 2.1 |
| 6 | D | 26 | GLY | 2.1 |
| 14 | L | 79 | ASP | 2.1 |
| 6 | D | 86 | THR | 2.1 |
| 8 | F | 49 | PHE | 2.0 |
| 8 | F | 15 | ASP | 2.0 |
| 6 | D | 40 | ILE | 2.0 |
| 16 | N | 175 | LEU | 2.0 |
| 14 | L | 89 | PHE | 2.0 |
| 8 | F | 119 | ARG | 2.0 |
| 8 | F | 20 | LEU | 2.0 |
| 11 | I | 87 | PRO | 2.0 |
| 21 | S | 70 | GLU | 2.0 |
| 6 | D | 45 | THR | 2.0 |
| 1 | 0 | 1195 | G | 2.0 |
| 3 | A | 31 | LYS | 2.0 |
| 6 | D | 75 | LEU | 2.0 |
| 16 | N | 185 | GLU | 2.0 |
| 27 | Y | 182 | PHE | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 1 | UR3 | 0 | 2619 | 21/22 | 0.98 | 0.14 | - | 40,42,43,46 | 0 |
| 1 | OMG | 0 | 2588 | 24/25 | 0.98 | 0.14 | - | 40,42,44,44 | 0 |
| 1 | 1MA | 0 | 628 | 23/24 | 0.99 | 0.16 | - | 32,37,39,39 | 0 |
| 1 | PSU | 0 | 2621 | 20/21 | 0.98 | 0.14 | - | 40,41,43,44 | 0 |
| 1 | OMU | 0 | 2587 | 21/22 | 0.98 | 0.14 | - | 39,42,43,46 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 34 | NA | 9 | 8583 | 1/1 | 0.89 | 0.64 | 67.19 | 71,71,71,71 | 0 |
| 35 | CL | 0 | 8815 | 1/1 | 0.71 | 0.75 | 64.08 | 112,112,112,112 | 0 |
| 34 | NA | 0 | 8578 | 1/1 | 0.94 | 0.59 | 43.70 | 77,77,77,77 | 0 |
| 34 | NA | 0 | 8568 | 1/1 | 0.49 | 0.45 | 43.24 | 84,84,84,84 | 0 |
| 34 | NA | 0 | 8574 | 1/1 | 0.93 | 0.80 | 40.37 | 63,63,63,63 | 0 |
| 34 | NA | 0 | 8526 | 1/1 | 0.65 | 0.82 | 37.47 | 78,78,78,78 | 0 |
| 34 | NA | L | 8580 | 1/1 | 0.85 | 0.71 | 36.83 | 72,72,72,72 | 0 |
| 34 | NA | 0 | 8556 | 1/1 | 0.70 | 0.68 | 33.92 | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8559 | 1/1 | 0.93 | 0.40 | 31.66 | 66,66,66,66 | 0 |
| 33 | K | 0 | 8401 | 1/1 | 0.96 | 0.41 | 27.93 | 91,91,91,91 | 0 |
| 34 | NA | 0 | 8521 | 1/1 | 0.95 | 0.39 | 27.33 | 73,73,73,73 | 0 |
| 34 | NA | 0 | 8571 | 1/1 | 0.75 | 0.27 | 23.84 | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8532 | 1/1 | 0.88 | 0.37 | 23.68 | 47,47,47,47 | 0 |
| 34 | NA | 0 | 8573 | 1/1 | 0.94 | 0.65 | 21.94 | 73,73,73,73 | 0 |
| 35 | CL | B | 8819 | 1/1 | 0.91 | 0.41 | 21.05 | 74,74,74,74 | 0 |
| 34 | NA | 0 | 8502 | 1/1 | 0.97 | 0.23 | 19.92 | 49,49,49,49 | 0 |
| 34 | NA | 0 | 8579 | 1/1 | 0.92 | 0.27 | 16.21 | 62,62,62,62 | 0 |
| 34 | NA | 0 | 8561 | 1/1 | 0.94 | 0.34 | 15.97 | 50,50,50,50 | 0 |
| 35 | CL | 0 | 8805 | 1/1 | 0.89 | 0.23 | 15.80 | 77,77,77,77 | 0 |
| 34 | NA | 0 | 8562 | 1/1 | 0.96 | 0.31 | 14.43 | 81,81,81,81 | 0 |
| 34 | NA | 0 | 8550 | 1/1 | 0.94 | 0.27 | 10.08 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 34 | NA | R | 8586 | 1/1 | 0.61 | 0.50 | 9.09 | 81,81,81,81 | 0 |
