# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 06:36 AM EST

| | | |
|---|---|---|
| PDB ID | : | 3CCS |
| Title | : | Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482A |
| Authors | : | Blaha, G.; Gurel, G. |
| Deposited on | : | 2008-02-26 |
| Resolution | : | 2.95 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

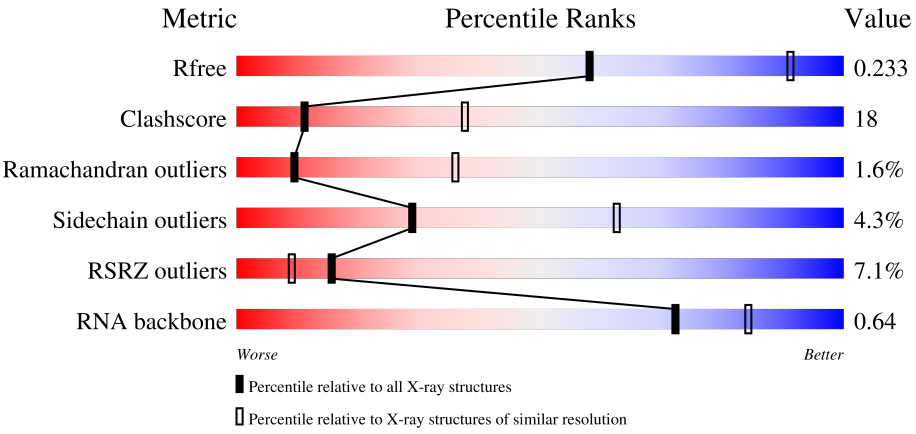
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 3104 (3.00-2.92) |
| Clashscore | 141614 | 3462 (3.00-2.92) |
| Ramachandran outliers | 138981 | 3340 (3.00-2.92) |
| Sidechain outliers | 138945 | 3343 (3.00-2.92) |
| RSRZ outliers | 127900 | 2986 (3.00-2.92) |
| RNA backbone | 3102 | 1065 (3.22-2.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | A | 240 | 3%, 66%, 28%, . . |
| 2 | B | 338 | 62%, 33%, . |
| 3 | C | 246 | 73%, 24%, . |
| 4 | D | 177 | 29%, 51%, 25%, ., 21% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | E | 178 | 2% 69% 26% |
| 6 | F | 120 | 12% 74% 24% |
| 7 | G | 348 | 5% 92% |
| 8 | H | 177 | 18% 68% 20% 10% |
| 9 | I | 162 | 31% 30% 12% 57% |
| 10 | J | 145 | 65% 31% |
| 11 | K | 132 | 72% 27% |
| 12 | L | 165 | 13% 60% 28% 12% |
| 13 | M | 196 | 10% 58% 37% |
| 14 | N | 187 | 14% 63% 33% |
| 15 | O | 116 | 78% 21% |
| 16 | P | 149 | 70% 23% |
| 17 | Q | 96 | 73% 25% |
| 18 | R | 155 | 70% 24% |
| 19 | S | 85 | 2% 72% 24% 5% |
| 20 | T | 120 | 4% 68% 29% |
| 21 | U | 67 | 75% 43% 31% 21% |
| 22 | V | 71 | 17% 58% 31% 8% |
| 23 | W | 154 | 62% 35% |
| 24 | X | 92 | 4% 60% 27% 11% |
| 25 | Y | 241 | 42% 16% 41% |
| 26 | Z | 116 | 51% 29% 29% 37% |
| 27 | 1 | 57 | 68% 30% |
| 28 | 2 | 50 | 6% 56% 36% 8% |
| 29 | 3 | 92 | 99% 43% 52% |

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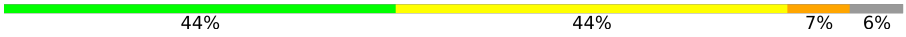
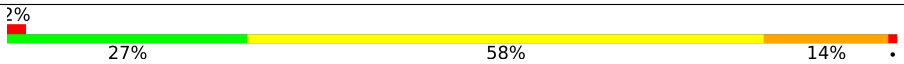
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 30 | 0 | 2923 |   |
| 31 | 9 | 122 |   |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 33 | CL | 0 | 8812 | - | - | X | - |
| 33 | CL | Y | 8820 | - | - | X | - |
| 34 | SR | 0 | 8982 | - | - | - | X |
| 34 | SR | 0 | 9004 | - | - | - | X |
| 34 | SR | 0 | 9006 | - | - | - | X |
| 34 | SR | 0 | 9007 | - | - | - | X |
| 35 | NA | 0 | 8528 | - | - | - | X |
| 37 | CD | 3 | 8704 | - | - | - | X |
| 37 | CD | Z | 8703 | - | - | - | X |

## 2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99121 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 protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 237 | 1753 | 1072 | 352 | 324 | 5 | 0 | 0 | 0 |

- Molecule 2 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | B | 337 | 2625 | 1616 | 493 | 511 | 5 | 0 | 0 | 0 |

- Molecule 3 is a protein called 50S ribosomal protein L4P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | C | 246 | 1860 | 1130 | 345 | 384 | 1 | 0 | 0 | 0 |

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | E | 172 | 1357 | 840 | 224 | 289 | 4 | 0 | 0 | 0 |

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | F | 119 | 890 | 551 | 141 | 197 | 1 | 0 | 0 | 0 |

- Molecule 7 is a protein called 50S ribosomal protein L10E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 240 | 149 | 39 | 51 | 1 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L10e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 160 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1282 | 798 | 240 | 238 | 6 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L11P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 519 | 323 | 81 | 114 | 1 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L13P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1120 | 696 | 199 | 222 | 3 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 994 | 609 | 189 | 192 | 4 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L15P.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 145 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1118 | 670 | 222 | 226 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L15e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | M | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1558 | 943 | 333 | 281 | 1 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L18P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | N | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 895 | 262 | 286 | 2 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | O | 115 | Total | C | N | O | 0 | 0 | 0 |
| | | | 865 | 529 | 161 | 175 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L19e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | P | 143 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1136 | 683 | 229 | 224 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | Q | 95 | Total | C | N | O | 0 | 0 | 0 |
| | | | 735 | 450 | 141 | 144 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 18 | R | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1149 | 713 | 209 | 223 | 4 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L23P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | S | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 641 | 389 | 111 | 138 | 3 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L24P.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | T | 119 | Total | C | N | O | 0 | 0 | 0 |
| | | | 950 | 568 | 180 | 202 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L24e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | U | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 410 | 244 | 75 | 86 | 5 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L29P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | V | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 499 | 304 | 94 | 100 | 1 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L30P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | W | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1196 | 737 | 209 | 244 | 6 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | X | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 654 | 402 | 129 | 122 | 1 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L32e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Y | 142 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1130 | 686 | 228 | 216 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | Z | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 573 | 343 | 113 | 112 | 5 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 431 | 258 | 86 | 83 | 4 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | 2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 396 | 239 | 89 | 67 | 1 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | 3 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 458 | 153 | 137 | 7 | | | |

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | 0 | 2754 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59019 | 26349 | 10873 | 19052 | 2745 | | | |

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | 9 | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2599 | 1160 | 471 | 847 | 121 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 32 | A | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 32 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | T | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 0 | 86 | Total | Mg | 0 | 0 |
| | | | 86 | 86 | | |
| 32 | 9 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 33 | A | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | B | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | J | 3 | Total Cl<br>3 3 | 0 | 0 |
| 33 | L | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | M | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | N | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | O | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | R | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | Y | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | 3 | 1 | Total Cl<br>1 1 | 0 | 0 |
| 33 | 0 | 10 | Total Cl<br>10 10 | 0 | 0 |

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 34 | A | 2 | Total Sr<br>2 2 | 0 | 0 |
| 34 | B | 2 | Total Sr<br>2 2 | 0 | 0 |
| 34 | F | 1 | Total Sr<br>1 1 | 0 | 0 |
| 34 | H | 1 | Total Sr<br>1 1 | 0 | 0 |
| 34 | L | 1 | Total Sr<br>1 1 | 0 | 0 |
| 34 | R | 1 | Total Sr<br>1 1 | 0 | 0 |
| 34 | S | 1 | Total Sr<br>1 1 | 0 | 0 |
| 34 | 1 | 2 | Total Sr<br>2 2 | 0 | 0 |
| 34 | 3 | 2 | Total Sr<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 34 | 0 | 92 | Total Sr<br>92 92 | 0 | 0 |
| 34 | 9 | 3 | Total Sr<br>3 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 35 | B | 1 | Total Na<br>1 1 | 0 | 0 |
| 35 | C | 1 | Total Na<br>1 1 | 0 | 0 |
| 35 | H | 1 | Total Na<br>1 1 | 0 | 0 |
| 35 | J | 1 | Total Na<br>1 1 | 0 | 0 |
| 35 | M | 1 | Total Na<br>1 1 | 0 | 0 |
| 35 | Q | 1 | Total Na<br>1 1 | 0 | 0 |
| 35 | R | 1 | Total Na<br>1 1 | 0 | 0 |
| 35 | S | 1 | Total Na<br>1 1 | 0 | 0 |
| 35 | 0 | 65 | Total Na<br>65 65 | 0 | 0 |
| 35 | 9 | 2 | Total Na<br>2 2 | 0 | 0 |

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 36 | M | 1 | Total K<br>1 1 | 0 | 0 |
| 36 | 0 | 1 | Total K<br>1 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 37 | O | 1 | Total Cd<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 37 | U | 1 | Total Cd<br>1 1 | 0 | 0 |
| 37 | Z | 1 | Total Cd<br>1 1 | 0 | 0 |
| 37 | 1 | 1 | Total Cd<br>1 1 | 0 | 0 |
| 37 | 3 | 1 | Total Cd<br>1 1 | 0 | 0 |

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 38 | A | 119 | Total O<br>119 119 | 0 | 0 |
| 38 | B | 152 | Total O<br>152 152 | 0 | 0 |
| 38 | C | 185 | Total O<br>185 185 | 0 | 0 |
| 38 | D | 42 | Total O<br>42 42 | 0 | 0 |
| 38 | E | 43 | Total O<br>43 43 | 0 | 0 |
| 38 | F | 26 | Total O<br>26 26 | 0 | 0 |
| 38 | G | 19 | Total O<br>19 19 | 0 | 0 |
| 38 | H | 65 | Total O<br>65 65 | 0 | 0 |
| 38 | I | 8 | Total O<br>8 8 | 0 | 0 |
| 38 | J | 53 | Total O<br>53 53 | 0 | 0 |
| 38 | K | 58 | Total O<br>58 58 | 0 | 0 |
| 38 | L | 85 | Total O<br>85 85 | 0 | 0 |
| 38 | M | 127 | Total O<br>127 127 | 0 | 0 |
| 38 | N | 59 | Total O<br>59 59 | 0 | 0 |
| 38 | O | 39 | Total O<br>39 39 | 0 | 0 |

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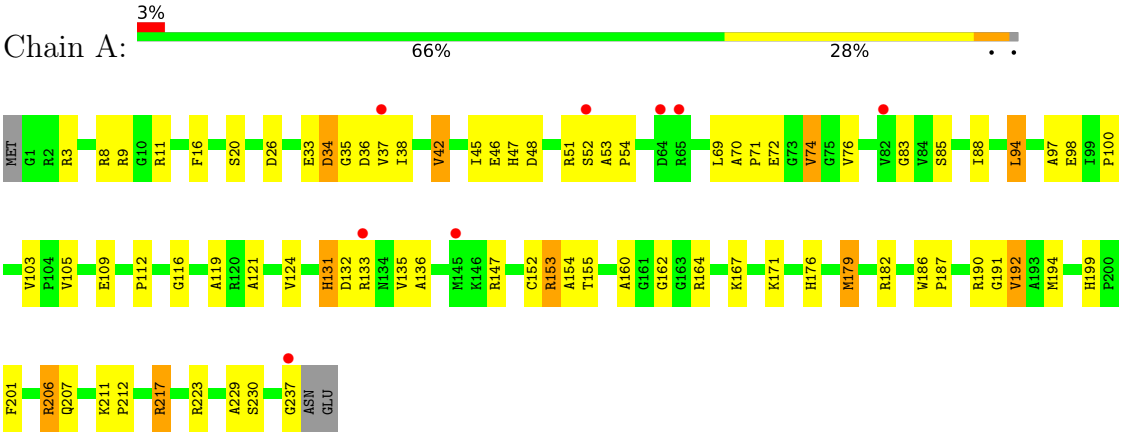
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 38 | P | 67 | Total O<br>67 67 | 0 | 0 |
| 38 | Q | 48 | Total O<br>48 48 | 0 | 0 |
| 38 | R | 77 | Total O<br>77 77 | 0 | 0 |
| 38 | S | 30 | Total O<br>30 30 | 0 | 0 |
| 38 | T | 36 | Total O<br>36 36 | 0 | 0 |
| 38 | U | 28 | Total O<br>28 28 | 0 | 0 |
| 38 | V | 13 | Total O<br>13 13 | 0 | 0 |
| 38 | W | 67 | Total O<br>67 67 | 0 | 0 |
| 38 | X | 21 | Total O<br>21 21 | 0 | 0 |
| 38 | Y | 100 | Total O<br>100 100 | 0 | 0 |
| 38 | Z | 31 | Total O<br>31 31 | 0 | 0 |
| 38 | 1 | 59 | Total O<br>59 59 | 0 | 0 |
| 38 | 2 | 43 | Total O<br>43 43 | 0 | 0 |
| 38 | 3 | 70 | Total O<br>70 70 | 0 | 0 |
| 38 | 0 | 5904 | Total O<br>5904 5904 | 0 | 0 |
| 38 | 9 | 149 | Total O<br>149 149 | 0 | 0 |

# 3 Residue-property plots (i)

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

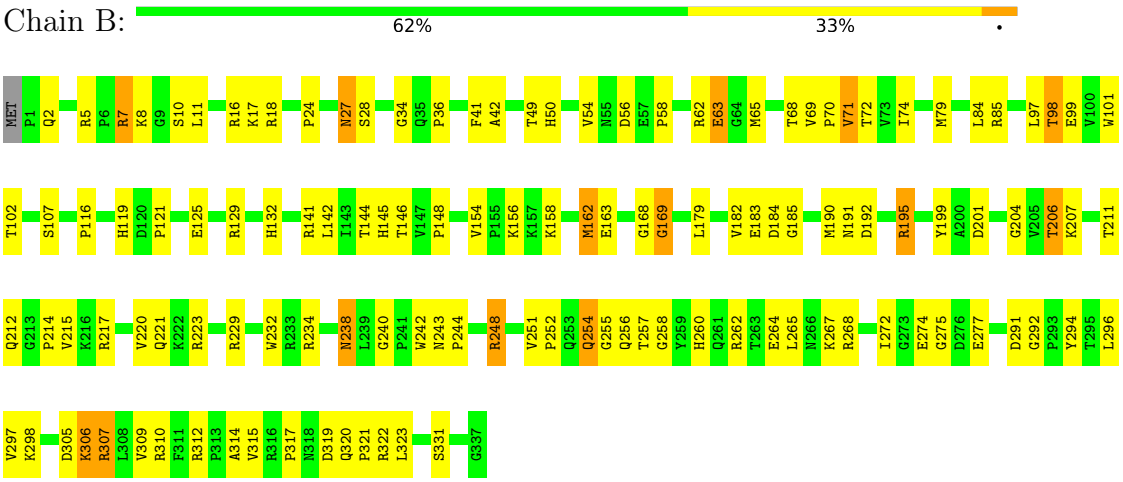
• Molecule 1: 50S ribosomal protein L2P

Chain A:



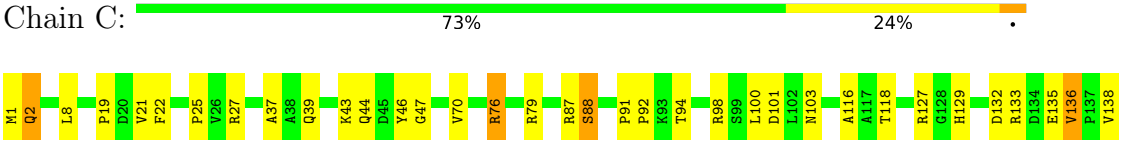

• Molecule 2: 50S ribosomal protein L3P

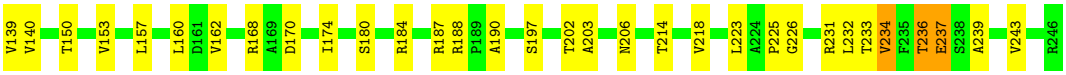
Chain B:




• Molecule 3: 50S ribosomal protein L4P

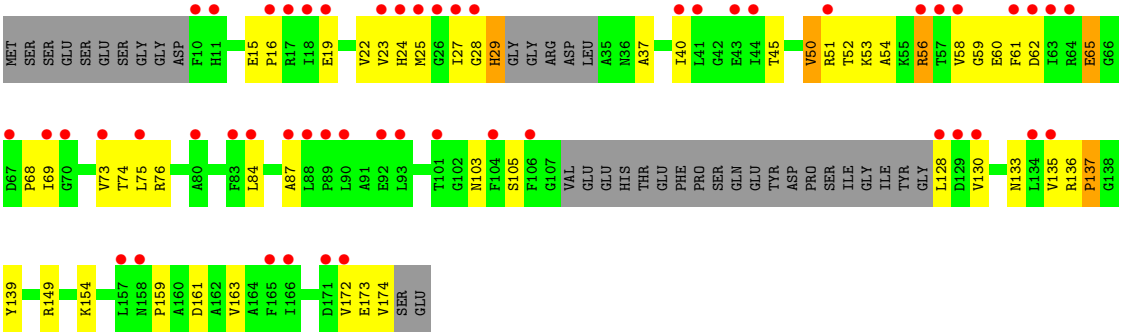
Chain C:





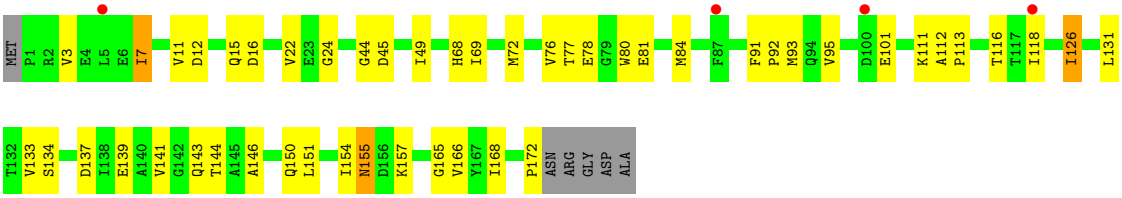

• Molecule 4: 50S ribosomal protein L5P

Chain D:

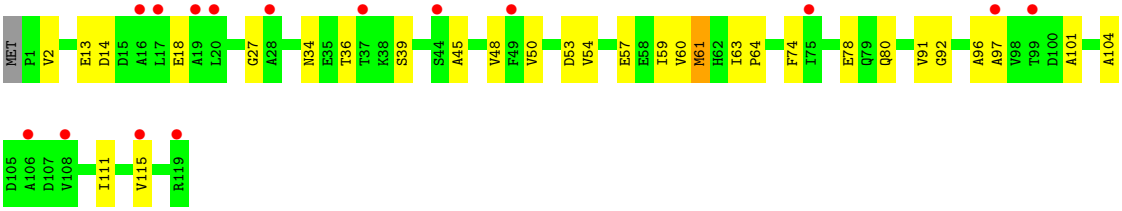

• Molecule 5: 50S ribosomal protein L6P

Chain E:

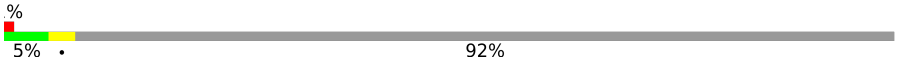

• Molecule 6: 50S ribosomal protein L7Ae

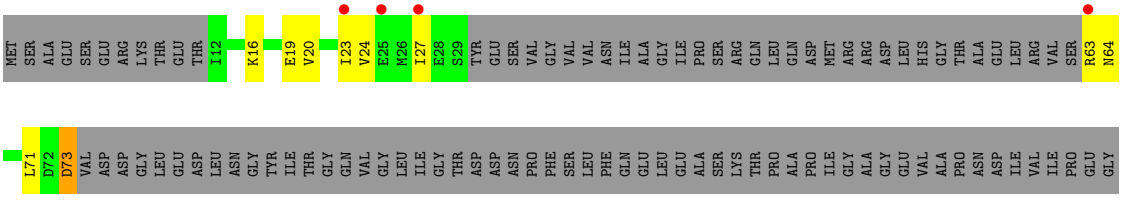
Chain F:

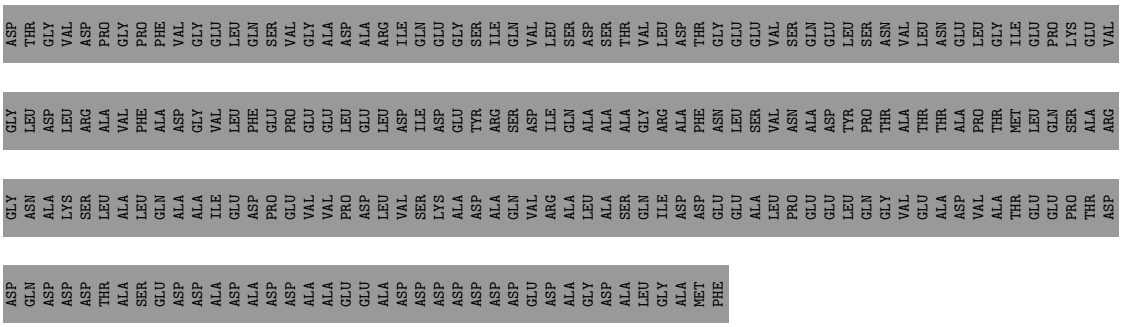




• Molecule 7: 50S ribosomal protein L10E

Chain G:

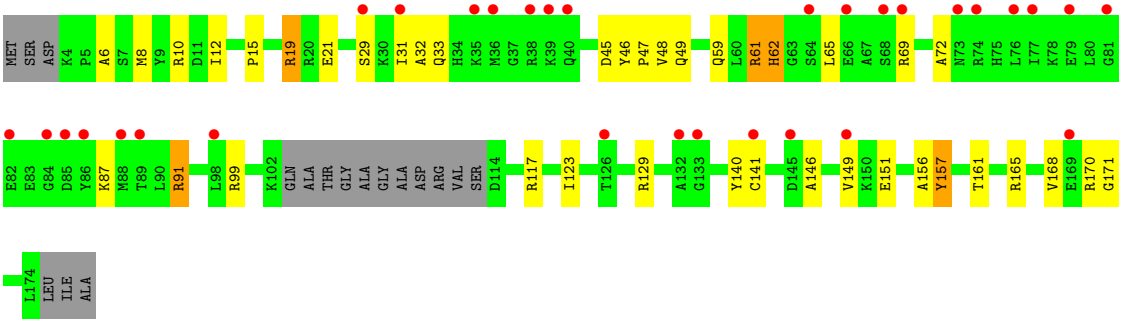




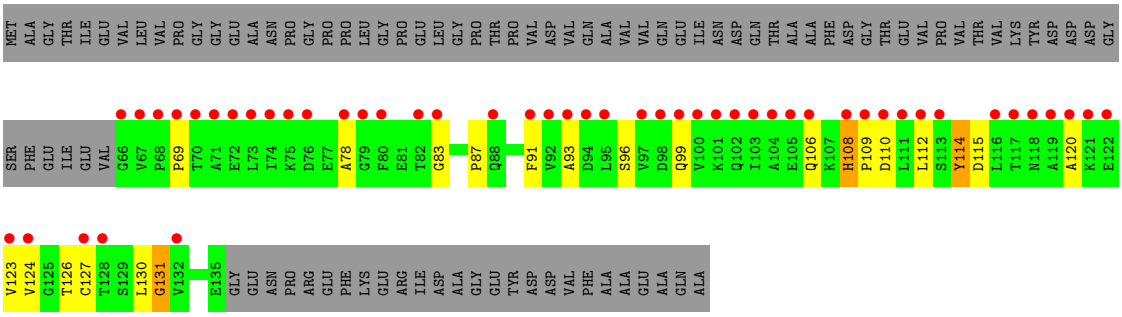
• Molecule 8: 50S ribosomal protein L10e

Chain H:

• Molecule 9: 50S ribosomal protein L11P

Chain I:

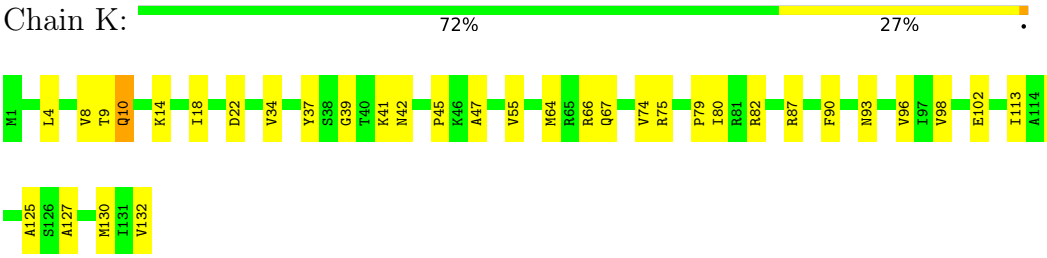



• Molecule 10: 50S ribosomal protein L13P

Chain J:

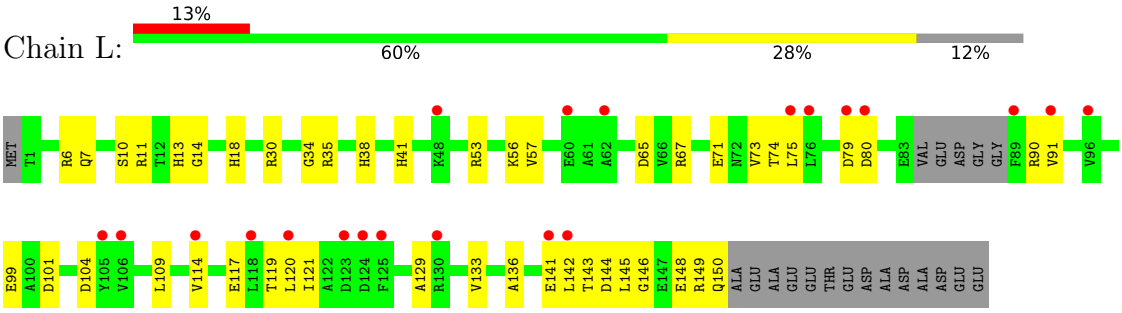

• Molecule 11: 50S ribosomal protein L14P

Chain K:



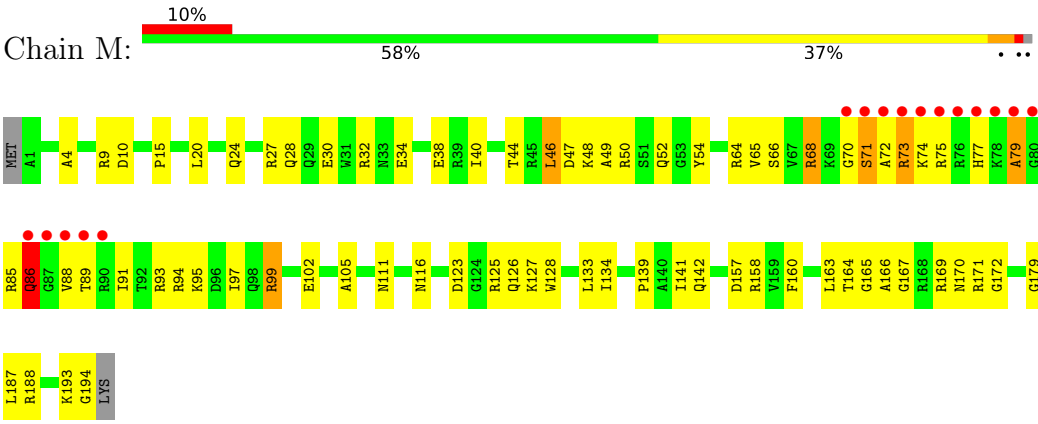

• Molecule 12: 50S ribosomal protein L15P

Chain L:



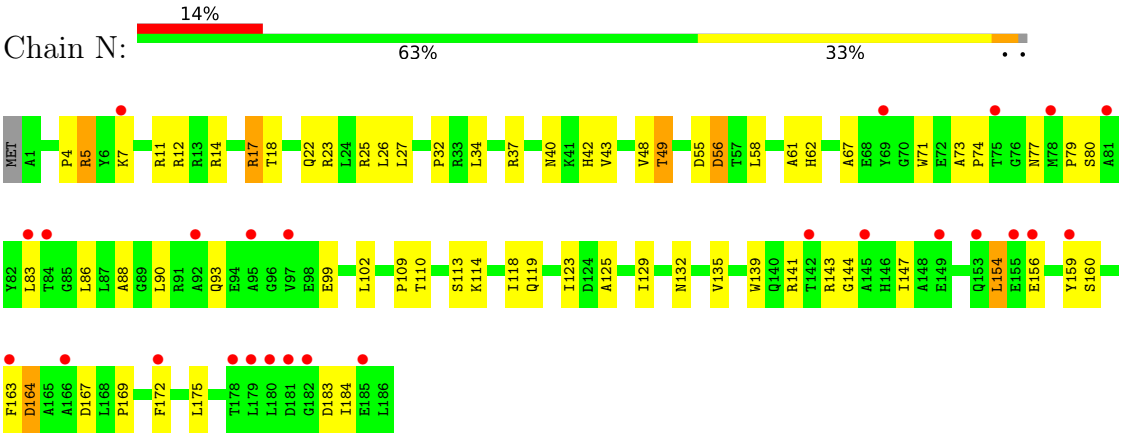

• Molecule 13: 50S ribosomal protein L15e

Chain M:



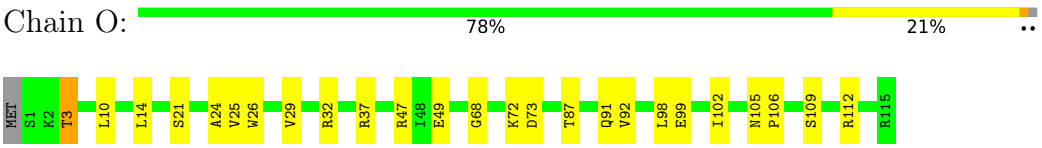

• Molecule 14: 50S ribosomal protein L18P

Chain N:



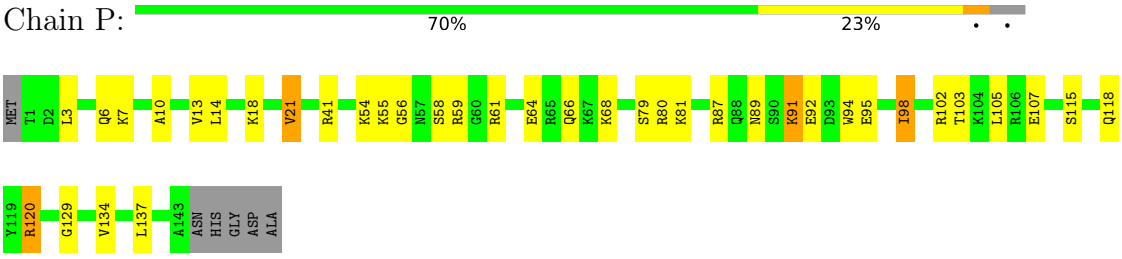

• Molecule 15: 50S ribosomal protein L18e

Chain O:



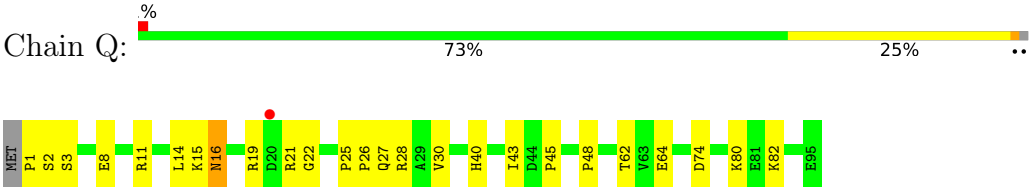

• Molecule 16: 50S ribosomal protein L19e

Chain P:



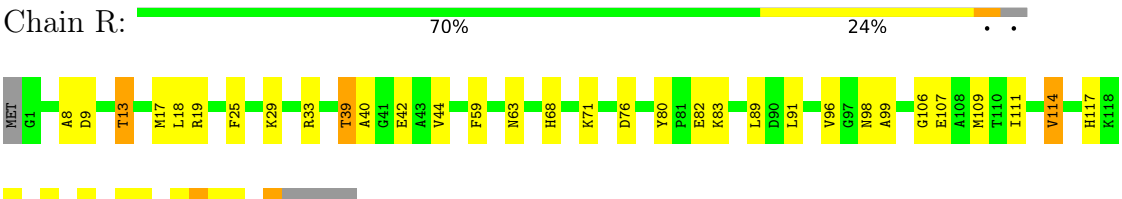

• Molecule 17: 50S ribosomal protein L21e

Chain Q:



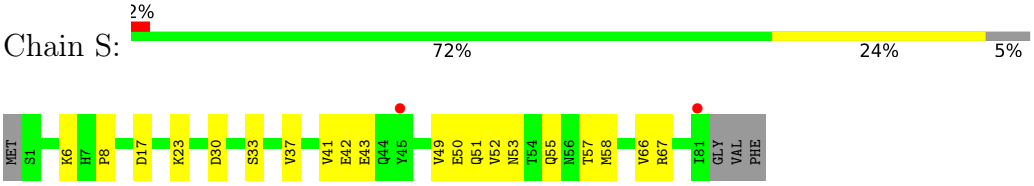

• Molecule 18: 50S ribosomal protein L22P

Chain R:



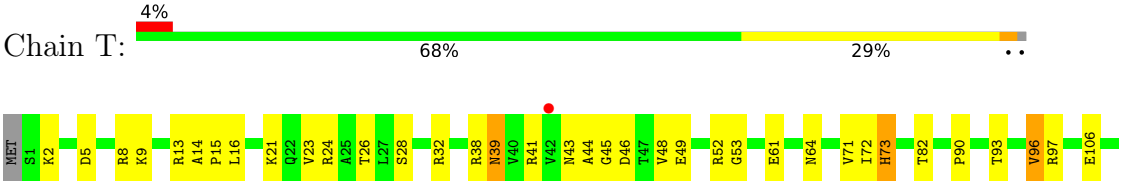

• Molecule 19: 50S ribosomal protein L23P

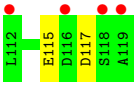
Chain S:



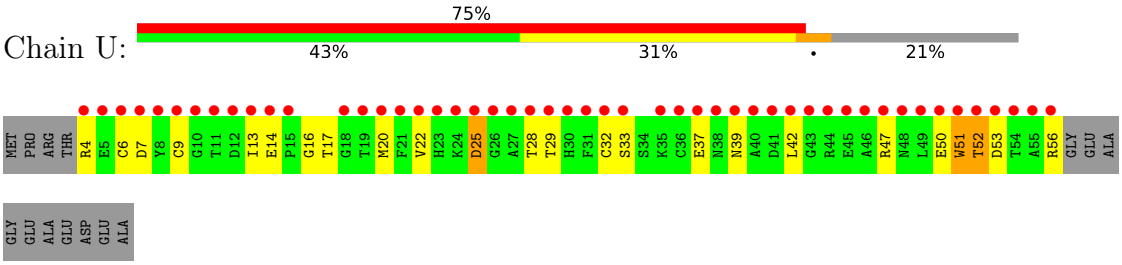

• Molecule 20: 50S ribosomal protein L24P

Chain T:





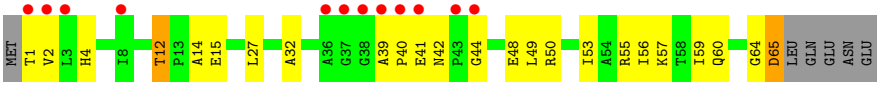

• Molecule 21: 50S ribosomal protein L24e



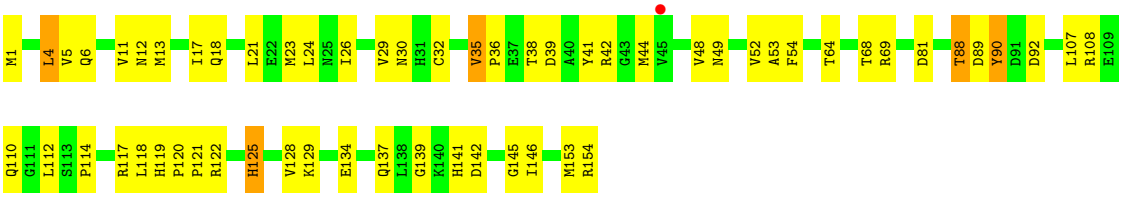




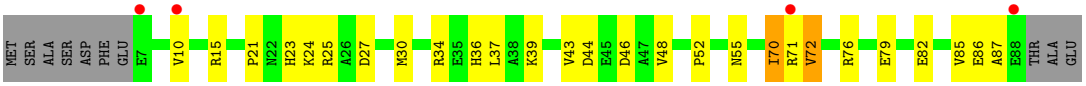
• Molecule 22: 50S ribosomal protein L29P

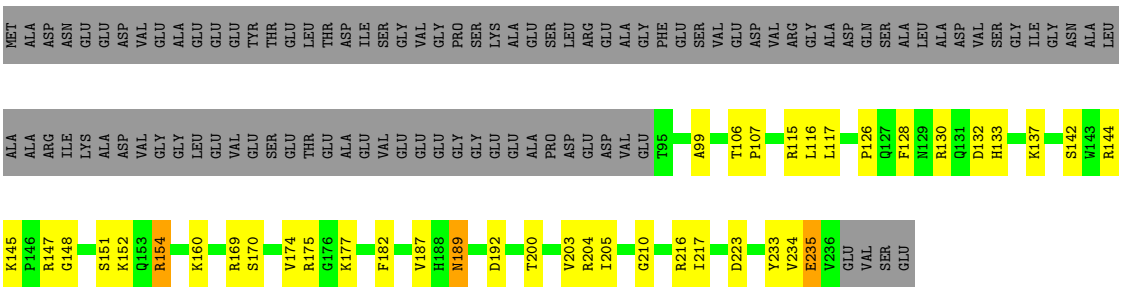

• Molecule 23: 50S ribosomal protein L30P


• Molecule 24: 50S ribosomal protein L31e

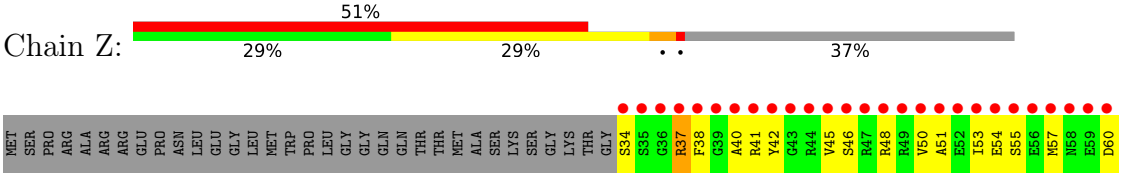



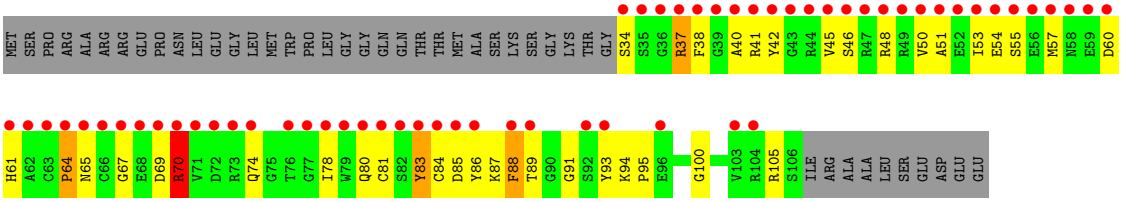

• Molecule 25: 50S ribosomal protein L32e

• Molecule 26: 50S ribosomal protein L37Ae

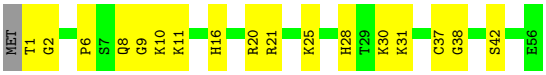
Chain Z:



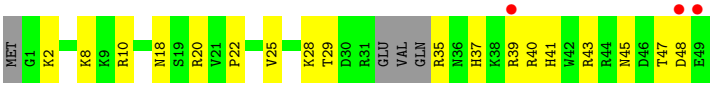

• Molecule 27: 50S ribosomal protein L37e

Chain 1:

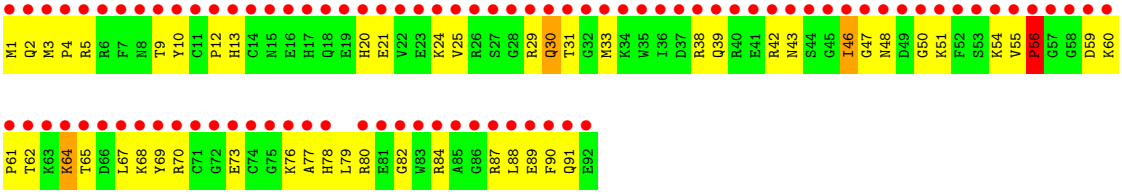

• Molecule 28: 50S ribosomal protein L39e

Chain 2:

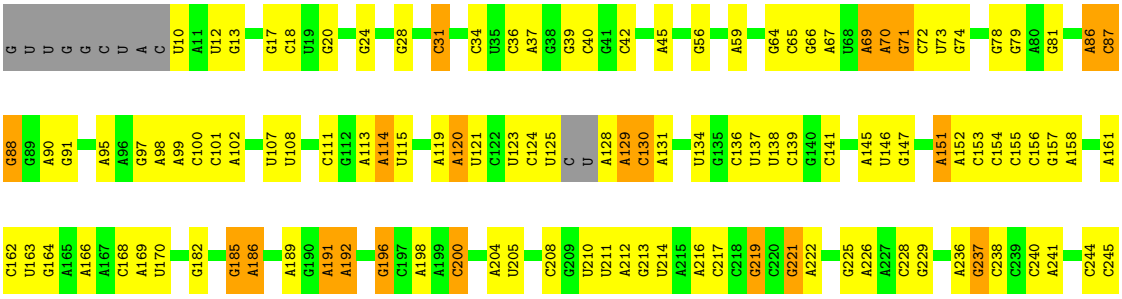

• Molecule 29: 50S ribosomal protein L44E

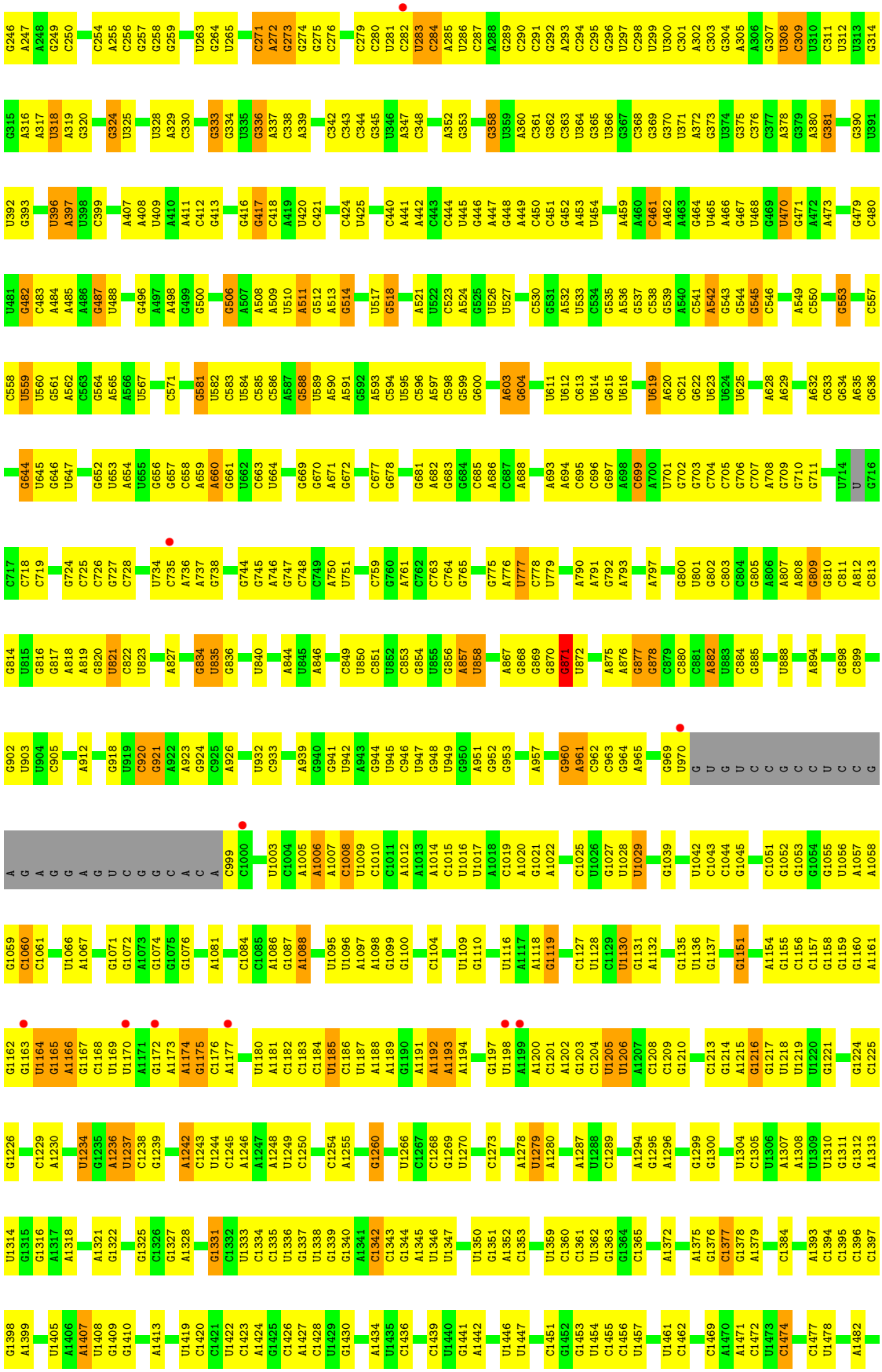
Chain 3:

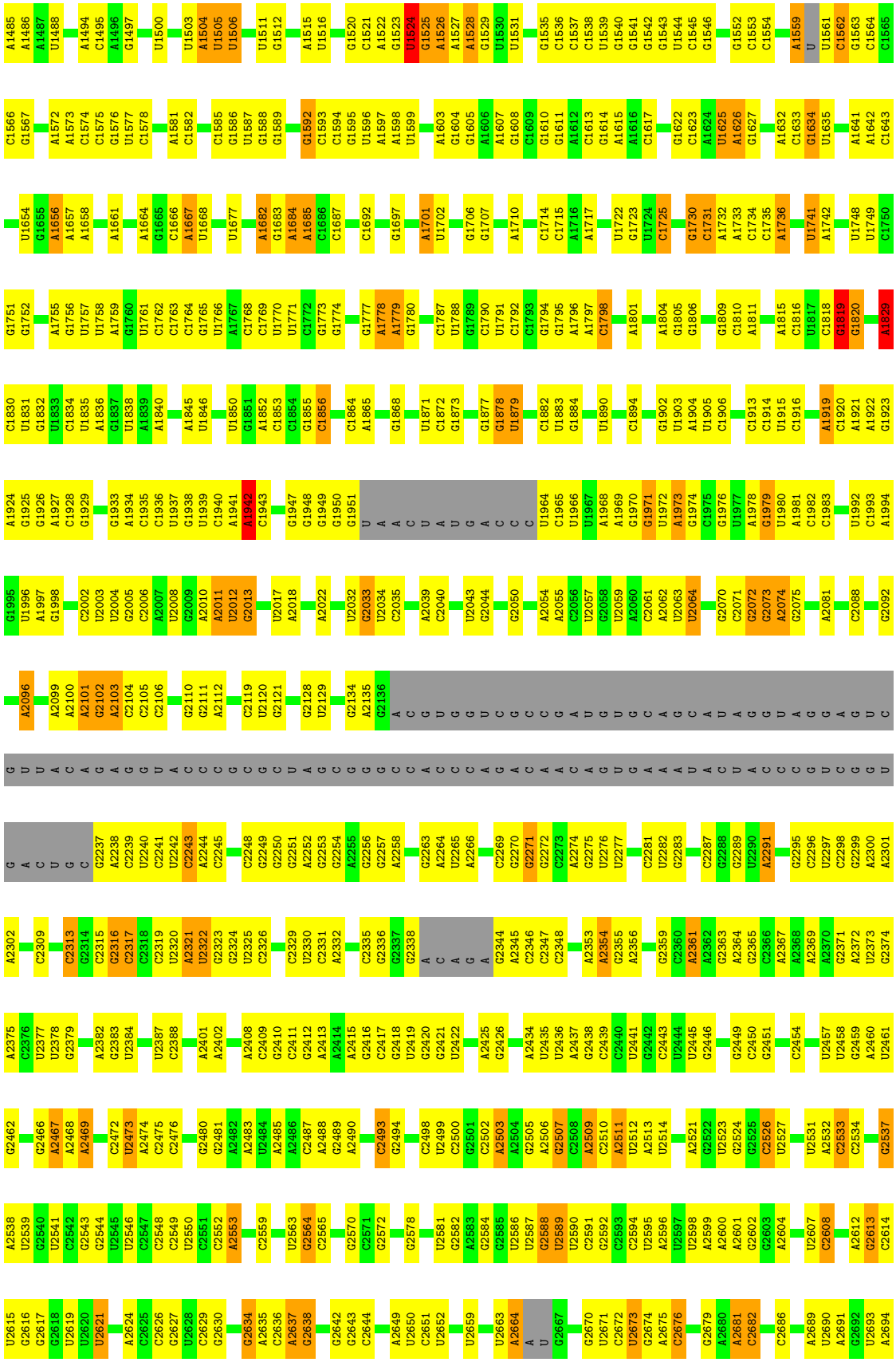



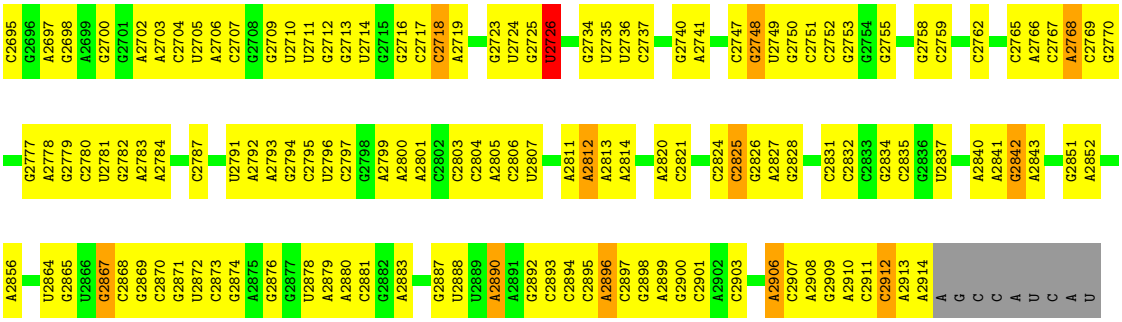

• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:








• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:


# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 212.24Å 299.19Å 575.16Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 2.95<br>85.59 – 2.40 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | (Not available) (50.00-2.95)<br>91.7 (85.59-2.40) | Depositor<br>EDS |
| $R_{merge}$ | 0.09 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.00 (at 2.40Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.179 , 0.238<br>0.177 , 0.233 | Depositor<br>DCC |
| $R_{free}$ test set | 6547 reflections (0.98%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 62.1 | Xtriage |
| Anisotropy | 0.128 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 79.8 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 99121 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 68.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, PSU, OMG, SR, K, CL, MG, 1MA, CD, OMU, NA

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 | A | 0.34 | 0/1786 | 0.64 | 0/2408 |
| 2 | B | 0.34 | 0/2690 | 0.64 | 0/3652 |
| 3 | C | 0.39 | 0/1885 | 0.65 | 0/2552 |
| 4 | D | 0.33 | 0/1111 | 0.57 | 0/1498 |
| 5 | E | 0.34 | 0/1382 | 0.56 | 0/1880 |
| 6 | F | 0.35 | 0/901 | 0.57 | 0/1224 |
| 7 | G | 0.32 | 0/241 | 0.47 | 0/324 |
| 8 | H | 0.33 | 0/1302 | 0.62 | 0/1743 |
| 9 | I | 0.32 | 0/526 | 0.54 | 0/716 |
| 10 | J | 0.39 | 0/1136 | 0.61 | 0/1530 |
| 11 | K | 0.37 | 0/1004 | 0.66 | 0/1351 |
| 12 | L | 0.34 | 0/1130 | 0.61 | 0/1509 |
| 13 | M | 0.40 | 0/1582 | 0.63 | 0/2116 |
| 14 | N | 0.32 | 0/1474 | 0.61 | 0/1999 |
| 15 | O | 0.37 | 0/874 | 0.62 | 0/1181 |
| 16 | P | 0.34 | 0/1147 | 0.53 | 0/1528 |
| 17 | Q | 0.33 | 0/749 | 0.64 | 0/1005 |
| 18 | R | 1.27 | 7/1172 (0.6%) | 1.10 | 6/1578 (0.4%) |
| 19 | S | 0.36 | 0/648 | 0.59 | 0/875 |
| 20 | T | 0.34 | 0/958 | 0.66 | 0/1289 |
| 21 | U | 0.45 | 0/417 | 0.60 | 0/562 |
| 22 | V | 0.34 | 0/502 | 0.53 | 0/675 |
| 23 | W | 0.38 | 0/1219 | 0.65 | 0/1655 |
| 24 | X | 0.36 | 0/664 | 0.61 | 0/895 |
| 25 | Y | 0.38 | 0/1146 | 0.62 | 0/1536 |
| 26 | Z | 0.43 | 0/584 | 0.63 | 0/781 |
| 27 | 1 | 0.47 | 0/438 | 0.64 | 0/578 |
| 28 | 2 | 0.36 | 0/401 | 0.61 | 0/529 |
| 29 | 3 | 0.46 | 0/771 | 0.60 | 0/1024 |
| 30 | 0 | 0.42 | 0/65956 | 0.68 | 7/102865 (0.0%) |
| 31 | 9 | 0.32 | 0/2904 | 0.67 | 1/4526 (0.0%) |
| All | All | 0.42 | 7/98700 (0.0%) | 0.67 | 14/147584 (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 |
|---|---|---|---|
| 18 | R | 1 | 0 |
| 23 | W | 0 | 1 |
| 30 | 0 | 0 | 34 |
| All | All | 1 | 35 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | R | 150 | PRO | CB-CG | 27.15 | 2.85 | 1.50 |
| 18 | R | 150 | PRO | CA-C | -18.51 | 1.15 | 1.52 |
| 18 | R | 150 | PRO | CG-CD | 13.84 | 1.96 | 1.50 |
| 18 | R | 150 | PRO | C-O | 11.87 | 1.47 | 1.23 |
| 18 | R | 150 | PRO | N-CA | 11.57 | 1.67 | 1.47 |
| 18 | R | 150 | PRO | N-CD | 10.73 | 1.62 | 1.47 |
| 18 | R | 150 | PRO | CA-CB | 7.84 | 1.69 | 1.53 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | R | 150 | PRO | CB-CA-C | -22.43 | 55.92 | 112.00 |
| 18 | R | 150 | PRO | N-CA-C | -19.45 | 61.53 | 112.10 |
| 18 | R | 150 | PRO | CA-N-CD | 12.27 | 128.88 | 111.70 |
| 18 | R | 150 | PRO | N-CA-CB | 10.98 | 116.47 | 103.30 |
| 18 | R | 150 | PRO | CA-C-O | -8.27 | 100.34 | 120.20 |
| 18 | R | 150 | PRO | CA-CB-CG | -6.08 | 92.45 | 104.00 |
| 30 | 0 | 871 | G | C5'-C4'-O4' | -5.70 | 102.26 | 109.10 |
| 30 | 0 | 1504 | A | C1'-O4'-C4' | -5.64 | 105.39 | 109.90 |
| 30 | 0 | 1942 | A | C5'-C4'-C3' | 5.59 | 124.94 | 116.00 |
| 30 | 0 | 1971 | G | N9-C1'-C2' | 5.38 | 121.00 | 114.00 |
| 30 | 0 | 1819 | G | C5'-C4'-C3' | 5.29 | 124.46 | 116.00 |
| 30 | 0 | 2726 | U | N1-C1'-C2' | 5.20 | 120.75 | 114.00 |
| 30 | 0 | 2313 | C | O4'-C4'-C3' | -5.12 | 98.88 | 104.00 |
| 31 | 9 | 39 | U | N1-C1'-C2' | 5.09 | 120.62 | 114.00 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 18 | R | 150 | PRO | CA |

All (35) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 30 | 0 | 1039 | G | Sidechain |
| 30 | 0 | 1236 | A | Sidechain |
| 30 | 0 | 1260 | G | Sidechain |
| 30 | 0 | 1430 | G | Sidechain |
| 30 | 0 | 1524 | U | Sidechain |
| 30 | 0 | 1599 | U | Sidechain |
| 30 | 0 | 1736 | A | Sidechain |
| 30 | 0 | 1741 | U | Sidechain |
| 30 | 0 | 1777 | G | Sidechain |
| 30 | 0 | 1819 | G | Sidechain |
| 30 | 0 | 1829 | A | Sidechain |
| 30 | 0 | 1878 | G | Sidechain |
| 30 | 0 | 196 | G | Sidechain |
| 30 | 0 | 1993 | C | Sidechain |
| 30 | 0 | 221 | G | Sidechain |
| 30 | 0 | 2316 | G | Sidechain |
| 30 | 0 | 2473 | U | Sidechain |
| 30 | 0 | 2493 | C | Sidechain |
| 30 | 0 | 2503 | A | Sidechain |
| 30 | 0 | 2552 | C | Sidechain |
| 30 | 0 | 2599 | A | Sidechain |
| 30 | 0 | 2630 | G | Sidechain |
| 30 | 0 | 2673 | U | Sidechain |
| 30 | 0 | 2726 | U | Sidechain |
| 30 | 0 | 2842 | G | Sidechain |
| 30 | 0 | 324 | G | Sidechain |
| 30 | 0 | 333 | G | Sidechain |
| 30 | 0 | 470 | U | Sidechain |
| 30 | 0 | 471 | G | Sidechain |
| 30 | 0 | 482 | G | Sidechain |
| 30 | 0 | 506 | G | Sidechain |
| 30 | 0 | 518 | G | Sidechain |
| 30 | 0 | 619 | U | Sidechain |
| 30 | 0 | 888 | U | Sidechain |
| 23 | W | 90 | TYR | Sidechain |

## 5.2 Too-close contacts (i)

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 | A | 1753 | 0 | 1766 | 85 | 0 |
| 2 | B | 2625 | 0 | 2533 | 108 | 0 |
| 3 | C | 1860 | 0 | 1813 | 63 | 0 |
| 4 | D | 1094 | 0 | 1085 | 37 | 0 |
| 5 | E | 1357 | 0 | 1266 | 39 | 0 |
| 6 | F | 890 | 0 | 843 | 19 | 0 |
| 7 | G | 240 | 0 | 231 | 8 | 0 |
| 8 | H | 1282 | 0 | 1292 | 33 | 0 |
| 9 | I | 519 | 0 | 500 | 14 | 0 |
| 10 | J | 1120 | 0 | 1098 | 44 | 0 |
| 11 | K | 994 | 0 | 1027 | 34 | 0 |
| 12 | L | 1118 | 0 | 1076 | 38 | 0 |
| 13 | M | 1558 | 0 | 1573 | 95 | 0 |
| 14 | N | 1445 | 0 | 1401 | 73 | 0 |
| 15 | O | 865 | 0 | 873 | 22 | 0 |
| 16 | P | 1136 | 0 | 1123 | 34 | 0 |
| 17 | Q | 735 | 0 | 729 | 28 | 0 |
| 18 | R | 1149 | 0 | 1122 | 41 | 0 |
| 19 | S | 641 | 0 | 605 | 15 | 0 |
| 20 | T | 950 | 0 | 924 | 36 | 0 |
| 21 | U | 410 | 0 | 368 | 26 | 0 |
| 22 | V | 499 | 0 | 511 | 21 | 0 |
| 23 | W | 1196 | 0 | 1137 | 58 | 0 |
| 24 | X | 654 | 0 | 653 | 20 | 0 |
| 25 | Y | 1130 | 0 | 1133 | 39 | 0 |
| 26 | Z | 573 | 0 | 535 | 50 | 0 |
| 27 | 1 | 431 | 0 | 426 | 21 | 0 |
| 28 | 2 | 396 | 0 | 413 | 21 | 0 |
| 29 | 3 | 755 | 0 | 732 | 57 | 0 |
| 30 | 0 | 59019 | 0 | 29809 | 1661 | 0 |
| 31 | 9 | 2599 | 0 | 1325 | 127 | 0 |
| 32 | 0 | 86 | 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 |
| 32 | K | 1 | 0 | 0 | 0 | 0 |
| 32 | T | 1 | 0 | 0 | 0 | 0 |
| 32 | Y | 1 | 0 | 0 | 0 | 0 |
| 33 | 0 | 10 | 0 | 0 | 3 | 0 |
| 33 | 3 | 1 | 0 | 0 | 1 | 0 |
| 33 | A | 1 | 0 | 0 | 0 | 0 |
| 33 | B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 33 | J | 3 | 0 | 0 | 2 | 0 |
| 33 | L | 1 | 0 | 0 | 0 | 0 |
| 33 | M | 1 | 0 | 0 | 0 | 0 |
| 33 | N | 1 | 0 | 0 | 0 | 0 |
| 33 | O | 1 | 0 | 0 | 0 | 0 |
| 33 | R | 1 | 0 | 0 | 0 | 0 |
| 33 | Y | 1 | 0 | 0 | 2 | 0 |
| 34 | 0 | 92 | 0 | 0 | 0 | 0 |
| 34 | 1 | 2 | 0 | 0 | 0 | 0 |
| 34 | 3 | 2 | 0 | 0 | 0 | 0 |
| 34 | 9 | 3 | 0 | 0 | 0 | 0 |
| 34 | A | 2 | 0 | 0 | 0 | 0 |
| 34 | B | 2 | 0 | 0 | 0 | 0 |
| 34 | F | 1 | 0 | 0 | 0 | 0 |
| 34 | H | 1 | 0 | 0 | 0 | 0 |
| 34 | L | 1 | 0 | 0 | 0 | 0 |
| 34 | R | 1 | 0 | 0 | 0 | 0 |
| 34 | S | 1 | 0 | 0 | 0 | 0 |
| 35 | 0 | 65 | 0 | 0 | 0 | 0 |
| 35 | 9 | 2 | 0 | 0 | 0 | 0 |
| 35 | B | 1 | 0 | 0 | 0 | 0 |
| 35 | C | 1 | 0 | 0 | 0 | 0 |
| 35 | H | 1 | 0 | 0 | 0 | 0 |
| 35 | J | 1 | 0 | 0 | 0 | 0 |
| 35 | M | 1 | 0 | 0 | 0 | 0 |
| 35 | Q | 1 | 0 | 0 | 0 | 0 |
| 35 | R | 1 | 0 | 0 | 0 | 0 |
| 35 | S | 1 | 0 | 0 | 0 | 0 |
| 36 | 0 | 1 | 0 | 0 | 0 | 0 |
| 36 | M | 1 | 0 | 0 | 0 | 0 |
| 37 | 1 | 1 | 0 | 0 | 0 | 0 |
| 37 | 3 | 1 | 0 | 0 | 0 | 0 |
| 37 | O | 1 | 0 | 0 | 0 | 0 |
| 37 | U | 1 | 0 | 0 | 0 | 0 |
| 37 | Z | 1 | 0 | 0 | 0 | 0 |
| 38 | 0 | 5904 | 0 | 0 | 251 | 0 |
| 38 | 1 | 59 | 0 | 0 | 3 | 0 |
| 38 | 2 | 43 | 0 | 0 | 2 | 0 |
| 38 | 3 | 70 | 0 | 0 | 3 | 0 |
| 38 | 9 | 149 | 0 | 0 | 10 | 0 |
| 38 | A | 119 | 0 | 0 | 7 | 0 |
| 38 | B | 152 | 0 | 0 | 16 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 38 | C | 185 | 0 | 0 | 18 | 0 |
| 38 | D | 42 | 0 | 0 | 4 | 0 |
| 38 | E | 43 | 0 | 0 | 1 | 0 |
| 38 | F | 26 | 0 | 0 | 1 | 0 |
| 38 | G | 19 | 0 | 0 | 1 | 0 |
| 38 | H | 65 | 0 | 0 | 4 | 0 |
| 38 | I | 8 | 0 | 0 | 1 | 0 |
| 38 | J | 53 | 0 | 0 | 1 | 0 |
| 38 | K | 58 | 0 | 0 | 3 | 0 |
| 38 | L | 85 | 0 | 0 | 9 | 0 |
| 38 | M | 127 | 0 | 0 | 13 | 0 |
| 38 | N | 59 | 0 | 0 | 2 | 0 |
| 38 | O | 39 | 0 | 0 | 2 | 0 |
| 38 | P | 67 | 0 | 0 | 3 | 0 |
| 38 | Q | 48 | 0 | 0 | 1 | 0 |
| 38 | R | 77 | 0 | 0 | 2 | 0 |
| 38 | S | 30 | 0 | 0 | 2 | 0 |
| 38 | T | 36 | 0 | 0 | 3 | 0 |
| 38 | U | 28 | 0 | 0 | 4 | 0 |
| 38 | V | 13 | 0 | 0 | 2 | 0 |
| 38 | W | 67 | 0 | 0 | 3 | 0 |
| 38 | X | 21 | 0 | 0 | 2 | 0 |
| 38 | Y | 100 | 0 | 0 | 5 | 0 |
| 38 | Z | 31 | 0 | 0 | 7 | 0 |
| All | All | 99121 | 0 | 59922 | 2675 | 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 18.