| 35 | CL | 0 | 8816 | 1/1 | 0.87 | 0.45 | 8.51 | 79,79,79,79 | 0 |
| 34 | NA | 0 | 8566 | 1/1 | 0.91 | 0.32 | 8.04 | 68,68,68,68 | 0 |
| 34 | NA | 0 | 8510 | 1/1 | 0.93 | 0.24 | 7.95 | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8582 | 1/1 | 0.86 | 0.25 | 6.56 | 78,78,78,78 | 0 |
| 34 | NA | 0 | 8503 | 1/1 | 0.97 | 0.22 | 6.06 | 70,70,70,70 | 0 |
| 32 | MG | 0 | 8038 | 1/1 | 0.84 | 0.21 | 5.77 | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8064 | 1/1 | 0.97 | 0.20 | 4.70 | 43,43,43,43 | 0 |
| 34 | NA | 0 | 8565 | 1/1 | 0.98 | 0.30 | 3.38 | 49,49,49,49 | 0 |
| 34 | NA | 0 | 8531 | 1/1 | 0.98 | 0.17 | 3.21 | 55,55,55,55 | 0 |
| 34 | NA | M | 8547 | 1/1 | 0.94 | 0.22 | 2.93 | 45,45,45,45 | 0 |
| 34 | NA | 0 | 8529 | 1/1 | 0.93 | 0.15 | 2.88 | 79,79,79,79 | 0 |
| 35 | CL | O | 8808 | 1/1 | 0.95 | 0.39 | 2.86 | 99,99,99,99 | 0 |
| 34 | NA | 0 | 8535 | 1/1 | 0.94 | 0.20 | 2.76 | 73,73,73,73 | 0 |
| 34 | NA | 0 | 8555 | 1/1 | 0.99 | 0.23 | 2.52 | 67,67,67,67 | 0 |
| 34 | NA | 0 | 8576 | 1/1 | 0.95 | 0.18 | 2.25 | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8564 | 1/1 | 0.83 | 0.17 | 1.80 | 40,40,40,40 | 0 |
| 35 | CL | 3 | 8804 | 1/1 | 0.92 | 0.29 | 1.71 | 74,74,74,74 | 0 |
| 34 | NA | 0 | 8505 | 1/1 | 0.96 | 0.17 | 1.56 | 49,49,49,49 | 0 |
| 32 | MG | 0 | 8044 | 1/1 | 0.95 | 0.16 | 1.02 | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8053 | 1/1 | 0.97 | 0.14 | 0.53 | 47,47,47,47 | 0 |
| 34 | NA | 0 | 8554 | 1/1 | 0.96 | 0.15 | 0.42 | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8057 | 1/1 | 0.98 | 0.18 | 0.31 | 67,67,67,67 | 0 |
| 35 | CL | M | 8818 | 1/1 | 0.98 | 0.19 | 0.16 | 60,60,60,60 | 0 |
| 34 | NA | 0 | 8533 | 1/1 | 0.94 | 0.14 | -0.01 | 49,49,49,49 | 0 |
| 34 | NA | Q | 8548 | 1/1 | 0.95 | 0.17 | -0.27 | 49,49,49,49 | 0 |
| 32 | MG | 0 | 8013 | 1/1 | 0.98 | 0.16 | -0.35 | 54,54,54,54 | 0 |
| 34 | NA | T | 8543 | 1/1 | 0.96 | 0.14 | -0.48 | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8091 | 1/1 | 0.96 | 0.13 | -0.66 | 53,53,53,53 | 0 |
| 35 | CL | 0 | 8812 | 1/1 | 0.97 | 0.14 | -0.73 | 65,65,65,65 | 0 |
| 36 | CD | Z | 8703 | 1/1 | 0.99 | 0.11 | -0.79 | 71,71,71,71 | 0 |
| 34 | NA | 0 | 8509 | 1/1 | 0.96 | 0.12 | -0.81 | 37,37,37,37 | 0 |
| 36 | CD | 3 | 8704 | 1/1 | 0.93 | 0.08 | -0.95 | 72,72,72,72 | 0 |
| 32 | MG | T | 8073 | 1/1 | 0.91 | 0.21 | -1.19 | 68,68,68,68 | 0 |
| 32 | MG | 0 | 8086 | 1/1 | 0.98 | 0.07 | -1.37 | 46,46,46,46 | 0 |
| 33 | K | 0 | 8402 | 1/1 | 0.96 | 0.13 | -1.37 | 69,69,69,69 | 0 |
| 32 | MG | 0 | 8060 | 1/1 | 0.99 | 0.13 | -1.37 | 50,50,50,50 | 0 |
| 36 | CD | U | 8701 | 1/1 | 0.99 | 0.10 | -1.39 | 76,76,76,76 | 0 |
| 32 | MG | Y | 8108 | 1/1 | 0.95 | 0.15 | -1.52 | 48,48,48,48 | 0 |
| 36 | CD | 1 | 8702 | 1/1 | 1.00 | 0.07 | -1.53 | 68,68,68,68 | 0 |
| 32 | MG | 0 | 8033 | 1/1 | 0.97 | 0.13 | -1.56 | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8113 | 1/1 | 0.95 | 0.12 | -1.56 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 34 | NA | 0 | 8527 | 1/1 | 0.97 | 0.13 | -1.56 | 69,69,69,69 | 0 |
| 34 | NA | 0 | 8517 | 1/1 | 0.96 | 0.10 | -1.60 | 52,52,52,52 | 0 |
| 34 | NA | 0 | 8538 | 1/1 | 0.88 | 0.09 | -2.20 | 61,61,61,61 | 0 |
| 32 | MG | 0 | 8027 | 1/1 | 0.96 | 0.09 | -2.31 | 63,63,63,63 | 0 |
| 35 | CL | J | 8821 | 1/1 | 0.97 | 0.10 | -2.56 | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8008 | 1/1 | 0.97 | 0.08 | -2.61 | 35,35,35,35 | 0 |
| 34 | NA | J | 8546 | 1/1 | 0.98 | 0.11 | -2.61 | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8012 | 1/1 | 0.99 | 0.10 | -2.63 | 33,33,33,33 | 0 |
| 34 | NA | 0 | 8553 | 1/1 | 0.99 | 0.10 | -2.65 | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8074 | 1/1 | 0.97 | 0.06 | -2.75 | 40,40,40,40 | 0 |
| 32 | MG | 3 | 8078 | 1/1 | 0.97 | 0.07 | -2.85 | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8004 | 1/1 | 0.96 | 0.07 | -2.92 | 43,43,43,43 | 0 |
| 34 | NA | A | 8545 | 1/1 | 0.96 | 0.10 | -3.02 | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8056 | 1/1 | 0.99 | 0.11 | -3.06 | 49,49,49,49 | 0 |
| 32 | MG | 0 | 8015 | 1/1 | 0.95 | 0.06 | -3.20 | 41,41,41,41 | 0 |
| 32 | MG | 0 | 8047 | 1/1 | 0.98 | 0.09 | -3.24 | 59,59,59,59 | 0 |
| 34 | NA | 0 | 8544 | 1/1 | 0.97 | 0.07 | -3.28 | 33,33,33,33 | 0 |
| 34 | NA | 0 | 8525 | 1/1 | 0.97 | 0.10 | -3.29 | 50,50,50,50 | 0 |
| 32 | MG | 0 | 8088 | 1/1 | 0.96 | 0.10 | -3.42 | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8077 | 1/1 | 0.98 | 0.07 | -3.60 | 32,32,32,32 | 0 |
| 32 | MG | 0 | 8010 | 1/1 | 0.98 | 0.10 | -3.61 | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8032 | 1/1 | 0.98 | 0.07 | -3.80 | 32,32,32,32 | 0 |
| 32 | MG | 0 | 8017 | 1/1 | 0.99 | 0.04 | -3.92 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8101 | 1/1 | 0.97 | 0.09 | -3.95 | 70,70,70,70 | 0 |
| 32 | MG | A | 8065 | 1/1 | 0.99 | 0.08 | -3.96 | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8054 | 1/1 | 0.99 | 0.10 | -4.28 | 43,43,43,43 | 0 |
| 32 | MG | B | 8055 | 1/1 | 0.99 | 0.06 | -4.29 | 46,46,46,46 | 0 |
| 34 | NA | 0 | 8539 | 1/1 | 0.97 | 0.10 | -4.32 | 26,26,26,26 | 0 |