All (2675) 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) |
|---|---|---|---|
| 18:R:150:PRO:CG | 18:R:150:PRO:CD | 1.96 | 1.41 |
| 30:0:871:G:C8 | 30:0:871:G:H5' | 1.77 | 1.19 |
| 10:J:82:THR:HG23 | 30:0:1242:A:H5' | 1.23 | 1.16 |
| 30:0:1165:G:H1' | 30:0:1174:A:H1' | 1.17 | 1.14 |
| 31:9:56:A:H2' | 31:9:57:A:H5" | 1.19 | 1.13 |
| 30:0:1559:A:H1' | 38:0:5849:HOH:O | 1.45 | 1.13 |
| 30:0:1160:G:C5' | 30:0:1161:A:H5' | 1.78 | 1.13 |
| 31:9:29:C:H2' | 31:9:30:C:H5' | 1.32 | 1.10 |
| 15:O:3:THR:HG22 | 30:0:656:G:H5' | 1.19 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:M:171:ARG:HD3 | 30:0:156:C:H5” | 1.28 | 1.09 |
| 30:0:1160:G:H5’ | 30:0:1161:A:C5’ | 1.80 | 1.09 |
| 10:J:52:GLN:HE22 | 30:0:1119:G:H2’ | 1.17 | 1.08 |
| 30:0:871:G:H5’ | 30:0:871:G:H8 | 0.99 | 1.08 |
| 10:J:52:GLN:NE2 | 30:0:1119:G:H2’ | 1.69 | 1.07 |
| 18:R:150:PRO:CG | 18:R:150:PRO:C | 2.22 | 1.07 |
| 31:9:76:G:H3’ | 31:9:77:A:H5” | 1.33 | 1.05 |
| 30:0:545:G:H5’ | 30:0:545:G:H8 | 1.22 | 1.05 |
| 14:N:37:ARG:NH1 | 31:9:6:C:H5” | 1.71 | 1.03 |
| 30:0:1603:A:H5’ | 30:0:1605:G:O4’ | 1.60 | 1.02 |
| 30:0:1641:A:H2’ | 30:0:1642:A:H5’ | 1.44 | 0.99 |
| 21:U:56:ARG:HD2 | 30:0:2890:A:C8 | 1.98 | 0.98 |
| 30:0:1666:C:O2’ | 30:0:1667:A:H5” | 1.63 | 0.98 |
| 26:Z:60:ASP:HB3 | 26:Z:69:ASP:HB3 | 1.43 | 0.98 |
| 11:K:10:GLN:HE21 | 11:K:10:GLN:H | 0.99 | 0.97 |
| 30:0:1979:G:H2’ | 38:0:9283:HOH:O | 1.65 | 0.97 |
| 30:0:381:G:H5” | 38:0:4317:HOH:O | 1.64 | 0.96 |
| 30:0:871:G:H8 | 30:0:871:G:C5’ | 1.78 | 0.96 |
| 30:0:1165:G:H21 | 30:0:1173:A:H5” | 1.30 | 0.96 |
| 13:M:70:GLY:HA3 | 13:M:73:ARG:NH2 | 1.80 | 0.96 |
| 17:Q:15:LYS:HD3 | 30:0:2364:A:H5” | 1.47 | 0.96 |
| 16:P:59:ARG:HH22 | 16:P:66:GLN:HE22 | 1.05 | 0.95 |
| 31:9:56:A:C2’ | 31:9:57:A:H5” | 1.95 | 0.95 |
| 30:0:1474:C:H6 | 30:0:1474:C:H5’ | 1.30 | 0.95 |
| 18:R:8:ALA:HB1 | 18:R:13:THR:HG21 | 1.50 | 0.94 |
| 31:9:14:G:H5’ | 31:9:14:G:H8 | 1.32 | 0.94 |
| 30:0:236:A:H4’ | 30:0:237:G:H5’ | 1.49 | 0.94 |
| 2:B:264:GLU:HG2 | 2:B:267:LYS:HE3 | 1.50 | 0.94 |
| 30:0:1165:G:H21 | 30:0:1173:A:C5’ | 1.81 | 0.93 |
| 16:P:115:SER:H | 16:P:118:GLN:HE21 | 1.11 | 0.93 |
| 30:0:2505:G:H2’ | 30:0:2506:A:H5’ | 1.50 | 0.93 |
| 30:0:2717:C:C2’ | 30:0:2718:C:H5” | 1.99 | 0.93 |
| 30:0:2502:C:H2’ | 30:0:2503:A:H5’ | 1.52 | 0.92 |
| 23:W:108:ARG:HH21 | 23:W:114:PRO:HG2 | 1.35 | 0.92 |
| 1:A:211:LYS:HB3 | 1:A:212:PRO:HD2 | 1.52 | 0.91 |
| 3:C:27:ARG:HG2 | 3:C:27:ARG:HH11 | 1.36 | 0.91 |
| 30:0:2321:A:H2 | 30:0:2378:U:H3 | 1.14 | 0.91 |
| 15:O:3:THR:CG2 | 30:0:656:G:H5’ | 2.00 | 0.91 |
| 30:0:282:C:O2’ | 30:0:283:U:H5’ | 1.71 | 0.90 |
| 30:0:2710:U:H1’ | 38:0:7613:HOH:O | 1.71 | 0.90 |
| 30:0:1118:A:H62 | 30:0:1244:U:H3 | 1.14 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:236:THR:HG22 | 3:C:239:ALA:H | 1.35 | 0.90 |
| 29:3:60:LYS:HG3 | 29:3:61:PRO:HD2 | 1.53 | 0.90 |
| 30:0:2506:A:HO2' | 30:0:2507:G:H8 | 0.90 | 0.90 |
| 30:0:2812:A:H2 | 30:0:2814:A:H62 | 1.19 | 0.90 |
| 30:0:1116:U:O2' | 30:0:1118:A:H2 | 1.54 | 0.90 |
| 30:0:545:G:H5' | 30:0:545:G:C8 | 2.06 | 0.89 |
| 30:0:2321:A:H8 | 30:0:2322:U:HO2' | 1.13 | 0.89 |
| 30:0:2502:C:C2' | 30:0:2503:A:H5' | 2.03 | 0.89 |
| 33:Y:8820:CL:CL | 38:0:4953:HOH:O | 2.27 | 0.88 |
| 30:0:870:G:H2' | 30:0:871:G:H5" | 1.53 | 0.88 |
| 23:W:137:GLN:HE21 | 23:W:141:HIS:HE1 | 1.20 | 0.88 |
| 30:0:1119:G:H22 | 30:0:1246:A:H2 | 1.16 | 0.88 |
| 30:0:2700:G:H3' | 38:0:3569:HOH:O | 1.73 | 0.88 |
| 13:M:79:ALA:HB3 | 13:M:81:ARG:HH12 | 1.38 | 0.88 |
| 31:9:92:G:H2' | 31:9:93:A:C8 | 2.07 | 0.88 |
| 30:0:1118:A:C8 | 30:0:1118:A:H3' | 2.08 | 0.88 |
| 30:0:1206:U:H5' | 30:0:1206:U:H6 | 1.39 | 0.88 |
| 15:O:47:ARG:HH11 | 15:O:47:ARG:HG3 | 1.35 | 0.88 |
| 30:0:506:G:H22 | 30:0:509:A:C5' | 1.85 | 0.87 |
| 30:0:1474:C:H5' | 30:0:1474:C:C6 | 2.10 | 0.87 |
| 30:0:542:A:H5' | 30:0:542:A:H8 | 1.39 | 0.87 |
| 30:0:1835:U:H5 | 30:0:1840:A:N7 | 1.73 | 0.87 |
| 30:0:1118:A:H3' | 30:0:1118:A:H8 | 1.39 | 0.87 |
| 30:0:2321:A:H4' | 30:0:2322:U:OP1 | 1.73 | 0.87 |
| 30:0:363:C:H1' | 38:0:5273:HOH:O | 1.75 | 0.86 |
| 30:0:1278:A:H4' | 30:0:1279:U:C4 | 2.10 | 0.86 |
| 30:0:2505:G:C2' | 30:0:2506:A:H5' | 2.04 | 0.86 |
| 1:A:70:ALA:HB1 | 26:Z:89:THR:HG21 | 1.57 | 0.86 |
| 30:0:1701:A:H4' | 30:0:1702:U:H5" | 1.55 | 0.86 |
| 13:M:70:GLY:HA2 | 30:0:2263:G:H4' | 1.59 | 0.85 |
| 23:W:6:GLN:HB2 | 23:W:26:ILE:HD11 | 1.58 | 0.85 |
| 30:0:506:G:H22 | 30:0:509:A:H5" | 1.42 | 0.85 |
| 26:Z:70:ARG:NH1 | 26:Z:83:TYR:HB2 | 1.91 | 0.85 |
| 30:0:1205:U:H2' | 30:0:1206:U:H5' | 1.58 | 0.85 |
| 30:0:1641:A:C2' | 30:0:1642:A:H5' | 2.06 | 0.85 |
| 30:0:2717:C:H2' | 30:0:2718:C:H5" | 1.59 | 0.85 |
| 30:0:1666:C:H2' | 30:0:1667:A:H5' | 1.58 | 0.84 |
| 30:0:2717:C:O2' | 30:0:2718:C:H5" | 1.76 | 0.84 |
| 29:3:68:LYS:HE2 | 30:0:2436:U:H5' | 1.60 | 0.84 |
| 30:0:2637:A:H4' | 38:0:4923:HOH:O | 1.78 | 0.83 |
| 2:B:217:ARG:HG3 | 2:B:257:THR:HG22 | 1.58 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2043:U:H3' | 38:0:6696:HOH:O | 1.76 | 0.83 |
| 23:W:125:HIS:NE2 | 30:0:1097:A:H5" | 1.93 | 0.83 |
| 30:0:2010:A:H2' | 38:0:5942:HOH:O | 1.77 | 0.83 |
| 1:A:167:LYS:HE2 | 26:Z:50:VAL:HG13 | 1.61 | 0.83 |
| 13:M:68:ARG:NH2 | 13:M:73:ARG:HD3 | 1.94 | 0.83 |
| 29:3:64:LYS:HA | 29:3:84:ARG:HA | 1.57 | 0.83 |
| 30:0:380:A:H2' | 38:0:7216:HOH:O | 1.77 | 0.83 |
| 11:K:10:GLN:H | 11:K:10:GLN:NE2 | 1.77 | 0.83 |
| 11:K:39:GLY:HA2 | 38:0:5215:HOH:O | 1.76 | 0.83 |
| 2:B:36:PRO:HA | 2:B:168:GLY:HA3 | 1.61 | 0.82 |
| 30:0:2454:C:H5" | 38:0:7719:HOH:O | 1.79 | 0.82 |
| 30:0:1189:A:H1' | 30:0:1209:C:O4' | 1.79 | 0.82 |
| 13:M:27:ARG:HH22 | 13:M:44:THR:HG23 | 1.44 | 0.82 |
| 30:0:1667:A:H5' | 30:0:1667:A:H8 | 1.44 | 0.82 |
| 30:0:541:C:C2' | 30:0:542:A:H5" | 2.09 | 0.82 |
| 30:0:541:C:H2' | 30:0:542:A:C5' | 2.08 | 0.82 |
| 29:3:31:THR:O | 30:0:1923:G:H4' | 1.79 | 0.81 |
| 30:0:1300:G:H1' | 38:0:4678:HOH:O | 1.80 | 0.81 |
| 30:0:1184:C:H1' | 38:0:7461:HOH:O | 1.80 | 0.81 |
| 11:K:10:GLN:HE21 | 11:K:10:GLN:N | 1.79 | 0.81 |
| 20:T:71:VAL:HG11 | 20:T:90:PRO:HB3 | 1.62 | 0.81 |
| 30:0:2769:C:O2' | 30:0:2770:G:H5' | 1.81 | 0.81 |
| 3:C:139:VAL:HG13 | 38:C:8658:HOH:O | 1.79 | 0.81 |
| 30:0:559:U:H6 | 30:0:559:U:H5' | 1.45 | 0.81 |
| 30:0:2005:G:H3' | 30:0:2005:G:OP2 | 1.80 | 0.81 |
| 31:9:29:C:C2' | 31:9:30:C:H5' | 2.08 | 0.81 |
| 8:H:59:GLN:HE21 | 8:H:129:ARG:HE | 1.25 | 0.81 |
| 18:R:39:THR:HG22 | 18:R:42:GLU:H | 1.46 | 0.81 |
| 30:0:1174:A:C6 | 30:0:1201:C:H4' | 2.14 | 0.81 |
| 30:0:681:G:N3 | 30:0:681:G:H5' | 1.96 | 0.81 |
| 30:0:1119:G:N2 | 30:0:1246:A:C2 | 2.47 | 0.81 |
| 30:0:1205:U:H2' | 30:0:1206:U:C5' | 2.10 | 0.81 |
| 30:0:1641:A:H2' | 30:0:1642:A:C5' | 2.09 | 0.81 |
| 30:0:1801:A:H3' | 38:0:7607:HOH:O | 1.81 | 0.80 |
| 28:2:43:ARG:HH22 | 30:0:1684:A:H1' | 1.47 | 0.80 |
| 30:0:2748:G:H2' | 38:0:7534:HOH:O | 1.81 | 0.80 |
| 20:T:9:LYS:HE3 | 20:T:13:ARG:NH1 | 1.96 | 0.80 |
| 28:2:41:HIS:H | 28:2:45:ASN:HD22 | 1.27 | 0.80 |
| 30:0:1593:C:H1' | 38:0:6089:HOH:O | 1.80 | 0.80 |
| 15:O:3:THR:HG22 | 30:0:656:G:C5' | 2.09 | 0.80 |
| 25:Y:115:ARG:NH2 | 30:0:1266:U:H4' | 1.97 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2783:A:H3' | 38:0:5225:HOH:O | 1.81 | 0.80 |
| 31:9:39:U:H1' | 31:9:44:A:H61 | 1.45 | 0.80 |
| 30:0:1603:A:H5" | 30:0:1605:G:H5' | 1.63 | 0.80 |
| 31:9:14:G:H5' | 31:9:14:G:C8 | 2.16 | 0.80 |
| 9:I:112:LEU:HD11 | 30:0:1162:G:H1' | 1.63 | 0.80 |
| 18:R:99:ALA:HB1 | 18:R:109:MET:HE1 | 1.62 | 0.80 |
| 30:0:586:C:H5" | 38:0:7275:HOH:O | 1.81 | 0.80 |
| 22:V:12:THR:HG22 | 22:V:15:GLU:HG3 | 1.63 | 0.79 |
| 13:M:27:ARG:NH2 | 13:M:44:THR:HG23 | 1.96 | 0.79 |
| 6:F:91:VAL:HG12 | 6:F:92:GLY:H | 1.46 | 0.79 |
| 38:N:8842:HOH:O | 31:9:49:G:H5" | 1.83 | 0.79 |
| 10:J:82:THR:CG2 | 30:0:1242:A:H5' | 2.09 | 0.79 |
| 30:0:2419:U:H5" | 30:0:2420:G:H5' | 1.65 | 0.79 |
| 30:0:2586:U:H3 | 30:0:2592:G:H22 | 1.28 | 0.79 |
| 30:0:255:A:H2' | 30:0:256:C:H6 | 1.48 | 0.79 |
| 30:0:1183:C:H2' | 38:0:6224:HOH:O | 1.82 | 0.79 |
| 3:C:1:MET:HG2 | 3:C:2:GLN:H | 1.47 | 0.78 |
| 30:0:2635:A:O2' | 30:0:2636:C:H5' | 1.82 | 0.78 |
| 2:B:320:GLN:HE21 | 2:B:321:PRO:HD2 | 1.48 | 0.78 |
| 30:0:308:U:H5' | 30:0:309:C:OP1 | 1.82 | 0.78 |
| 30:0:659:A:H5" | 38:0:7089:HOH:O | 1.83 | 0.78 |
| 4:D:154:LYS:H | 4:D:154:LYS:HD2 | 1.48 | 0.78 |
| 30:0:123:U:H5' | 38:0:6637:HOH:O | 1.82 | 0.78 |
| 30:0:1372:A:H3' | 38:0:7180:HOH:O | 1.81 | 0.78 |
| 30:0:2485:A:H3' | 38:0:5838:HOH:O | 1.82 | 0.78 |
| 13:M:99:ARG:HE | 13:M:170:ASN:HD22 | 1.31 | 0.78 |
| 13:M:134:ILE:HG23 | 13:M:141:ILE:HD13 | 1.66 | 0.78 |
| 16:P:59:ARG:NH2 | 16:P:66:GLN:HE22 | 1.80 | 0.78 |
| 30:0:960:G:H4' | 38:0:7423:HOH:O | 1.83 | 0.78 |
| 30:0:1595:G:O2' | 30:0:1596:U:H5' | 1.84 | 0.78 |
| 30:0:2291:A:C8 | 30:0:2309:C:H5' | 2.19 | 0.78 |
| 8:H:59:GLN:NE2 | 8:H:129:ARG:HE | 1.82 | 0.78 |
| 30:0:541:C:H2' | 30:0:542:A:H5" | 1.65 | 0.77 |
| 30:0:2469:A:H1' | 38:0:3229:HOH:O | 1.83 | 0.77 |
| 30:0:871:G:C8 | 30:0:871:G:C5' | 2.58 | 0.77 |
| 30:0:1189:A:H3' | 38:0:7669:HOH:O | 1.83 | 0.77 |
| 30:0:2420:G:O2' | 30:0:2421:G:H5' | 1.85 | 0.77 |
| 30:0:558:C:C2' | 30:0:559:U:H5" | 2.14 | 0.77 |
| 30:0:1116:U:H3 | 30:0:1246:A:H62 | 1.33 | 0.77 |
| 30:0:564:G:H1' | 38:0:6295:HOH:O | 1.84 | 0.77 |
| 30:0:558:C:O2' | 30:0:559:U:H5" | 1.85 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2769:C:C2’ | 30:0:2770:G:H5’ | 2.15 | 0.77 |
| 30:0:1632:A:H2’ | 30:0:1633:C:H5’ | 1.67 | 0.76 |
| 30:0:1973:A:H5’ | 30:0:1973:A:H8 | 1.48 | 0.76 |
| 30:0:2703:A:H2’ | 30:0:2704:C:H6 | 1.50 | 0.76 |
| 30:0:283:U:H5 | 30:0:284:C:C4 | 2.02 | 0.76 |
| 30:0:1175:G:H1’ | 30:0:1193:A:H2’ | 1.65 | 0.76 |
| 31:9:1:U:H4’ | 31:9:3:A:OP1 | 1.84 | 0.76 |
| 30:0:2468:A:H3’ | 38:0:5449:HOH:O | 1.84 | 0.76 |
| 2:B:221:GLN:HE22 | 11:K:42:ASN:HD22 | 1.33 | 0.76 |
| 24:X:37:LEU:HD13 | 24:X:85:VAL:HG21 | 1.68 | 0.76 |
| 30:0:2506:A:O2’ | 30:0:2507:G:H8 | 1.68 | 0.76 |
| 38:C:8633:HOH:O | 30:0:338:C:H5” | 1.86 | 0.76 |
| 30:0:969:G:H1 | 30:0:999:C:H42 | 1.34 | 0.76 |
| 13:M:71:SER:HB3 | 30:0:2264:A:OP1 | 1.85 | 0.75 |
| 30:0:899:C:H5’ | 38:0:3190:HOH:O | 1.85 | 0.75 |
| 4:D:105:SER:OG | 30:0:2338:G:H1’ | 1.85 | 0.75 |
| 10:J:75:PRO:HG2 | 10:J:105:LEU:HD21 | 1.66 | 0.75 |
| 14:N:132:ASN:HD22 | 30:0:2413:A:H4’ | 1.52 | 0.75 |
| 30:0:282:C:H1’ | 30:0:368:C:N4 | 2.01 | 0.75 |
| 30:0:2505:G:H2’ | 30:0:2506:A:C5’ | 2.17 | 0.75 |
| 30:0:1170:U:H2’ | 30:0:1172:G:OP2 | 1.87 | 0.75 |
| 26:Z:70:ARG:HB2 | 26:Z:70:ARG:HH11 | 1.51 | 0.74 |
| 30:0:2908:A:H2’ | 30:0:2909:G:O4’ | 1.87 | 0.74 |
| 30:0:544:G:H2’ | 30:0:545:G:H5” | 1.68 | 0.74 |
| 30:0:1741:U:O2’ | 30:0:2723:G:H4’ | 1.87 | 0.74 |
| 24:X:76:ARG:HH11 | 24:X:76:ARG:HG3 | 1.52 | 0.74 |
| 3:C:218:VAL:HG12 | 38:C:8637:HOH:O | 1.87 | 0.74 |
| 22:V:57:LYS:HA | 22:V:60:GLN:HE21 | 1.52 | 0.74 |
| 30:0:1834:C:H2’ | 30:0:1840:A:N6 | 2.02 | 0.74 |
| 33:0:8813:CL:CL | 38:0:4678:HOH:O | 2.43 | 0.74 |
| 23:W:4:LEU:HD23 | 23:W:54:PHE:HB3 | 1.69 | 0.74 |
| 30:0:2781:U:C2’ | 30:0:2782:G:H5’ | 2.18 | 0.74 |
| 30:0:2793:A:H1’ | 38:0:6312:HOH:O | 1.88 | 0.74 |
| 14:N:11:ARG:HD3 | 31:9:114:G:O6 | 1.88 | 0.74 |
| 25:Y:235:GLU:CD | 25:Y:235:GLU:H | 1.92 | 0.73 |
| 3:C:140:VAL:HB | 38:C:8660:HOH:O | 1.86 | 0.73 |
| 4:D:22:VAL:HG22 | 4:D:74:THR:HG22 | 1.70 | 0.73 |
| 18:R:98:ASN:HD21 | 30:0:500:G:H21 | 1.36 | 0.73 |
| 30:0:1525:G:H5’ | 30:0:1526:A:OP2 | 1.89 | 0.73 |
| 30:0:2578:G:H5’ | 30:0:2578:G:H8 | 1.52 | 0.73 |
| 31:9:92:G:H2’ | 31:9:93:A:H8 | 1.50 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:56:ASP:HB2 | 2:B:322:ARG:HE | 1.52 | 0.73 |
| 21:U:56:ARG:HH11 | 21:U:56:ARG:HG3 | 1.54 | 0.73 |
| 11:K:14:LYS:HB2 | 11:K:45:PRO:HG2 | 1.70 | 0.73 |
| 30:0:2748:G:H1' | 38:0:7889:HOH:O | 1.88 | 0.73 |
| 30:0:1279:U:O2 | 30:0:1279:U:H2' | 1.89 | 0.72 |
| 30:0:619:U:H3' | 38:0:3270:HOH:O | 1.88 | 0.72 |
| 30:0:2768:A:O2' | 30:0:2769:C:H5' | 1.89 | 0.72 |
| 14:N:37:ARG:HH12 | 31:9:6:C:H5" | 1.55 | 0.72 |
| 30:0:2524:G:H21 | 30:0:2526:C:N4 | 1.85 | 0.72 |
| 30:0:2871:G:H2' | 30:0:2872:U:H6 | 1.54 | 0.72 |
| 30:0:271:C:H41 | 30:0:378:A:H2 | 1.33 | 0.72 |
| 30:0:558:C:H2' | 30:0:559:U:C5' | 2.20 | 0.72 |
| 2:B:179:LEU:O | 2:B:183:GLU:HG2 | 1.89 | 0.72 |
| 30:0:1921:A:O2' | 30:0:1922:A:H5' | 1.89 | 0.72 |
| 30:0:2766:A:H5' | 38:0:9565:HOH:O | 1.88 | 0.72 |
| 30:0:1166:A:P | 30:0:1174:A:H4' | 2.29 | 0.72 |
| 31:9:29:C:H2' | 31:9:30:C:C5' | 2.17 | 0.72 |
| 30:0:877:G:H5' | 30:0:878:G:OP1 | 1.89 | 0.72 |
| 30:0:2533:C:H5' | 30:0:2533:C:H6 | 1.53 | 0.72 |
| 13:M:15:PRO:HA | 13:M:20:LEU:HD23 | 1.70 | 0.72 |
| 13:M:79:ALA:H | 13:M:81:ARG:HH22 | 1.37 | 0.72 |
| 30:0:544:G:C2' | 30:0:545:G:H5" | 2.20 | 0.72 |
| 30:0:836:G:H5" | 38:0:9285:HOH:O | 1.89 | 0.72 |
| 30:0:2712:G:H5' | 38:0:5215:HOH:O | 1.90 | 0.72 |
| 2:B:145:HIS:HD2 | 2:B:146:THR:O | 1.73 | 0.71 |
| 13:M:66:SER:HB3 | 13:M:128:TRP:CD1 | 2.24 | 0.71 |
| 29:3:2:GLN:O | 30:0:2320:U:H2' | 1.90 | 0.71 |
| 31:9:54:A:O2' | 31:9:55:U:H5' | 1.89 | 0.71 |
| 14:N:159:TYR:HE1 | 31:9:50:G:H5" | 1.55 | 0.71 |
| 14:N:67:ALA:HA | 14:N:71:TRP:HB3 | 1.72 | 0.71 |
| 30:0:281:U:H2' | 30:0:282:C:O4' | 1.90 | 0.71 |
| 30:0:702:G:O2' | 30:0:703:G:H5' | 1.90 | 0.71 |
| 30:0:821:U:H3' | 38:0:3759:HOH:O | 1.90 | 0.71 |
| 30:0:2534:C:H1' | 38:0:3477:HOH:O | 1.91 | 0.71 |
| 30:0:2426:G:H1' | 38:0:6075:HOH:O | 1.90 | 0.71 |
| 30:0:221:G:H5" | 38:0:5725:HOH:O | 1.90 | 0.71 |
| 30:0:1165:G:N2 | 30:0:1173:A:C5' | 2.53 | 0.71 |
| 2:B:307:ARG:HH11 | 2:B:307:ARG:HG3 | 1.55 | 0.71 |
| 38:I:6825:HOH:O | 30:0:1166:A:H2 | 1.73 | 0.71 |
| 30:0:1835:U:C5 | 30:0:1840:A:N7 | 2.57 | 0.71 |
| 30:0:1132:A:N6 | 30:0:1229:C:H2' | 2.06 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:5:ARG:HB2 | 14:N:5:ARG:HH11 | 1.56 | 0.71 |
| 30:0:1589:G:N2 | 30:0:1605:G:H1' | 2.05 | 0.71 |
| 30:0:1979:G:H3' | 38:0:3282:HOH:O | 1.88 | 0.71 |
| 30:0:2487:C:H5 | 38:0:4880:HOH:O | 1.73 | 0.70 |
| 14:N:143:ARG:HH21 | 14:N:169:PRO:HB2 | 1.56 | 0.70 |
| 30:0:2514:U:OP1 | 30:0:2572:G:H1' | 1.90 | 0.70 |
| 14:N:17:ARG:HB3 | 14:N:17:ARG:HH11 | 1.55 | 0.70 |
| 30:0:2505:G:O2' | 30:0:2506:A:H5' | 1.90 | 0.70 |
| 11:K:98:VAL:CG1 | 11:K:102:GLU:HA | 2.20 | 0.70 |
| 26:Z:70:ARG:HH12 | 26:Z:83:TYR:HB2 | 1.55 | 0.70 |
| 30:0:1666:C:H2' | 30:0:1667:A:C5' | 2.21 | 0.70 |
| 17:Q:11:ARG:NH2 | 30:0:2297:U:H4' | 2.07 | 0.70 |
| 30:0:1189:A:H1' | 30:0:1209:C:C1' | 2.21 | 0.70 |
| 18:R:132:ARG:NH2 | 30:0:2055:A:H4' | 2.06 | 0.70 |
| 30:0:1209:C:H2' | 30:0:1210:G:H8 | 1.57 | 0.70 |
| 30:0:2237:G:H1' | 30:0:2238:A:C8 | 2.27 | 0.70 |
| 13:M:188:ARG:HD3 | 30:0:155:C:OP2 | 1.92 | 0.70 |
| 26:Z:80:GLN:HG3 | 26:Z:81:CYS:H | 1.56 | 0.70 |
| 30:0:31:C:H2' | 38:0:7677:HOH:O | 1.90 | 0.70 |
| 38:Q:6286:HOH:O | 30:0:1019:C:H5' | 1.91 | 0.69 |
| 3:C:127:ARG:NH2 | 3:C:225:PRO:HG2 | 2.07 | 0.69 |
| 30:0:2251:G:H2' | 30:0:2252:A:C8 | 2.27 | 0.69 |
| 2:B:36:PRO:HG3 | 2:B:169:GLY:H | 1.57 | 0.69 |
| 30:0:42:C:H3' | 38:0:4166:HOH:O | 1.92 | 0.69 |
| 30:0:138:U:H5" | 30:0:139:C:OP2 | 1.93 | 0.69 |
| 30:0:1451:C:H5' | 30:0:1505:U:C5 | 2.27 | 0.69 |
| 30:0:1562:C:O2 | 30:0:1562:C:H2' | 1.91 | 0.69 |
| 1:A:94:LEU:HD12 | 1:A:98:GLU:HB2 | 1.74 | 0.69 |
| 5:E:143:GLN:HE21 | 30:0:2780:C:H1' | 1.57 | 0.69 |
| 9:I:91:PHE:HD2 | 9:I:131:GLY:HA2 | 1.55 | 0.69 |
| 14:N:49:THR:HB | 14:N:58:LEU:HD11 | 1.74 | 0.69 |
| 4:D:28:GLY:HA2 | 4:D:69:ILE:HG23 | 1.72 | 0.69 |
| 13:M:79:ALA:HB3 | 13:M:81:ARG:NH1 | 2.06 | 0.69 |
| 30:0:287:C:H42 | 30:0:365:G:H1 | 1.41 | 0.69 |
| 30:0:407:A:H2' | 30:0:408:A:C8 | 2.28 | 0.69 |
| 30:0:961:A:H4' | 38:0:6759:HOH:O | 1.91 | 0.69 |
| 30:0:1666:C:C2' | 30:0:1667:A:C5' | 2.70 | 0.69 |
| 30:0:2102:G:H4' | 38:0:5631:HOH:O | 1.92 | 0.69 |
| 30:0:2102:G:N2 | 30:0:2103:A:N1 | 2.40 | 0.69 |
| 30:0:2871:G:H2' | 30:0:2872:U:C6 | 2.28 | 0.69 |
| 10:J:26:VAL:HG13 | 10:J:36:VAL:HG11 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:141:ARG:HH21 | 31:9:48:C:H4' | 1.57 | 0.69 |
| 2:B:206:THR:HG21 | 30:0:2716:G:H5" | 1.73 | 0.69 |
| 12:L:91:VAL:HG13 | 12:L:120:LEU:HD23 | 1.75 | 0.69 |
| 31:9:39:U:H3' | 31:9:40:C:H5" | 1.75 | 0.69 |
| 2:B:18:ARG:HE | 2:B:256:GLN:HE21 | 1.41 | 0.69 |
| 30:0:2511:A:H2' | 30:0:2512:U:O4' | 1.93 | 0.69 |
| 30:0:2781:U:H2' | 30:0:2782:G:H5' | 1.73 | 0.69 |
| 13:M:68:ARG:O | 13:M:68:ARG:HD3 | 1.93 | 0.69 |
| 30:0:969:G:H1 | 30:0:999:C:N4 | 1.91 | 0.69 |
| 30:0:1589:G:H22 | 30:0:1605:G:H1' | 1.55 | 0.69 |
| 4:D:51:ARG:HH11 | 4:D:68:PRO:HB3 | 1.59 | 0.68 |
| 10:J:18:ILE:HD13 | 30:0:1244:U:OP1 | 1.92 | 0.68 |
| 22:V:50:ARG:HH12 | 30:0:56:G:H5" | 1.58 | 0.68 |
| 30:0:317:A:H5' | 38:0:3761:HOH:O | 1.91 | 0.68 |
| 30:0:1474:C:H6 | 30:0:1474:C:C5' | 2.06 | 0.68 |
| 30:0:2781:U:O2' | 30:0:2782:G:H5' | 1.93 | 0.68 |
| 14:N:40:ASN:ND2 | 31:9:28:U:H5" | 2.08 | 0.68 |
| 16:P:59:ARG:HH22 | 16:P:66:GLN:NE2 | 1.87 | 0.68 |
| 30:0:870:G:C2' | 30:0:871:G:H5" | 2.22 | 0.68 |
| 2:B:254:GLN:HG3 | 38:0:9697:HOH:O | 1.92 | 0.68 |
| 13:M:99:ARG:HD2 | 13:M:167:GLY:HA2 | 1.75 | 0.68 |
| 29:3:59:ASP:HA | 30:0:2460:A:H5" | 1.74 | 0.68 |
| 30:0:962:C:H2' | 30:0:963:C:H5' | 1.74 | 0.68 |
| 10:J:131:THR:HB | 10:J:134:GLU:HG3 | 1.75 | 0.68 |
| 28:2:35:ARG:HB2 | 38:2:2691:HOH:O | 1.92 | 0.68 |
| 30:0:255:A:H2' | 30:0:256:C:C6 | 2.29 | 0.68 |
| 30:0:390:G:H5' | 38:0:7539:HOH:O | 1.94 | 0.68 |
| 30:0:283:U:H5 | 30:0:284:C:N3 | 1.91 | 0.68 |
| 30:0:1527:A:H1' | 30:0:1528:A:C8 | 2.28 | 0.68 |
| 30:0:1634:G:H2' | 30:0:1635:U:H6 | 1.57 | 0.68 |
| 30:0:1702:U:H1' | 38:0:5758:HOH:O | 1.93 | 0.68 |
| 12:L:6:ARG:HD3 | 30:0:1299:G:O6 | 1.94 | 0.68 |
| 13:M:171:ARG:CD | 30:0:156:C:H5" | 2.15 | 0.68 |
| 30:0:440:C:H2' | 30:0:441:A:C8 | 2.29 | 0.68 |
| 30:0:2374:G:H2' | 30:0:2375:A:C8 | 2.29 | 0.68 |
| 13:M:83:SER:HA | 38:M:8877:HOH:O | 1.94 | 0.68 |
| 24:X:25:ARG:HD2 | 38:X:5356:HOH:O | 1.91 | 0.68 |
| 26:Z:70:ARG:HB3 | 38:Z:8728:HOH:O | 1.93 | 0.68 |
| 2:B:264:GLU:CG | 2:B:267:LYS:HE3 | 2.24 | 0.67 |
| 27:1:8:GLN:HE22 | 27:1:11:LYS:NZ | 1.93 | 0.67 |
| 30:0:1666:C:C2' | 30:0:1667:A:H5" | 2.23 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:72:ALA:HB2 | 8:H:156:ALA:HB2 | 1.75 | 0.67 |
| 23:W:137:GLN:HE21 | 23:W:141:HIS:CE1 | 2.08 | 0.67 |
| 30:0:1158:G:C2' | 30:0:1159:G:H5' | 2.24 | 0.67 |
| 10:J:90:LYS:HB2 | 33:J:8802:CL:CL | 2.31 | 0.67 |
| 23:W:88:THR:HG23 | 23:W:110:GLN:HB3 | 1.76 | 0.67 |
| 30:0:1634:G:H2' | 30:0:1635:U:C6 | 2.29 | 0.67 |
| 6:F:63:ILE:HB | 6:F:64:PRO:HD3 | 1.74 | 0.67 |
| 31:9:24:U:H3' | 31:9:25:G:H5' | 1.75 | 0.67 |
| 20:T:2:LYS:HG2 | 30:0:447:A:OP1 | 1.95 | 0.67 |
| 30:0:283:U:C5 | 30:0:284:C:C4 | 2.83 | 0.67 |
| 30:0:735:C:C5 | 30:0:736:A:C4 | 2.82 | 0.67 |
| 30:0:1632:A:C2' | 30:0:1633:C:H5' | 2.24 | 0.67 |
| 30:0:1762:C:O2' | 30:0:1763:C:H5' | 1.95 | 0.67 |
| 31:9:91:C:H1' | 38:9:9143:HOH:O | 1.95 | 0.67 |
| 30:0:541:C:H2' | 30:0:542:A:H5' | 1.75 | 0.67 |
| 30:0:1268:C:H2' | 30:0:1269:G:H8 | 1.59 | 0.67 |
| 1:A:72:GLU:HG2 | 26:Z:100:GLY:HA3 | 1.76 | 0.67 |
| 14:N:7:LYS:HE3 | 17:Q:21:ARG:O | 1.95 | 0.67 |
| 18:R:150:PRO:CG | 18:R:150:PRO:O | 2.42 | 0.67 |
| 30:0:221:G:H2' | 30:0:222:A:C8 | 2.30 | 0.67 |
| 30:0:603:A:H5" | 30:0:604:G:OP1 | 1.94 | 0.67 |
| 9:I:96:SER:H | 9:I:99:GLN:NE2 | 1.93 | 0.66 |
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:HB3 | 1.77 | 0.66 |
| 30:0:2073:G:OP2 | 30:0:2490:A:H5' | 1.95 | 0.66 |
| 12:L:121:ILE:HG12 | 12:L:141:GLU:HB2 | 1.78 | 0.66 |
| 23:W:44:MET:CE | 30:0:944:G:H21 | 2.09 | 0.66 |
| 30:0:506:G:H22 | 30:0:509:A:H5' | 1.60 | 0.66 |
| 30:0:613:C:H2' | 30:0:614:U:H6 | 1.61 | 0.66 |
| 30:0:2488:A:C2 | 38:0:7265:HOH:O | 2.48 | 0.66 |
| 11:K:18:ILE:HG22 | 11:K:93:ASN:HB2 | 1.77 | 0.66 |
| 30:0:451:C:O2' | 30:0:452:G:H5' | 1.95 | 0.66 |
| 18:R:18:LEU:HB2 | 18:R:143:VAL:HG13 | 1.76 | 0.66 |
| 30:0:1158:G:O2' | 30:0:1159:G:H5' | 1.96 | 0.66 |
| 22:V:50:ARG:NH1 | 30:0:56:G:H5" | 2.10 | 0.66 |
| 30:0:849:C:H1' | 38:0:6602:HOH:O | 1.95 | 0.66 |
| 31:9:55:U:H4' | 31:9:56:A:C8 | 2.31 | 0.66 |
| 25:Y:169:ARG:HD2 | 30:0:1328:A:OP1 | 1.96 | 0.66 |
| 30:0:2461:U:O2 | 30:0:2466:G:H1' | 1.96 | 0.66 |
| 30:0:735:C:H2' | 30:0:736:A:O4' | 1.96 | 0.66 |
| 30:0:2321:A:C2 | 30:0:2378:U:N3 | 2.57 | 0.66 |
| 8:H:32:ALA:HB3 | 8:H:69:ARG:HH12 | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:I:87:PRO:HD2 | 30:0:1180:U:H1' | 1.77 | 0.66 |
| 30:0:558:C:H2' | 30:0:559:U:H5' | 1.78 | 0.66 |
| 2:B:162:MET:HG3 | 2:B:310:ARG:NH1 | 2.10 | 0.65 |
| 9:I:110:ASP:O | 30:0:1163:G:H5' | 1.96 | 0.65 |
| 3:C:233:THR:HG22 | 3:C:234:VAL:H | 1.61 | 0.65 |
| 4:D:103:ASN:HD22 | 4:D:133:ASN:HA | 1.60 | 0.65 |
| 4:D:103:ASN:ND2 | 4:D:133:ASN:HA | 2.11 | 0.65 |
| 21:U:56:ARG:NE | 30:0:2890:A:H1' | 2.11 | 0.65 |
| 30:0:567:U:H5" | 38:0:5280:HOH:O | 1.97 | 0.65 |
| 30:0:635:A:H2' | 30:0:636:G:H5" | 1.77 | 0.65 |
| 30:0:1477:C:H5' | 30:0:1868:G:C5' | 2.26 | 0.65 |
| 30:0:1940:C:H1' | 38:0:9376:HOH:O | 1.96 | 0.65 |
| 30:0:1950:G:H2' | 30:0:1951:G:C8 | 2.32 | 0.65 |
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:CB | 2.27 | 0.65 |
| 30:0:625:U:H5" | 30:0:1044:C:N4 | 2.11 | 0.65 |
| 30:0:1925:G:O2' | 30:0:1926:G:H5' | 1.96 | 0.65 |
| 5:E:139:GLU:OE2 | 30:0:2781:U:H1' | 1.97 | 0.65 |
| 30:0:2869:G:H2' | 30:0:2870:C:C6 | 2.31 | 0.65 |
| 14:N:144:GLY:O | 14:N:147:ILE:HG22 | 1.97 | 0.65 |
| 22:V:39:ALA:N | 22:V:40:PRO:HD2 | 2.12 | 0.65 |
| 30:0:1165:G:H1' | 30:0:1174:A:C1' | 2.11 | 0.65 |
| 30:0:1972:U:H2' | 30:0:1973:A:C5' | 2.27 | 0.65 |
| 17:Q:19:ARG:HH21 | 31:9:11:A:P | 2.19 | 0.64 |
| 23:W:21:LEU:HD21 | 23:W:48:VAL:HG11 | 1.78 | 0.64 |
| 30:0:2458:U:H3' | 38:0:3239:HOH:O | 1.96 | 0.64 |
| 30:0:128:A:O2' | 30:0:129:A:H5' | 1.97 | 0.64 |
| 30:0:583:C:H2' | 30:0:584:U:H6 | 1.62 | 0.64 |
| 30:0:1165:G:H21 | 30:0:1173:A:H5' | 1.63 | 0.64 |
| 30:0:2672:C:O2' | 30:0:2673:U:H5' | 1.97 | 0.64 |
| 30:0:2896:A:H5" | 38:0:6082:HOH:O | 1.96 | 0.64 |
| 11:K:74:VAL:HG11 | 11:K:113:ILE:HG12 | 1.79 | 0.64 |
| 30:0:69:A:H5' | 30:0:69:A:C8 | 2.32 | 0.64 |
| 30:0:125:U:H2' | 38:0:3755:HOH:O | 1.97 | 0.64 |
| 30:0:369:G:O2' | 30:0:370:G:H5' | 1.98 | 0.64 |
| 30:0:660:A:H4' | 30:0:661:G:O5' | 1.98 | 0.64 |
| 2:B:312:ARG:HD3 | 2:B:315:VAL:HG13 | 1.79 | 0.64 |
| 30:0:200:C:H2' | 38:0:3428:HOH:O | 1.96 | 0.64 |
| 30:0:2488:A:H2 | 38:0:7265:HOH:O | 1.81 | 0.64 |
| 19:S:17:ASP:HB3 | 19:S:23:LYS:HB2 | 1.79 | 0.64 |
| 30:0:1167:G:H2' | 30:0:1168:C:O4' | 1.98 | 0.64 |
| 13:M:70:GLY:CA | 30:0:2263:G:H4' | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:9:36:C:H5' | 38:9:9047:HOH:O | 1.98 | 0.64 |
| 30:0:285:A:H2' | 30:0:286:U:O4' | 1.97 | 0.64 |
| 30:0:1119:G:N2 | 30:0:1246:A:H2 | 1.89 | 0.64 |
| 30:0:2781:U:H2' | 30:0:2782:G:C5' | 2.27 | 0.64 |
| 15:O:47:ARG:HG3 | 15:O:47:ARG:NH1 | 2.12 | 0.64 |
| 30:0:441:A:H1' | 30:0:442:A:N7 | 2.13 | 0.64 |
| 30:0:1181:A:H2' | 30:0:1182:C:H5' | 1.78 | 0.64 |