| 32 | MG | 0 | 8111 | 1/1 | 0.94 | 0.07 | -4.50 | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8084 | 1/1 | 0.99 | 0.07 | -5.00 | 54,54,54,54 | 0 |
| 34 | NA | 0 | 8523 | 1/1 | 0.96 | 0.10 | -5.36 | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8052 | 1/1 | 0.96 | 0.06 | -5.55 | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8001 | 1/1 | 0.99 | 0.09 | -5.87 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8106 | 1/1 | 0.99 | 0.09 | -6.15 | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8058 | 1/1 | 1.00 | 0.09 | -6.19 | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8003 | 1/1 | 0.96 | 0.10 | -6.39 | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8080 | 1/1 | 0.99 | 0.09 | -6.85 | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8020 | 1/1 | 1.00 | 0.06 | -7.55 | 31,31,31,31 | 0 |
| 32 | MG | 0 | 8006 | 1/1 | 0.99 | 0.06 | -7.69 | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8019 | 1/1 | 0.99 | 0.03 | -7.83 | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8035 | 1/1 | 0.98 | 0.03 | -8.14 | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8520 | 1/1 | 0.98 | 0.07 | -8.17 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 32 | MG | 0 | 8007 | 1/1 | 0.97 | 0.09 | -8.66 | 29,29,29,29 | 0 |
| 32 | MG | 0 | 8002 | 1/1 | 0.99 | 0.06 | -10.31 | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8109 | 1/1 | 0.95 | 0.05 | -10.36 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8067 | 1/1 | 1.00 | 0.07 | -10.54 | 54,54,54,54 | 0 |
| 34 | NA | 0 | 8516 | 1/1 | 0.96 | 0.23 | - | 61,61,61,61 | 0 |
| 35 | CL | 0 | 8814 | 1/1 | 0.94 | 0.17 | - | 71,71,71,71 | 0 |
| 34 | NA | 0 | 8558 | 1/1 | 0.97 | 0.70 | - | 107,107,107,107 | 0 |
| 34 | NA | R | 8537 | 1/1 | 0.87 | 0.13 | - | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8048 | 1/1 | 0.96 | 0.09 | - | 62,62,62,62 | 0 |
| 32 | MG | 0 | 8036 | 1/1 | 0.98 | 0.08 | - | 44,44,44,44 | 0 |
| 34 | NA | 0 | 8570 | 1/1 | 0.93 | 0.16 | - | 66,66,66,66 | 0 |
| 32 | MG | 0 | 8025 | 1/1 | 0.97 | 0.12 | - | 58,58,58,58 | 0 |
| 35 | CL | 0 | 8803 | 1/1 | 0.94 | 0.20 | - | 80,80,80,80 | 0 |
| 32 | MG | 0 | 8031 | 1/1 | 0.70 | 0.19 | - | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8079 | 1/1 | 0.99 | 0.11 | - | 43,43,43,43 | 0 |
| 34 | NA | 0 | 8567 | 1/1 | 0.86 | 0.17 | - | 70,70,70,70 | 0 |
| 32 | MG | 0 | 8026 | 1/1 | 0.99 | 0.09 | - | 28,28,28,28 | 0 |
| 34 | NA | 9 | 8551 | 1/1 | 0.85 | 0.18 | - | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8081 | 1/1 | 0.97 | 0.14 | - | 74,74,74,74 | 0 |
| 32 | MG | 0 | 8034 | 1/1 | 0.99 | 0.10 | - | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8524 | 1/1 | 0.86 | 0.26 | - | 68,68,68,68 | 0 |
| 36 | CD | O | 8705 | 1/1 | 0.98 | 0.08 | - | 98,98,98,98 | 0 |
| 34 | NA | 0 | 8542 | 1/1 | 0.97 | 0.20 | - | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8100 | 1/1 | 0.96 | 0.14 | - | 66,66,66,66 | 0 |
| 35 | CL | 0 | 8822 | 1/1 | 0.92 | 0.20 | - | 79,79,79,79 | 0 |
| 34 | NA | 0 | 8563 | 1/1 | 0.79 | 0.46 | - | 51,51,51,51 | 0 |
| 35 | CL | Q | 8811 | 1/1 | 0.96 | 0.17 | - | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8005 | 1/1 | 0.99 | 0.09 | - | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8021 | 1/1 | 0.99 | 0.10 | - | 31,31,31,31 | 0 |
| 34 | NA | 0 | 8508 | 1/1 | 0.89 | 0.23 | - | 73,73,73,73 | 0 |
| 34 | NA | 0 | 8557 | 1/1 | 0.94 | 0.11 | - | 65,65,65,65 | 0 |
| 32 | MG | 0 | 8022 | 1/1 | 0.98 | 0.06 | - | 42,42,42,42 | 0 |
| 32 | MG | 0 | 8085 | 1/1 | 0.91 | 0.13 | - | 62,62,62,62 | 0 |
| 32 | MG | 0 | 8039 | 1/1 | 1.00 | 0.07 | - | 44,44,44,44 | 0 |
| 35 | CL | 0 | 8817 | 1/1 | 0.89 | 0.16 | - | 74,74,74,74 | 0 |
| 32 | MG | 0 | 8042 | 1/1 | 0.95 | 0.11 | - | 55,55,55,55 | 0 |
| 34 | NA | 0 | 8581 | 1/1 | 0.91 | 0.14 | - | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8011 | 1/1 | 0.98 | 0.11 | - | 32,32,32,32 | 0 |
| 32 | MG | A | 8066 | 1/1 | 0.98 | 0.06 | - | 88,88,88,88 | 0 |
| 34 | NA | C | 8504 | 1/1 | 0.89 | 0.34 | - | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8093 | 1/1 | 0.95 | 0.19 | - | 50,50,50,50 | 0 |
| 32 | MG | 0 | 8043 | 1/1 | 0.88 | 0.12 | - | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32 | MG | 0 | 8110 | 1/1 | 0.98 | 0.04 | - | 59,59,59,59 | 0 |
| 32 | MG | 0 | 8089 | 1/1 | 0.94 | 0.08 | - | 69,69,69,69 | 0 |
| 32 | MG | 0 | 8040 | 1/1 | 0.90 | 0.12 | - | 57,57,57,57 | 0 |
| 34 | NA | S | 8512 | 1/1 | 0.92 | 0.14 | - | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8041 | 1/1 | 0.87 | 0.22 | - | 59,59,59,59 | 0 |
| 32 | MG | 0 | 8092 | 1/1 | 0.92 | 0.23 | - | 80,80,80,80 | 0 |
| 34 | NA | 0 | 8507 | 1/1 | 0.82 | 0.46 | - | 61,61,61,61 | 0 |
| 35 | CL | 0 | 8813 | 1/1 | 0.97 | 0.10 | - | 67,67,67,67 | 0 |
| 35 | CL | N | 8807 | 1/1 | 0.88 | 0.33 | - | 74,74,74,74 | 0 |
| 32 | MG | 0 | 8059 | 1/1 | 0.96 | 0.10 | - | 44,44,44,44 | 0 |
| 34 | NA | 0 | 8501 | 1/1 | 0.97 | 0.11 | - | 29,29,29,29 | 0 |
| 34 | NA | 0 | 8577 | 1/1 | 0.96 | 0.20 | - | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8046 | 1/1 | 0.97 | 0.06 | - | 55,55,55,55 | 0 |