| 31:9:5:G:O2' | 31:9:6:C:H5' | 1.97 | 0.64 |
| 18:R:132:ARG:HH21 | 30:0:2055:A:H4' | 1.61 | 0.64 |
| 30:0:1213:C:O2' | 30:0:1214:G:H5' | 1.98 | 0.64 |
| 30:0:2436:U:H2' | 30:0:2437:A:C8 | 2.33 | 0.64 |
| 30:0:2878:U:H5" | 38:0:4165:HOH:O | 1.98 | 0.64 |
| 30:0:2887:G:H2' | 30:0:2888:U:C6 | 2.32 | 0.64 |
| 12:L:143:THR:HG22 | 12:L:144:ASP:H | 1.62 | 0.63 |
| 30:0:2377:U:O2' | 30:0:2378:U:H5' | 1.98 | 0.63 |
| 30:0:2613:G:O2' | 30:0:2614:C:H5' | 1.99 | 0.63 |
| 31:9:24:U:H3' | 31:9:25:G:C5' | 2.28 | 0.63 |
| 30:0:2281:C:C2' | 30:0:2282:U:H5' | 2.28 | 0.63 |
| 3:C:162:VAL:HG22 | 3:C:232:LEU:HD21 | 1.81 | 0.63 |
| 14:N:141:ARG:NH2 | 31:9:48:C:H4' | 2.13 | 0.63 |
| 21:U:4:ARG:O | 21:U:13:ILE:HG22 | 1.98 | 0.63 |
| 30:0:585:C:H5" | 38:0:4864:HOH:O | 1.98 | 0.63 |
| 30:0:2831:C:C2' | 30:0:2832:C:H5' | 2.28 | 0.63 |
| 13:M:99:ARG:HE | 13:M:170:ASN:ND2 | 1.96 | 0.63 |
| 30:0:281:U:O2' | 30:0:282:C:H5' | 1.97 | 0.63 |
| 30:0:1170:U:H1' | 30:0:1172:G:N7 | 2.13 | 0.63 |
| 30:0:2869:G:H5' | 38:0:5487:HOH:O | 1.97 | 0.63 |
| 13:M:81:ARG:HB3 | 13:M:85:ARG:HB2 | 1.80 | 0.63 |
| 30:0:1204:C:H1' | 38:0:4741:HOH:O | 1.98 | 0.63 |
| 30:0:1268:C:H2' | 30:0:1269:G:C8 | 2.34 | 0.63 |
| 30:0:1904:A:C2 | 30:0:1905:U:H1' | 2.34 | 0.63 |
| 30:0:2336:G:H2' | 38:0:6280:HOH:O | 1.98 | 0.63 |
| 30:0:2868:C:H1' | 38:0:7114:HOH:O | 1.97 | 0.63 |
| 2:B:262:ARG:HG3 | 30:0:2716:G:H5' | 1.79 | 0.63 |
| 3:C:174:ILE:CD1 | 30:0:338:C:H4' | 2.29 | 0.63 |
| 29:3:55:VAL:HB | 29:3:56:PRO:HD2 | 1.81 | 0.63 |
| 30:0:820:G:H5' | 30:0:821:U:H5' | 1.80 | 0.63 |
| 30:0:424:C:H2' | 30:0:425:U:H6 | 1.64 | 0.63 |
| 30:0:1528:A:H2' | 30:0:1529:G:O4' | 1.98 | 0.63 |
| 30:0:2321:A:H8 | 30:0:2322:U:O2' | 1.80 | 0.63 |
| 30:0:2831:C:H2' | 30:0:2832:C:H5' | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:25:MET:SD | 4:D:40:ILE:HD11 | 2.39 | 0.63 |
| 30:0:280:C:H2' | 30:0:281:U:O4' | 1.99 | 0.63 |
| 30:0:1950:G:H2' | 30:0:1951:G:H8 | 1.64 | 0.63 |
| 30:0:2401:A:H2' | 30:0:2402:A:C8 | 2.34 | 0.63 |
| 31:9:2:U:OP2 | 31:9:3:A:H5' | 1.99 | 0.63 |
| 31:9:36:C:C5 | 31:9:37:C:C5 | 2.87 | 0.63 |
| 18:R:9:ASP:O | 18:R:13:THR:HB | 1.99 | 0.62 |
| 30:0:558:C:C2' | 30:0:559:U:C5' | 2.77 | 0.62 |
| 2:B:238:ASN:HD22 | 2:B:240:GLY:H | 1.45 | 0.62 |
| 2:B:272:ILE:HG22 | 38:B:9132:HOH:O | 2.00 | 0.62 |
| 12:L:79:ASP:HB3 | 38:L:9022:HOH:O | 1.98 | 0.62 |
| 13:M:179:GLY:O | 30:0:399:C:H5' | 1.98 | 0.62 |
| 18:R:39:THR:HG23 | 18:R:107:GLU:O | 1.99 | 0.62 |
| 30:0:834:G:H4' | 30:0:835:U:OP2 | 1.99 | 0.62 |
| 30:0:2594:C:O2' | 30:0:2595:U:H5' | 1.99 | 0.62 |
| 30:0:2827:A:H2' | 30:0:2828:G:O4' | 1.99 | 0.62 |
| 30:0:2894:C:O2' | 30:0:2895:C:H5' | 1.99 | 0.62 |
| 11:K:66:ARG:HH22 | 30:0:1994:A:P | 2.21 | 0.62 |
| 30:0:308:U:C4 | 30:0:342:C:H1' | 2.34 | 0.62 |
| 30:0:1829:A:H2' | 30:0:1830:C:H5' | 1.81 | 0.62 |
| 30:0:2505:G:C2' | 30:0:2506:A:C5' | 2.76 | 0.62 |
| 15:O:10:LEU:HD13 | 15:O:99:GLU:HG3 | 1.82 | 0.62 |
| 30:0:249:G:O2' | 30:0:250:C:H5' | 1.99 | 0.62 |
| 30:0:256:C:H2' | 30:0:257:G:O4' | 2.00 | 0.62 |
| 30:0:1797:A:H4' | 30:0:1798:C:C5 | 2.33 | 0.62 |
| 25:Y:204:ARG:HH22 | 30:0:553:G:P | 2.22 | 0.62 |
| 30:0:506:G:N2 | 30:0:509:A:H5" | 2.14 | 0.62 |
| 17:Q:11:ARG:HH21 | 30:0:2297:U:H4' | 1.62 | 0.62 |
| 23:W:48:VAL:HG12 | 23:W:52:VAL:HB | 1.81 | 0.62 |
| 30:0:1087:G:H4' | 30:0:1088:A:OP1 | 2.00 | 0.62 |
| 30:0:1230:A:H8 | 30:0:1230:A:OP1 | 1.83 | 0.62 |
| 30:0:2705:U:H2' | 30:0:2706:A:C8 | 2.35 | 0.62 |
| 30:0:418:C:H5 | 38:0:5765:HOH:O | 1.82 | 0.62 |
| 1:A:47:HIS:CD2 | 30:0:1654:U:H2' | 2.35 | 0.62 |
| 13:M:24:GLN:HE21 | 13:M:27:ARG:HH11 | 1.48 | 0.62 |
| 17:Q:27:GLN:HE21 | 31:9:8:G:C5' | 2.11 | 0.62 |
| 30:0:1625:U:H5" | 38:0:6005:HOH:O | 2.00 | 0.62 |
| 30:0:2248:C:H3' | 38:0:5435:HOH:O | 1.98 | 0.62 |
| 15:O:37:ARG:HD2 | 30:0:656:G:OP2 | 2.00 | 0.62 |
| 30:0:303:C:O2' | 30:0:304:G:H5' | 2.00 | 0.62 |
| 30:0:1165:G:N2 | 30:0:1173:A:H5" | 2.09 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:168:VAL:HG13 | 38:H:9006:HOH:O | 2.00 | 0.62 |
| 13:M:79:ALA:H | 13:M:81:ARG:NH2 | 1.96 | 0.62 |
| 30:0:289:G:O2' | 30:0:290:C:H5' | 1.98 | 0.62 |
| 30:0:1477:C:H5' | 30:0:1868:G:H5' | 1.81 | 0.62 |
| 23:W:44:MET:HE2 | 30:0:944:G:H21 | 1.63 | 0.61 |
| 31:9:110:G:C6 | 31:9:111:U:C5 | 2.88 | 0.61 |
| 19:S:52:VAL:HG22 | 19:S:66:VAL:HG22 | 1.82 | 0.61 |
| 25:Y:126:PRO:HG2 | 25:Y:128:PHE:CE1 | 2.34 | 0.61 |
| 30:0:545:G:H8 | 30:0:545:G:C5' | 2.08 | 0.61 |
| 30:0:807:A:O2' | 30:0:808:A:H5' | 1.99 | 0.61 |
| 3:C:27:ARG:HG2 | 3:C:27:ARG:NH1 | 2.12 | 0.61 |
| 10:J:75:PRO:HG2 | 10:J:105:LEU:CD2 | 2.31 | 0.61 |
| 12:L:90:ARG:HA | 12:L:119:THR:HB | 1.82 | 0.61 |
| 14:N:83:LEU:HD13 | 14:N:175:LEU:HD23 | 1.82 | 0.61 |
| 20:T:9:LYS:HD2 | 38:0:3744:HOH:O | 2.00 | 0.61 |
| 28:2:41:HIS:HE1 | 30:0:1439:C:H5" | 1.65 | 0.61 |
| 30:0:39:G:N2 | 30:0:444:C:C2 | 2.68 | 0.61 |
| 30:0:1596:U:H2' | 30:0:1598:A:OP2 | 2.00 | 0.61 |
| 30:0:2102:G:N2 | 30:0:2104:C:C2 | 2.69 | 0.61 |
| 31:9:107:C:O2' | 31:9:108:C:H5' | 2.00 | 0.61 |
| 3:C:129:HIS:CE1 | 3:C:231:ARG:HA | 2.35 | 0.61 |
| 30:0:1245:C:O5' | 30:0:1245:C:H6 | 1.84 | 0.61 |
| 13:M:102:GLU:OE1 | 13:M:164:THR:HG21 | 2.00 | 0.61 |
| 30:0:1015:C:H2' | 30:0:1016:U:H6 | 1.64 | 0.61 |
| 3:C:1:MET:HG2 | 3:C:2:GLN:N | 2.15 | 0.61 |
| 3:C:236:THR:HG22 | 3:C:239:ALA:N | 2.12 | 0.61 |
| 26:Z:40:ALA:HA | 30:0:1773:G:C8 | 2.35 | 0.61 |
| 30:0:138:U:OP2 | 30:0:139:C:H5 | 1.84 | 0.61 |
| 30:0:2502:C:H2' | 30:0:2503:A:C5' | 2.29 | 0.61 |
| 30:0:2717:C:H2' | 30:0:2718:C:C5' | 2.30 | 0.61 |
| 4:D:173:GLU:HG3 | 4:D:174:VAL:HG23 | 1.83 | 0.61 |
| 29:3:60:LYS:CG | 29:3:61:PRO:HD2 | 2.29 | 0.61 |
| 30:0:24:G:N2 | 30:0:518:G:H1' | 2.16 | 0.61 |
| 30:0:559:U:H5' | 30:0:559:U:C6 | 2.32 | 0.61 |
| 16:P:98:ILE:HD12 | 16:P:102:ARG:NE | 2.16 | 0.61 |
| 26:Z:78:ILE:HD12 | 38:Z:8714:HOH:O | 2.01 | 0.61 |
| 30:0:272:A:H5' | 30:0:273:G:OP2 | 2.01 | 0.61 |
| 30:0:424:C:H2' | 30:0:425:U:C6 | 2.35 | 0.61 |
| 30:0:735:C:H5 | 30:0:736:A:C4 | 2.18 | 0.61 |
| 30:0:2766:A:O2' | 30:0:2767:C:H5' | 2.00 | 0.61 |
| 29:3:4:PRO:HA | 29:3:91:GLN:HB2 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:657:G:H2' | 30:0:658:C:H6 | 1.64 | 0.61 |
| 30:0:946:C:H2' | 30:0:947:U:H6 | 1.65 | 0.61 |
| 30:0:1015:C:H2' | 30:0:1016:U:C6 | 2.36 | 0.61 |
| 27:1:8:GLN:HE22 | 27:1:11:LYS:HZ2 | 1.49 | 0.60 |
| 30:0:1741:U:H5' | 30:0:1742:A:OP1 | 2.01 | 0.60 |
| 15:O:32:ARG:O | 15:O:32:ARG:HD3 | 2.01 | 0.60 |
| 30:0:1165:G:N2 | 30:0:1173:A:H5' | 2.15 | 0.60 |
| 30:0:1972:U:H2' | 30:0:1973:A:H5' | 1.83 | 0.60 |
| 30:0:2769:C:H2' | 30:0:2770:G:H5' | 1.82 | 0.60 |
| 2:B:207:LYS:HG3 | 30:0:2717:C:OP1 | 2.01 | 0.60 |
| 5:E:154:ILE:HD11 | 5:E:157:LYS:HE2 | 1.83 | 0.60 |
| 28:2:10:ARG:NH2 | 30:0:121:U:OP2 | 2.34 | 0.60 |
| 30:0:1181:A:C2' | 30:0:1182:C:H5' | 2.30 | 0.60 |
| 30:0:1603:A:C5' | 30:0:1605:G:H5' | 2.29 | 0.60 |
| 8:H:29:SER:HA | 8:H:62:HIS:HD2 | 1.66 | 0.60 |
| 30:0:192:A:H5' | 38:0:7634:HOH:O | 1.99 | 0.60 |
| 30:0:272:A:H3' | 38:0:7522:HOH:O | 2.00 | 0.60 |
| 30:0:1183:C:N4 | 30:0:1184:C:H41 | 1.98 | 0.60 |
| 30:0:1603:A:C5' | 30:0:1605:G:O4' | 2.45 | 0.60 |
| 30:0:1622:G:H2' | 30:0:1623:C:H5' | 1.83 | 0.60 |
| 30:0:2102:G:C8 | 30:0:2538:A:O4' | 2.54 | 0.60 |
| 30:0:2281:C:H2' | 30:0:2282:U:H5' | 1.83 | 0.60 |
| 31:9:20:G:O2' | 31:9:21:G:H5' | 2.02 | 0.60 |
| 31:9:76:G:C3' | 31:9:77:A:H5" | 2.21 | 0.60 |
| 10:J:107:ASN:HD22 | 10:J:109:TYR:H | 1.48 | 0.60 |
| 13:M:84:LYS:HA | 29:3:46:ILE:O | 2.01 | 0.60 |
| 18:R:96:VAL:HG13 | 18:R:106:GLY:HA3 | 1.84 | 0.60 |
| 29:3:25:VAL:HG22 | 29:3:68:LYS:HG3 | 1.84 | 0.60 |
| 30:0:396:U:H3' | 38:0:3920:HOH:O | 2.00 | 0.60 |
| 30:0:851:C:O2 | 30:0:2022:A:H2 | 1.85 | 0.60 |
| 13:M:77:HIS:HB2 | 13:M:81:ARG:HH21 | 1.66 | 0.60 |
| 29:3:3:MET:SD | 29:3:88:LEU:HD11 | 2.41 | 0.60 |
| 30:0:182:G:H5' | 38:0:5152:HOH:O | 2.01 | 0.60 |
| 30:0:282:C:O2' | 30:0:283:U:C5' | 2.48 | 0.60 |
| 30:0:333:G:O2' | 30:0:334:G:H5' | 2.01 | 0.60 |
| 30:0:946:C:H2' | 30:0:947:U:C6 | 2.35 | 0.60 |
| 30:0:2659:U:H5" | 38:0:4122:HOH:O | 2.02 | 0.60 |
| 5:E:24:GLY:HA3 | 5:E:76:VAL:HB | 1.82 | 0.60 |
| 16:P:115:SER:N | 16:P:118:GLN:HE21 | 1.92 | 0.60 |
| 30:0:228:C:H2' | 30:0:229:G:H5' | 1.82 | 0.60 |
| 30:0:90:A:H2' | 30:0:91:G:O4' | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:671:A:O2' | 30:0:672:G:H2' | 2.02 | 0.60 |
| 1:A:217:ARG:HG2 | 1:A:229:ALA:HB2 | 1.84 | 0.60 |
| 19:S:33:SER:O | 19:S:37:VAL:HG23 | 2.02 | 0.60 |
| 23:W:6:GLN:CB | 23:W:26:ILE:HD11 | 2.30 | 0.60 |
| 30:0:293:A:O2' | 30:0:294:C:H5' | 2.02 | 0.60 |
| 30:0:2793:A:H2' | 38:0:4488:HOH:O | 2.02 | 0.60 |
| 3:C:184:ARG:NH2 | 30:0:450:C:OP1 | 2.29 | 0.60 |
| 26:Z:37:ARG:HB2 | 30:0:819:A:C4' | 2.32 | 0.60 |
| 26:Z:53:ILE:O | 26:Z:57:MET:HB2 | 2.02 | 0.60 |
| 30:0:453:A:H5" | 38:0:3254:HOH:O | 2.02 | 0.60 |
| 30:0:1183:C:H42 | 30:0:1184:C:H41 | 1.50 | 0.60 |
| 30:0:2769:C:H2' | 30:0:2770:G:C5' | 2.31 | 0.60 |
| 1:A:35:GLY:O | 1:A:36:ASP:HB3 | 2.02 | 0.59 |
| 11:K:4:LEU:HD22 | 11:K:116:GLU:HB3 | 1.83 | 0.59 |
| 21:U:39:ASN:HB3 | 38:U:3805:HOH:O | 2.02 | 0.59 |
| 27:1:9:GLY:HA2 | 30:0:1687:C:O2 | 2.02 | 0.59 |
| 2:B:154:VAL:CG1 | 2:B:156:LYS:HG2 | 2.31 | 0.59 |
| 2:B:258:GLY:H | 2:B:260:HIS:CE1 | 2.20 | 0.59 |
| 30:0:2812:A:H1' | 38:0:5773:HOH:O | 2.01 | 0.59 |
| 31:9:63:C:O2' | 31:9:64:C:H5' | 2.02 | 0.59 |
| 14:N:159:TYR:CE1 | 31:9:50:G:H5" | 2.37 | 0.59 |
| 27:1:1:THR:HB | 38:0:7134:HOH:O | 2.02 | 0.59 |
| 27:1:10:LYS:HG3 | 38:1:2979:HOH:O | 2.01 | 0.59 |
| 30:0:1058:A:H2' | 30:0:1060:C:H5" | 1.83 | 0.59 |
| 30:0:1819:G:H2' | 30:0:1820:G:H4' | 1.82 | 0.59 |
| 30:0:1973:A:H5' | 30:0:1973:A:C8 | 2.35 | 0.59 |
| 30:0:747:G:H5' | 38:0:4947:HOH:O | 2.02 | 0.59 |
| 30:0:2321:A:H2 | 30:0:2378:U:N3 | 1.92 | 0.59 |
| 30:0:2472:C:O2' | 30:0:2634:G:H4' | 2.02 | 0.59 |
| 31:9:39:U:H1' | 31:9:44:A:N6 | 2.15 | 0.59 |
| 9:I:112:LEU:CD1 | 30:0:1162:G:H1' | 2.32 | 0.59 |
| 30:0:247:A:H2' | 38:0:3921:HOH:O | 2.02 | 0.59 |
| 30:0:2498:C:O2' | 30:0:2499:U:H5' | 2.03 | 0.59 |
| 30:0:2670:G:O2' | 30:0:2671:U:H5' | 2.02 | 0.59 |
| 30:0:2689:A:H2' | 30:0:2690:U:H5' | 1.85 | 0.59 |
| 3:C:174:ILE:HD11 | 30:0:338:C:H4' | 1.85 | 0.59 |
| 13:M:9:ARG:HD2 | 30:0:380:A:OP2 | 2.02 | 0.59 |
| 17:Q:11:ARG:NH2 | 30:0:2363:G:H4' | 2.18 | 0.59 |
| 18:R:17:MET:HE3 | 18:R:19:ARG:NH2 | 2.17 | 0.59 |
| 21:U:6:CYS:SG | 21:U:32:CYS:HB3 | 2.43 | 0.59 |
| 26:Z:64:PRO:HB2 | 26:Z:86:TYR:CE2 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:3:51:LYS:HB3 | 30:0:219:G:O2' | 2.03 | 0.59 |
| 30:0:468:U:H3' | 38:0:7561:HOH:O | 2.03 | 0.59 |
| 30:0:1201:C:H5" | 38:0:6132:HOH:O | 2.02 | 0.59 |
| 30:0:1904:A:H2' | 30:0:1905:U:O4' | 2.02 | 0.59 |
| 17:Q:26:PRO:O | 17:Q:30:VAL:HG22 | 2.02 | 0.59 |
| 30:0:214:U:H5' | 38:0:6123:HOH:O | 2.01 | 0.59 |
| 30:0:1116:U:HO2' | 30:0:1118:A:H2 | 0.72 | 0.59 |
| 30:0:1377:C:H5' | 30:0:1377:C:H6 | 1.67 | 0.59 |
| 4:D:62:ASP:HA | 38:D:4233:HOH:O | 2.03 | 0.59 |
| 30:0:319:A:H4' | 30:0:338:C:C4 | 2.38 | 0.59 |
| 30:0:1187:U:H2' | 38:0:6882:HOH:O | 2.02 | 0.59 |
| 30:0:1634:G:H3' | 38:0:3889:HOH:O | 2.02 | 0.59 |
| 30:0:2250:G:H2' | 30:0:2251:G:O4' | 2.03 | 0.59 |
| 15:O:25:VAL:HG12 | 30:0:709:G:O2' | 2.03 | 0.59 |
| 30:0:827:A:H1' | 38:0:6196:HOH:O | 2.02 | 0.59 |
| 2:B:68:THR:HG21 | 21:U:16:GLY:HA3 | 1.85 | 0.58 |
| 18:R:40:ALA:O | 18:R:44:VAL:HG23 | 2.03 | 0.58 |
| 20:T:48:VAL:HG11 | 20:T:96:VAL:HG13 | 1.85 | 0.58 |
| 29:3:3:MET:O | 29:3:90:PHE:HA | 2.03 | 0.58 |
| 30:0:1118:A:C8 | 30:0:1118:A:C3' | 2.74 | 0.58 |
| 30:0:1175:G:H1' | 30:0:1193:A:C2' | 2.31 | 0.58 |
| 2:B:195:ARG:HE | 2:B:323:LEU:HD13 | 1.68 | 0.58 |
| 30:0:542:A:H5' | 30:0:542:A:C8 | 2.29 | 0.58 |
| 30:0:1603:A:H5' | 30:0:1605:G:C4' | 2.33 | 0.58 |
| 30:0:2353:A:H4' | 30:0:2354:A:O5' | 2.02 | 0.58 |
| 2:B:256:GLN:HG2 | 38:B:9129:HOH:O | 2.03 | 0.58 |
| 4:D:25:MET:HE3 | 4:D:37:ALA:HB1 | 1.84 | 0.58 |
| 30:0:482:G:H4' | 30:0:508:A:N1 | 2.18 | 0.58 |
| 30:0:669:G:O2' | 30:0:670:G:H5' | 2.03 | 0.58 |
| 30:0:918:G:H5" | 38:0:9099:HOH:O | 2.01 | 0.58 |
| 30:0:1393:A:H2' | 30:0:1394:C:C6 | 2.38 | 0.58 |
| 30:0:1929:G:H1' | 38:0:5153:HOH:O | 2.03 | 0.58 |
| 31:9:54:A:C2' | 31:9:55:U:H5' | 2.33 | 0.58 |
| 1:A:199:HIS:CD2 | 1:A:201:PHE:H | 2.21 | 0.58 |
| 30:0:657:G:H2' | 30:0:658:C:C6 | 2.38 | 0.58 |
| 30:0:1127:C:C5 | 30:0:1128:U:C4 | 2.91 | 0.58 |
| 30:0:1161:A:O5' | 30:0:1161:A:H8 | 1.85 | 0.58 |
| 2:B:307:ARG:HG3 | 2:B:307:ARG:NH1 | 2.19 | 0.58 |
| 3:C:2:GLN:HB3 | 38:C:8594:HOH:O | 2.04 | 0.58 |
| 12:L:30:ARG:HD2 | 30:0:164:G:H5" | 1.85 | 0.58 |
| 12:L:133:VAL:HA | 38:L:9035:HOH:O | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:M:68:ARG:HH21 | 13:M:73:ARG:HD3 | 1.65 | 0.58 |
| 30:0:812:A:H2' | 30:0:813:C:C6 | 2.38 | 0.58 |
| 30:0:962:C:H2' | 30:0:963:C:C5' | 2.33 | 0.58 |
| 2:B:41:PHE:CZ | 2:B:79:MET:HG3 | 2.39 | 0.58 |
| 7:G:64:ASN:HD22 | 7:G:64:ASN:N | 1.99 | 0.58 |
| 12:L:80:ASP:HB2 | 12:L:90:ARG:O | 2.03 | 0.58 |
| 13:M:157:ASP:HB3 | 13:M:160:PHE:HD1 | 1.68 | 0.58 |
| 30:0:69:A:H5' | 30:0:69:A:H8 | 1.69 | 0.58 |
| 30:0:416:G:H3' | 38:0:9910:HOH:O | 2.02 | 0.58 |
| 30:0:696:C:O2' | 30:0:697:G:H5' | 2.03 | 0.58 |
| 30:0:814:G:H4' | 38:0:3124:HOH:O | 2.03 | 0.58 |
| 30:0:858:U:H5 | 38:0:5421:HOH:O | 1.86 | 0.58 |
| 30:0:2256:G:O2' | 30:0:2257:G:H5' | 2.04 | 0.58 |
| 30:0:2878:U:H2' | 30:0:2879:A:O4' | 2.02 | 0.58 |
| 30:0:2900:G:H2' | 30:0:2901:C:O4' | 2.03 | 0.58 |
| 2:B:125:GLU:O | 2:B:129:ARG:HG3 | 2.03 | 0.58 |
| 3:C:236:THR:HA | 38:C:8660:HOH:O | 2.04 | 0.58 |
| 25:Y:133:HIS:HD2 | 38:Y:8886:HOH:O | 1.85 | 0.58 |
| 28:2:41:HIS:CD2 | 28:2:43:ARG:H | 2.22 | 0.58 |
| 30:0:244:C:H6 | 30:0:244:C:O5' | 1.87 | 0.58 |
| 30:0:541:C:O2' | 30:0:542:A:H5" | 2.03 | 0.58 |
| 30:0:2276:U:H1' | 38:0:9608:HOH:O | 2.04 | 0.58 |
| 1:A:109:GLU:HG2 | 1:A:116:GLY:H | 1.69 | 0.58 |
| 13:M:30:GLU:O | 13:M:34:GLU:HG3 | 2.04 | 0.58 |
| 13:M:81:ARG:HG3 | 30:0:161:A:OP1 | 2.04 | 0.58 |
| 30:0:1221:G:H8 | 38:0:5971:HOH:O | 1.87 | 0.58 |
| 30:0:1819:G:H2' | 30:0:1820:G:C5' | 2.34 | 0.58 |
| 30:0:2064:U:H5' | 30:0:2652:U:H4' | 1.86 | 0.58 |
| 31:9:1:U:C4' | 31:9:3:A:OP1 | 2.52 | 0.58 |
| 29:3:60:LYS:HB2 | 30:0:2460:A:OP1 | 2.04 | 0.58 |
| 31:9:64:C:C2' | 31:9:65:A:H5' | 2.33 | 0.58 |
| 13:M:28:GLN:O | 13:M:32:ARG:HG3 | 2.02 | 0.58 |
| 22:V:1:THR:HG23 | 22:V:2:VAL:H | 1.69 | 0.58 |
| 23:W:64:THR:O | 23:W:68:THR:HG22 | 2.04 | 0.58 |
| 30:0:316:A:N3 | 30:0:336:G:O2' | 2.35 | 0.58 |
| 30:0:1205:U:C2' | 30:0:1206:U:C5' | 2.81 | 0.58 |
| 30:0:2867:G:H2' | 30:0:2868:C:C6 | 2.39 | 0.58 |
| 3:C:25:PRO:HG2 | 38:C:8522:HOH:O | 2.03 | 0.57 |
| 5:E:143:GLN:NE2 | 30:0:2779:G:H21 | 2.01 | 0.57 |
| 18:R:71:LYS:HE2 | 30:0:2831:C:O3' | 2.04 | 0.57 |
| 26:Z:80:GLN:HG3 | 26:Z:81:CYS:N | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1829:A:C2' | 30:0:1830:C:H5' | 2.34 | 0.57 |
| 31:9:12:C:H5' | 31:9:70:U:O4' | 2.04 | 0.57 |
| 30:0:553:G:H5' | 38:0:3481:HOH:O | 2.04 | 0.57 |
| 30:0:695:C:O2' | 30:0:696:C:H5' | 2.04 | 0.57 |
| 30:0:1626:A:H2' | 30:0:1627:G:C5' | 2.35 | 0.57 |
| 30:0:1664:A:H8 | 30:0:1664:A:OP1 | 1.87 | 0.57 |
| 30:0:2499:U:H2' | 30:0:2500:C:H6 | 1.69 | 0.57 |
| 31:9:108:C:H2' | 31:9:109:G:C8 | 2.38 | 0.57 |
| 4:D:58:VAL:HB | 4:D:62:ASP:HB2 | 1.86 | 0.57 |
| 12:L:14:GLY:O | 30:0:1295:G:H5" | 2.04 | 0.57 |
| 30:0:1197:G:H1' | 30:0:1203:G:N2 | 2.19 | 0.57 |
| 30:0:1494:A:C4 | 30:0:1495:C:C5 | 2.93 | 0.57 |
| 16:P:81:LYS:O | 30:0:1761:U:H5' | 2.04 | 0.57 |
| 19:S:55:GLN:NE2 | 30:0:1446:U:H2' | 2.19 | 0.57 |
| 20:T:26:THR:HA | 20:T:39:ASN:HB3 | 1.86 | 0.57 |
| 29:3:69:TYR:HD1 | 29:3:78:HIS:O | 1.87 | 0.57 |
| 30:0:544:G:C3' | 30:0:545:G:H5" | 2.35 | 0.57 |
| 30:0:558:C:H2' | 30:0:559:U:H5" | 1.81 | 0.57 |
| 30:0:1395:C:H2' | 30:0:1396:C:C6 | 2.39 | 0.57 |
| 30:0:2269:C:C2' | 30:0:2270:G:H5' | 2.34 | 0.57 |
| 31:9:49:G:O2' | 31:9:50:G:H5' | 2.05 | 0.57 |
| 1:A:192:VAL:CG1 | 1:A:207:GLN:HB3 | 2.34 | 0.57 |
| 30:0:318:U:H5' | 30:0:339:A:C2 | 2.39 | 0.57 |
| 30:0:2563:U:H2' | 30:0:2565:C:O5' | 2.04 | 0.57 |
| 30:0:2840:A:H3' | 38:0:7638:HOH:O | 2.04 | 0.57 |
| 19:S:51:GLN:HE21 | 19:S:53:ASN:HD21 | 1.52 | 0.57 |
| 30:0:1919:A:H4' | 38:0:4844:HOH:O | 2.04 | 0.57 |
| 30:0:2300:A:H4' | 30:0:2301:A:O5' | 2.05 | 0.57 |
| 5:E:81:GLU:HG2 | 5:E:134:SER:HB3 | 1.85 | 0.57 |
| 9:I:126:THR:O | 9:I:130:LEU:HG | 2.03 | 0.57 |
| 25:Y:130:ARG:HD2 | 38:Y:8857:HOH:O | 2.04 | 0.57 |
| 30:0:957:A:H8 | 30:0:957:A:O5' | 1.88 | 0.57 |
| 30:0:1165:G:O3' | 30:0:1174:A:H4' | 2.04 | 0.57 |
| 30:0:1201:C:H2' | 30:0:1202:A:H5' | 1.85 | 0.57 |
| 3:C:101:ASP:HB2 | 30:0:750:A:O3' | 2.05 | 0.57 |
| 8:H:146:ALA:O | 8:H:149:VAL:HG12 | 2.04 | 0.57 |
| 14:N:4:PRO:HD2 | 38:0:6759:HOH:O | 2.04 | 0.57 |
| 30:0:2531:U:O2' | 30:0:2532:A:H5' | 2.05 | 0.57 |
| 31:9:114:G:H2' | 31:9:115:C:C6 | 2.39 | 0.57 |
| 4:D:65:GLU:HA | 38:D:6752:HOH:O | 2.05 | 0.57 |
| 5:E:69:ILE:HA | 5:E:72:MET:HE3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:O:73:ASP:HA | 15:O:92:VAL:O | 2.05 | 0.57 |
| 20:T:53:GLY:HA3 | 38:T:6384:HOH:O | 2.04 | 0.57 |
| 23:W:81:ASP:OD1 | 23:W:92:ASP:HB2 | 2.05 | 0.57 |
| 30:0:1200:A:H3' | 38:0:5738:HOH:O | 2.05 | 0.57 |
| 30:0:1482:A:H1' | 38:0:9425:HOH:O | 2.04 | 0.57 |
| 30:0:2032:U:H2' | 30:0:2033:G:C5' | 2.35 | 0.57 |
| 2:B:102:THR:HG23 | 2:B:182:VAL:HG12 | 1.85 | 0.57 |
| 23:W:137:GLN:NE2 | 23:W:141:HIS:HE1 | 1.99 | 0.57 |
| 29:3:25:VAL:HG12 | 38:0:9267:HOH:O | 2.04 | 0.57 |
| 30:0:1697:G:H4' | 38:0:9342:HOH:O | 2.05 | 0.57 |
| 30:0:2437:A:H2' | 30:0:2438:G:C8 | 2.40 | 0.57 |
| 30:0:2768:A:H2' | 30:0:2769:C:O4' | 2.05 | 0.57 |
| 30:0:2831:C:H2' | 30:0:2832:C:C5' | 2.35 | 0.57 |
| 2:B:307:ARG:HB3 | 38:B:9126:HOH:O | 2.04 | 0.56 |
| 30:0:589:U:H2' | 30:0:590:A:H8 | 1.69 | 0.56 |
| 30:0:1202:A:H2' | 30:0:1203:G:C5' | 2.34 | 0.56 |
| 30:0:1748:U:C5 | 30:0:1749:U:C5 | 2.92 | 0.56 |
| 30:0:2324:G:H1' | 38:0:6095:HOH:O | 2.04 | 0.56 |
| 2:B:229:ARG:HD2 | 38:0:9111:HOH:O | 2.04 | 0.56 |
| 2:B:297:VAL:HB | 38:B:9075:HOH:O | 2.03 | 0.56 |
| 3:C:214:THR:HG23 | 38:C:8649:HOH:O | 2.04 | 0.56 |
| 4:D:135:VAL:HG21 | 4:D:139:TYR:CD1 | 2.39 | 0.56 |
| 22:V:39:ALA:H | 22:V:40:PRO:HD2 | 1.69 | 0.56 |
| 26:Z:45:VAL:HA | 26:Z:48:ARG:HB3 | 1.87 | 0.56 |
| 30:0:1511:U:O2' | 30:0:1512:G:H5' | 2.05 | 0.56 |
| 30:0:2032:U:O2' | 30:0:2033:G:H5" | 2.04 | 0.56 |
| 30:0:2758:G:H2' | 30:0:2759:C:C6 | 2.40 | 0.56 |
| 30:0:2824:C:O3' | 30:0:2825:C:H6 | 1.88 | 0.56 |
| 2:B:212:GLN:HB2 | 2:B:257:THR:HG21 | 1.87 | 0.56 |
| 2:B:244:PRO:HB3 | 30:0:1234:U:N3 | 2.20 | 0.56 |
| 3:C:88:SER:HB3 | 3:C:91:PRO:HB3 | 1.87 | 0.56 |
| 3:C:138:VAL:HG11 | 3:C:160:LEU:HD13 | 1.87 | 0.56 |
| 8:H:31:ILE:HD11 | 8:H:65:LEU:HD23 | 1.87 | 0.56 |
| 8:H:49:GLN:HG3 | 8:H:140:TYR:CE2 | 2.40 | 0.56 |
| 14:N:61:ALA:HB3 | 14:N:88:ALA:HB2 | 1.88 | 0.56 |
| 21:U:56:ARG:HD2 | 30:0:2890:A:N9 | 2.20 | 0.56 |
| 24:X:71:ARG:HD3 | 38:X:2171:HOH:O | 2.04 | 0.56 |
| 30:0:594:C:O2' | 30:0:595:U:H5' | 2.05 | 0.56 |
| 30:0:708:A:H2' | 30:0:709:G:O4' | 2.05 | 0.56 |
| 30:0:962:C:C2' | 30:0:963:C:H5' | 2.35 | 0.56 |
| 30:0:1206:U:H6 | 30:0:1206:U:C5' | 2.14 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1426:C:H2' | 38:0:9592:HOH:O | 2.04 | 0.56 |
| 31:9:18:U:H2' | 31:9:19:G:C8 | 2.40 | 0.56 |
| 31:9:38:A:H2' | 31:9:39:U:C6 | 2.41 | 0.56 |
| 30:0:28:G:H1' | 38:0:4676:HOH:O | 2.04 | 0.56 |
| 30:0:31:C:H4' | 38:0:7417:HOH:O | 2.04 | 0.56 |
| 30:0:1202:A:C2' | 30:0:1203:G:H5' | 2.35 | 0.56 |
| 30:0:1236:A:C2' | 30:0:1237:U:H5' | 2.36 | 0.56 |
| 5:E:93:MET:HE1 | 5:E:165:GLY:N | 2.21 | 0.56 |
| 29:3:67:LEU:HD21 | 29:3:88:LEU:HD21 | 1.86 | 0.56 |
| 30:0:941:G:C5 | 30:0:942:U:C4 | 2.94 | 0.56 |
| 30:0:1523:G:H2' | 30:0:1524:U:C6 | 2.41 | 0.56 |
| 30:0:2248:C:H2' | 30:0:2249:G:H8 | 1.70 | 0.56 |
| 30:0:2703:A:H2' | 30:0:2704:C:C6 | 2.37 | 0.56 |
| 38:B:9106:HOH:O | 30:0:2672:C:H1' | 2.05 | 0.56 |
| 14:N:58:LEU:N | 14:N:58:LEU:HD12 | 2.20 | 0.56 |
| 20:T:61:GLU:HG2 | 38:T:3851:HOH:O | 2.06 | 0.56 |
| 22:V:55:ARG:O | 22:V:59:ILE:HG12 | 2.06 | 0.56 |
| 26:Z:37:ARG:H | 26:Z:37:ARG:HD3 | 1.71 | 0.56 |
| 30:0:1559:A:OP2 | 30:0:1559:A:H8 | 1.87 | 0.56 |
| 13:M:24:GLN:HE21 | 13:M:27:ARG:NH1 | 2.03 | 0.56 |
| 30:0:711:G:C2 | 30:0:718:C:C2 | 2.93 | 0.56 |
| 30:0:1342:C:C2' | 30:0:1343:C:H5' | 2.35 | 0.56 |
| 30:0:1504:A:H5' | 38:0:4410:HOH:O | 2.06 | 0.56 |
| 31:9:52:A:O2' | 31:9:53:G:H5' | 2.06 | 0.56 |
| 19:S:37:VAL:O | 19:S:41:VAL:HG23 | 2.04 | 0.56 |
| 21:U:56:ARG:HG3 | 21:U:56:ARG:NH1 | 2.18 | 0.56 |
| 26:Z:51:ALA:O | 26:Z:55:SER:HB2 | 2.05 | 0.56 |
| 30:0:119:A:H2' | 30:0:120:A:H5" | 1.87 | 0.56 |
| 30:0:1537:C:H1' | 38:0:6573:HOH:O | 2.05 | 0.56 |
| 30:0:1574:C:H2' | 30:0:1575:C:H6 | 1.70 | 0.56 |
| 30:0:2559:C:H4' | 38:0:7245:HOH:O | 2.06 | 0.56 |
| 10:J:70:PHE:CE1 | 30:0:2676:C:H4' | 2.40 | 0.56 |
| 19:S:51:GLN:NE2 | 19:S:53:ASN:HD21 | 2.04 | 0.56 |
| 28:2:41:HIS:CE1 | 30:0:1439:C:H5" | 2.41 | 0.56 |
| 30:0:1202:A:H2' | 30:0:1203:G:O4' | 2.06 | 0.56 |
| 30:0:1574:C:H2' | 30:0:1575:C:C6 | 2.41 | 0.56 |
| 30:0:1622:G:C2' | 30:0:1623:C:H5' | 2.36 | 0.56 |
| 30:0:1850:U:O4' | 30:0:1941:A:C2 | 2.59 | 0.56 |
| 30:0:2795:C:O2' | 30:0:2796:U:H5' | 2.05 | 0.56 |
| 30:0:2897:C:O2' | 30:0:2898:G:H5' | 2.06 | 0.56 |
| 30:0:290:C:O2' | 30:0:291:C:H5' | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1060:C:H6 | 30:0:1060:C:H5' | 1.71 | 0.56 |
| 30:0:1159:G:H21 | 30:0:1189:A:H8 | 1.53 | 0.56 |
| 30:0:1778:A:H2' | 30:0:1779:A:H5' | 1.87 | 0.56 |
| 30:0:2004:U:H2' | 30:0:2004:U:O2 | 2.05 | 0.56 |
| 30:0:2291:A:N9 | 30:0:2309:C:H5' | 2.21 | 0.56 |
| 1:A:112:PRO:HD3 | 1:A:152:CYS:SG | 2.46 | 0.55 |
| 8:H:59:GLN:HE21 | 8:H:129:ARG:NE | 2.01 | 0.55 |
| 26:Z:34:SER:HA | 30:0:797:A:H4' | 1.88 | 0.55 |
| 29:3:12:PRO:HD3 | 38:3:9032:HOH:O | 2.05 | 0.55 |
| 30:0:2316:G:H4' | 38:0:6075:HOH:O | 2.06 | 0.55 |
| 30:0:2906:A:H5' | 30:0:2907:C:O4' | 2.07 | 0.55 |
| 3:C:46:TYR:CE2 | 3:C:98:ARG:NH1 | 2.75 | 0.55 |
| 13:M:77:HIS:HB2 | 13:M:81:ARG:HE | 1.72 | 0.55 |
| 14:N:49:THR:HG22 | 14:N:56:ASP:HB3 | 1.88 | 0.55 |
| 22:V:42:ASN:HB3 | 38:V:7247:HOH:O | 2.06 | 0.55 |
| 24:X:23:HIS:HE1 | 30:0:2044:G:OP1 | 1.89 | 0.55 |
| 30:0:299:U:C2 | 30:0:300:U:C6 | 2.95 | 0.55 |
| 30:0:304:G:H1' | 30:0:347:A:N6 | 2.21 | 0.55 |
| 30:0:485:A:N3 | 30:0:487:G:H5" | 2.20 | 0.55 |
| 30:0:595:U:O2' | 30:0:596:C:H5' | 2.05 | 0.55 |
| 30:0:1594:C:O2' | 30:0:1607:A:H4' | 2.07 | 0.55 |
| 12:L:30:ARG:HD3 | 30:0:164:G:H4' | 1.87 | 0.55 |
| 30:0:1972:U:C2' | 30:0:1973:A:H5" | 2.36 | 0.55 |
| 30:0:2718:C:H6 | 30:0:2718:C:H5' | 1.71 | 0.55 |
| 30:0:2887:G:H2' | 30:0:2888:U:O4' | 2.07 | 0.55 |
| 22:V:4:HIS:HB3 | 38:V:6622:HOH:O | 2.06 | 0.55 |
| 26:Z:81:CYS:O | 26:Z:85:ASP:HA | 2.05 | 0.55 |
| 30:0:12:U:H2' | 30:0:13:G:H5' | 1.88 | 0.55 |
| 30:0:1361:C:H2' | 30:0:1362:U:H6 | 1.72 | 0.55 |