| 32 | MG | 0 | 8016 | 1/1 | 0.97 | 0.13 | - | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8045 | 1/1 | 0.98 | 0.10 | - | 59,59,59,59 | 0 |
| 32 | MG | 0 | 8051 | 1/1 | 0.96 | 0.15 | - | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8009 | 1/1 | 0.99 | 0.04 | - | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8536 | 1/1 | 0.96 | 0.09 | - | 52,52,52,52 | 0 |
| 34 | NA | 0 | 8560 | 1/1 | 0.93 | 0.64 | - | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8518 | 1/1 | 0.97 | 0.18 | - | 32,32,32,32 | 0 |
| 32 | MG | 0 | 8099 | 1/1 | 0.88 | 0.14 | - | 62,62,62,62 | 0 |
| 32 | MG | 0 | 8096 | 1/1 | 0.97 | 0.11 | - | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8098 | 1/1 | 0.99 | 0.11 | - | 30,30,30,30 | 0 |
| 32 | MG | 0 | 8062 | 1/1 | 0.93 | 0.14 | - | 65,65,65,65 | 0 |
| 34 | NA | 0 | 8528 | 1/1 | 0.89 | 0.74 | - | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8522 | 1/1 | 0.88 | 0.19 | - | 68,68,68,68 | 0 |
| 32 | MG | 0 | 8082 | 1/1 | 0.91 | 0.10 | - | 76,76,76,76 | 0 |
| 34 | NA | 0 | 8506 | 1/1 | 0.88 | 0.71 | - | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8575 | 1/1 | 0.96 | 0.25 | - | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8569 | 1/1 | 0.91 | 0.59 | - | 66,66,66,66 | 0 |
| 34 | NA | 0 | 8515 | 1/1 | 0.95 | 0.26 | - | 65,65,65,65 | 0 |
| 35 | CL | J | 8801 | 1/1 | 0.95 | 0.10 | - | 67,67,67,67 | 0 |
| 34 | NA | 0 | 8541 | 1/1 | 0.87 | 0.23 | - | 53,53,53,53 | 0 |
| 35 | CL | R | 8806 | 1/1 | 0.89 | 0.18 | - | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8070 | 1/1 | 0.94 | 0.12 | - | 54,54,54,54 | 0 |
| 34 | NA | 0 | 8513 | 1/1 | 0.60 | 0.17 | - | 72,72,72,72 | 0 |
| 34 | NA | 0 | 8572 | 1/1 | 0.85 | 0.31 | - | 69,69,69,69 | 0 |
| 32 | MG | 0 | 8115 | 1/1 | 0.91 | 0.14 | - | 70,70,70,70 | 0 |
| 32 | MG | 0 | 8023 | 1/1 | 0.99 | 0.08 | - | 42,42,42,42 | 0 |
| 32 | MG | 0 | 8075 | 1/1 | 0.98 | 0.09 | - | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8083 | 1/1 | 0.98 | 0.04 | - | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8107 | 1/1 | 0.89 | 0.19 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32 | MG | 0 | 8087 | 1/1 | 0.96 | 0.10 | - | 81,81,81,81 | 0 |
| 32 | MG | 0 | 8114 | 1/1 | 0.90 | 0.16 | - | 47,47,47,47 | 0 |
| 34 | NA | 0 | 8584 | 1/1 | 0.94 | 0.17 | - | 70,70,70,70 | 0 |
| 34 | NA | 0 | 8549 | 1/1 | 0.95 | 0.16 | - | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8049 | 1/1 | 0.90 | 0.31 | - | 70,70,70,70 | 0 |
| 35 | CL | A | 8809 | 1/1 | 0.94 | 0.23 | - | 82,82,82,82 | 0 |
| 32 | MG | 0 | 8105 | 1/1 | 0.97 | 0.08 | - | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8030 | 1/1 | 0.99 | 0.13 | - | 34,34,34,34 | 0 |