| 1:A:211:LYS:HB3 | 1:A:212:PRO:CD | 2.32 | 0.55 |
| 13:M:82:ARG:H | 13:M:82:ARG:HD3 | 1.72 | 0.55 |
| 23:W:38:THR:HG22 | 23:W:39:ASP:H | 1.72 | 0.55 |
| 29:3:2:GLN:HA | 29:3:89:GLU:O | 2.07 | 0.55 |
| 30:0:136:C:H2' | 30:0:137:U:O4' | 2.07 | 0.55 |
| 30:0:536:A:H3' | 38:0:5040:HOH:O | 2.06 | 0.55 |
| 30:0:699:C:C2 | 30:0:744:G:C2 | 2.95 | 0.55 |
| 30:0:1809:G:H1' | 38:0:7682:HOH:O | 2.06 | 0.55 |
| 30:0:1913:C:H2' | 30:0:1914:C:C6 | 2.41 | 0.55 |
| 1:A:54:PRO:HG2 | 1:A:160:ALA:HB3 | 1.89 | 0.55 |
| 1:A:88:ILE:HD13 | 1:A:100:PRO:HD3 | 1.88 | 0.55 |
| 13:M:164:THR:HG22 | 13:M:166:ALA:H | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:17:ARG:HB3 | 14:N:17:ARG:NH1 | 2.21 | 0.55 |
| 29:3:48:ASN:O | 30:0:170:U:H4' | 2.07 | 0.55 |
| 30:0:1342:C:O2' | 30:0:1343:C:H5' | 2.06 | 0.55 |
| 30:0:1762:C:H2' | 30:0:1763:C:H6 | 1.71 | 0.55 |
| 30:0:2451:G:H8 | 38:0:5174:HOH:O | 1.90 | 0.55 |
| 30:0:2812:A:C2 | 30:0:2814:A:N6 | 2.71 | 0.55 |
| 2:B:74:ILE:HD13 | 2:B:309:VAL:HG21 | 1.89 | 0.55 |
| 8:H:29:SER:HA | 8:H:62:HIS:CD2 | 2.41 | 0.55 |
| 12:L:56:LYS:HE3 | 30:0:2443:C:H1' | 1.89 | 0.55 |
| 30:0:876:A:H2' | 30:0:876:A:N3 | 2.22 | 0.55 |
| 30:0:2480:G:H3' | 38:0:4182:HOH:O | 2.07 | 0.55 |
| 6:F:59:ILE:CD1 | 30:0:263:U:C2 | 2.90 | 0.55 |
| 18:R:114:VAL:HA | 18:R:144:GLU:O | 2.06 | 0.55 |
| 30:0:945:U:H2' | 30:0:946:C:C6 | 2.42 | 0.55 |
| 30:0:1174:A:C5 | 30:0:1201:C:H4' | 2.41 | 0.55 |
| 30:0:1202:A:C8 | 30:0:1203:G:C8 | 2.95 | 0.55 |
| 30:0:1204:C:H2' | 30:0:1205:U:O4' | 2.06 | 0.55 |
| 30:0:1236:A:O2' | 30:0:1237:U:H5' | 2.07 | 0.55 |
| 30:0:1667:A:H5' | 30:0:1667:A:C8 | 2.34 | 0.55 |
| 30:0:2240:U:O2' | 30:0:2241:C:H5' | 2.06 | 0.55 |
| 19:S:57:THR:HG22 | 19:S:58:MET:N | 2.21 | 0.55 |
| 25:Y:182:PHE:HD2 | 25:Y:200:THR:O | 1.89 | 0.55 |
| 30:0:154:C:H2' | 30:0:155:C:H6 | 1.72 | 0.55 |
| 30:0:2416:G:H2' | 30:0:2417:C:C6 | 2.42 | 0.55 |
| 31:9:59:C:H4' | 38:9:9127:HOH:O | 2.06 | 0.55 |
| 1:A:192:VAL:HG12 | 38:A:9012:HOH:O | 2.06 | 0.55 |
| 2:B:41:PHE:HA | 2:B:79:MET:HE2 | 1.89 | 0.55 |
| 22:V:64:GLY:O | 22:V:65:ASP:HB2 | 2.07 | 0.55 |
| 30:0:807:A:H2' | 30:0:808:A:C8 | 2.41 | 0.55 |
| 30:0:2102:G:N3 | 30:0:2103:A:C6 | 2.75 | 0.55 |
| 1:A:237:GLY:O | 30:0:1939:U:H5" | 2.06 | 0.54 |
| 3:C:188:ARG:HD3 | 38:C:8571:HOH:O | 2.07 | 0.54 |
| 11:K:74:VAL:CG1 | 11:K:113:ILE:HG12 | 2.37 | 0.54 |
| 30:0:204:A:H2' | 30:0:205:U:H5' | 1.89 | 0.54 |
| 30:0:368:C:H2' | 30:0:369:G:H5' | 1.88 | 0.54 |
| 30:0:1377:C:H5' | 30:0:1377:C:C6 | 2.42 | 0.54 |
| 30:0:2869:G:H2' | 30:0:2870:C:H6 | 1.73 | 0.54 |
| 3:C:233:THR:HG22 | 3:C:234:VAL:N | 2.21 | 0.54 |
| 16:P:54:LYS:HB2 | 30:0:1717:A:H5" | 1.90 | 0.54 |
| 26:Z:46:SER:O | 26:Z:50:VAL:HB | 2.07 | 0.54 |
| 30:0:1878:G:C4' | 38:0:6104:HOH:O | 2.55 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:R:150:PRO:CG | 18:R:150:PRO:CB | 2.85 | 0.54 |
| 30:0:963:C:O2 | 30:0:1005:A:N1 | 2.39 | 0.54 |
| 30:0:1183:C:N3 | 30:0:1184:C:N4 | 2.55 | 0.54 |
| 30:0:1334:C:O2' | 30:0:1335:C:H5' | 2.07 | 0.54 |
| 30:0:2372:A:H2' | 30:0:2373:U:C6 | 2.43 | 0.54 |
| 30:0:2872:U:H2' | 30:0:2873:C:H6 | 1.73 | 0.54 |
| 2:B:201:ASP:HB2 | 2:B:312:ARG:HD2 | 1.88 | 0.54 |
| 25:Y:169:ARG:NE | 33:Y:8820:CL:CL | 2.73 | 0.54 |
| 30:0:561:G:H2' | 30:0:562:A:H8 | 1.73 | 0.54 |
| 30:0:1188:A:C5 | 30:0:1189:A:C2 | 2.95 | 0.54 |
| 30:0:1902:G:N2 | 30:0:1936:C:C2 | 2.75 | 0.54 |
| 20:T:52:ARG:HD2 | 30:0:317:A:H5" | 1.90 | 0.54 |
| 25:Y:216:ARG:HD2 | 38:Y:8874:HOH:O | 2.06 | 0.54 |
| 30:0:951:A:C2' | 30:0:952:G:H5' | 2.37 | 0.54 |
| 30:0:1969:A:O2' | 30:0:1970:G:H5' | 2.08 | 0.54 |
| 1:A:199:HIS:HD2 | 1:A:201:PHE:H | 1.55 | 0.54 |
| 4:D:76:ARG:NE | 31:9:44:A:O4' | 2.41 | 0.54 |
| 14:N:5:ARG:HB2 | 14:N:5:ARG:NH1 | 2.21 | 0.54 |
| 14:N:43:VAL:CG1 | 14:N:118:ILE:HD11 | 2.38 | 0.54 |
| 18:R:80:TYR:O | 30:0:2050:G:H5" | 2.08 | 0.54 |
| 30:0:314:G:N2 | 30:0:317:A:C8 | 2.75 | 0.54 |
| 30:0:703:G:O2' | 30:0:704:C:H5' | 2.07 | 0.54 |
| 30:0:2102:G:C2 | 30:0:2103:A:C6 | 2.95 | 0.54 |
| 1:A:211:LYS:HG2 | 38:0:7019:HOH:O | 2.08 | 0.54 |
| 6:F:2:VAL:HG22 | 6:F:57:GLU:OE1 | 2.06 | 0.54 |
| 7:G:20:VAL:O | 7:G:24:VAL:HG23 | 2.07 | 0.54 |
| 15:O:14:LEU:HG | 15:O:102:ILE:HD11 | 1.89 | 0.54 |
| 16:P:115:SER:H | 16:P:118:GLN:NE2 | 1.92 | 0.54 |
| 18:R:18:LEU:HB2 | 18:R:143:VAL:CG1 | 2.36 | 0.54 |
| 27:1:42:SER:HB2 | 38:1:354:HOH:O | 2.08 | 0.54 |
| 29:3:79:LEU:HD13 | 30:0:2457:U:H1' | 1.88 | 0.54 |
| 30:0:255:A:C5 | 30:0:256:C:C5 | 2.96 | 0.54 |
| 30:0:2321:A:H2' | 30:0:2321:A:N3 | 2.22 | 0.54 |
| 31:9:55:U:H4' | 31:9:56:A:H8 | 1.73 | 0.54 |
| 12:L:18:HIS:HD2 | 30:0:902:G:N7 | 2.05 | 0.54 |
| 12:L:41:HIS:H | 12:L:41:HIS:CD2 | 2.25 | 0.54 |
| 27:1:1:THR:HA | 38:0:9360:HOH:O | 2.07 | 0.54 |
| 30:0:120:A:H2' | 30:0:120:A:N3 | 2.22 | 0.54 |
| 30:0:535:G:C5 | 30:0:2063:U:C4 | 2.95 | 0.54 |
| 1:A:176:HIS:CD2 | 30:0:857:A:H4' | 2.43 | 0.54 |
| 1:A:190:ARG:HD2 | 30:0:1884:G:O6 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:J:39:VAL:HG13 | 10:J:106:GLY:O | 2.08 | 0.54 |
| 23:W:26:ILE:HB | 38:W:5420:HOH:O | 2.06 | 0.54 |
| 30:0:1130:U:H2' | 30:0:1131:G:O4' | 2.08 | 0.54 |
| 30:0:1202:A:O2' | 30:0:1203:G:H5' | 2.08 | 0.54 |
| 30:0:2326:C:H4' | 30:0:2412:G:C4' | 2.38 | 0.54 |
| 30:0:2589:U:H2' | 30:0:2590:U:C6 | 2.42 | 0.54 |
| 30:0:2638:G:H5' | 38:0:4923:HOH:O | 2.07 | 0.54 |
| 1:A:179:MET:HG2 | 1:A:186:TRP:HB2 | 1.89 | 0.54 |
| 2:B:98:THR:HG22 | 2:B:99:GLU:H | 1.73 | 0.54 |
| 3:C:237:GLU:HA | 38:C:8643:HOH:O | 2.08 | 0.54 |
| 11:K:82:ARG:NH2 | 11:K:115:ARG:HG2 | 2.22 | 0.54 |
| 14:N:4:PRO:HB2 | 30:0:1010:C:H4' | 1.89 | 0.54 |
| 14:N:147:ILE:HD11 | 31:9:49:G:O3' | 2.07 | 0.54 |
| 30:0:1163:G:H1 | 30:0:1184:C:N4 | 2.06 | 0.54 |
| 30:0:1176:C:H5 | 38:0:5727:HOH:O | 1.91 | 0.54 |
| 30:0:1714:C:O2' | 30:0:1715:C:H5' | 2.08 | 0.54 |
| 30:0:2344:G:H8 | 38:0:6641:HOH:O | 1.91 | 0.54 |
| 3:C:135:GLU:HB3 | 38:C:8586:HOH:O | 2.08 | 0.53 |
| 6:F:53:ASP:OD1 | 6:F:80:GLN:HB2 | 2.08 | 0.53 |
| 6:F:96:ALA:HA | 38:F:3111:HOH:O | 2.08 | 0.53 |
| 8:H:15:PRO:HG3 | 30:0:1053:G:OP1 | 2.08 | 0.53 |
| 14:N:37:ARG:NH1 | 31:9:6:C:C5' | 2.60 | 0.53 |
| 14:N:67:ALA:HA | 14:N:71:TRP:CB | 2.37 | 0.53 |
| 21:U:33:SER:O | 21:U:37:GLU:HG3 | 2.08 | 0.53 |
| 29:3:33:MET:SD | 30:0:2450:C:H4' | 2.48 | 0.53 |
| 30:0:1706:G:C6 | 30:0:1707:G:C6 | 2.96 | 0.53 |
| 30:0:2335:C:H2' | 30:0:2336:G:C8 | 2.43 | 0.53 |
| 21:U:51:TRP:HA | 21:U:56:ARG:HE | 1.72 | 0.53 |
| 29:3:48:ASN:HB3 | 30:0:170:U:H5' | 1.91 | 0.53 |
| 30:0:480:C:H4' | 38:0:7715:HOH:O | 2.08 | 0.53 |
| 30:0:962:C:H5" | 38:0:4907:HOH:O | 2.06 | 0.53 |
| 30:0:1379:A:H1' | 38:0:9690:HOH:O | 2.08 | 0.53 |
| 30:0:1506:U:H6 | 30:0:1506:U:H5' | 1.73 | 0.53 |
| 30:0:2347:C:H2' | 30:0:2348:C:H6 | 1.73 | 0.53 |
| 30:0:2712:G:H1' | 38:0:5829:HOH:O | 2.08 | 0.53 |
| 1:A:36:ASP:HB2 | 1:A:85:SER:H | 1.73 | 0.53 |
| 3:C:180:SER:HB2 | 38:C:8656:HOH:O | 2.06 | 0.53 |
| 10:J:107:ASN:HD21 | 10:J:109:TYR:HB2 | 1.74 | 0.53 |
| 11:K:98:VAL:HG13 | 11:K:102:GLU:HA | 1.90 | 0.53 |
| 23:W:88:THR:HG22 | 23:W:89:ASP:H | 1.74 | 0.53 |
| 30:0:311:C:H2' | 30:0:312:U:C6 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2546:U:H4' | 38:0:6160:HOH:O | 2.09 | 0.53 |
| 1:A:47:HIS:HD2 | 30:0:1654:U:H2' | 1.72 | 0.53 |
| 1:A:109:GLU:HG2 | 1:A:116:GLY:N | 2.23 | 0.53 |
| 14:N:55:ASP:OD2 | 31:9:7:G:H4' | 2.08 | 0.53 |
| 17:Q:40:HIS:HE1 | 30:0:949:U:O2' | 1.91 | 0.53 |
| 24:X:43:VAL:HG11 | 24:X:82:GLU:HA | 1.89 | 0.53 |
| 30:0:185:G:H4' | 30:0:186:A:OP1 | 2.08 | 0.53 |
| 31:9:13:A:O2' | 31:9:14:G:H5" | 2.09 | 0.53 |
| 31:9:39:U:H3' | 31:9:40:C:C5' | 2.39 | 0.53 |
| 31:9:60:C:O2' | 31:9:61:C:H5' | 2.08 | 0.53 |
| 31:9:117:G:H2' | 31:9:118:C:C6 | 2.44 | 0.53 |
| 13:M:164:THR:HG22 | 13:M:166:ALA:N | 2.23 | 0.53 |
| 30:0:1205:U:H2' | 30:0:1206:U:H5" | 1.88 | 0.53 |
| 30:0:2265:U:H2' | 30:0:2266:A:C8 | 2.43 | 0.53 |
| 31:9:64:C:H2' | 31:9:65:A:H5' | 1.90 | 0.53 |
| 6:F:13:GLU:OE2 | 6:F:78:GLU:HG2 | 2.09 | 0.53 |
| 30:0:363:C:O2' | 30:0:364:U:H5' | 2.09 | 0.53 |
| 30:0:517:U:H2' | 30:0:518:G:H5' | 1.90 | 0.53 |
| 30:0:1014:A:H5" | 31:9:101:G:O2' | 2.09 | 0.53 |
| 30:0:1269:G:H2' | 30:0:1270:U:C6 | 2.44 | 0.53 |
| 30:0:1523:G:C6 | 30:0:1524:U:O4 | 2.62 | 0.53 |
| 30:0:1553:C:H2' | 30:0:1554:C:H6 | 1.74 | 0.53 |
| 30:0:2112:A:C8 | 38:0:6930:HOH:O | 2.54 | 0.53 |
| 13:M:68:ARG:HG3 | 30:0:1469:C:OP1 | 2.09 | 0.53 |
| 18:R:39:THR:HB | 18:R:42:GLU:HG3 | 1.91 | 0.53 |
| 30:0:10:U:O4 | 30:0:532:A:OP2 | 2.27 | 0.53 |
| 30:0:2371:G:H5' | 38:0:5000:HOH:O | 2.07 | 0.53 |
| 2:B:102:THR:HG21 | 2:B:182:VAL:O | 2.09 | 0.53 |
| 16:P:134:VAL:O | 16:P:137:LEU:HB3 | 2.09 | 0.53 |
| 30:0:734:U:O2' | 30:0:736:A:N7 | 2.35 | 0.53 |
| 30:0:2578:G:H5' | 30:0:2578:G:C8 | 2.40 | 0.53 |
| 31:9:39:U:H3 | 31:9:42:C:H5" | 1.72 | 0.53 |
| 31:9:76:G:H3' | 31:9:77:A:C5' | 2.23 | 0.53 |
| 14:N:132:ASN:O | 14:N:135:VAL:HG12 | 2.09 | 0.53 |
| 30:0:312:U:C2 | 30:0:320:G:N2 | 2.77 | 0.53 |
| 30:0:454:U:C2 | 38:0:9033:HOH:O | 2.53 | 0.53 |
| 30:0:1224:G:H2' | 30:0:1225:C:C6 | 2.43 | 0.53 |
| 30:0:1940:C:H4' | 38:0:7336:HOH:O | 2.08 | 0.53 |
| 2:B:62:ARG:HA | 2:B:65:MET:CE | 2.39 | 0.53 |
| 2:B:199:TYR:HE2 | 2:B:268:ARG:HB2 | 1.74 | 0.53 |
| 14:N:42:HIS:HB3 | 14:N:62:HIS:HE1 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:160:SER:CB | 31:9:51:A:H5' | 2.39 | 0.53 |
| 23:W:13:MET:HE1 | 23:W:18:GLN:HA | 1.90 | 0.53 |
| 25:Y:152:LYS:HB3 | 25:Y:160:LYS:HG3 | 1.91 | 0.53 |
| 29:3:70:ARG:HA | 29:3:77:ALA:HB2 | 1.91 | 0.53 |
| 30:0:10:U:C4 | 30:0:532:A:C8 | 2.97 | 0.53 |
| 30:0:279:C:O2' | 30:0:280:C:H5' | 2.09 | 0.53 |
| 30:0:821:U:H2' | 30:0:822:C:H6 | 1.73 | 0.53 |
| 30:0:1515:A:H2' | 30:0:1516:U:C6 | 2.43 | 0.53 |
| 1:A:51:ARG:NH2 | 1:A:53:ALA:HB3 | 2.25 | 0.52 |
| 2:B:211:THR:HG23 | 30:0:2840:A:OP1 | 2.08 | 0.52 |
| 26:Z:61:HIS:HB3 | 38:Z:8710:HOH:O | 2.07 | 0.52 |
| 30:0:72:C:H5' | 38:0:5876:HOH:O | 2.10 | 0.52 |
| 30:0:853:C:H3' | 38:0:4548:HOH:O | 2.08 | 0.52 |
| 30:0:2438:G:H2' | 30:0:2439:C:O4' | 2.09 | 0.52 |
| 1:A:33:GLU:O | 1:A:34:ASP:HB2 | 2.09 | 0.52 |
| 3:C:94:THR:HG22 | 38:C:8687:HOH:O | 2.09 | 0.52 |
| 9:I:108:HIS:H | 9:I:109:PRO:HD2 | 1.74 | 0.52 |
| 24:X:30:MET:HE1 | 24:X:55:ASN:HA | 1.91 | 0.52 |
| 25:Y:154:ARG:HH22 | 30:0:1071:G:H4' | 1.74 | 0.52 |
| 27:1:2:GLY:O | 27:1:6:PRO:HG2 | 2.09 | 0.52 |
| 30:0:1180:U:H2' | 30:0:1181:A:O4' | 2.10 | 0.52 |
| 30:0:1201:C:H6 | 38:0:5738:HOH:O | 1.93 | 0.52 |
| 30:0:2506:A:N6 | 30:0:2511:A:O2' | 2.42 | 0.52 |
| 30:0:2748:G:H5' | 38:0:7534:HOH:O | 2.08 | 0.52 |
| 2:B:298:LYS:HD3 | 38:B:9095:HOH:O | 2.08 | 0.52 |
| 12:L:145:LEU:O | 12:L:148:GLU:HG3 | 2.09 | 0.52 |
| 14:N:32:PRO:HD2 | 14:N:99:GLU:O | 2.10 | 0.52 |
| 17:Q:21:ARG:HH12 | 30:0:2353:A:H1' | 1.74 | 0.52 |
| 23:W:68:THR:HG23 | 23:W:69:ARG:HG2 | 1.91 | 0.52 |
| 30:0:705:C:O2 | 30:0:705:C:H2' | 2.08 | 0.52 |
| 30:0:960:G:N3 | 30:0:960:G:H2' | 2.23 | 0.52 |
| 30:0:1311:G:C2 | 30:0:1312:G:C8 | 2.96 | 0.52 |
| 30:0:1441:G:O2' | 30:0:1442:A:H5' | 2.09 | 0.52 |
| 30:0:2499:U:H2' | 30:0:2500:C:C6 | 2.44 | 0.52 |
| 2:B:18:ARG:HE | 2:B:256:GLN:NE2 | 2.06 | 0.52 |
| 13:M:73:ARG:HD2 | 13:M:73:ARG:N | 2.24 | 0.52 |
| 14:N:12:ARG:HD3 | 14:N:18:THR:OG1 | 2.10 | 0.52 |
| 30:0:324:G:O2' | 30:0:325:U:H5' | 2.09 | 0.52 |
| 30:0:506:G:N2 | 30:0:509:A:C5' | 2.66 | 0.52 |
| 30:0:1928:C:H2' | 30:0:1929:G:O4' | 2.09 | 0.52 |
| 30:0:2295:G:N3 | 30:0:2361:A:C2 | 2.77 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2864:U:O2' | 30:0:2865:G:H5' | 2.09 | 0.52 |
| 1:A:94:LEU:HD23 | 1:A:94:LEU:N | 2.24 | 0.52 |
| 4:D:58:VAL:CG1 | 4:D:60:GLU:HG2 | 2.40 | 0.52 |
| 5:E:80:TRP:O | 5:E:134:SER:HA | 2.10 | 0.52 |
| 20:T:28:SER:O | 20:T:32:ARG:HG3 | 2.10 | 0.52 |
| 23:W:38:THR:O | 23:W:42:ARG:HB2 | 2.09 | 0.52 |
| 30:0:107:U:H2' | 30:0:108:U:H5' | 1.92 | 0.52 |
| 30:0:1375:A:C2' | 30:0:1376:G:H5' | 2.39 | 0.52 |
| 30:0:2032:U:H2' | 30:0:2033:G:H5' | 1.91 | 0.52 |
| 30:0:2831:C:O2' | 30:0:2832:C:H5' | 2.10 | 0.52 |
| 31:9:56:A:C3' | 31:9:57:A:H5" | 2.39 | 0.52 |
| 5:E:118:ILE:HG23 | 5:E:144:THR:HG21 | 1.92 | 0.52 |
| 21:U:6:CYS:SG | 21:U:13:ILE:HD12 | 2.49 | 0.52 |
| 23:W:52:VAL:HG22 | 23:W:53:ALA:H | 1.75 | 0.52 |
| 30:0:297:U:H2' | 30:0:298:C:C6 | 2.43 | 0.52 |
| 2:B:49:THR:HG21 | 2:B:331:SER:O | 2.10 | 0.52 |
| 3:C:70:VAL:HG21 | 30:0:1361:C:H5' | 1.91 | 0.52 |
| 4:D:128:LEU:HB2 | 38:D:6007:HOH:O | 2.10 | 0.52 |
| 13:M:77:HIS:CE1 | 13:M:86:GLN:HG3 | 2.44 | 0.52 |
| 13:M:91:ILE:HG12 | 38:0:7539:HOH:O | 2.10 | 0.52 |
| 20:T:9:LYS:HE3 | 20:T:13:ARG:CZ | 2.40 | 0.52 |
| 30:0:64:G:H2' | 30:0:65:C:O4' | 2.10 | 0.52 |
| 30:0:694:A:H2' | 30:0:695:C:H5' | 1.90 | 0.52 |
| 30:0:1182:C:H1' | 30:0:1192:A:H8 | 1.74 | 0.52 |
| 30:0:1183:C:H2' | 30:0:1183:C:O2 | 2.08 | 0.52 |
| 30:0:1269:G:H2' | 30:0:1270:U:H6 | 1.75 | 0.52 |
| 30:0:1667:A:H2' | 30:0:1668:U:C6 | 2.44 | 0.52 |
| 30:0:2326:C:H4' | 30:0:2412:G:H4' | 1.91 | 0.52 |
| 13:M:46:LEU:HG | 38:M:8918:HOH:O | 2.08 | 0.52 |
| 13:M:89:THR:HA | 38:M:8851:HOH:O | 2.10 | 0.52 |
| 30:0:101:C:H2' | 30:0:102:A:C8 | 2.45 | 0.52 |
| 30:0:506:G:N2 | 30:0:508:A:H3' | 2.25 | 0.52 |
| 30:0:952:G:N3 | 30:0:2302:A:H2' | 2.25 | 0.52 |
| 30:0:1845:A:O2' | 30:0:1846:U:H5' | 2.10 | 0.52 |
| 30:0:1972:U:H2' | 30:0:1973:A:H5" | 1.90 | 0.52 |
| 30:0:1992:U:H2' | 30:0:1994:A:OP2 | 2.10 | 0.52 |
| 30:0:2111:G:H1' | 38:0:9051:HOH:O | 2.09 | 0.52 |
| 30:0:2420:G:C2' | 30:0:2421:G:H5' | 2.39 | 0.52 |
| 30:0:2584:G:H4' | 38:0:7109:HOH:O | 2.08 | 0.52 |
| 30:0:2689:A:C2' | 30:0:2690:U:H5' | 2.40 | 0.52 |
| 1:A:100:PRO:HG2 | 1:A:103:VAL:HG21 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:3:51:LYS:HA | 29:3:54:LYS:HD2 | 1.92 | 0.52 |
| 30:0:208:C:H3' | 38:0:6388:HOH:O | 2.10 | 0.52 |
| 30:0:553:G:O4' | 30:0:1325:G:H5' | 2.10 | 0.52 |
| 30:0:2549:C:O2' | 30:0:2550:U:H5' | 2.09 | 0.52 |
| 7:G:27:ILE:HD13 | 7:G:71:LEU:HD23 | 1.92 | 0.52 |
| 11:K:8:VAL:HG13 | 11:K:80:ILE:HG22 | 1.91 | 0.52 |
| 11:K:118:ALA:HA | 11:K:125:ALA:HB2 | 1.91 | 0.52 |
| 14:N:11:ARG:HG3 | 14:N:14:ARG:NH1 | 2.24 | 0.52 |
| 14:N:119:GLN:O | 14:N:123:ILE:HG13 | 2.10 | 0.52 |
| 18:R:119:VAL:HG21 | 18:R:142:ASP:CG | 2.31 | 0.52 |
| 23:W:4:LEU:HD22 | 23:W:52:VAL:HG21 | 1.91 | 0.52 |
| 23:W:4:LEU:O | 23:W:32:CYS:HA | 2.10 | 0.52 |
| 30:0:293:A:C4 | 30:0:360:A:C2 | 2.98 | 0.52 |
| 30:0:365:G:C6 | 30:0:366:U:C4 | 2.98 | 0.52 |
| 30:0:541:C:C2' | 30:0:542:A:C5' | 2.75 | 0.52 |
| 31:9:18:U:H2' | 31:9:19:G:H8 | 1.74 | 0.52 |
| 2:B:214:PRO:HD2 | 38:0:9078:HOH:O | 2.10 | 0.51 |
| 26:Z:42:TYR:HA | 30:0:1829:A:H61 | 1.74 | 0.51 |
| 29:3:64:LYS:HD2 | 30:0:2459:G:OP2 | 2.11 | 0.51 |
| 30:0:523:C:H2' | 30:0:524:A:C8 | 2.45 | 0.51 |
| 30:0:960:G:N3 | 30:0:960:G:C2' | 2.73 | 0.51 |
| 30:0:1189:A:H1' | 30:0:1209:C:H1' | 1.92 | 0.51 |
| 30:0:1495:C:H1' | 30:0:1573:A:H1' | 1.93 | 0.51 |
| 30:0:2526:C:O2' | 30:0:2527:U:H5' | 2.10 | 0.51 |
| 3:C:226:GLY:HA3 | 30:0:1308:A:O4' | 2.10 | 0.51 |
| 14:N:4:PRO:CB | 30:0:1010:C:H4' | 2.40 | 0.51 |
| 17:Q:45:PRO:O | 30:0:2365:G:H4' | 2.10 | 0.51 |
| 29:3:42:ARG:NH1 | 30:0:396:U:H5' | 2.25 | 0.51 |
| 30:0:1682:A:O2' | 30:0:1683:G:H5" | 2.10 | 0.51 |
| 31:9:22:G:H5' | 31:9:23:U:OP1 | 2.10 | 0.51 |
| 5:E:22:VAL:O | 5:E:76:VAL:HG11 | 2.10 | 0.51 |
| 11:K:41:LYS:HA | 30:0:2582:G:O3' | 2.11 | 0.51 |
| 14:N:102:LEU:HD13 | 14:N:119:GLN:HB2 | 1.92 | 0.51 |
| 22:V:44:GLY:O | 22:V:48:GLU:HG2 | 2.10 | 0.51 |
| 30:0:78:G:C6 | 30:0:79:G:C6 | 2.99 | 0.51 |
| 30:0:1185:U:H5' | 38:0:7461:HOH:O | 2.10 | 0.51 |
| 30:0:1805:G:O2' | 30:0:1806:G:H5' | 2.10 | 0.51 |
| 30:0:2004:U:H4' | 38:0:5299:HOH:O | 2.09 | 0.51 |
| 30:0:2344:G:H2' | 30:0:2344:G:N3 | 2.24 | 0.51 |
| 5:E:143:GLN:NE2 | 30:0:2780:C:H1' | 2.26 | 0.51 |
| 13:M:81:ARG:HG2 | 38:M:8926:HOH:O | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:O:105:ASN:HD21 | 15:O:109:SER:H | 1.58 | 0.51 |
| 30:0:255:A:C4 | 30:0:256:C:C6 | 2.98 | 0.51 |
| 30:0:282:C:C2' | 30:0:283:U:H5' | 2.40 | 0.51 |
| 30:0:2088:C:H1' | 30:0:2841:A:N1 | 2.25 | 0.51 |
| 30:0:2239:C:H2' | 30:0:2240:U:C6 | 2.46 | 0.51 |
| 30:0:2269:C:O2' | 30:0:2270:G:H5' | 2.10 | 0.51 |
| 30:0:2769:C:C2' | 30:0:2770:G:C5' | 2.88 | 0.51 |
| 3:C:150:THR:HA | 3:C:203:ALA:O | 2.11 | 0.51 |
| 8:H:141:CYS:HB2 | 38:H:8991:HOH:O | 2.10 | 0.51 |
| 28:2:2:LYS:HG3 | 30:0:1486:A:C5 | 2.45 | 0.51 |
| 30:0:1361:C:H2' | 30:0:1362:U:C6 | 2.45 | 0.51 |
| 30:0:1563:G:H4' | 38:0:4227:HOH:O | 2.10 | 0.51 |
| 30:0:1788:U:C2 | 30:0:1805:G:N2 | 2.79 | 0.51 |
| 30:0:2269:C:H2' | 30:0:2270:G:O4' | 2.09 | 0.51 |
| 1:A:97:ALA:HA | 1:A:131:HIS:NE2 | 2.26 | 0.51 |
| 22:V:12:THR:HG23 | 22:V:14:ALA:H | 1.75 | 0.51 |
| 26:Z:37:ARG:HB2 | 30:0:819:A:H4' | 1.92 | 0.51 |
| 30:0:343:C:O2' | 30:0:344:C:H5' | 2.11 | 0.51 |
| 30:0:466:A:H2' | 30:0:467:G:O4' | 2.10 | 0.51 |
| 30:0:646:G:H2' | 30:0:647:U:C6 | 2.46 | 0.51 |
| 30:0:1061:C:H1' | 30:0:2283:G:O6 | 2.10 | 0.51 |
| 30:0:1304:U:H2' | 30:0:1305:C:C6 | 2.46 | 0.51 |
| 30:0:2851:G:O2' | 30:0:2852:A:H5' | 2.11 | 0.51 |
| 3:C:21:VAL:HG13 | 38:C:8606:HOH:O | 2.09 | 0.51 |
| 13:M:24:GLN:NE2 | 13:M:27:ARG:NH1 | 2.58 | 0.51 |
| 13:M:86:GLN:HE22 | 30:0:2274:A:H1' | 1.74 | 0.51 |
| 14:N:163:PHE:HB3 | 38:N:8829:HOH:O | 2.11 | 0.51 |
| 21:U:47:ARG:HG3 | 38:U:4381:HOH:O | 2.10 | 0.51 |
| 22:V:56:ILE:O | 22:V:60:GLN:HG3 | 2.10 | 0.51 |
| 24:X:76:ARG:HG3 | 24:X:76:ARG:NH1 | 2.24 | 0.51 |
| 30:0:42:C:H1' | 38:0:4670:HOH:O | 2.09 | 0.51 |
| 30:0:1855:G:H4' | 30:0:1856:C:O5' | 2.10 | 0.51 |
| 30:0:1878:G:H1' | 38:0:6104:HOH:O | 2.11 | 0.51 |
| 30:0:2099:A:H2 | 38:0:3918:HOH:O | 1.93 | 0.51 |
| 30:0:2507:G:H2' | 30:0:2510:C:H42 | 1.75 | 0.51 |
| 30:0:2899:A:O2' | 30:0:2900:G:H5' | 2.10 | 0.51 |
| 31:9:3:A:OP2 | 31:9:25:G:N2 | 2.43 | 0.51 |
| 31:9:45:A:C5 | 31:9:46:C:C5 | 2.98 | 0.51 |
| 31:9:117:G:H2' | 31:9:118:C:H6 | 1.75 | 0.51 |
| 2:B:162:MET:HG3 | 2:B:310:ARG:HH11 | 1.75 | 0.51 |
| 5:E:133:VAL:HG12 | 5:E:141:VAL:HG13 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:137:ASP:O | 5:E:141:VAL:HG23 | 2.10 | 0.51 |
| 6:F:39:SER:OG | 6:F:45:ALA:HB2 | 2.11 | 0.51 |
| 10:J:70:PHE:CD1 | 30:0:2676:C:H4' | 2.46 | 0.51 |
| 14:N:114:LYS:O | 14:N:118:ILE:HG13 | 2.10 | 0.51 |
| 30:0:124:C:H3' | 38:0:7649:HOH:O | 2.10 | 0.51 |
| 30:0:703:G:H2' | 30:0:704:C:H6 | 1.76 | 0.51 |
| 30:0:1020:A:H1' | 38:0:7218:HOH:O | 2.11 | 0.51 |
| 30:0:1056:U:H2' | 30:0:1057:A:O4' | 2.10 | 0.51 |
| 30:0:1581:A:C5 | 30:0:1582:C:C5 | 2.99 | 0.51 |
| 30:0:1626:A:O2' | 30:0:1627:G:H5' | 2.10 | 0.51 |
| 30:0:2354:A:H5' | 30:0:2355:G:N7 | 2.26 | 0.51 |
| 30:0:2842:G:H2' | 30:0:2843:A:H5' | 1.92 | 0.51 |
| 1:A:132:ASP:CG | 1:A:133:ARG:H | 2.14 | 0.51 |
| 1:A:223:ARG:HG3 | 38:A:9021:HOH:O | 2.11 | 0.51 |
| 3:C:76:ARG:NH2 | 30:0:1363:G:OP1 | 2.44 | 0.51 |
| 17:Q:25:PRO:HB2 | 38:9:9082:HOH:O | 2.11 | 0.51 |
| 29:3:10:TYR:HD1 | 30:0:2408:A:HO2' | 1.52 | 0.51 |
| 30:0:615:G:H2' | 30:0:616:U:C6 | 2.46 | 0.51 |
| 30:0:920:C:H5' | 30:0:921:G:C4 | 2.46 | 0.51 |
| 30:0:1279:U:O2 | 30:0:1279:U:C2' | 2.58 | 0.51 |
| 30:0:1562:C:O2 | 30:0:1562:C:C2' | 2.59 | 0.51 |
| 30:0:1701:A:H5" | 30:0:1702:U:H3' | 1.93 | 0.51 |
| 1:A:207:GLN:HA | 38:A:8981:HOH:O | 2.10 | 0.51 |
| 5:E:116:THR:HG22 | 5:E:151:LEU:HD22 | 1.92 | 0.51 |
| 17:Q:28:ARG:HG2 | 38:9:9082:HOH:O | 2.11 | 0.51 |
| 20:T:71:VAL:HG11 | 20:T:90:PRO:CB | 2.38 | 0.51 |
| 30:0:168:C:O5' | 30:0:168:C:H6 | 1.92 | 0.51 |
| 30:0:255:A:C5 | 30:0:256:C:C4 | 2.99 | 0.51 |
| 30:0:1202:A:H2' | 30:0:1203:G:H5' | 1.92 | 0.51 |
| 30:0:1218:U:H2' | 30:0:1219:U:C6 | 2.46 | 0.51 |
| 30:0:1972:U:C2' | 30:0:1973:A:C5' | 2.89 | 0.51 |
| 30:0:2345:A:H3' | 30:0:2346:C:C6 | 2.45 | 0.51 |
| 6:F:34:ASN:HA | 13:M:4:ALA:HB2 | 1.93 | 0.50 |
| 14:N:164:ASP:OD1 | 14:N:167:ASP:HA | 2.11 | 0.50 |
| 17:Q:11:ARG:HH22 | 30:0:2363:G:C5' | 2.24 | 0.50 |
| 20:T:72:ILE:HD13 | 20:T:93:THR:HG22 | 1.92 | 0.50 |
| 26:Z:80:GLN:CG | 26:Z:81:CYS:H | 2.22 | 0.50 |
| 30:0:291:C:H2' | 30:0:292:G:O4' | 2.11 | 0.50 |
| 30:0:407:A:H5' | 38:0:6009:HOH:O | 2.11 | 0.50 |
| 30:0:1626:A:C2' | 30:0:1627:G:H5' | 2.41 | 0.50 |
| 1:A:179:MET:HG2 | 1:A:186:TRP:CB | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:72:THR:HB | 38:B:9075:HOH:O | 2.10 | 0.50 |
| 2:B:320:GLN:HE21 | 2:B:321:PRO:CD | 2.20 | 0.50 |
| 3:C:46:TYR:CE1 | 30:0:450:C:H4' | 2.45 | 0.50 |
| 30:0:151:A:H2' | 30:0:152:A:O4' | 2.11 | 0.50 |
| 30:0:1213:C:C2' | 30:0:1214:G:H5' | 2.42 | 0.50 |
| 30:0:2506:A:O2' | 30:0:2507:G:C8 | 2.49 | 0.50 |
| 33:0:8812:CL:CL | 38:0:5117:HOH:O | 2.57 | 0.50 |
| 2:B:238:ASN:HD22 | 2:B:240:GLY:N | 2.10 | 0.50 |
| 30:0:396:U:O2' | 30:0:397:A:P | 2.70 | 0.50 |
| 30:0:1589:G:H4' | 38:0:6843:HOH:O | 2.10 | 0.50 |
| 30:0:1934:A:C8 | 30:0:1935:C:C5 | 3.00 | 0.50 |
| 30:0:2758:G:H2' | 30:0:2759:C:H6 | 1.76 | 0.50 |
| 1:A:162:GLY:N | 26:Z:91:GLY:HA2 | 2.26 | 0.50 |
| 3:C:47:GLY:HA2 | 3:C:92:PRO:HB2 | 1.93 | 0.50 |
| 38:C:8676:HOH:O | 30:0:2100:A:H5' | 2.12 | 0.50 |
| 5:E:81:GLU:O | 5:E:172:PRO:HD3 | 2.12 | 0.50 |
| 13:M:139:PRO:HA | 13:M:142:GLN:HB2 | 1.93 | 0.50 |
| 21:U:9:CYS:HB2 | 38:U:6796:HOH:O | 2.12 | 0.50 |
| 23:W:5:VAL:HG22 | 23:W:32:CYS:HB2 | 1.94 | 0.50 |
| 25:Y:115:ARG:HH22 | 30:0:1266:U:H4' | 1.72 | 0.50 |
| 30:0:99:A:C8 | 30:0:100:C:C5 | 2.99 | 0.50 |
| 30:0:549:A:O2' | 30:0:550:C:H5' | 2.11 | 0.50 |
| 30:0:1189:A:O2' | 30:0:1208:C:H2' | 2.12 | 0.50 |
| 30:0:2533:C:H5' | 30:0:2533:C:C6 | 2.42 | 0.50 |
| 30:0:2724:U:H2' | 30:0:2725:G:O4' | 2.12 | 0.50 |
| 30:0:2896:A:N3 | 30:0:2896:A:H2' | 2.26 | 0.50 |
| 1:A:135:VAL:HG21 | 1:A:147:ARG:HB3 | 1.94 | 0.50 |
| 28:2:8:LYS:NZ | 30:0:1677:U:OP2 | 2.44 | 0.50 |
| 30:0:693:A:H2' | 30:0:694:A:C8 | 2.46 | 0.50 |
| 30:0:920:C:H4' | 30:0:921:G:C2 | 2.46 | 0.50 |
| 30:0:1118:A:H8 | 30:0:1119:G:H5" | 1.75 | 0.50 |
| 3:C:197:SER:HB3 | 38:C:8583:HOH:O | 2.12 | 0.50 |
| 13:M:72:ALA:HB3 | 38:M:8944:HOH:O | 2.12 | 0.50 |
| 13:M:184:ARG:HG3 | 13:M:185:PRO:HA | 1.93 | 0.50 |
| 16:P:41:ARG:HH22 | 30:0:1500:U:P | 2.34 | 0.50 |
| 17:Q:11:ARG:NH1 | 30:0:2363:G:O3' | 2.45 | 0.50 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:HG23 | 1.94 | 0.50 |
| 30:0:216:A:O2' | 30:0:217:C:H5' | 2.12 | 0.50 |
| 30:0:1180:U:O2' | 30:0:1181:A:H5' | 2.11 | 0.50 |
| 30:0:1183:C:N3 | 30:0:1184:C:C5 | 2.79 | 0.50 |
| 30:0:1759:A:N3 | 30:0:1818:C:H2' | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2072:G:C6 | 30:0:2533:C:H1' | 2.47 | 0.50 |
| 2:B:158:LYS:HB2 | 38:0:4101:HOH:O | 2.11 | 0.50 |
| 5:E:11:VAL:HG12 | 5:E:12:ASP:N | 2.27 | 0.50 |
| 6:F:36:THR:HG23 | 6:F:97:ALA:HB2 | 1.94 | 0.50 |
| 10:J:75:PRO:HD3 | 10:J:136:SER:OG | 2.12 | 0.50 |
| 23:W:4:LEU:CD2 | 23:W:54:PHE:HB3 | 2.39 | 0.50 |
| 30:0:39:G:C2 | 30:0:444:C:C2 | 3.00 | 0.50 |
| 30:0:559:U:H6 | 30:0:559:U:C5' | 2.20 | 0.50 |
| 30:0:820:G:H5' | 30:0:821:U:C5' | 2.41 | 0.50 |
| 30:0:1158:G:H2' | 30:0:1159:G:H5' | 1.93 | 0.50 |
| 30:0:1395:C:H2' | 30:0:1396:C:H6 | 1.77 | 0.50 |
| 30:0:1494:A:H1' | 30:0:1495:C:C6 | 2.47 | 0.50 |
| 30:0:1819:G:H2' | 30:0:1820:G:C4' | 2.42 | 0.50 |
| 30:0:2416:G:H2' | 30:0:2417:C:H6 | 1.76 | 0.50 |
| 30:0:2781:U:C2' | 30:0:2782:G:C5' | 2.89 | 0.50 |
| 10:J:82:THR:HG23 | 30:0:1242:A:C5' | 2.17 | 0.50 |
| 10:J:88:PRO:HD3 | 30:0:1104:C:H4' | 1.94 | 0.50 |
| 11:K:34:VAL:HG22 | 11:K:47:ALA:HB2 | 1.94 | 0.50 |
| 14:N:160:SER:HB3 | 31:9:51:A:H5' | 1.93 | 0.50 |
| 23:W:121:PRO:CA | 23:W:153:MET:HG2 | 2.42 | 0.50 |
| 30:0:204:A:C2' | 30:0:205:U:H5' | 2.41 | 0.50 |
| 30:0:441:A:C2 | 30:0:442:A:N6 | 2.80 | 0.50 |
| 30:0:523:C:H2' | 30:0:524:A:H8 | 1.77 | 0.50 |
| 30:0:1610:G:H2' | 30:0:1611:G:O4' | 2.12 | 0.50 |
| 30:0:1765:G:H1' | 30:0:1780:G:N2 | 2.26 | 0.50 |
| 30:0:2354:A:H5' | 30:0:2355:G:C5 | 2.46 | 0.50 |
| 30:0:2598:U:O2 | 30:0:2600:A:H8 | 1.95 | 0.50 |
| 31:9:61:C:H2' | 31:9:62:A:H8 | 1.76 | 0.50 |
| 10:J:22:VAL:O | 10:J:26:VAL:HG23 | 2.12 | 0.50 |
| 10:J:76:ASP:HA | 38:J:8863:HOH:O | 2.11 | 0.50 |
| 14:N:169:PRO:O | 14:N:172:PHE:HB3 | 2.12 | 0.50 |
| 27:1:28:HIS:HE1 | 30:0:776:A:OP1 | 1.95 | 0.50 |
| 30:0:932:U:H2' | 30:0:933:C:C6 | 2.47 | 0.50 |
| 30:0:1160:G:H5' | 30:0:1161:A:H5' | 0.83 | 0.50 |
| 30:0:1226:G:H5' | 38:0:4526:HOH:O | 2.11 | 0.50 |
| 30:0:1398:G:H2' | 30:0:1399:A:C8 | 2.47 | 0.50 |
| 30:0:1947:G:H2' | 30:0:1948:G:H8 | 1.77 | 0.50 |
| 30:0:2269:C:H2' | 30:0:2270:G:C5' | 2.42 | 0.50 |
| 30:0:2330:U:H4' | 30:0:2331:C:OP1 | 2.11 | 0.50 |
| 31:9:58:G:C8 | 31:9:59:C:C5 | 3.00 | 0.50 |
| 27:1:28:HIS:HD2 | 27:1:30:LYS:H | 1.58 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:88:G:H8 | 30:0:88:G:H5' | 1.76 | 0.49 |
| 30:0:299:U:N3 | 30:0:300:U:C5 | 2.80 | 0.49 |
| 30:0:1365:C:H4' | 38:0:4606:HOH:O | 2.12 | 0.49 |
| 30:0:1541:G:O2' | 30:0:1542:G:H5' | 2.11 | 0.49 |
| 30:0:1791:U:O2' | 30:0:1792:C:H5' | 2.12 | 0.49 |
| 30:0:2502:C:O2' | 30:0:2503:A:H5' | 2.12 | 0.49 |
| 1:A:153:ARG:HB2 | 1:A:153:ARG:HH11 | 1.77 | 0.49 |
| 6:F:48:VAL:HG23 | 6:F:74:PHE:CB | 2.41 | 0.49 |
| 13:M:94:ARG:HD2 | 30:0:158:A:OP2 | 2.11 | 0.49 |
| 15:O:24:ALA:HB3 | 30:0:710:G:OP1 | 2.12 | 0.49 |
| 18:R:117:HIS:HD2 | 30:0:20:G:H21 | 1.61 | 0.49 |
| 30:0:249:G:N2 | 30:0:250:C:C2 | 2.80 | 0.49 |
| 30:0:951:A:O2' | 30:0:952:G:H5' | 2.12 | 0.49 |
| 30:0:1188:A:C6 | 30:0:1189:A:C6 | 3.00 | 0.49 |
| 30:0:1964:U:H2' | 30:0:1964:U:O2 | 2.10 | 0.49 |
| 30:0:2705:U:H2' | 30:0:2706:A:H8 | 1.73 | 0.49 |
| 31:9:114:G:H2' | 31:9:115:C:H6 | 1.76 | 0.49 |
| 2:B:24:PRO:HG3 | 2:B:204:GLY:HA2 | 1.94 | 0.49 |
| 4:D:76:ARG:NH1 | 31:9:42:C:O2 | 2.45 | 0.49 |
| 5:E:15:GLN:HG2 | 5:E:16:ASP:N | 2.28 | 0.49 |
| 11:K:8:VAL:HG12 | 11:K:9:THR:N | 2.26 | 0.49 |
| 18:R:111:ILE:HG23 | 18:R:145:LEU:HD11 | 1.94 | 0.49 |
| 30:0:699:C:O2' | 30:0:744:G:H1' | 2.12 | 0.49 |
| 30:0:876:A:N3 | 30:0:876:A:C2' | 2.75 | 0.49 |
| 30:0:2002:C:H2' | 30:0:2003:U:H5' | 1.94 | 0.49 |
| 31:9:20:G:H3' | 38:9:9055:HOH:O | 2.12 | 0.49 |
| 31:9:49:G:H2' | 31:9:50:G:O4' | 2.12 | 0.49 |
| 23:W:11:VAL:HG11 | 30:0:1086:A:C6 | 2.48 | 0.49 |
| 23:W:90:TYR:N | 23:W:90:TYR:CD1 | 2.80 | 0.49 |
| 24:X:21:PRO:HG2 | 24:X:24:LYS:HD3 | 1.94 | 0.49 |
| 26:Z:38:PHE:HB3 | 26:Z:42:TYR:HD1 | 1.78 | 0.49 |
| 30:0:816:G:H5' | 30:0:1598:A:H4' | 1.94 | 0.49 |
| 30:0:1191:A:H2' | 30:0:1193:A:H5' | 1.95 | 0.49 |
| 30:0:1453:G:H2' | 30:0:1454:U:O4' | 2.13 | 0.49 |
| 30:0:2316:G:H8 | 38:0:5642:HOH:O | 1.95 | 0.49 |
| 2:B:212:GLN:HA | 30:0:1733:A:H4' | 1.94 | 0.49 |
| 6:F:50:VAL:HG13 | 6:F:60:VAL:HG11 | 1.95 | 0.49 |
| 11:K:22:ASP:HB2 | 38:K:5264:HOH:O | 2.13 | 0.49 |
| 14:N:18:THR:HG21 | 38:9:9099:HOH:O | 2.12 | 0.49 |
| 15:O:25:VAL:HG23 | 15:O:26:TRP:N | 2.27 | 0.49 |
| 23:W:119:HIS:HE1 | 38:0:9557:HOH:O | 1.96 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:3:38:ARG:CB | 29:3:42:ARG:HH12 | 2.25 | 0.49 |
| 30:0:445:U:O2' | 30:0:446:G:H5' | 2.12 | 0.49 |
| 30:0:514:G:OP1 | 30:0:514:G:H2' | 2.12 | 0.49 |
| 30:0:1206:U:H5' | 30:0:1206:U:C6 | 2.31 | 0.49 |
| 30:0:1526:A:H4' | 30:0:1527:A:H5' | 1.95 | 0.49 |
| 30:0:1942:A:O2' | 30:0:1943:C:H5' | 2.11 | 0.49 |
| 30:0:2612:A:H4' | 38:0:3666:HOH:O | 2.13 | 0.49 |
| 2:B:28:SER:HB2 | 30:0:2807:U:OP2 | 2.13 | 0.49 |
| 2:B:199:TYR:CE2 | 2:B:268:ARG:HB2 | 2.48 | 0.49 |
| 11:K:98:VAL:HG11 | 11:K:102:GLU:HA | 1.94 | 0.49 |
| 24:X:43:VAL:HG12 | 24:X:44:ASP:N | 2.27 | 0.49 |
| 30:0:314:G:C2 | 30:0:317:A:C8 | 3.01 | 0.49 |
| 30:0:352:A:H2' | 30:0:353:G:C8 | 2.48 | 0.49 |
| 30:0:1159:G:H2' | 30:0:1160:G:O4' | 2.11 | 0.49 |
| 30:0:1375:A:H2' | 30:0:1376:G:H5' | 1.95 | 0.49 |
| 31:9:7:G:H5' | 38:9:9099:HOH:O | 2.11 | 0.49 |
| 8:H:19:ARG:HH12 | 30:0:1008:C:H5" | 1.78 | 0.49 |
| 14:N:77:ASN:OD1 | 14:N:79:PRO:HD2 | 2.13 | 0.49 |
| 27:1:16:HIS:HD2 | 30:0:470:U:O2' | 1.95 | 0.49 |
| 29:3:48:ASN:ND2 | 30:0:169:A:H1' | 2.27 | 0.49 |
| 30:0:128:A:C8 | 30:0:128:A:H3' | 2.47 | 0.49 |
| 30:0:2135:A:O4' | 30:0:2243:C:N4 | 2.45 | 0.49 |
| 30:0:2265:U:H2' | 30:0:2266:A:H8 | 1.77 | 0.49 |
| 30:0:2820:A:H2' | 30:0:2821:C:C6 | 2.46 | 0.49 |
| 7:G:16:LYS:O | 7:G:20:VAL:HG23 | 2.13 | 0.49 |
| 21:U:9:CYS:HA | 21:U:52:THR:HG22 | 1.94 | 0.49 |
| 30:0:661:G:C5 | 30:0:686:A:C2 | 3.01 | 0.49 |
| 30:0:1181:A:C2 | 30:0:1192:A:C8 | 3.00 | 0.49 |
| 30:0:1209:C:H2' | 30:0:1210:G:C8 | 2.42 | 0.49 |
| 30:0:1572:A:H3' | 38:0:4098:HOH:O | 2.13 | 0.49 |
| 30:0:1765:G:O2' | 30:0:1766:U:H5' | 2.12 | 0.49 |
| 30:0:1976:G:H1' | 30:0:2005:G:N2 | 2.28 | 0.49 |
| 30:0:2237:G:H1' | 30:0:2238:A:H8 | 1.77 | 0.49 |
| 30:0:2707:C:O2 | 30:0:2707:C:H2' | 2.13 | 0.49 |
| 30:0:2805:A:C8 | 30:0:2806:C:C5 | 3.01 | 0.49 |
| 31:9:52:A:H2' | 31:9:53:G:H8 | 1.76 | 0.49 |
| 38:L:9036:HOH:O | 30:0:196:G:H2' | 2.12 | 0.49 |
| 13:M:133:LEU:O | 13:M:134:ILE:HD13 | 2.13 | 0.49 |
| 30:0:264:G:H1' | 30:0:265:U:H5 | 1.78 | 0.49 |
| 30:0:1521:C:H2' | 30:0:1522:A:H8 | 1.78 | 0.49 |
| 30:0:2254:G:H1' | 38:0:5527:HOH:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2359:G:H3' | 38:0:5674:HOH:O | 2.13 | 0.49 |
| 30:0:2635:A:C2' | 30:0:2636:C:H5' | 2.41 | 0.49 |
| 10:J:19:MET:HE1 | 10:J:132:LEU:HD21 | 1.93 | 0.49 |
| 14:N:132:ASN:HD22 | 30:0:2413:A:C4' | 2.25 | 0.49 |
| 19:S:49:VAL:HG13 | 19:S:66:VAL:HG13 | 1.95 | 0.49 |
| 26:Z:64:PRO:HB2 | 26:Z:86:TYR:HE2 | 1.78 | 0.49 |
| 29:3:68:LYS:HE3 | 30:0:2435:U:O2' | 2.12 | 0.49 |
| 30:0:526:U:H2' | 30:0:527:U:C6 | 2.48 | 0.49 |
| 30:0:727:G:H3' | 30:0:728:C:H6 | 1.78 | 0.49 |
| 30:0:1118:A:C8 | 30:0:1119:G:H5" | 2.47 | 0.49 |
| 30:0:1118:A:N6 | 30:0:1244:U:H3 | 1.95 | 0.49 |
| 30:0:1566:C:O2' | 30:0:1567:G:H5' | 2.12 | 0.49 |
| 30:0:1586:G:O2' | 30:0:1587:U:H5' | 2.13 | 0.49 |
| 30:0:1913:C:H2' | 30:0:1914:C:H6 | 1.76 | 0.49 |
| 30:0:2289:G:O2' | 30:0:2291:A:N6 | 2.45 | 0.49 |
| 30:0:2911:C:H2' | 30:0:2912:C:C6 | 2.48 | 0.49 |
| 2:B:7:ARG:HG2 | 2:B:7:ARG:HH11 | 1.77 | 0.48 |
| 4:D:23:VAL:HG12 | 4:D:130:VAL:HG22 | 1.95 | 0.48 |
| 6:F:91:VAL:HG12 | 6:F:92:GLY:N | 2.22 | 0.48 |
| 17:Q:11:ARG:HH22 | 30:0:2363:G:H5" | 1.78 | 0.48 |
| 25:Y:174:VAL:HG23 | 25:Y:177:LYS:HD2 | 1.94 | 0.48 |
| 30:0:10:U:O4 | 30:0:532:A:H8 | 1.96 | 0.48 |
| 30:0:59:A:H5' | 38:0:4330:HOH:O | 2.13 | 0.48 |
| 30:0:146:U:O2' | 30:0:147:G:H5' | 2.12 | 0.48 |
| 30:0:2269:C:H2' | 30:0:2270:G:H5' | 1.95 | 0.48 |
| 2:B:71:VAL:HG21 | 2:B:296:LEU:HB3 | 1.95 | 0.48 |
| 3:C:236:THR:H | 3:C:239:ALA:HB3 | 1.78 | 0.48 |
| 16:P:64:GLU:HG2 | 38:P:169:HOH:O | 2.13 | 0.48 |
| 21:U:50:GLU:O | 21:U:56:ARG:HG2 | 2.13 | 0.48 |
| 25:Y:235:GLU:CD | 25:Y:235:GLU:N | 2.65 | 0.48 |
| 29:3:5:ARG:O | 29:3:21:GLU:HA | 2.12 | 0.48 |
| 30:0:1447:U:H3' | 30:0:1506:U:O2 | 2.12 | 0.48 |
| 30:0:1641:A:O2' | 30:0:1642:A:H5' | 2.13 | 0.48 |
| 30:0:2061:C:C2' | 30:0:2062:A:H5' | 2.43 | 0.48 |
| 30:0:2073:G:C6 | 30:0:2489:G:H4' | 2.48 | 0.48 |
| 30:0:2710:U:O2' | 30:0:2711:U:H5' | 2.13 | 0.48 |
| 1:A:212:PRO:HB2 | 38:A:8985:HOH:O | 2.13 | 0.48 |
| 2:B:49:THR:HG22 | 2:B:50:HIS:H | 1.79 | 0.48 |
| 11:K:74:VAL:HG21 | 11:K:96:VAL:HG23 | 1.95 | 0.48 |
| 13:M:70:GLY:HA3 | 13:M:73:ARG:CZ | 2.42 | 0.48 |
| 13:M:164:THR:CG2 | 13:M:165:GLY:N | 2.75 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:T:8:ARG:NH1 | 30:0:31:C:OP2 | 2.46 | 0.48 |
| 25:Y:145:LYS:O | 25:Y:147:ARG:HG2 | 2.13 | 0.48 |
| 30:0:305:A:C5 | 30:0:329:A:C2 | 3.02 | 0.48 |
| 30:0:311:C:H2' | 30:0:312:U:H6 | 1.77 | 0.48 |
| 30:0:344:C:H2' | 30:0:345:G:O4' | 2.12 | 0.48 |
| 30:0:598:C:H2' | 30:0:599:G:H8 | 1.77 | 0.48 |
| 30:0:682:A:H2' | 30:0:683:G:O4' | 2.13 | 0.48 |
| 30:0:1461:U:H2' | 30:0:1462:C:C6 | 2.48 | 0.48 |
| 30:0:1566:C:H2' | 30:0:1567:G:H8 | 1.78 | 0.48 |
| 30:0:1922:A:N1 | 30:0:2449:G:O2' | 2.46 | 0.48 |
| 30:0:2509:A:H2' | 30:0:2510:C:O4' | 2.13 | 0.48 |
| 30:0:2512:U:H4' | 30:0:2514:U:O4 | 2.13 | 0.48 |
| 30:0:2616:G:H1' | 38:0:9428:HOH:O | 2.12 | 0.48 |
| 12:L:143:THR:HG22 | 12:L:144:ASP:N | 2.28 | 0.48 |
| 30:0:370:G:O2' | 30:0:371:U:H5' | 2.14 | 0.48 |
| 30:0:1706:G:C6 | 30:0:1707:G:N1 | 2.81 | 0.48 |
| 30:0:2271:G:N3 | 30:0:2271:G:H2' | 2.27 | 0.48 |
| 13:M:48:LYS:HE3 | 13:M:52:GLN:HE21 | 1.78 | 0.48 |
| 18:R:18:LEU:HG | 18:R:91:LEU:HD13 | 1.95 | 0.48 |
| 26:Z:37:ARG:HB2 | 30:0:819:A:O4' | 2.14 | 0.48 |
| 29:3:64:LYS:HA | 29:3:84:ARG:CA | 2.38 | 0.48 |
| 30:0:645:U:O2 | 30:0:761:A:H2 | 1.97 | 0.48 |
| 30:0:809:G:H2' | 30:0:810:G:H8 | 1.78 | 0.48 |
| 30:0:816:G:C6 | 30:0:817:G:N1 | 2.82 | 0.48 |
| 30:0:1188:A:H5' | 38:0:7418:HOH:O | 2.12 | 0.48 |
| 30:0:1626:A:H2' | 30:0:1627:G:H5' | 1.96 | 0.48 |
| 30:0:1835:U:H3' | 38:0:5569:HOH:O | 2.12 | 0.48 |
| 30:0:2511:A:H2' | 30:0:2512:U:C6 | 2.47 | 0.48 |
| 30:0:2626:C:H2' | 30:0:2627:G:C8 | 2.49 | 0.48 |
| 30:0:2651:C:H2' | 30:0:2652:U:O4' | 2.13 | 0.48 |
| 30:0:2673:U:C4 | 30:0:2674:G:C6 | 3.01 | 0.48 |
| 11:K:130:MET:SD | 21:U:25:ASP:O | 2.71 | 0.48 |
| 13:M:74:LYS:O | 13:M:88:VAL:HG13 | 2.13 | 0.48 |
| 14:N:48:VAL:CG1 | 14:N:55:ASP:HB3 | 2.43 | 0.48 |
| 20:T:48:VAL:HG12 | 20:T:49:GLU:N | 2.29 | 0.48 |
| 23:W:6:GLN:HB2 | 23:W:26:ILE:CD1 | 2.36 | 0.48 |
| 26:Z:74:GLN:HG2 | 26:Z:80:GLN:HB2 | 1.95 | 0.48 |
| 29:3:64:LYS:HD3 | 29:3:82:GLY:O | 2.13 | 0.48 |
| 30:0:421:C:H4' | 30:0:1919:A:C6 | 2.49 | 0.48 |
| 30:0:1187:U:O2' | 30:0:1188:A:C8 | 2.64 | 0.48 |
| 30:0:1684:A:O2' | 30:0:1685:A:H5" | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1905:U:H2' | 30:0:1906:C:H6 | 1.79 | 0.48 |
| 30:0:2713:G:O2' | 30:0:2714:U:H5' | 2.13 | 0.48 |
| 1:A:72:GLU:HG2 | 26:Z:100:GLY:CA | 2.40 | 0.48 |
| 1:A:171:LYS:HB2 | 30:0:820:G:C5 | 2.49 | 0.48 |
| 2:B:74:ILE:HG13 | 38:B:9075:HOH:O | 2.13 | 0.48 |
| 5:E:101:GLU:HB2 | 5:E:116:THR:O | 2.13 | 0.48 |
| 12:L:65:ASP:HA | 12:L:109:LEU:O | 2.14 | 0.48 |
| 18:R:33:ARG:NH1 | 38:R:8944:HOH:O | 2.47 | 0.48 |
| 25:Y:170:SER:OG | 25:Y:175:ARG:HG3 | 2.14 | 0.48 |
| 30:0:154:C:H2' | 30:0:155:C:C6 | 2.49 | 0.48 |
| 30:0:696:C:HO2' | 30:0:697:G:H5' | 1.78 | 0.48 |
| 30:0:1343:C:H2' | 30:0:1344:G:O5' | 2.12 | 0.48 |
| 30:0:2608:C:H2' | 38:0:3561:HOH:O | 2.13 | 0.48 |
| 31:9:23:U:O2 | 31:9:23:U:H2' | 2.14 | 0.48 |
| 2:B:84:LEU:HD23 | 2:B:142:LEU:HD23 | 1.96 | 0.48 |
| 10:J:75:PRO:HB3 | 10:J:132:LEU:HB3 | 1.96 | 0.48 |
| 10:J:135:ILE:O | 10:J:139:LEU:HG | 2.14 | 0.48 |
| 13:M:73:ARG:HH22 | 30:0:2263:G:H5" | 1.77 | 0.48 |
| 17:Q:27:GLN:HE21 | 31:9:8:G:H5" | 1.75 | 0.48 |
| 23:W:107:LEU:O | 23:W:112:LEU:HB2 | 2.13 | 0.48 |
| 30:0:228:C:C2' | 30:0:229:G:H5' | 2.44 | 0.48 |
| 30:0:284:C:H4' | 30:0:285:A:H8 | 1.79 | 0.48 |
| 30:0:533:U:H3' | 38:0:3736:HOH:O | 2.13 | 0.48 |
| 30:0:589:U:H2' | 30:0:590:A:C8 | 2.47 | 0.48 |
| 30:0:1168:C:H5 | 38:0:7488:HOH:O | 1.96 | 0.48 |
| 30:0:1422:U:H2' | 30:0:1423:C:C6 | 2.49 | 0.48 |
| 30:0:1632:A:C3' | 30:0:1633:C:H5' | 2.44 | 0.48 |
| 30:0:2524:G:N2 | 30:0:2526:C:N4 | 2.57 | 0.48 |
| 38:2:3526:HOH:O | 30:0:1413:A:H5" | 2.14 | 0.48 |
| 30:0:581:G:O2' | 30:0:582:U:H5' | 2.13 | 0.48 |
| 30:0:1795:G:H2' | 30:0:1796:A:O4' | 2.13 | 0.48 |
| 30:0:1965:C:H2' | 30:0:1966:U:C6 | 2.49 | 0.48 |
| 30:0:2614:C:O2' | 30:0:2615:U:H5' | 2.13 | 0.48 |
| 31:9:38:A:H2 | 31:9:43:G:H5" | 1.77 | 0.48 |
| 1:A:36:ASP:HA | 1:A:83:GLY:HA3 | 1.96 | 0.48 |
| 2:B:24:PRO:CG | 2:B:204:GLY:HA2 | 2.44 | 0.48 |
| 2:B:36:PRO:CA | 2:B:168:GLY:HA3 | 2.40 | 0.48 |
| 3:C:206:ASN:HB2 | 30:0:329:A:OP2 | 2.13 | 0.48 |
| 4:D:52:THR:HG21 | 30:0:2346:C:O2' | 2.13 | 0.48 |
| 13:M:40:ILE:HG21 | 13:M:64:ARG:NH2 | 2.29 | 0.48 |
| 14:N:139:TRP:HA | 14:N:139:TRP:CE3 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:T:38:ARG:NH1 | 38:0:6667:HOH:O | 2.47 | 0.48 |
| 23:W:134:GLU:OE2 | 31:9:97:U:H1' | 2.14 | 0.48 |
| 24:X:85:VAL:HG12 | 24:X:86:GLU:N | 2.29 | 0.48 |
| 30:0:113:A:C8 | 30:0:114:A:C8 | 3.02 | 0.48 |
| 30:0:138:U:OP2 | 30:0:139:C:C5 | 2.67 | 0.48 |
| 30:0:542:A:H2' | 30:0:543:G:O4' | 2.14 | 0.48 |
| 30:0:1592:G:C4 | 30:0:1593:C:C5 | 3.02 | 0.48 |
| 30:0:1706:G:C5 | 30:0:1707:G:C6 | 3.02 | 0.48 |
| 30:0:1790:C:H2' | 30:0:1791:U:H6 | 1.79 | 0.48 |
| 30:0:2296:C:H2' | 30:0:2297:U:H6 | 1.79 | 0.48 |
| 30:0:2842:G:C2' | 30:0:2843:A:H5' | 2.44 | 0.48 |
| 31:9:5:G:C2' | 31:9:6:C:H5' | 2.43 | 0.48 |
| 1:A:36:ASP:O | 1:A:38:ILE:N | 2.44 | 0.47 |
| 1:A:42:VAL:HG21 | 1:A:74:VAL:CG1 | 2.44 | 0.47 |
| 5:E:154:ILE:HD11 | 5:E:157:LYS:HB2 | 1.96 | 0.47 |
| 11:K:37:TYR:HB3 | 38:K:7169:HOH:O | 2.14 | 0.47 |
| 14:N:22:GLN:O | 14:N:26:LEU:HB2 | 2.14 | 0.47 |
| 18:R:39:THR:HB | 18:R:42:GLU:CG | 2.44 | 0.47 |
| 23:W:11:VAL:O | 23:W:12:ASN:HB2 | 2.14 | 0.47 |
| 30:0:764:C:H2' | 30:0:765:G:O4' | 2.14 | 0.47 |
| 30:0:1735:C:H2' | 30:0:1736:A:C8 | 2.49 | 0.47 |
| 30:0:1878:G:C1' | 38:0:6104:HOH:O | 2.62 | 0.47 |
| 30:0:2074:A:H2' | 38:0:3520:HOH:O | 2.13 | 0.47 |
| 10:J:107:ASN:ND2 | 10:J:109:TYR:H | 2.11 | 0.47 |
| 16:P:102:ARG:NH2 | 30:0:1596:U:C5 | 2.82 | 0.47 |
| 29:3:38:ARG:HB3 | 29:3:42:ARG:HH12 | 1.79 | 0.47 |
| 30:0:24:G:H22 | 30:0:518:G:H1' | 1.79 | 0.47 |
| 30:0:45:A:N6 | 30:0:147:G:C4 | 2.83 | 0.47 |
| 30:0:844:A:C6 | 30:0:882:A:C6 | 3.02 | 0.47 |
| 30:0:2864:U:C2' | 30:0:2865:G:H5' | 2.44 | 0.47 |
| 2:B:41:PHE:HB3 | 2:B:190:MET:CE | 2.44 | 0.47 |
| 2:B:54:VAL:HB | 38:B:9084:HOH:O | 2.13 | 0.47 |
| 4:D:58:VAL:HG12 | 4:D:60:GLU:HG2 | 1.96 | 0.47 |
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:HB2 | 1.96 | 0.47 |
| 26:Z:65:ASN:HD22 | 26:Z:84:CYS:HB2 | 1.80 | 0.47 |
| 27:1:20:ARG:HG2 | 30:0:111:C:O2' | 2.14 | 0.47 |
| 28:2:29:THR:HG22 | 30:0:86:A:O4' | 2.14 | 0.47 |
| 30:0:301:C:H2' | 30:0:302:A:H8 | 1.79 | 0.47 |
| 30:0:703:G:H2' | 30:0:704:C:C6 | 2.49 | 0.47 |
| 30:0:1205:U:C2' | 30:0:1206:U:H5" | 2.44 | 0.47 |
| 30:0:1787:C:H4' | 30:0:2883:A:O4' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2241:C:O2' | 30:0:2242:U:H5' | 2.14 | 0.47 |
| 30:0:2890:A:H2' | 30:0:2890:A:N3 | 2.29 | 0.47 |
| 31:9:52:A:H2' | 31:9:53:G:O4' | 2.13 | 0.47 |
| 2:B:305:ASP:O | 2:B:306:LYS:HB2 | 2.15 | 0.47 |
| 3:C:153:VAL:O | 3:C:157:LEU:HG | 2.15 | 0.47 |
| 16:P:55:LYS:HG3 | 16:P:56:GLY:N | 2.29 | 0.47 |
| 20:T:48:VAL:HG13 | 20:T:97:ARG:O | 2.14 | 0.47 |
| 25:Y:106:THR:HG23 | 25:Y:107:PRO:HD2 | 1.96 | 0.47 |
| 29:3:10:TYR:HE2 | 30:0:2382:A:H1' | 1.80 | 0.47 |
| 30:0:95:A:H5" | 30:0:97:G:O4' | 2.14 | 0.47 |
| 30:0:1561:U:H5' | 38:0:7421:HOH:O | 2.13 | 0.47 |
| 30:0:1603:A:H5" | 30:0:1604:G:H3' | 1.96 | 0.47 |
| 30:0:2032:U:C2' | 30:0:2033:G:C5' | 2.93 | 0.47 |
| 30:0:2784:A:O5' | 30:0:2784:A:H8 | 1.98 | 0.47 |
| 31:9:108:C:H2' | 31:9:109:G:H8 | 1.79 | 0.47 |
| 1:A:45:ILE:HG22 | 26:Z:78:ILE:HG12 | 1.96 | 0.47 |
| 10:J:54:VAL:HG11 | 10:J:138:THR:HG21 | 1.95 | 0.47 |
| 13:M:75:ARG:HB2 | 38:M:8905:HOH:O | 2.14 | 0.47 |
| 20:T:64:ASN:HB3 | 20:T:73:HIS:HB2 | 1.96 | 0.47 |
| 30:0:292:G:H2' | 30:0:358:G:N2 | 2.30 | 0.47 |
| 30:0:599:G:H2' | 30:0:600:G:H8 | 1.79 | 0.47 |
| 30:0:810:G:H2' | 30:0:811:C:C6 | 2.49 | 0.47 |
| 30:0:1217:G:C2 | 30:0:1218:U:C2 | 3.03 | 0.47 |
| 30:0:1942:A:H3' | 38:0:7336:HOH:O | 2.14 | 0.47 |
| 30:0:2336:G:C2' | 38:0:6280:HOH:O | 2.60 | 0.47 |
| 30:0:2697:A:H2' | 30:0:2698:G:O4' | 2.15 | 0.47 |
| 30:0:2908:A:O5' | 30:0:2908:A:H8 | 1.97 | 0.47 |
| 1:A:186:TRP:CG | 1:A:187:PRO:HA | 2.50 | 0.47 |
| 2:B:5:ARG:NH2 | 30:0:2548:C:OP2 | 2.47 | 0.47 |
| 5:E:69:ILE:HA | 5:E:72:MET:CE | 2.44 | 0.47 |
| 6:F:50:VAL:HG21 | 6:F:63:ILE:HG21 | 1.97 | 0.47 |
| 10:J:131:THR:HG22 | 10:J:133:GLY:H | 1.79 | 0.47 |
| 13:M:65:VAL:HG21 | 13:M:105:ALA:HB2 | 1.97 | 0.47 |
| 13:M:91:ILE:HD11 | 38:M:8830:HOH:O | 2.15 | 0.47 |
| 23:W:119:HIS:HD2 | 23:W:120:PRO:O | 1.97 | 0.47 |
| 23:W:120:PRO:HG2 | 30:0:1095:U:O2 | 2.14 | 0.47 |
| 29:3:46:ILE:HG12 | 38:0:3138:HOH:O | 2.14 | 0.47 |
| 29:3:79:LEU:HB2 | 38:0:6581:HOH:O | 2.14 | 0.47 |
| 30:0:371:U:H2' | 30:0:372:A:C8 | 2.49 | 0.47 |
| 30:0:960:G:N3 | 30:0:960:G:H3' | 2.30 | 0.47 |
| 30:0:1181:A:H2' | 30:0:1182:C:C5' | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1318:A:H4' | 30:0:1343:C:H4' | 1.96 | 0.47 |
| 30:0:1359:U:C5 | 30:0:2101:A:C8 | 3.03 | 0.47 |
| 30:0:2510:C:H5' | 30:0:2511:A:OP2 | 2.13 | 0.47 |
| 2:B:98:THR:HG23 | 30:0:2820:A:OP1 | 2.15 | 0.47 |
| 18:R:68:HIS:CD2 | 18:R:76:ASP:HB2 | 2.50 | 0.47 |
| 23:W:88:THR:HB | 38:W:6679:HOH:O | 2.14 | 0.47 |
| 23:W:121:PRO:HA | 23:W:153:MET:HG2 | 1.96 | 0.47 |
| 29:3:50:GLY:HA3 | 38:0:9164:HOH:O | 2.14 | 0.47 |
| 30:0:282:C:H1' | 30:0:368:C:H41 | 1.78 | 0.47 |
| 30:0:484:A:N1 | 30:0:506:G:H4' | 2.30 | 0.47 |
| 30:0:512:G:O3' | 30:0:513:A:H8 | 1.97 | 0.47 |
| 30:0:677:C:O2' | 30:0:678:G:H5' | 2.14 | 0.47 |
| 30:0:1042:U:O2' | 30:0:1043:C:H5' | 2.15 | 0.47 |
| 30:0:1173:A:H4' | 30:0:1174:A:C8 | 2.49 | 0.47 |
| 30:0:1523:G:C6 | 30:0:1524:U:C4 | 3.03 | 0.47 |
| 30:0:1769:C:O2' | 30:0:1770:U:H5' | 2.15 | 0.47 |
| 30:0:1790:C:H2' | 30:0:1791:U:C6 | 2.50 | 0.47 |
| 30:0:1864:C:H2' | 30:0:1865:A:O4' | 2.14 | 0.47 |
| 30:0:1882:C:H2' | 30:0:1883:U:H6 | 1.80 | 0.47 |
| 30:0:2598:U:O2 | 30:0:2600:A:C8 | 2.68 | 0.47 |
| 30:0:2686:C:C2 | 30:0:2709:G:N2 | 2.82 | 0.47 |
| 1:A:121:ALA:O | 1:A:124:VAL:HG22 | 2.14 | 0.47 |
| 3:C:127:ARG:HD3 | 3:C:129:HIS:HE1 | 1.80 | 0.47 |
| 17:Q:14:LEU:HD21 | 17:Q:43:ILE:HD12 | 1.97 | 0.47 |
| 20:T:24:ARG:HH21 | 20:T:39:ASN:HD22 | 1.63 | 0.47 |
| 22:V:39:ALA:N | 22:V:40:PRO:CD | 2.77 | 0.47 |
| 23:W:29:VAL:O | 23:W:30:ASN:HB2 | 2.13 | 0.47 |
| 29:3:24:LYS:HE3 | 29:3:90:PHE:CE1 | 2.50 | 0.47 |
| 30:0:304:G:H8 | 30:0:304:G:O5' | 1.98 | 0.47 |
| 30:0:1183:C:C2 | 30:0:1184:C:C5 | 3.03 | 0.47 |
| 30:0:1187:U:O2' | 30:0:1189:A:H2 | 1.98 | 0.47 |
| 30:0:1377:C:H6 | 30:0:1377:C:C5' | 2.28 | 0.47 |
| 30:0:2134:G:N2 | 30:0:2242:U:C2 | 2.83 | 0.47 |
| 30:0:2253:G:H2' | 30:0:2254:G:H8 | 1.80 | 0.47 |
| 30:0:2329:C:O2' | 30:0:2330:U:H5' | 2.14 | 0.47 |
| 30:0:2383:G:C6 | 30:0:2384:U:C4 | 3.03 | 0.47 |
| 30:0:2752:C:O2' | 30:0:2753:G:H5' | 2.15 | 0.47 |
| 8:H:91:ARG:HB2 | 30:0:1003:U:OP1 | 2.15 | 0.47 |
| 25:Y:99:ALA:HB2 | 25:Y:233:TYR:CZ | 2.50 | 0.47 |
| 25:Y:137:LYS:HD2 | 30:0:521:A:H5" | 1.97 | 0.47 |
| 30:0:36:C:C2 | 30:0:447:A:C2 | 3.03 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:371:U:H2' | 30:0:372:A:H8 | 1.80 | 0.47 |
| 30:0:447:A:O2' | 30:0:448:G:H5' | 2.15 | 0.47 |
| 30:0:1966:U:O5' | 30:0:1966:U:H6 | 1.98 | 0.47 |
| 30:0:2096:A:H2' | 30:0:2539:U:O4' | 2.14 | 0.47 |
| 30:0:2769:C:H2' | 30:0:2770:G:O4' | 2.14 | 0.47 |
| 3:C:103:ASN:ND2 | 30:0:663:C:H5" | 2.29 | 0.47 |
| 13:M:111:ASN:HB2 | 38:M:8849:HOH:O | 2.14 | 0.47 |
| 17:Q:11:ARG:CZ | 30:0:2363:G:H4' | 2.44 | 0.47 |
| 18:R:82:GLU:HG3 | 18:R:83:LYS:N | 2.29 | 0.47 |
| 23:W:154:ARG:NH1 | 30:0:588:G:O6 | 2.47 | 0.47 |
| 30:0:613:C:H2' | 30:0:614:U:C6 | 2.46 | 0.47 |
| 30:0:805:G:N2 | 30:0:807:A:H3' | 2.30 | 0.47 |
| 30:0:1878:G:O2' | 30:0:1879:U:C5 | 2.66 | 0.47 |
| 30:0:2604:A:H5' | 38:0:5775:HOH:O | 2.14 | 0.47 |
| 3:C:127:ARG:CZ | 3:C:225:PRO:HG2 | 2.44 | 0.46 |
| 5:E:7:ILE:HG23 | 5:E:45:ASP:O | 2.15 | 0.46 |
| 5:E:93:MET:HE1 | 5:E:165:GLY:H | 1.79 | 0.46 |
| 30:0:1350:U:H4' | 38:0:5115:HOH:O | 2.15 | 0.46 |
| 30:0:1477:C:C5' | 30:0:1868:G:H5" | 2.45 | 0.46 |
| 30:0:1477:C:H4' | 30:0:1868:G:OP1 | 2.15 | 0.46 |
| 30:0:1969:A:C2' | 30:0:1970:G:H5' | 2.45 | 0.46 |
| 2:B:79:MET:HE1 | 38:B:9096:HOH:O | 2.15 | 0.46 |
| 11:K:34:VAL:HB | 38:K:7169:HOH:O | 2.15 | 0.46 |
| 16:P:120:ARG:HD2 | 30:0:1594:C:OP2 | 2.14 | 0.46 |
| 29:3:69:TYR:O | 29:3:77:ALA:HA | 2.15 | 0.46 |
| 30:0:629:A:C2 | 30:0:2074:A:C2 | 3.03 | 0.46 |
| 30:0:735:C:H3' | 30:0:736:A:C8 | 2.50 | 0.46 |
| 30:0:877:G:C5' | 30:0:878:G:OP1 | 2.62 | 0.46 |
| 30:0:921:G:H4' | 30:0:924:G:N1 | 2.30 | 0.46 |
| 30:0:1116:U:C2 | 30:0:1246:A:N6 | 2.83 | 0.46 |
| 30:0:1163:G:N1 | 30:0:1184:C:N4 | 2.64 | 0.46 |
| 30:0:1634:G:H2' | 38:0:3889:HOH:O | 2.15 | 0.46 |
| 30:0:1701:A:H4' | 30:0:1702:U:C5' | 2.37 | 0.46 |
| 30:0:1838:U:O2' | 30:0:2644:C:H5' | 2.15 | 0.46 |
| 30:0:1949:G:H22 | 30:0:1964:U:H1' | 1.79 | 0.46 |
| 3:C:129:HIS:HE1 | 3:C:231:ARG:HA | 1.77 | 0.46 |
| 7:G:63:ARG:N | 38:G:2569:HOH:O | 2.48 | 0.46 |
| 16:P:87:ARG:HG2 | 38:P:186:HOH:O | 2.15 | 0.46 |
| 18:R:99:ALA:HB1 | 18:R:109:MET:CE | 2.37 | 0.46 |
| 20:T:32:ARG:NH1 | 20:T:38:ARG:HH12 | 2.13 | 0.46 |
| 22:V:27:LEU:HA | 22:V:49:LEU:HD13 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:130:C:O2' | 30:0:131:A:N7 | 2.46 | 0.46 |
| 30:0:530:C:H4' | 30:0:612:U:H4' | 1.97 | 0.46 |
| 30:0:790:A:H2' | 30:0:791:A:O4' | 2.16 | 0.46 |
| 30:0:1197:G:H1' | 30:0:1203:G:C2 | 2.51 | 0.46 |
| 30:0:1545:C:H1' | 30:0:1641:A:N6 | 2.29 | 0.46 |
| 30:0:1617:C:C5 | 30:0:1643:C:H4' | 2.50 | 0.46 |
| 30:0:1797:A:O3' | 30:0:1798:C:C6 | 2.69 | 0.46 |
| 30:0:1928:C:C2' | 30:0:1929:G:H5' | 2.45 | 0.46 |
| 30:0:2102:G:C2 | 30:0:2103:A:N6 | 2.83 | 0.46 |
| 30:0:2256:G:H2' | 30:0:2257:G:C5' | 2.46 | 0.46 |
| 30:0:2347:C:H2' | 30:0:2348:C:C6 | 2.50 | 0.46 |
| 30:0:2526:C:C6 | 30:0:2526:C:H5' | 2.50 | 0.46 |
| 4:D:29:HIS:ND1 | 4:D:29:HIS:N | 2.61 | 0.46 |
| 5:E:84:MET:HG2 | 5:E:168:ILE:HA | 1.98 | 0.46 |
| 21:U:13:ILE:HG13 | 38:U:3194:HOH:O | 2.15 | 0.46 |
| 27:1:25:LYS:O | 27:1:25:LYS:HG2 | 2.16 | 0.46 |
| 29:3:47:GLY:HA2 | 30:0:2121:G:H4' | 1.97 | 0.46 |
| 30:0:238:C:H4' | 30:0:287:C:OP1 | 2.16 | 0.46 |
| 30:0:254:C:O2 | 30:0:254:C:H2' | 2.14 | 0.46 |
| 30:0:834:G:C4' | 30:0:835:U:OP2 | 2.61 | 0.46 |
| 30:0:2297:U:H1' | 38:0:5172:HOH:O | 2.16 | 0.46 |
| 30:0:2438:G:H2' | 30:0:2439:C:C6 | 2.50 | 0.46 |
| 30:0:2445:U:H2' | 30:0:2446:G:C8 | 2.51 | 0.46 |
| 1:A:171:LYS:HB2 | 30:0:820:G:C6 | 2.50 | 0.46 |
| 6:F:111:ILE:O | 6:F:115:VAL:HG23 | 2.15 | 0.46 |
| 10:J:80:LYS:HE3 | 10:J:101:VAL:O | 2.14 | 0.46 |
| 12:L:10:SER:O | 12:L:11:ARG:HB3 | 2.16 | 0.46 |
| 13:M:102:GLU:CD | 13:M:164:THR:HG21 | 2.36 | 0.46 |
| 21:U:56:ARG:HD2 | 30:0:2890:A:C1' | 2.46 | 0.46 |
| 30:0:2434:A:H2' | 30:0:2435:U:O4' | 2.15 | 0.46 |
| 29:3:1:MET:HG2 | 29:3:87:ARG:O | 2.16 | 0.46 |