| 34 | NA | 0 | 8540 | 1/1 | 0.93 | 0.24 | - | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8072 | 1/1 | 0.99 | 0.11 | - | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8530 | 1/1 | 0.86 | 0.30 | - | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8028 | 1/1 | 0.98 | 0.06 | - | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8102 | 1/1 | 0.97 | 0.19 | - | 71,71,71,71 | 0 |
| 32 | MG | 0 | 8071 | 1/1 | 0.99 | 0.07 | - | 80,80,80,80 | 0 |
| 32 | MG | 0 | 8103 | 1/1 | 0.92 | 0.16 | - | 67,67,67,67 | 0 |
| 32 | MG | 2 | 8076 | 1/1 | 0.92 | 0.16 | - | 69,69,69,69 | 0 |
| 34 | NA | 0 | 8552 | 1/1 | 0.73 | 0.65 | - | 62,62,62,62 | 0 |
| 32 | MG | 0 | 8116 | 1/1 | 0.97 | 0.08 | - | 39,39,39,39 | 0 |
| 35 | CL | J | 8802 | 1/1 | 0.92 | 0.12 | - | 75,75,75,75 | 0 |
| 32 | MG | 0 | 8068 | 1/1 | 0.96 | 0.05 | - | 70,70,70,70 | 0 |
| 32 | MG | 9 | 8095 | 1/1 | 0.82 | 0.09 | - | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8104 | 1/1 | 0.78 | 0.29 | - | 61,61,61,61 | 0 |
| 32 | MG | 0 | 8090 | 1/1 | 0.99 | 0.10 | - | 59,59,59,59 | 0 |
| 32 | MG | 0 | 8061 | 1/1 | 0.99 | 0.10 | - | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8585 | 1/1 | 0.86 | 0.53 | - | 60,60,60,60 | 0 |
| 34 | NA | 0 | 8514 | 1/1 | 0.95 | 0.09 | - | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8037 | 1/1 | 0.98 | 0.08 | - | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8094 | 1/1 | 0.97 | 0.04 | - | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8024 | 1/1 | 0.95 | 0.14 | - | 45,45,45,45 | 0 |
| 35 | CL | Y | 8820 | 1/1 | 0.92 | 0.14 | - | 55,55,55,55 | 0 |
| 34 | NA | 0 | 8534 | 1/1 | 0.97 | 0.11 | - | 55,55,55,55 | 0 |
| 34 | NA | 0 | 8519 | 1/1 | 0.97 | 0.07 | - | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8097 | 1/1 | 0.87 | 0.19 | - | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8014 | 1/1 | 0.96 | 0.10 | - | 20,20,20,20 | 0 |
| 35 | CL | L | 8810 | 1/1 | 0.94 | 0.13 | - | 73,73,73,73 | 0 |
| 32 | MG | 0 | 8018 | 1/1 | 0.98 | 0.11 | - | 50,50,50,50 | 0 |
| 34 | NA | 0 | 8511 | 1/1 | 0.92 | 0.13 | - | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8112 | 1/1 | 0.94 | 0.18 | - | 64,64,64,64 | 0 |
| 32 | MG | 0 | 8029 | 1/1 | 0.98 | 0.11 | - | 55,55,55,55 | 0 |
| 32 | MG | K | 8069 | 1/1 | 0.95 | 0.09 | - | 62,62,62,62 | 0 |
| 32 | MG | 0 | 8063 | 1/1 | 0.96 | 0.23 | - | 73,73,73,73 | 0 |
| 32 | MG | 0 | 8050 | 1/1 | 0.80 | 0.12 | - | 97,97,97,97 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.