| 30:0:100:C:H2' | 30:0:101:C:H6 | 1.80 | 0.46 |
| 30:0:101:C:H2' | 30:0:102:A:H8 | 1.80 | 0.46 |
| 30:0:461:C:N3 | 30:0:479:G:H5' | 2.31 | 0.46 |
| 30:0:660:A:N6 | 30:0:746:A:O4' | 2.49 | 0.46 |
| 30:0:1154:A:H2' | 30:0:1155:G:C8 | 2.50 | 0.46 |
| 30:0:1434:A:H2' | 30:0:1436:C:C5 | 2.51 | 0.46 |
| 31:9:14:G:H8 | 31:9:14:G:C5' | 2.16 | 0.46 |
| 2:B:144:THR:HG22 | 2:B:145:HIS:N | 2.31 | 0.46 |
| 8:H:48:VAL:HA | 8:H:170:ARG:O | 2.15 | 0.46 |
| 10:J:69:TYR:CE1 | 30:0:2081:A:H4' | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:11:ARG:NH1 | 31:9:8:G:O6 | 2.48 | 0.46 |
| 16:P:115:SER:OG | 16:P:118:GLN:HG3 | 2.16 | 0.46 |
| 27:1:16:HIS:HE1 | 30:0:775:G:OP1 | 1.97 | 0.46 |
| 28:2:43:ARG:NH2 | 30:0:1684:A:H1' | 2.25 | 0.46 |
| 30:0:17:G:H2' | 30:0:18:C:C6 | 2.51 | 0.46 |
| 30:0:134:U:C2 | 30:0:145:A:C2 | 3.04 | 0.46 |
| 30:0:365:G:C5 | 30:0:366:U:C5 | 3.04 | 0.46 |
| 30:0:517:U:C2' | 30:0:518:G:H5' | 2.46 | 0.46 |
| 30:0:561:G:O2' | 30:0:562:A:H5' | 2.15 | 0.46 |
| 30:0:1503:U:H2' | 30:0:1504:A:O4' | 2.16 | 0.46 |
| 30:0:1878:G:O2' | 30:0:1879:U:OP2 | 2.33 | 0.46 |
| 2:B:85:ARG:NH1 | 38:B:9106:HOH:O | 2.47 | 0.46 |
| 2:B:232:TRP:CZ3 | 30:0:2614:C:H5" | 2.51 | 0.46 |
| 12:L:34:GLY:HA2 | 38:L:9017:HOH:O | 2.16 | 0.46 |
| 13:M:47:ASP:CG | 13:M:48:LYS:N | 2.70 | 0.46 |
| 19:S:43:GLU:HB3 | 38:S:7106:HOH:O | 2.16 | 0.46 |
| 26:Z:41:ARG:HH12 | 30:0:821:U:H4' | 1.81 | 0.46 |
| 29:3:30:GLN:HB3 | 38:3:9051:HOH:O | 2.16 | 0.46 |
| 30:0:241:A:C2 | 30:0:378:A:H4' | 2.51 | 0.46 |
| 30:0:1526:A:H4' | 30:0:1527:A:C5' | 2.45 | 0.46 |
| 30:0:1764:C:O2' | 30:0:1765:G:H5' | 2.15 | 0.46 |
| 30:0:1845:A:C2' | 30:0:1846:U:H5' | 2.45 | 0.46 |
| 30:0:1871:U:O4' | 30:0:1873:G:C8 | 2.69 | 0.46 |
| 30:0:1894:C:N4 | 30:0:1939:U:H2' | 2.30 | 0.46 |
| 30:0:2537:G:H5" | 30:0:2538:A:H5" | 1.98 | 0.46 |
| 30:0:2812:A:N7 | 38:0:7508:HOH:O | 2.36 | 0.46 |
| 31:9:3:A:H2 | 31:9:21:G:N3 | 2.14 | 0.46 |
| 31:9:47:A:C2 | 31:9:48:C:C2 | 3.04 | 0.46 |
| 1:A:230:SER:HB2 | 30:0:1852:A:H4' | 1.97 | 0.46 |
| 3:C:43:LYS:HG2 | 30:0:449:A:N7 | 2.31 | 0.46 |
| 14:N:22:GLN:HG3 | 30:0:2415:A:C2 | 2.51 | 0.46 |
| 20:T:16:LEU:HB2 | 30:0:100:C:H4' | 1.98 | 0.46 |
| 25:Y:189:ASN:HA | 25:Y:217:ILE:HD11 | 1.97 | 0.46 |
| 30:0:545:G:C8 | 30:0:545:G:C5' | 2.88 | 0.46 |
| 30:0:594:C:C2' | 30:0:595:U:H5' | 2.46 | 0.46 |
| 30:0:1021:G:O2' | 30:0:1022:A:H5' | 2.16 | 0.46 |
| 30:0:1132:A:H61 | 30:0:1229:C:H2' | 1.80 | 0.46 |
| 30:0:1294:A:H2' | 30:0:1295:G:O4' | 2.16 | 0.46 |
| 30:0:1346:U:H2' | 30:0:1347:U:C6 | 2.50 | 0.46 |
| 30:0:1634:G:C4 | 30:0:1635:U:C5 | 3.03 | 0.46 |
| 30:0:2624:A:H1' | 38:0:9764:HOH:O | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:C:8575:HOH:O | 20:T:2:LYS:HE2 | 2.15 | 0.46 |
| 13:M:169:ARG:HD2 | 38:M:8885:HOH:O | 2.16 | 0.46 |
| 30:0:372:A:H2' | 30:0:373:G:C8 | 2.51 | 0.46 |
| 30:0:483:C:C4 | 30:0:484:A:C6 | 3.04 | 0.46 |
| 30:0:603:A:H4' | 30:0:604:G:O5' | 2.15 | 0.46 |
| 30:0:1012:A:H8 | 30:0:1012:A:O5' | 1.99 | 0.46 |
| 30:0:1166:A:C6 | 30:0:1181:A:C2 | 3.04 | 0.46 |
| 30:0:1588:G:C6 | 30:0:1589:G:N1 | 2.84 | 0.46 |
| 30:0:1615:A:H4' | 38:0:5868:HOH:O | 2.16 | 0.46 |
| 30:0:1615:A:H5' | 38:0:4181:HOH:O | 2.15 | 0.46 |
| 30:0:2017:U:O2' | 30:0:2018:A:C8 | 2.66 | 0.46 |
| 30:0:2276:U:H2' | 30:0:2277:U:C6 | 2.51 | 0.46 |
| 30:0:2488:A:H1' | 38:0:9096:HOH:O | 2.16 | 0.46 |
| 31:9:65:A:C2' | 31:9:66:G:OP2 | 2.64 | 0.46 |
| 25:Y:151:SER:HB3 | 25:Y:154:ARG:HB3 | 1.98 | 0.45 |
| 30:0:71:G:H8 | 38:0:3908:HOH:O | 1.98 | 0.45 |
| 30:0:255:A:C4 | 30:0:256:C:C5 | 3.05 | 0.45 |
| 30:0:1029:U:O2' | 30:0:1273:C:OP1 | 2.31 | 0.45 |
| 30:0:1052:G:H2' | 30:0:1052:G:N3 | 2.31 | 0.45 |
| 30:0:1119:G:C5 | 30:0:1243:C:C4 | 3.04 | 0.45 |
| 30:0:1409:G:C2 | 30:0:1410:G:C8 | 3.04 | 0.45 |
| 30:0:1520:G:C6 | 30:0:1521:C:C4 | 3.05 | 0.45 |
| 30:0:1756:G:H1' | 38:0:6244:HOH:O | 2.15 | 0.45 |
| 30:0:1890:U:H4' | 30:0:2010:A:C6 | 2.51 | 0.45 |
| 30:0:2740:G:H2' | 30:0:2741:A:O4' | 2.15 | 0.45 |
| 14:N:37:ARG:NH1 | 31:9:6:C:OP1 | 2.48 | 0.45 |
| 28:2:28:LYS:O | 30:0:87:C:H2' | 2.17 | 0.45 |
| 30:0:293:A:C5 | 30:0:360:A:C2 | 3.04 | 0.45 |
| 30:0:633:C:O2' | 30:0:634:G:H5' | 2.15 | 0.45 |
| 30:0:810:G:H2' | 30:0:811:C:H6 | 1.81 | 0.45 |
| 30:0:1625:U:H4' | 38:0:4661:HOH:O | 2.15 | 0.45 |
| 30:0:1768:C:H2' | 30:0:1769:C:O4' | 2.16 | 0.45 |
| 30:0:2057:U:O5' | 30:0:2057:U:H6 | 1.98 | 0.45 |
| 30:0:2717:C:C2' | 30:0:2718:C:C5' | 2.84 | 0.45 |
| 17:Q:25:PRO:HA | 17:Q:26:PRO:HD3 | 1.65 | 0.45 |
| 27:1:11:LYS:HG2 | 30:0:777:U:O2' | 2.17 | 0.45 |
| 29:3:70:ARG:NH2 | 29:3:77:ALA:HB3 | 2.31 | 0.45 |
| 30:0:612:U:H2' | 30:0:613:C:C6 | 2.52 | 0.45 |
| 30:0:1131:G:C6 | 30:0:1230:A:C4 | 3.04 | 0.45 |
| 30:0:1310:U:C2' | 30:0:1311:G:O5' | 2.64 | 0.45 |
| 30:0:1588:G:C6 | 30:0:1589:G:C6 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1730:G:H4' | 30:0:1731:C:H6 | 1.82 | 0.45 |
| 30:0:1856:C:H1' | 38:0:5858:HOH:O | 2.17 | 0.45 |
| 30:0:1882:C:H2' | 30:0:1883:U:C6 | 2.51 | 0.45 |
| 30:0:1902:G:O2' | 30:0:1903:U:H5' | 2.16 | 0.45 |
| 30:0:2298:C:O2' | 30:0:2299:G:H5' | 2.17 | 0.45 |
| 31:9:28:U:O2 | 31:9:57:A:N6 | 2.50 | 0.45 |
| 1:A:192:VAL:HG13 | 1:A:207:GLN:HB3 | 1.99 | 0.45 |
| 2:B:275:GLY:O | 2:B:291:ASP:HA | 2.16 | 0.45 |
| 12:L:142:LEU:HG | 12:L:146:GLY:HA3 | 1.99 | 0.45 |
| 13:M:88:VAL:HG13 | 38:M:8902:HOH:O | 2.16 | 0.45 |
| 14:N:34:LEU:HD22 | 14:N:129:ILE:HD13 | 1.98 | 0.45 |
| 18:R:128:ARG:NH2 | 30:0:2054:A:C2 | 2.84 | 0.45 |
| 26:Z:34:SER:HA | 30:0:797:A:C4' | 2.46 | 0.45 |
| 30:0:670:G:H2' | 30:0:671:A:C8 | 2.51 | 0.45 |
| 30:0:1342:C:H2' | 30:0:1343:C:H5' | 1.99 | 0.45 |
| 30:0:2438:G:H2' | 30:0:2439:C:H6 | 1.81 | 0.45 |
| 3:C:236:THR:CG2 | 3:C:239:ALA:H | 2.17 | 0.45 |
| 11:K:115:ARG:HG3 | 11:K:116:GLU:N | 2.32 | 0.45 |
| 14:N:40:ASN:HD22 | 31:9:28:U:H5" | 1.82 | 0.45 |
| 29:3:9:THR:HG23 | 29:3:20:HIS:ND1 | 2.32 | 0.45 |
| 30:0:169:A:HO2' | 30:0:170:U:H6 | 1.63 | 0.45 |
| 30:0:1187:U:C2 | 30:0:1189:A:OP2 | 2.70 | 0.45 |
| 30:0:1540:G:C4 | 30:0:1541:G:C8 | 3.05 | 0.45 |
| 30:0:1613:C:H2' | 30:0:1614:G:O4' | 2.15 | 0.45 |
| 30:0:1758:U:O2' | 30:0:1759:A:H5' | 2.15 | 0.45 |
| 30:0:2032:U:C2' | 30:0:2033:G:H5" | 2.46 | 0.45 |
| 30:0:2315:C:H4' | 30:0:2425:A:C6 | 2.51 | 0.45 |
| 1:A:9:ARG:HG2 | 1:A:16:PHE:CD2 | 2.52 | 0.45 |
| 8:H:123:ILE:HD12 | 8:H:123:ILE:N | 2.32 | 0.45 |
| 8:H:165:ARG:HD2 | 38:H:9029:HOH:O | 2.16 | 0.45 |
| 8:H:170:ARG:HD2 | 38:H:8987:HOH:O | 2.15 | 0.45 |
| 10:J:42:GLU:HG2 | 10:J:43:ARG:HG3 | 1.98 | 0.45 |
| 12:L:75:LEU:HD21 | 38:O:7543:HOH:O | 2.17 | 0.45 |
| 15:O:87:THR:O | 15:O:91:GLN:HG3 | 2.17 | 0.45 |
| 21:U:14:GLU:O | 21:U:17:THR:HB | 2.16 | 0.45 |
| 25:Y:142:SER:HB2 | 38:Y:8903:HOH:O | 2.16 | 0.45 |
| 30:0:1016:U:H2' | 30:0:1017:U:O4' | 2.17 | 0.45 |
| 30:0:1278:A:H4' | 30:0:1279:U:C5 | 2.49 | 0.45 |
| 30:0:1535:G:H2' | 30:0:1536:C:C6 | 2.52 | 0.45 |
| 30:0:1603:A:H5" | 30:0:1605:G:C5' | 2.39 | 0.45 |
| 30:0:2104:C:O2 | 30:0:2485:A:N1 | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2505:G:H3' | 38:0:5626:HOH:O | 2.17 | 0.45 |
| 30:0:2591:C:H2' | 30:0:2592:G:O4' | 2.16 | 0.45 |
| 2:B:254:GLN:HG2 | 2:B:255:GLY:N | 2.31 | 0.45 |
| 8:H:12:ILE:HG23 | 8:H:129:ARG:CZ | 2.47 | 0.45 |
| 8:H:99:ARG:NH1 | 30:0:1055:G:OP2 | 2.50 | 0.45 |
| 21:U:6:CYS:SG | 21:U:13:ILE:HB | 2.57 | 0.45 |
| 24:X:30:MET:HG2 | 30:0:1384:C:H5' | 1.98 | 0.45 |
| 30:0:212:A:O4' | 30:0:214:U:C6 | 2.70 | 0.45 |
| 30:0:352:A:H2' | 30:0:353:G:H8 | 1.79 | 0.45 |
| 30:0:2321:A:C4 | 30:0:2323:G:C8 | 3.05 | 0.45 |
| 30:0:2778:A:C2 | 30:0:2797:C:O2 | 2.70 | 0.45 |
| 1:A:47:HIS:HD2 | 30:0:1654:U:C2' | 2.30 | 0.45 |
| 1:A:105:VAL:CG1 | 1:A:154:ALA:HB1 | 2.47 | 0.45 |
| 3:C:170:ASP:OD2 | 30:0:330:C:H5 | 2.00 | 0.45 |
| 14:N:86:LEU:HD12 | 14:N:125:ALA:HB2 | 1.99 | 0.45 |
| 14:N:110:THR:HB | 14:N:113:SER:OG | 2.17 | 0.45 |
| 18:R:132:ARG:HG2 | 18:R:133:ALA:N | 2.31 | 0.45 |
| 23:W:129:LYS:HE2 | 30:0:1098:A:O3' | 2.17 | 0.45 |
| 30:0:213:G:N2 | 30:0:225:G:H2' | 2.31 | 0.45 |
| 30:0:226:A:H1' | 30:0:393:G:C5 | 2.51 | 0.45 |
| 30:0:644:G:H1' | 38:0:6390:HOH:O | 2.16 | 0.45 |
| 30:0:727:G:C2 | 30:0:728:C:C2 | 3.05 | 0.45 |
| 30:0:867:A:H2 | 30:0:880:C:O2 | 2.00 | 0.45 |
| 30:0:921:G:H4' | 30:0:924:G:C6 | 2.52 | 0.45 |
| 30:0:1151:G:H2' | 38:0:5008:HOH:O | 2.17 | 0.45 |
| 30:0:1346:U:H2' | 30:0:1347:U:H6 | 1.82 | 0.45 |
| 30:0:2071:C:H5' | 38:0:9532:HOH:O | 2.17 | 0.45 |
| 30:0:2679:G:H2' | 30:0:2681:A:OP2 | 2.17 | 0.45 |
| 31:9:26:C:H5" | 38:9:9049:HOH:O | 2.17 | 0.45 |
| 2:B:252:PRO:HD2 | 30:0:2548:C:H5' | 1.99 | 0.45 |
| 3:C:27:ARG:HH11 | 3:C:27:ARG:CG | 2.15 | 0.45 |
| 4:D:154:LYS:HD2 | 4:D:154:LYS:N | 2.22 | 0.45 |
| 12:L:136:ALA:HB3 | 38:L:9035:HOH:O | 2.17 | 0.45 |
| 13:M:68:ARG:HD3 | 13:M:68:ARG:C | 2.37 | 0.45 |
| 16:P:91:LYS:O | 16:P:95:GLU:HG3 | 2.17 | 0.45 |
| 25:Y:132:ASP:OD2 | 30:0:621:C:H5' | 2.17 | 0.45 |
| 30:0:113:A:H3' | 30:0:114:A:H5" | 1.98 | 0.45 |
| 30:0:282:C:H2' | 30:0:283:U:O4' | 2.16 | 0.45 |
| 30:0:482:G:O4' | 30:0:511:A:C2 | 2.70 | 0.45 |
| 30:0:559:U:H2' | 30:0:560:U:O4' | 2.17 | 0.45 |
| 30:0:941:G:C6 | 30:0:942:U:C4 | 3.05 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1755:A:H2' | 30:0:1756:G:O4' | 2.16 | 0.45 |
| 30:0:2596:A:H2 | 33:0:8812:CL:CL | 2.37 | 0.45 |
| 30:0:2650:U:O2' | 30:0:2651:C:H5' | 2.16 | 0.45 |
| 30:0:2691:A:H5' | 30:0:2693:U:H1' | 1.99 | 0.45 |
| 30:0:2735:U:H2' | 30:0:2736:U:C6 | 2.52 | 0.45 |
| 31:9:82:U:H2' | 31:9:83:G:C8 | 2.52 | 0.45 |
| 1:A:76:VAL:HG23 | 26:Z:87:LYS:O | 2.17 | 0.45 |
| 2:B:5:ARG:HD2 | 2:B:8:LYS:HE2 | 1.99 | 0.45 |
| 3:C:39:GLN:O | 3:C:43:LYS:HD3 | 2.17 | 0.45 |
| 18:R:25:PHE:CE2 | 18:R:29:LYS:HE2 | 2.51 | 0.45 |
| 25:Y:142:SER:OG | 30:0:1331:G:OP2 | 2.32 | 0.45 |
| 30:0:792:G:O2' | 30:0:793:A:H5' | 2.16 | 0.45 |
| 30:0:1249:U:H2' | 30:0:1250:C:H6 | 1.82 | 0.45 |
| 30:0:1878:G:O2' | 30:0:1879:U:P | 2.74 | 0.45 |
| 30:0:2010:A:C2' | 38:0:5942:HOH:O | 2.51 | 0.45 |
| 30:0:2252:A:C5 | 30:0:2253:G:H1' | 2.51 | 0.45 |
| 13:M:72:ALA:C | 13:M:74:LYS:H | 2.20 | 0.44 |
| 14:N:25:ARG:HG2 | 30:0:2416:G:O2' | 2.17 | 0.44 |
| 15:O:98:LEU:O | 15:O:102:ILE:HG13 | 2.17 | 0.44 |
| 16:P:68:LYS:HE2 | 30:0:1787:C:OP1 | 2.16 | 0.44 |
| 18:R:114:VAL:HG13 | 18:R:114:VAL:O | 2.18 | 0.44 |
| 28:2:41:HIS:H | 28:2:45:ASN:ND2 | 2.04 | 0.44 |
| 30:0:65:C:O2' | 30:0:66:G:H5' | 2.16 | 0.44 |
| 30:0:152:A:H2' | 30:0:153:C:C6 | 2.52 | 0.44 |
| 30:0:699:C:C2 | 30:0:744:G:N2 | 2.85 | 0.44 |
| 30:0:797:A:N6 | 30:0:816:G:H1' | 2.32 | 0.44 |
| 30:0:1209:C:C2 | 30:0:1210:G:C8 | 3.04 | 0.44 |
| 30:0:1268:C:O2' | 30:0:1269:G:H5' | 2.16 | 0.44 |
| 30:0:2301:A:H5" | 30:0:2302:A:H5' | 1.99 | 0.44 |
| 30:0:2335:C:H2' | 30:0:2336:G:H8 | 1.80 | 0.44 |
| 30:0:2837:U:H2' | 38:0:6825:HOH:O | 2.15 | 0.44 |
| 31:9:1:U:O3' | 31:9:3:A:C5' | 2.65 | 0.44 |
| 1:A:51:ARG:C | 1:A:53:ALA:H | 2.20 | 0.44 |
| 1:A:206:ARG:HH21 | 30:0:2629:C:N4 | 2.16 | 0.44 |
| 8:H:46:TYR:HA | 8:H:47:PRO:HD3 | 1.81 | 0.44 |
| 18:R:106:GLY:HA2 | 18:R:109:MET:HE3 | 1.99 | 0.44 |
| 21:U:42:LEU:O | 30:0:1810:C:H5' | 2.17 | 0.44 |
| 23:W:35:VAL:HG23 | 23:W:41:TYR:CD2 | 2.52 | 0.44 |
| 30:0:365:G:C5 | 30:0:366:U:C4 | 3.05 | 0.44 |
| 30:0:598:C:H2' | 30:0:599:G:C8 | 2.51 | 0.44 |
| 30:0:1310:U:H2' | 30:0:1311:G:O5' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1949:G:N2 | 30:0:1964:U:H1' | 2.32 | 0.44 |
| 30:0:2074:A:H1' | 38:0:9875:HOH:O | 2.16 | 0.44 |
| 30:0:2250:G:C2 | 30:0:2251:G:H1' | 2.52 | 0.44 |
| 30:0:2493:C:O2 | 30:0:2493:C:H2' | 2.17 | 0.44 |
| 30:0:2734:G:O2' | 30:0:2735:U:H5' | 2.17 | 0.44 |
| 31:9:1:U:O3' | 31:9:3:A:H5" | 2.16 | 0.44 |
| 38:B:9136:HOH:O | 21:U:17:THR:HG21 | 2.16 | 0.44 |
| 5:E:3:VAL:HG22 | 5:E:49:ILE:HB | 2.00 | 0.44 |
| 7:G:64:ASN:N | 7:G:64:ASN:ND2 | 2.65 | 0.44 |
| 14:N:11:ARG:HG3 | 14:N:14:ARG:HH12 | 1.82 | 0.44 |
| 23:W:24:LEU:O | 23:W:26:ILE:HG22 | 2.18 | 0.44 |
| 26:Z:65:ASN:HB2 | 26:Z:84:CYS:SG | 2.58 | 0.44 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:CG2 | 2.48 | 0.44 |
| 30:0:40:C:O5' | 30:0:40:C:H6 | 2.01 | 0.44 |
| 30:0:307:G:C2 | 30:0:309:C:C4 | 3.05 | 0.44 |
| 30:0:734:U:H2' | 30:0:736:A:OP2 | 2.17 | 0.44 |
| 30:0:970:U:H2' | 38:0:6313:HOH:O | 2.16 | 0.44 |
| 30:0:1206:U:C6 | 30:0:1206:U:C3' | 3.01 | 0.44 |
| 30:0:1279:U:C5' | 30:0:1280:A:OP2 | 2.65 | 0.44 |
| 30:0:1461:U:H2' | 30:0:1462:C:H6 | 1.83 | 0.44 |
| 30:0:1735:C:O2' | 30:0:1736:A:H5' | 2.17 | 0.44 |
| 30:0:2004:U:H2' | 30:0:2005:G:OP1 | 2.17 | 0.44 |
| 30:0:2410:G:O2' | 30:0:2411:C:H5' | 2.18 | 0.44 |
| 30:0:2642:G:H2' | 30:0:2643:G:O4' | 2.16 | 0.44 |
| 30:0:2777:G:O2' | 30:0:2778:A:H5' | 2.17 | 0.44 |
| 3:C:226:GLY:HA3 | 30:0:1308:A:C4' | 2.48 | 0.44 |
| 4:D:22:VAL:HA | 4:D:73:VAL:O | 2.17 | 0.44 |
| 4:D:154:LYS:H | 4:D:154:LYS:CD | 2.24 | 0.44 |
| 5:E:84:MET:HG2 | 5:E:168:ILE:HD13 | 1.98 | 0.44 |
| 13:M:73:ARG:NH2 | 30:0:2263:G:H5" | 2.32 | 0.44 |
| 20:T:71:VAL:HG12 | 20:T:72:ILE:N | 2.32 | 0.44 |
| 30:0:161:A:H2' | 30:0:162:C:C6 | 2.52 | 0.44 |
| 30:0:664:U:O4 | 30:0:681:G:H5" | 2.16 | 0.44 |
| 30:0:711:G:C2 | 30:0:718:C:O2 | 2.70 | 0.44 |
| 30:0:1928:C:O2' | 30:0:1929:G:H5' | 2.17 | 0.44 |
| 30:0:2663:U:N3 | 30:0:2664:A:N6 | 2.65 | 0.44 |
| 30:0:2755:G:H1' | 38:0:4677:HOH:O | 2.17 | 0.44 |
| 1:A:11:ARG:HD3 | 38:0:9221:HOH:O | 2.17 | 0.44 |
| 3:C:162:VAL:CG2 | 3:C:232:LEU:HD21 | 2.47 | 0.44 |
| 4:D:159:PRO:O | 4:D:163:VAL:HG23 | 2.17 | 0.44 |
| 5:E:95:VAL:HG11 | 5:E:131:LEU:HD11 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:48:VAL:HG23 | 6:F:74:PHE:HB3 | 1.99 | 0.44 |
| 18:R:125:ARG:HG2 | 38:R:8942:HOH:O | 2.17 | 0.44 |
| 20:T:23:VAL:HG23 | 20:T:41:ARG:HG3 | 2.00 | 0.44 |
| 30:0:1076:G:C2 | 30:0:1084:C:C2 | 3.06 | 0.44 |
| 30:0:1477:C:H5' | 30:0:1868:G:H5" | 1.98 | 0.44 |
| 30:0:2245:C:H6 | 30:0:2245:C:O5' | 2.00 | 0.44 |
| 31:9:82:U:H2' | 31:9:83:G:H8 | 1.82 | 0.44 |
| 1:A:46:GLU:C | 26:Z:78:ILE:HD11 | 2.38 | 0.44 |
| 3:C:37:ALA:HA | 3:C:100:LEU:HD12 | 2.00 | 0.44 |
| 9:I:114:TYR:CD1 | 9:I:114:TYR:N | 2.86 | 0.44 |
| 10:J:63:ILE:CD1 | 30:0:1236:A:C8 | 3.01 | 0.44 |
| 12:L:129:ALA:O | 12:L:133:VAL:HG23 | 2.17 | 0.44 |
| 13:M:97:ILE:HD13 | 13:M:127:LYS:HD2 | 2.00 | 0.44 |
| 13:M:123:ASP:OD1 | 13:M:126:GLN:HG2 | 2.18 | 0.44 |
| 14:N:93:GLN:HA | 14:N:93:GLN:HE21 | 1.82 | 0.44 |
| 15:O:49:GLU:OE1 | 15:O:72:LYS:HG3 | 2.17 | 0.44 |
| 16:P:18:LYS:O | 16:P:21:VAL:HG13 | 2.18 | 0.44 |
| 19:S:57:THR:CG2 | 19:S:58:MET:N | 2.79 | 0.44 |
| 21:U:7:ASP:HB2 | 21:U:29:THR:HG23 | 2.00 | 0.44 |
| 30:0:81:G:N3 | 30:0:98:A:C2 | 2.85 | 0.44 |
| 30:0:549:A:C2 | 30:0:550:C:C2 | 3.06 | 0.44 |
| 30:0:737:A:H2' | 30:0:738:G:O4' | 2.18 | 0.44 |
| 30:0:1028:U:H1' | 38:0:3631:HOH:O | 2.18 | 0.44 |
| 30:0:1067:A:H5' | 38:0:4344:HOH:O | 2.18 | 0.44 |
| 30:0:1116:U:C2' | 30:0:1118:A:H2 | 2.28 | 0.44 |
| 30:0:2119:C:O2' | 30:0:2120:U:H5' | 2.18 | 0.44 |
| 30:0:2313:C:H4' | 38:0:6558:HOH:O | 2.18 | 0.44 |
| 30:0:2325:U:O2' | 30:0:2411:C:H1' | 2.18 | 0.44 |
| 30:0:2887:G:H2' | 30:0:2888:U:H6 | 1.79 | 0.44 |
| 4:D:56:ARG:NH2 | 30:0:2332:A:H5' | 2.32 | 0.44 |
| 12:L:149:ARG:O | 12:L:150:GLN:HB2 | 2.17 | 0.44 |
| 13:M:171:ARG:NH2 | 30:0:189:A:OP1 | 2.50 | 0.44 |
| 16:P:41:ARG:NH2 | 30:0:1500:U:OP2 | 2.49 | 0.44 |
| 17:Q:3:SER:O | 17:Q:8:GLU:HG3 | 2.18 | 0.44 |
| 25:Y:116:LEU:HD23 | 25:Y:116:LEU:HA | 1.80 | 0.44 |
| 27:1:1:THR:O | 30:0:1836:A:H1' | 2.17 | 0.44 |
| 29:3:62:THR:HG21 | 30:0:2317:C:H5' | 1.98 | 0.44 |
| 30:0:295:C:H2' | 30:0:296:G:O4' | 2.18 | 0.44 |
| 30:0:462:A:H2' | 38:0:4875:HOH:O | 2.18 | 0.44 |
| 30:0:615:G:H2' | 30:0:616:U:H6 | 1.83 | 0.44 |
| 30:0:725:C:H2' | 30:0:726:C:O5' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:912:A:C4 | 30:0:1294:A:C2 | 3.05 | 0.44 |
| 30:0:1014:A:H2' | 30:0:1015:C:H5' | 1.99 | 0.44 |
| 30:0:1249:U:H2' | 30:0:1250:C:C6 | 2.53 | 0.44 |
| 30:0:1597:A:C4 | 30:0:1598:A:C8 | 3.05 | 0.44 |
| 30:0:1883:U:C2' | 30:0:1884:G:H5' | 2.48 | 0.44 |
| 2:B:119:HIS:O | 2:B:121:PRO:HD3 | 2.18 | 0.44 |
| 14:N:73:ALA:HB1 | 14:N:74:PRO:CD | 2.48 | 0.44 |
| 15:O:21:SER:OG | 15:O:106:PRO:HB2 | 2.18 | 0.44 |
| 23:W:122:ARG:NH2 | 23:W:154:ARG:HG2 | 2.33 | 0.44 |
| 25:Y:234:VAL:HG12 | 25:Y:235:GLU:N | 2.33 | 0.44 |
| 30:0:368:C:C2' | 30:0:369:G:H5' | 2.48 | 0.44 |
| 30:0:1246:A:C4 | 30:0:1248:A:C8 | 3.06 | 0.44 |
| 30:0:1307:A:H2' | 30:0:1308:A:C8 | 2.53 | 0.44 |
| 30:0:1603:A:C5' | 30:0:1605:G:C5' | 2.96 | 0.44 |
| 30:0:1730:G:H4' | 30:0:1731:C:C6 | 2.52 | 0.44 |
| 30:0:1771:U:O2' | 30:0:1773:G:N7 | 2.50 | 0.44 |
| 30:0:1773:G:C2' | 30:0:1774:G:H5' | 2.48 | 0.44 |
| 30:0:2105:C:H2' | 30:0:2106:C:C6 | 2.53 | 0.44 |
| 30:0:2128:G:C5 | 30:0:2129:U:C5 | 3.06 | 0.44 |
| 30:0:2276:U:O2' | 30:0:2277:U:H5' | 2.18 | 0.44 |
| 30:0:2457:U:O2' | 30:0:2458:U:H5' | 2.17 | 0.44 |
| 30:0:2588:OMG:HM23 | 30:0:2617:G:C2 | 2.53 | 0.44 |
| 30:0:2793:A:H2' | 30:0:2794:G:H5' | 2.00 | 0.44 |
| 1:A:26:ASP:OD2 | 30:0:1872:C:H4' | 2.18 | 0.44 |
| 2:B:242:TRP:CZ2 | 30:0:2607:U:C4 | 3.06 | 0.44 |
| 3:C:27:ARG:HD2 | 38:O:327:HOH:O | 2.17 | 0.44 |
| 8:H:157:TYR:HD1 | 8:H:157:TYR:C | 2.21 | 0.44 |
| 13:M:95:LYS:HE2 | 30:0:157:G:H4' | 1.99 | 0.44 |
| 14:N:147:ILE:HD11 | 31:9:50:G:OP1 | 2.18 | 0.44 |
| 17:Q:62:THR:O | 17:Q:64:GLU:HG2 | 2.18 | 0.44 |
| 27:1:21:ARG:HD2 | 27:1:37:CYS:SG | 2.57 | 0.44 |
| 30:0:416:G:H2' | 38:0:9910:HOH:O | 2.16 | 0.44 |
| 30:0:559:U:C6 | 30:0:559:U:C3' | 3.01 | 0.44 |
| 30:0:1066:U:H2' | 30:0:1067:A:C8 | 2.53 | 0.44 |
| 30:0:1254:C:O2' | 30:0:1255:A:H5' | 2.18 | 0.44 |
| 30:0:1657:A:H2' | 30:0:1658:A:C8 | 2.53 | 0.44 |
| 30:0:2072:G:H3' | 30:0:2073:G:C5' | 2.48 | 0.44 |
| 30:0:2473:U:O2' | 30:0:2474:A:H5" | 2.18 | 0.44 |
| 4:D:59:GLY:HA3 | 38:D:4886:HOH:O | 2.17 | 0.43 |
| 12:L:117:GLU:HB3 | 38:L:9018:HOH:O | 2.18 | 0.43 |
| 13:M:102:GLU:OE2 | 13:M:164:THR:HG21 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:M:134:ILE:CG2 | 13:M:141:ILE:HD13 | 2.42 | 0.43 |
| 20:T:48:VAL:CG1 | 20:T:49:GLU:N | 2.81 | 0.43 |
| 24:X:72:VAL:HG22 | 24:X:85:VAL:HG12 | 2.00 | 0.43 |
| 30:0:297:U:H2' | 30:0:298:C:H6 | 1.83 | 0.43 |
| 30:0:590:A:H2' | 30:0:591:A:O4' | 2.18 | 0.43 |
| 30:0:653:U:H2' | 30:0:654:A:C8 | 2.52 | 0.43 |
| 30:0:1198:U:C6 | 30:0:1200:A:OP2 | 2.71 | 0.43 |
| 30:0:1592:G:H1' | 30:0:1593:C:C6 | 2.53 | 0.43 |
| 30:0:2256:G:C2' | 30:0:2257:G:H5' | 2.48 | 0.43 |
| 1:A:182:ARG:HG2 | 1:A:182:ARG:HH11 | 1.83 | 0.43 |
| 2:B:41:PHE:HB3 | 2:B:190:MET:HE2 | 2.00 | 0.43 |
| 2:B:223:ARG:HG3 | 2:B:232:TRP:O | 2.17 | 0.43 |
| 2:B:305:ASP:O | 2:B:306:LYS:CB | 2.66 | 0.43 |
| 3:C:118:THR:O | 3:C:136:VAL:HG13 | 2.18 | 0.43 |
| 4:D:45:THR:HB | 4:D:75:LEU:HD21 | 1.99 | 0.43 |
| 5:E:111:LYS:HE3 | 30:0:2690:U:H4' | 1.99 | 0.43 |
| 12:L:41:HIS:CD2 | 30:0:926:A:O2' | 2.71 | 0.43 |
| 16:P:10:ALA:HA | 16:P:13:VAL:HG12 | 2.01 | 0.43 |
| 17:Q:1:PRO:HA | 30:0:2299:G:O6 | 2.18 | 0.43 |
| 19:S:50:GLU:HB3 | 19:S:67:ARG:NH2 | 2.33 | 0.43 |
| 20:T:38:ARG:HG3 | 20:T:38:ARG:HH11 | 1.83 | 0.43 |
| 30:0:549:A:C6 | 30:0:550:C:C4 | 3.07 | 0.43 |
| 30:0:596:C:H2' | 30:0:597:A:C8 | 2.53 | 0.43 |
| 30:0:1477:C:O2' | 30:0:1478:U:H5' | 2.17 | 0.43 |
| 30:0:1973:A:H2' | 30:0:1974:G:O4' | 2.17 | 0.43 |
| 30:0:2387:U:H2' | 30:0:2388:C:C6 | 2.52 | 0.43 |
| 30:0:2543:G:H2' | 30:0:2544:G:O4' | 2.18 | 0.43 |
| 31:9:64:C:O2' | 31:9:65:A:H5' | 2.18 | 0.43 |
| 1:A:211:LYS:HB2 | 38:A:9038:HOH:O | 2.18 | 0.43 |
| 2:B:18:ARG:HG3 | 2:B:256:GLN:HG3 | 2.00 | 0.43 |
| 14:N:67:ALA:CA | 14:N:71:TRP:HB3 | 2.44 | 0.43 |
| 20:T:48:VAL:HG11 | 20:T:96:VAL:CG1 | 2.46 | 0.43 |
| 25:Y:144:ARG:NH1 | 38:Y:8882:HOH:O | 2.51 | 0.43 |
| 25:Y:148:GLY:HA3 | 30:0:622:G:P | 2.59 | 0.43 |
| 30:0:107:U:C2' | 30:0:108:U:H5' | 2.48 | 0.43 |
| 30:0:1362:U:H5' | 38:0:3253:HOH:O | 2.18 | 0.43 |
| 30:0:1702:U:H5" | 38:0:7207:HOH:O | 2.19 | 0.43 |
| 30:0:2321:A:N1 | 30:0:2378:U:O2 | 2.52 | 0.43 |
| 2:B:42:ALA:CB | 2:B:162:MET:HE3 | 2.48 | 0.43 |
| 2:B:199:TYR:HE1 | 2:B:319:ASP:HB2 | 1.83 | 0.43 |
| 2:B:234:ARG:HG3 | 30:0:1735:C:OP2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:157:TYR:C | 8:H:157:TYR:CD1 | 2.90 | 0.43 |
| 14:N:154:LEU:C | 14:N:156:GLU:H | 2.20 | 0.43 |
| 22:V:50:ARG:HH12 | 30:0:56:G:C5' | 2.30 | 0.43 |
| 26:Z:94:LYS:HA | 38:Z:8719:HOH:O | 2.18 | 0.43 |
| 30:0:275:G:N2 | 30:0:376:C:C2 | 2.87 | 0.43 |
| 30:0:496:G:H3' | 38:0:7658:HOH:O | 2.18 | 0.43 |
| 30:0:853:C:H2' | 30:0:854:G:O4' | 2.17 | 0.43 |
| 30:0:920:C:H5" | 30:0:921:G:O5' | 2.18 | 0.43 |
| 30:0:1183:C:H41 | 30:0:1192:A:P | 2.42 | 0.43 |
| 30:0:1878:G:O2' | 30:0:1879:U:C6 | 2.60 | 0.43 |
| 30:0:2474:A:H4' | 30:0:2475:C:O5' | 2.18 | 0.43 |
| 30:0:2834:G:H2' | 30:0:2835:C:O5' | 2.18 | 0.43 |
| 12:L:34:GLY:HA3 | 12:L:38:HIS:CE1 | 2.52 | 0.43 |
| 23:W:13:MET:HE3 | 23:W:17:ILE:HG22 | 1.99 | 0.43 |
| 23:W:118:LEU:HD12 | 23:W:153:MET:HE3 | 2.00 | 0.43 |
| 29:3:39:GLN:HG2 | 29:3:43:ASN:OD1 | 2.19 | 0.43 |
| 30:0:40:C:H4' | 38:0:6993:HOH:O | 2.18 | 0.43 |
| 30:0:1809:G:H2' | 30:0:1811:A:OP2 | 2.19 | 0.43 |
| 30:0:2355:G:H5" | 30:0:2356:A:OP2 | 2.19 | 0.43 |
| 6:F:14:ASP:O | 6:F:18:GLU:HG3 | 2.18 | 0.43 |
| 10:J:19:MET:HE2 | 10:J:79:PHE:HA | 2.01 | 0.43 |
| 13:M:49:ALA:C | 13:M:54:TYR:HB3 | 2.38 | 0.43 |
| 14:N:86:LEU:O | 14:N:90:LEU:HG | 2.19 | 0.43 |
| 20:T:43:ASN:C | 20:T:45:GLY:H | 2.22 | 0.43 |
| 22:V:49:LEU:O | 22:V:53:ILE:HG13 | 2.18 | 0.43 |
| 30:0:557:C:O2' | 30:0:558:C:H5' | 2.19 | 0.43 |
| 30:0:1185:U:H2' | 30:0:1186:C:C6 | 2.54 | 0.43 |
| 30:0:1471:A:H2' | 30:0:1472:C:C6 | 2.54 | 0.43 |
| 30:0:2039:A:H2' | 30:0:2040:C:C6 | 2.53 | 0.43 |
| 30:0:2102:G:N2 | 30:0:2104:C:N3 | 2.67 | 0.43 |
| 30:0:2346:C:C6 | 30:0:2346:C:O5' | 2.72 | 0.43 |
| 30:0:2718:C:H5' | 30:0:2718:C:C6 | 2.52 | 0.43 |
| 1:A:51:ARG:HH21 | 1:A:53:ALA:HB3 | 1.82 | 0.43 |
| 1:A:190:ARG:NH2 | 1:A:207:GLN:OE1 | 2.52 | 0.43 |
| 1:A:217:ARG:HG2 | 1:A:229:ALA:CB | 2.48 | 0.43 |
| 10:J:107:ASN:HD22 | 10:J:107:ASN:C | 2.22 | 0.43 |
| 11:K:66:ARG:NH2 | 30:0:1994:A:OP1 | 2.52 | 0.43 |
| 20:T:82:THR:HG21 | 30:0:488:U:O2' | 2.19 | 0.43 |
| 24:X:15:ARG:NH1 | 30:0:2896:A:OP1 | 2.51 | 0.43 |
| 25:Y:117:LEU:HB2 | 25:Y:174:VAL:HG21 | 1.99 | 0.43 |
| 28:2:20:ARG:NH1 | 28:2:39:ARG:HH21 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:2:40:ARG:HG3 | 28:2:45:ASN:CB | 2.48 | 0.43 |
| 30:0:328:U:C2 | 30:0:348:C:H4' | 2.53 | 0.43 |
| 30:0:459:A:H4' | 38:0:9455:HOH:O | 2.17 | 0.43 |
| 30:0:750:A:H2' | 30:0:751:U:C6 | 2.54 | 0.43 |
| 30:0:878:G:H4' | 30:0:1835:U:H4' | 2.00 | 0.43 |
| 30:0:1173:A:H4' | 30:0:1174:A:H8 | 1.83 | 0.43 |
| 30:0:1427:A:C2' | 30:0:1428:C:H5' | 2.49 | 0.43 |
| 30:0:1566:C:H2' | 30:0:1567:G:C8 | 2.54 | 0.43 |
| 30:0:1773:G:H4' | 38:0:3505:HOH:O | 2.19 | 0.43 |
| 30:0:2103:A:N3 | 30:0:2103:A:H2' | 2.33 | 0.43 |
| 30:0:2379:G:N3 | 30:0:2418:G:H2' | 2.34 | 0.43 |
| 30:0:2564:G:OP2 | 30:0:2565:C:H5" | 2.18 | 0.43 |
| 31:9:45:A:N7 | 31:9:46:C:C5 | 2.87 | 0.43 |
| 1:A:192:VAL:O | 1:A:207:GLN:HG2 | 2.18 | 0.43 |
| 3:C:132:ASP:O | 3:C:133:ARG:HG3 | 2.19 | 0.43 |
| 4:D:103:ASN:ND2 | 4:D:133:ASN:HD22 | 2.17 | 0.43 |
| 5:E:91:PHE:HE1 | 30:0:2694:A:H4' | 1.83 | 0.43 |
| 38:M:8865:HOH:O | 30:0:2244:A:H1' | 2.18 | 0.43 |
| 14:N:49:THR:HG22 | 14:N:56:ASP:CB | 2.49 | 0.43 |
| 14:N:109:PRO:HB3 | 30:0:2413:A:N7 | 2.34 | 0.43 |
| 18:R:59:PHE:O | 18:R:63:ASN:HB3 | 2.18 | 0.43 |
| 23:W:122:ARG:HG3 | 23:W:122:ARG:HH11 | 1.84 | 0.43 |
| 26:Z:95:PRO:HD2 | 38:Z:8719:HOH:O | 2.18 | 0.43 |
| 30:0:119:A:H2' | 30:0:120:A:C5' | 2.49 | 0.43 |
| 30:0:361:C:H2' | 30:0:362:G:O4' | 2.19 | 0.43 |
| 30:0:2681:A:H4' | 30:0:2682:C:OP1 | 2.19 | 0.43 |
| 30:0:2694:A:H3' | 30:0:2695:C:H6 | 1.84 | 0.43 |
| 31:9:110:G:C2 | 31:9:111:U:C6 | 3.07 | 0.43 |
| 31:9:110:G:C5 | 31:9:111:U:C5 | 3.07 | 0.43 |
| 2:B:116:PRO:HG3 | 30:0:2821:C:H4' | 2.01 | 0.43 |
| 2:B:215:VAL:HB | 38:B:9090:HOH:O | 2.19 | 0.43 |
| 8:H:6:ALA:HB3 | 30:0:2521:A:OP2 | 2.19 | 0.43 |
| 8:H:6:ALA:HA | 8:H:61:ARG:NH1 | 2.34 | 0.43 |
| 9:I:69:PRO:HA | 30:0:1164:U:OP1 | 2.19 | 0.43 |
| 26:Z:40:ALA:O | 30:0:2018:A:H2 | 2.02 | 0.43 |
| 26:Z:88:PHE:CD2 | 26:Z:88:PHE:N | 2.86 | 0.43 |
| 30:0:636:G:H5' | 30:0:2059:U:OP2 | 2.19 | 0.43 |
| 30:0:802:G:H2' | 30:0:803:C:C6 | 2.54 | 0.43 |
| 30:0:920:C:C5 | 30:0:2467:A:OP1 | 2.72 | 0.43 |
| 30:0:1099:G:H2' | 30:0:1100:G:O4' | 2.19 | 0.43 |
| 30:0:1156:C:O2' | 30:0:1157:C:H5' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1592:G:HO2' | 30:0:1593:C:H6 | 1.67 | 0.43 |
| 30:0:1937:U:O2' | 30:0:1938:G:H5' | 2.18 | 0.43 |
| 30:0:2487:C:C5 | 38:0:4880:HOH:O | 2.57 | 0.43 |
| 30:0:2523:U:H2' | 30:0:2524:G:O4' | 2.18 | 0.43 |
| 30:0:2581:U:H1' | 38:0:4466:HOH:O | 2.17 | 0.43 |
| 1:A:48:ASP:HB3 | 1:A:51:ARG:HG3 | 2.00 | 0.43 |
| 1:A:230:SER:CB | 30:0:1852:A:H4' | 2.49 | 0.43 |
| 4:D:136:ARG:HA | 4:D:137:PRO:HD3 | 1.84 | 0.43 |
| 5:E:91:PHE:HA | 5:E:92:PRO:HD3 | 1.86 | 0.43 |
| 10:J:93:ARG:HB3 | 10:J:93:ARG:HH11 | 1.84 | 0.43 |
| 16:P:58:SER:HB3 | 38:0:5616:HOH:O | 2.18 | 0.43 |
| 16:P:129:GLY:HA2 | 38:P:153:HOH:O | 2.18 | 0.43 |
| 23:W:122:ARG:NH2 | 38:0:5280:HOH:O | 2.51 | 0.43 |
| 24:X:15:ARG:NH2 | 30:0:2856:A:OP1 | 2.52 | 0.43 |
| 24:X:34:ARG:NH1 | 24:X:48:VAL:O | 2.51 | 0.43 |
| 29:3:13:HIS:HD2 | 29:3:76:LYS:HB3 | 1.83 | 0.43 |
| 30:0:236:A:H8 | 30:0:236:A:OP1 | 2.02 | 0.43 |
| 30:0:301:C:H2' | 30:0:302:A:C8 | 2.54 | 0.43 |
| 30:0:308:U:C4 | 30:0:342:C:C1' | 3.01 | 0.43 |
| 30:0:1456:C:H2' | 30:0:1457:U:C6 | 2.53 | 0.43 |
| 30:0:1561:U:C5' | 38:0:7421:HOH:O | 2.67 | 0.43 |
| 30:0:1758:U:H2' | 30:0:1759:A:O4' | 2.19 | 0.43 |
| 30:0:1923:G:H2' | 30:0:1924:A:H8 | 1.83 | 0.43 |
| 30:0:2252:A:H2' | 30:0:2253:G:O4' | 2.19 | 0.43 |
| 31:9:3:A:N6 | 31:9:22:G:H1' | 2.34 | 0.43 |
| 2:B:141:ARG:HD2 | 2:B:163:GLU:OE2 | 2.19 | 0.42 |
| 10:J:131:THR:HG22 | 10:J:133:GLY:N | 2.34 | 0.42 |
| 12:L:117:GLU:HG3 | 12:L:117:GLU:O | 2.19 | 0.42 |
| 12:L:150:GLN:HB3 | 38:L:9032:HOH:O | 2.18 | 0.42 |
| 30:0:290:C:C2' | 30:0:291:C:H5' | 2.49 | 0.42 |
| 30:0:412:C:O2' | 30:0:413:G:H5' | 2.18 | 0.42 |
| 30:0:612:U:H2' | 30:0:613:C:H6 | 1.84 | 0.42 |
| 30:0:1095:U:H2' | 30:0:1096:U:O4' | 2.18 | 0.42 |
| 30:0:1552:G:C6 | 30:0:1634:G:C6 | 3.07 | 0.42 |
| 30:0:1748:U:C5 | 30:0:1749:U:C4 | 3.07 | 0.42 |
| 30:0:1882:C:O2' | 30:0:2012:U:OP2 | 2.32 | 0.42 |
| 30:0:2070:G:H2' | 30:0:2072:G:OP1 | 2.19 | 0.42 |
| 30:0:2499:U:H1' | 38:0:9433:HOH:O | 2.19 | 0.42 |
| 30:0:2553:A:H2' | 30:0:2553:A:N3 | 2.34 | 0.42 |
| 30:0:2587:OMU:H2' | 30:0:2589:U:H5" | 2.01 | 0.42 |
| 31:9:65:A:N6 | 31:9:112:U:C6 | 2.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:135:VAL:HG22 | 1:A:136:ALA:N | 2.35 | 0.42 |
| 5:E:146:ALA:O | 5:E:150:GLN:HG2 | 2.19 | 0.42 |
| 15:O:105:ASN:HD21 | 15:O:109:SER:N | 2.17 | 0.42 |
| 15:O:112:ARG:NH2 | 30:0:719:C:O2' | 2.52 | 0.42 |
| 17:Q:64:GLU:HG3 | 17:Q:74:ASP:OD2 | 2.18 | 0.42 |
| 30:0:271:C:C2 | 30:0:273:G:O4' | 2.73 | 0.42 |
| 30:0:696:C:H4' | 38:0:7268:HOH:O | 2.19 | 0.42 |
| 30:0:706:G:N2 | 30:0:707:C:H41 | 2.17 | 0.42 |
| 30:0:1562:C:N4 | 38:0:5849:HOH:O | 2.49 | 0.42 |
| 30:0:1878:G:H4' | 38:0:6104:HOH:O | 2.19 | 0.42 |
| 30:0:1878:G:H5" | 38:0:5160:HOH:O | 2.18 | 0.42 |
| 30:0:2061:C:H2' | 30:0:2062:A:H5' | 1.99 | 0.42 |
| 30:0:2415:A:H2' | 30:0:2416:G:H5' | 2.01 | 0.42 |
| 30:0:2842:G:H2' | 30:0:2843:A:C5' | 2.48 | 0.42 |
| 1:A:8:ARG:HG2 | 38:A:8978:HOH:O | 2.20 | 0.42 |
| 2:B:8:LYS:HG3 | 2:B:220:VAL:HG12 | 2.01 | 0.42 |
| 2:B:17:LYS:O | 2:B:260:HIS:HD2 | 2.02 | 0.42 |
| 2:B:62:ARG:HA | 2:B:65:MET:HE2 | 2.01 | 0.42 |
| 2:B:217:ARG:HG3 | 2:B:257:THR:CG2 | 2.41 | 0.42 |
| 12:L:11:ARG:O | 30:0:903:U:C2 | 2.72 | 0.42 |
| 13:M:84:LYS:HB2 | 30:0:170:U:OP1 | 2.18 | 0.42 |
| 16:P:105:LEU:HD21 | 16:P:137:LEU:HD11 | 2.01 | 0.42 |
| 17:Q:2:SER:HA | 38:0:6711:HOH:O | 2.19 | 0.42 |
| 23:W:142:ASP:HB3 | 23:W:145:GLY:H | 1.83 | 0.42 |
| 27:1:25:LYS:HD2 | 28:2:48:ASP:HA | 2.02 | 0.42 |
| 30:0:113:A:H3' | 30:0:114:A:C5' | 2.48 | 0.42 |
| 30:0:128:A:C8 | 30:0:128:A:C3' | 2.99 | 0.42 |
| 30:0:276:C:H6 | 30:0:276:C:O5' | 2.02 | 0.42 |
| 30:0:1206:U:C6 | 30:0:1206:U:H3' | 2.55 | 0.42 |
| 30:0:1345:A:H2' | 30:0:1346:U:C6 | 2.54 | 0.42 |
| 30:0:1407:A:O2' | 30:0:1408:U:H3' | 2.20 | 0.42 |
| 30:0:1544:U:O2' | 30:0:1545:C:H5' | 2.19 | 0.42 |
| 30:0:1757:U:H6 | 30:0:1757:U:O5' | 2.03 | 0.42 |
| 30:0:2035:C:O5' | 30:0:2035:C:H6 | 2.02 | 0.42 |
| 30:0:2787:C:H5 | 38:0:4627:HOH:O | 2.02 | 0.42 |
| 1:A:70:ALA:HA | 1:A:71:PRO:HD3 | 1.73 | 0.42 |
| 1:A:135:VAL:HG11 | 1:A:147:ARG:NH2 | 2.34 | 0.42 |
| 4:D:50:VAL:HG13 | 31:9:41:C:O4' | 2.19 | 0.42 |
| 4:D:54:ALA:HB2 | 30:0:2346:C:H5' | 2.01 | 0.42 |
| 5:E:126:ILE:HA | 5:E:131:LEU:HD23 | 2.00 | 0.42 |
| 11:K:79:PRO:HB3 | 11:K:87:ARG:HB3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:L:7:GLN:HB3 | 12:L:13:HIS:CE1 | 2.54 | 0.42 |
| 13:M:97:ILE:HG21 | 13:M:127:LYS:HD2 | 2.01 | 0.42 |
| 18:R:68:HIS:O | 30:0:2842:G:H5' | 2.19 | 0.42 |
| 29:3:3:MET:HA | 29:3:4:PRO:HD2 | 1.86 | 0.42 |
| 30:0:707:C:C2 | 30:0:708:A:C8 | 3.07 | 0.42 |
| 30:0:1173:A:C2 | 30:0:1177:A:C8 | 3.07 | 0.42 |
| 30:0:1393:A:N1 | 30:0:1725:C:O2' | 2.44 | 0.42 |
| 30:0:1585:C:H2' | 30:0:1586:G:H8 | 1.84 | 0.42 |
| 30:0:1804:A:H2' | 30:0:1805:G:C8 | 2.53 | 0.42 |
| 30:0:1902:G:C2 | 30:0:1936:C:C2 | 3.07 | 0.42 |
| 30:0:2709:G:N2 | 38:0:7613:HOH:O | 2.53 | 0.42 |
| 30:0:2828:G:O5' | 30:0:2828:G:H8 | 2.03 | 0.42 |
| 2:B:310:ARG:HB3 | 38:B:9121:HOH:O | 2.19 | 0.42 |
| 10:J:45:VAL:CG2 | 10:J:129:PHE:HD1 | 2.32 | 0.42 |
| 11:K:64:MET:HA | 11:K:67:GLN:HE21 | 1.84 | 0.42 |
| 12:L:53:ARG:NH2 | 12:L:57:VAL:HG12 | 2.34 | 0.42 |
| 16:P:103:THR:O | 16:P:107:GLU:HG3 | 2.19 | 0.42 |
| 19:S:6:LYS:HD3 | 38:S:2519:HOH:O | 2.20 | 0.42 |
| 23:W:128:VAL:HG22 | 30:0:1098:A:OP1 | 2.19 | 0.42 |
| 30:0:407:A:H3' | 38:0:4452:HOH:O | 2.19 | 0.42 |
| 30:0:420:U:O4' | 30:0:1920:C:C4 | 2.73 | 0.42 |
| 30:0:727:G:H3' | 30:0:728:C:C6 | 2.54 | 0.42 |
| 30:0:849:C:H2' | 30:0:850:U:O4' | 2.20 | 0.42 |
| 30:0:939:A:N1 | 30:0:1027:G:O2' | 2.45 | 0.42 |
| 30:0:1321:A:H2' | 30:0:1322:G:C8 | 2.55 | 0.42 |
| 30:0:1420:C:O2 | 30:0:1420:C:H2' | 2.19 | 0.42 |
| 30:0:1933:G:O2' | 30:0:1934:A:H5' | 2.19 | 0.42 |
| 30:0:2480:G:O2' | 30:0:2481:G:H5' | 2.19 | 0.42 |
| 31:9:58:G:H3' | 31:9:59:C:C6 | 2.54 | 0.42 |
| 2:B:101:TRP:HB2 | 2:B:119:HIS:CD2 | 2.54 | 0.42 |
| 2:B:145:HIS:CD2 | 2:B:146:THR:O | 2.63 | 0.42 |
| 2:B:215:VAL:HA | 2:B:220:VAL:HG22 | 2.00 | 0.42 |
| 2:B:234:ARG:NH2 | 30:0:2039:A:OP2 | 2.53 | 0.42 |
| 5:E:112:ALA:HA | 5:E:113:PRO:HD3 | 1.77 | 0.42 |
| 5:E:137:ASP:OD1 | 5:E:139:GLU:HB2 | 2.19 | 0.42 |
| 8:H:61:ARG:HH11 | 8:H:61:ARG:HG3 | 1.85 | 0.42 |
| 13:M:188:ARG:NH1 | 30:0:154:C:H3' | 2.35 | 0.42 |
| 29:3:29:ARG:HG2 | 29:3:30:GLN:N | 2.35 | 0.42 |
| 30:0:154:C:O2' | 30:0:155:C:H5' | 2.18 | 0.42 |
| 30:0:273:G:H2' | 30:0:274:G:O4' | 2.20 | 0.42 |
| 30:0:299:U:C2 | 30:0:300:U:C5 | 3.08 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:571:C:O5' | 30:0:571:C:H6 | 2.02 | 0.42 |
| 30:0:1006:A:H2' | 30:0:1007:A:C8 | 2.55 | 0.42 |
| 30:0:1559:A:OP2 | 30:0:1559:A:C8 | 2.70 | 0.42 |
| 1:A:217:ARG:NH2 | 30:0:1853:C:O2' | 2.53 | 0.42 |
| 2:B:314:ALA:HB3 | 2:B:317:PRO:HG3 | 2.02 | 0.42 |
| 8:H:117:ARG:HH12 | 30:0:2287:C:N4 | 2.17 | 0.42 |
| 13:M:46:LEU:HD22 | 13:M:50:ARG:CD | 2.50 | 0.42 |
| 13:M:172:GLY:HA2 | 38:0:9086:HOH:O | 2.19 | 0.42 |
| 14:N:143:ARG:HG2 | 14:N:172:PHE:CD2 | 2.54 | 0.42 |
| 30:0:17:G:H2' | 30:0:18:C:H6 | 1.84 | 0.42 |
| 30:0:137:U:OP1 | 30:0:259:G:O2' | 2.36 | 0.42 |
| 30:0:947:U:O2' | 30:0:948:G:H5' | 2.20 | 0.42 |
| 30:0:1168:C:C5 | 30:0:1169:U:C4 | 3.08 | 0.42 |
| 30:0:1454:U:H5" | 30:0:1455:C:OP2 | 2.19 | 0.42 |
| 30:0:1883:U:O2' | 30:0:1884:G:H5' | 2.19 | 0.42 |
| 30:0:1924:A:H1' | 38:0:5731:HOH:O | 2.19 | 0.42 |
| 30:0:2274:A:H2' | 30:0:2275:G:C8 | 2.54 | 0.42 |
| 30:0:2321:A:C5 | 30:0:2323:G:C8 | 3.07 | 0.42 |
| 1:A:190:ARG:NH1 | 30:0:1845:A:OP2 | 2.53 | 0.42 |
| 2:B:252:PRO:HD3 | 38:0:9818:HOH:O | 2.18 | 0.42 |
| 8:H:151:GLU:OE1 | 8:H:151:GLU:HA | 2.19 | 0.42 |
| 11:K:132:VAL:HG11 | 21:U:22:VAL:HG22 | 2.02 | 0.42 |
| 13:M:74:LYS:HB3 | 38:M:8944:HOH:O | 2.20 | 0.42 |
| 19:S:8:PRO:HD2 | 22:V:32:ALA:HA | 2.02 | 0.42 |
| 20:T:106:GLU:HG3 | 38:T:4913:HOH:O | 2.20 | 0.42 |
| 22:V:39:ALA:C | 22:V:41:GLU:H | 2.22 | 0.42 |
| 24:X:70:ILE:O | 24:X:70:ILE:HG23 | 2.20 | 0.42 |
| 26:Z:42:TYR:HA | 30:0:1829:A:N6 | 2.35 | 0.42 |
| 29:3:64:LYS:HB3 | 29:3:82:GLY:O | 2.20 | 0.42 |
| 30:0:162:C:H2' | 30:0:163:U:H5' | 2.02 | 0.42 |
| 30:0:644:G:H5' | 30:0:644:G:N3 | 2.35 | 0.42 |
| 30:0:918:G:C2 | 30:0:926:A:C2 | 3.08 | 0.42 |
| 30:0:1188:A:C5 | 30:0:1189:A:N1 | 2.88 | 0.42 |
| 30:0:1539:U:O2' | 30:0:1540:G:H5' | 2.20 | 0.42 |
| 30:0:1576:G:H2' | 30:0:1577:U:C6 | 2.54 | 0.42 |
| 30:0:1815:A:H2' | 30:0:1816:C:O4' | 2.20 | 0.42 |
| 30:0:2354:A:C2 | 30:0:2367:A:C8 | 3.08 | 0.42 |
| 30:0:2671:U:C2' | 30:0:2672:C:O5' | 2.68 | 0.42 |
| 30:0:2673:U:O2' | 30:0:2674:G:H5' | 2.20 | 0.42 |
| 30:0:2690:U:C4 | 30:0:2691:A:C5 | 3.07 | 0.42 |
| 31:9:91:C:H2' | 31:9:92:G:O4' | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:9:116:C:O2' | 31:9:117:G:H5' | 2.20 | 0.42 |
| 8:H:10:ARG:HD2 | 8:H:161:THR:HG21 | 2.01 | 0.42 |
| 10:J:74:ARG:O | 10:J:78:ILE:HG12 | 2.20 | 0.42 |
| 13:M:48:LYS:HE3 | 13:M:52:GLN:NE2 | 2.34 | 0.42 |
| 13:M:187:LEU:HD22 | 13:M:194:GLY:HA3 | 2.01 | 0.42 |
| 25:Y:160:LYS:HD3 | 25:Y:160:LYS:HA | 1.87 | 0.42 |
| 25:Y:189:ASN:C | 25:Y:189:ASN:HD22 | 2.23 | 0.42 |
| 28:2:43:ARG:HH22 | 30:0:1684:A:C1' | 2.26 | 0.42 |
| 30:0:151:A:H2' | 30:0:152:A:C8 | 2.55 | 0.42 |
| 30:0:710:G:O2' | 30:0:711:G:H5' | 2.20 | 0.42 |
| 30:0:820:G:O2' | 30:0:856:G:H4' | 2.20 | 0.42 |
| 30:0:1198:U:H2' | 30:0:1200:A:OP2 | 2.20 | 0.42 |
| 30:0:1200:A:H4' | 38:0:7330:HOH:O | 2.19 | 0.42 |
| 30:0:1474:C:C6 | 30:0:1474:C:C5' | 2.89 | 0.42 |
| 30:0:1573:A:H2' | 30:0:1574:C:O4' | 2.20 | 0.42 |
| 30:0:2332:A:H2' | 38:0:5623:HOH:O | 2.19 | 0.42 |
| 30:0:2458:U:O2' | 30:0:2459:G:H5' | 2.20 | 0.42 |
| 30:0:2474:A:N7 | 30:0:2621:PSU:H4' | 2.34 | 0.42 |
| 30:0:2893:C:O2' | 30:0:2894:C:H5' | 2.19 | 0.42 |
| 1:A:94:LEU:HD12 | 1:A:98:GLU:CB | 2.47 | 0.42 |
| 10:J:52:GLN:HE21 | 30:0:1119:G:H5' | 1.84 | 0.42 |
| 18:R:89:LEU:HD23 | 18:R:89:LEU:HA | 1.82 | 0.42 |
| 18:R:98:ASN:ND2 | 30:0:500:G:H21 | 2.11 | 0.42 |
| 20:T:48:VAL:CG1 | 20:T:96:VAL:HG13 | 2.50 | 0.42 |
| 23:W:139:GLY:O | 23:W:141:HIS:CD2 | 2.73 | 0.42 |
| 24:X:10:VAL:HG11 | 24:X:36:HIS:HE1 | 1.85 | 0.42 |
| 30:0:191:A:H2' | 30:0:237:G:O6 | 2.20 | 0.42 |
| 30:0:364:U:H2' | 30:0:365:G:O4' | 2.20 | 0.42 |
| 30:0:1158:G:H2' | 30:0:1159:G:C5' | 2.50 | 0.42 |
| 30:0:1181:A:N1 | 30:0:1192:A:O2' | 2.45 | 0.42 |
| 30:0:1314:U:H5" | 30:0:1316:G:O4' | 2.19 | 0.42 |
| 30:0:1538:C:O2' | 30:0:1539:U:H5' | 2.19 | 0.42 |
| 30:0:1585:C:H2' | 30:0:1586:G:C8 | 2.54 | 0.42 |
| 30:0:1794:G:N2 | 30:0:1796:A:H3' | 2.35 | 0.42 |
| 31:9:29:C:C5 | 31:9:30:C:C6 | 3.08 | 0.42 |
| 1:A:20:SER:HB3 | 30:0:1872:C:H5 | 1.85 | 0.41 |
| 2:B:49:THR:HG22 | 2:B:331:SER:HB3 | 2.02 | 0.41 |
| 6:F:54:VAL:HG13 | 30:0:263:U:C4 | 2.55 | 0.41 |
| 9:I:91:PHE:CD2 | 9:I:131:GLY:HA2 | 2.44 | 0.41 |
| 10:J:42:GLU:HG2 | 10:J:43:ARG:N | 2.34 | 0.41 |
| 23:W:21:LEU:HD21 | 23:W:48:VAL:CG1 | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:Z:41:ARG:HD3 | 38:Z:8717:HOH:O | 2.19 | 0.41 |
| 30:0:299:U:H2' | 30:0:300:U:H6 | 1.85 | 0.41 |
| 30:0:1135:G:H5' | 38:0:5913:HOH:O | 2.19 | 0.41 |
| 30:0:1316:G:H5" | 38:0:5311:HOH:O | 2.20 | 0.41 |
| 30:0:1345:A:H2' | 30:0:1346:U:H6 | 1.85 | 0.41 |
| 30:0:1359:U:C5 | 30:0:2101:A:H8 | 2.38 | 0.41 |
| 30:0:1531:U:O2 | 30:0:1661:A:C2 | 2.73 | 0.41 |
| 30:0:1734:C:O5' | 30:0:1734:C:H6 | 2.03 | 0.41 |
| 31:9:73:A:N1 | 31:9:108:C:O2 | 2.53 | 0.41 |
| 1:A:135:VAL:HG11 | 1:A:147:ARG:HH21 | 1.85 | 0.41 |
| 11:K:41:LYS:O | 11:K:42:ASN:HB2 | 2.21 | 0.41 |
| 16:P:61:ARG:NH2 | 30:0:2737:C:OP2 | 2.45 | 0.41 |
| 20:T:14:ALA:HA | 20:T:15:PRO:HD3 | 1.89 | 0.41 |
| 20:T:52:ARG:O | 30:0:317:A:OP1 | 2.37 | 0.41 |
| 25:Y:154:ARG:NH2 | 30:0:1071:G:H4' | 2.36 | 0.41 |
| 26:Z:65:ASN:ND2 | 26:Z:84:CYS:SG | 2.91 | 0.41 |
| 30:0:34:C:H1' | 38:0:9175:HOH:O | 2.18 | 0.41 |
| 30:0:257:G:N2 | 30:0:258:G:C4 | 2.88 | 0.41 |
| 30:0:559:U:C4 | 30:0:560:U:C4 | 3.08 | 0.41 |
| 30:0:567:U:H5" | 38:0:6387:HOH:O | 2.19 | 0.41 |
| 30:0:820:G:N3 | 30:0:1831:U:H1' | 2.35 | 0.41 |
| 30:0:1333:U:H2' | 30:0:1334:C:C6 | 2.54 | 0.41 |
| 30:0:1405:U:H2' | 38:0:6827:HOH:O | 2.20 | 0.41 |
| 30:0:1441:G:H1' | 38:0:7755:HOH:O | 2.19 | 0.41 |
| 30:0:1572:A:C2 | 30:0:1573:A:C4 | 3.08 | 0.41 |
| 30:0:1832:G:H5" | 38:0:9044:HOH:O | 2.19 | 0.41 |
| 30:0:1926:G:C4 | 30:0:1927:A:C8 | 3.08 | 0.41 |
| 30:0:1980:U:O2' | 30:0:1981:A:H5' | 2.20 | 0.41 |
| 30:0:1997:A:C6 | 30:0:1998:G:C5 | 3.09 | 0.41 |
| 31:9:3:A:C8 | 31:9:26:C:O2 | 2.72 | 0.41 |
| 1:A:51:ARG:NH2 | 1:A:69:LEU:HD11 | 2.36 | 0.41 |
| 3:C:19:PRO:HG2 | 3:C:22:PHE:CE1 | 2.56 | 0.41 |
| 5:E:101:GLU:HA | 5:E:118:ILE:HG13 | 2.01 | 0.41 |
| 15:O:29:VAL:HG11 | 15:O:98:LEU:HD21 | 2.02 | 0.41 |
| 20:T:71:VAL:CG1 | 20:T:90:PRO:HB3 | 2.40 | 0.41 |
| 28:2:40:ARG:HD2 | 28:2:47:THR:HG22 | 2.01 | 0.41 |
| 30:0:282:C:O2' | 30:0:283:U:C4' | 2.69 | 0.41 |
| 30:0:778:C:C4 | 30:0:779:U:C4 | 3.08 | 0.41 |
| 30:0:818:A:C6 | 30:0:819:A:C2 | 3.07 | 0.41 |
| 30:0:1116:U:C2' | 30:0:1118:A:C2 | 3.04 | 0.41 |
| 30:0:1168:C:C5 | 30:0:1169:U:C5 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1168:C:C4 | 30:0:1169:U:C4 | 3.08 | 0.41 |
| 30:0:2675:A:H1' | 30:0:2813:A:C2 | 2.56 | 0.41 |
| 30:0:2909:G:H2' | 30:0:2910:A:H8 | 1.85 | 0.41 |
| 31:9:39:U:C2' | 31:9:40:C:OP1 | 2.68 | 0.41 |
| 31:9:119:C:H2' | 31:9:120:A:C8 | 2.55 | 0.41 |
| 14:N:40:ASN:HD21 | 31:9:28:U:H5" | 1.83 | 0.41 |
| 14:N:42:HIS:CB | 14:N:62:HIS:HE1 | 2.33 | 0.41 |
| 29:3:69:TYR:CE1 | 29:3:80:ARG:HB2 | 2.55 | 0.41 |
| 30:0:271:C:N4 | 30:0:378:A:C2 | 2.76 | 0.41 |
| 30:0:546:C:O5' | 30:0:546:C:H6 | 2.03 | 0.41 |
| 30:0:820:G:C5' | 30:0:821:U:H5' | 2.46 | 0.41 |
| 30:0:1015:C:C2 | 30:0:1016:U:C5 | 3.09 | 0.41 |
| 30:0:1246:A:C5 | 30:0:1248:A:C5 | 3.09 | 0.41 |
| 30:0:1607:A:C4 | 30:0:1608:G:C8 | 3.08 | 0.41 |
| 30:0:2011:A:H5' | 30:0:2013:G:H1' | 2.01 | 0.41 |
| 30:0:2092:G:H5" | 30:0:2613:G:OP1 | 2.21 | 0.41 |
| 30:0:2874:G:H3' | 38:0:9578:HOH:O | 2.21 | 0.41 |
| 31:9:7:G:C5' | 38:9:9099:HOH:O | 2.68 | 0.41 |
| 31:9:31:C:O2' | 31:9:32:G:H5' | 2.20 | 0.41 |
| 9:I:123:VAL:O | 9:I:127:CYS:SG | 2.78 | 0.41 |
| 10:J:116:LEU:HB2 | 10:J:119:THR:HG21 | 2.02 | 0.41 |
| 13:M:68:ARG:CZ | 13:M:73:ARG:HD3 | 2.51 | 0.41 |
| 16:P:3:LEU:HA | 16:P:6:GLN:OE1 | 2.21 | 0.41 |
| 17:Q:21:ARG:HG2 | 17:Q:22:GLY:H | 1.86 | 0.41 |
| 22:V:12:THR:H | 22:V:15:GLU:HB2 | 1.85 | 0.41 |
| 23:W:117:ARG:HD3 | 30:0:1287:A:O4' | 2.20 | 0.41 |
| 25:Y:187:VAL:HG13 | 25:Y:205:ILE:HA | 2.02 | 0.41 |
| 29:3:46:ILE:HA | 38:0:7897:HOH:O | 2.20 | 0.41 |
| 30:0:293:A:P | 30:0:358:G:H22 | 2.43 | 0.41 |
| 30:0:488:U:H2' | 38:0:4003:HOH:O | 2.20 | 0.41 |
| 30:0:652:G:H8 | 38:0:3003:HOH:O | 2.03 | 0.41 |
| 30:0:932:U:H1' | 30:0:1296:A:H1' | 2.02 | 0.41 |
| 30:0:1183:C:O2 | 30:0:1183:C:C2' | 2.68 | 0.41 |
| 30:0:1191:A:H8 | 30:0:1191:A:H3' | 1.84 | 0.41 |
| 30:0:1335:C:H2' | 30:0:1336:U:C6 | 2.56 | 0.41 |
| 30:0:1545:C:H2' | 30:0:1546:G:O4' | 2.20 | 0.41 |
| 30:0:2799:A:N6 | 30:0:2801:A:C2 | 2.89 | 0.41 |
| 31:9:1:U:O3' | 31:9:3:A:OP1 | 2.39 | 0.41 |
| 31:9:9:C:H2' | 31:9:10:C:H5' | 2.03 | 0.41 |
| 31:9:112:U:H2' | 31:9:113:C:H5' | 2.02 | 0.41 |
| 1:A:194:MET:CE | 1:A:199:HIS:HB2 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:27:ARG:NH1 | 3:C:27:ARG:CG | 2.79 | 0.41 |
| 7:G:71:LEU:C | 7:G:73:ASP:H | 2.23 | 0.41 |
| 11:K:34:VAL:CG2 | 11:K:47:ALA:HB2 | 2.51 | 0.41 |
| 12:L:6:ARG:NH1 | 30:0:1299:G:N7 | 2.68 | 0.41 |
| 13:M:77:HIS:CG | 13:M:81:ARG:HB2 | 2.56 | 0.41 |
| 14:N:23:ARG:O | 14:N:27:LEU:HG | 2.21 | 0.41 |
| 16:P:80:ARG:HG2 | 16:P:87:ARG:CZ | 2.50 | 0.41 |
| 17:Q:16:ASN:HD22 | 17:Q:16:ASN:HA | 1.67 | 0.41 |
| 18:R:17:MET:HE3 | 18:R:19:ARG:HH21 | 1.86 | 0.41 |
| 23:W:24:LEU:HD21 | 23:W:44:MET:SD | 2.61 | 0.41 |
| 27:1:16:HIS:CD2 | 30:0:470:U:O2' | 2.72 | 0.41 |
| 28:2:2:LYS:HG3 | 30:0:1486:A:C4 | 2.55 | 0.41 |
| 29:3:73:GLU:HB3 | 38:3:9056:HOH:O | 2.21 | 0.41 |
| 30:0:69:A:H2' | 30:0:70:A:OP2 | 2.20 | 0.41 |
| 30:0:69:A:C2' | 30:0:70:A:OP2 | 2.69 | 0.41 |
| 30:0:822:C:C2 | 30:0:823:U:C5 | 3.08 | 0.41 |
| 30:0:1362:U:H2' | 30:0:1363:G:C8 | 2.55 | 0.41 |
| 30:0:1427:A:O2' | 30:0:1428:C:H5' | 2.21 | 0.41 |
| 30:0:1563:G:H4' | 30:0:1564:C:H5' | 2.01 | 0.41 |
| 30:0:1757:U:H5 | 38:0:3211:HOH:O | 2.03 | 0.41 |
| 30:0:1903:U:O2' | 30:0:1904:A:C8 | 2.73 | 0.41 |
| 30:0:1915:U:H2' | 30:0:1916:C:O4' | 2.21 | 0.41 |
| 30:0:2092:G:H2' | 30:0:2613:G:OP1 | 2.21 | 0.41 |
| 30:0:2409:C:H5" | 38:0:4005:HOH:O | 2.20 | 0.41 |
| 4:D:84:LEU:HA | 4:D:87:ALA:HB3 | 2.02 | 0.41 |
| 5:E:77:THR:OG1 | 5:E:78:GLU:N | 2.52 | 0.41 |
| 5:E:155:ASN:ND2 | 5:E:155:ASN:H | 2.17 | 0.41 |
| 16:P:13:VAL:HG13 | 16:P:14:LEU:N | 2.36 | 0.41 |
| 23:W:23:MET:O | 30:0:1025:C:H5' | 2.21 | 0.41 |
| 23:W:38:THR:HG22 | 38:W:3580:HOH:O | 2.21 | 0.41 |
| 30:0:130:C:H2' | 38:0:3150:HOH:O | 2.21 | 0.41 |
| 30:0:186:A:OP1 | 30:0:186:A:H4' | 2.21 | 0.41 |
| 30:0:396:U:H1' | 30:0:397:A:OP1 | 2.20 | 0.41 |
| 30:0:536:A:N1 | 30:0:2075:G:O2' | 2.50 | 0.41 |
| 30:0:964:G:C4 | 30:0:965:A:C8 | 3.08 | 0.41 |
| 30:0:1051:C:H2' | 30:0:1052:G:O4' | 2.20 | 0.41 |
| 30:0:1339:G:C6 | 30:0:1340:G:N1 | 2.89 | 0.41 |
| 30:0:1947:G:H2' | 30:0:1948:G:C8 | 2.55 | 0.41 |
| 30:0:2872:U:C2 | 30:0:2873:C:C6 | 3.08 | 0.41 |
| 30:0:2880:A:H2' | 30:0:2881:C:H5' | 2.02 | 0.41 |
| 31:9:70:U:H2' | 31:9:71:C:O4' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:22:PHE:HA | 3:C:116:ALA:HA | 2.02 | 0.41 |
| 30:0:73:U:O2' | 30:0:74:G:H5' | 2.21 | 0.41 |
| 30:0:240:C:O2 | 30:0:240:C:H2' | 2.20 | 0.41 |
| 30:0:397:A:H1' | 30:0:417:G:H1' | 2.03 | 0.41 |
| 30:0:706:G:O2' | 30:0:707:C:H6 | 2.03 | 0.41 |
| 30:0:800:G:H2' | 30:0:801:U:C6 | 2.56 | 0.41 |
| 30:0:1215:A:O3' | 30:0:1216:G:C4' | 2.69 | 0.41 |
| 30:0:1337:G:C6 | 30:0:1338:U:C4 | 3.09 | 0.41 |
| 30:0:1682:A:H5" | 38:0:9458:HOH:O | 2.20 | 0.41 |
| 30:0:2780:C:C4 | 30:0:2781:U:C4 | 3.09 | 0.41 |
| 30:0:2892:G:C6 | 30:0:2893:C:C4 | 3.09 | 0.41 |
| 1:A:45:ILE:HD12 | 26:Z:89:THR:HG23 | 2.02 | 0.41 |
| 2:B:27:ASN:HD21 | 30:0:2807:U:P | 2.43 | 0.41 |
| 2:B:58:PRO:HA | 2:B:63:GLU:CD | 2.40 | 0.41 |
| 2:B:69:VAL:HA | 2:B:70:PRO:HD3 | 1.82 | 0.41 |
| 2:B:274:GLU:HA | 2:B:292:GLY:O | 2.21 | 0.41 |
| 3:C:44:GLN:HA | 38:C:8614:HOH:O | 2.21 | 0.41 |
| 3:C:87:ARG:NH2 | 30:0:894:A:C2 | 2.89 | 0.41 |
| 4:D:15:GLU:HA | 4:D:16:PRO:HD3 | 1.73 | 0.41 |
| 6:F:57:GLU:O | 6:F:61:MET:HG3 | 2.21 | 0.41 |
| 10:J:45:VAL:HG21 | 10:J:129:PHE:CD1 | 2.56 | 0.41 |
| 11:K:75:ARG:HD2 | 11:K:90:PHE:CD2 | 2.55 | 0.41 |
| 12:L:53:ARG:HD2 | 30:0:2441:U:H4' | 2.02 | 0.41 |
| 14:N:48:VAL:HG11 | 14:N:55:ASP:HB3 | 2.02 | 0.41 |
| 20:T:32:ARG:NH1 | 20:T:38:ARG:NH1 | 2.68 | 0.41 |
| 26:Z:54:GLU:HB3 | 38:Z:8731:HOH:O | 2.21 | 0.41 |
| 29:3:88:LEU:HD22 | 33:3:8804:CL:CL | 2.58 | 0.41 |
| 30:0:37:A:C2 | 30:0:446:G:C2 | 3.09 | 0.41 |
| 30:0:99:A:C8 | 30:0:100:C:C6 | 3.09 | 0.41 |
| 30:0:210:U:O2' | 30:0:211:U:H5' | 2.21 | 0.41 |
| 30:0:565:A:N6 | 30:0:593:A:C8 | 2.88 | 0.41 |
| 30:0:1244:U:H4' | 30:0:1246:A:O4' | 2.21 | 0.41 |
| 30:0:1351:G:H1' | 38:0:4673:HOH:O | 2.21 | 0.41 |
| 30:0:1423:C:O2' | 30:0:1424:A:H5' | 2.20 | 0.41 |
| 30:0:1523:G:C5 | 30:0:1524:U:C4 | 3.08 | 0.41 |
| 30:0:1819:G:C2' | 30:0:1820:G:H5' | 2.50 | 0.41 |
| 30:0:1834:C:H2' | 30:0:1840:A:H62 | 1.82 | 0.41 |
| 30:0:2296:C:H2' | 30:0:2297:U:C6 | 2.56 | 0.41 |
| 30:0:2345:A:H3' | 30:0:2346:C:C5 | 2.56 | 0.41 |
| 30:0:2438:G:C6 | 30:0:2439:C:C4 | 3.08 | 0.41 |
| 31:9:75:G:H1 | 31:9:106:U:H3 | 1.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:33:GLU:H | 1:A:33:GLU:CD | 2.24 | 0.41 |
| 1:A:47:HIS:CD2 | 30:0:1654:U:C2' | 3.02 | 0.41 |
| 1:A:191:GLY:HA2 | 1:A:194:MET:HE2 | 2.02 | 0.41 |
| 2:B:243:ASN:HA | 2:B:244:PRO:C | 2.41 | 0.41 |
| 2:B:244:PRO:HG3 | 2:B:248:ARG:NH2 | 2.35 | 0.41 |
| 3:C:127:ARG:HD3 | 3:C:129:HIS:CE1 | 2.56 | 0.41 |
| 4:D:53:LYS:HE3 | 31:9:40:C:H42 | 1.85 | 0.41 |
| 13:M:158:ARG:HB2 | 13:M:163:LEU:HB2 | 2.02 | 0.41 |
| 13:M:193:LYS:HB3 | 30:0:392:U:C5' | 2.51 | 0.41 |
| 14:N:22:GLN:HG3 | 30:0:2415:A:H2 | 1.85 | 0.41 |
| 15:O:68:GLY:HA3 | 30:0:745:G:O6 | 2.20 | 0.41 |
| 16:P:81:LYS:HG2 | 38:0:9540:HOH:O | 2.20 | 0.41 |
| 21:U:20:MET:HG3 | 21:U:28:THR:HG23 | 2.03 | 0.41 |
| 24:X:43:VAL:HG12 | 24:X:44:ASP:H | 1.84 | 0.41 |
| 25:Y:126:PRO:HG2 | 25:Y:128:PHE:CZ | 2.56 | 0.41 |
| 27:1:38:GLY:HA3 | 38:1:6935:HOH:O | 2.20 | 0.41 |
| 30:0:39:G:C2 | 30:0:444:C:N3 | 2.89 | 0.41 |
| 30:0:375:G:C4 | 30:0:411:A:C6 | 3.09 | 0.41 |
| 30:0:407:A:H8 | 38:0:4452:HOH:O | 2.04 | 0.41 |
| 30:0:622:G:O2' | 30:0:623:U:H5' | 2.21 | 0.41 |
| 30:0:685:C:O2 | 30:0:748:C:H4' | 2.21 | 0.41 |
| 30:0:1193:A:C2 | 30:0:1194:A:N6 | 2.89 | 0.41 |
| 30:0:1419:U:H2' | 30:0:1685:A:C2 | 2.56 | 0.41 |
| 30:0:1769:C:C2' | 30:0:1770:U:H5' | 2.51 | 0.41 |
| 30:0:2002:C:C2' | 30:0:2003:U:H5' | 2.50 | 0.41 |
| 30:0:2064:U:H5' | 30:0:2652:U:O3' | 2.21 | 0.41 |
| 4:D:172:VAL:HG12 | 4:D:173:GLU:N | 2.36 | 0.40 |
| 8:H:12:ILE:HG12 | 8:H:59:GLN:HG3 | 2.02 | 0.40 |
| 10:J:47:THR:O | 10:J:53:ILE:HD11 | 2.21 | 0.40 |
| 13:M:46:LEU:HD22 | 13:M:50:ARG:HD2 | 2.03 | 0.40 |
| 13:M:95:LYS:HA | 13:M:170:ASN:HD21 | 1.86 | 0.40 |
| 19:S:42:GLU:HG2 | 19:S:49:VAL:HG23 | 2.03 | 0.40 |
| 26:Z:53:ILE:HG23 | 26:Z:93:TYR:HB3 | 2.02 | 0.40 |
| 26:Z:65:ASN:HD22 | 26:Z:84:CYS:CB | 2.33 | 0.40 |
| 30:0:375:G:C2 | 30:0:411:A:C2 | 3.08 | 0.40 |
| 30:0:1008:C:H2' | 30:0:1009:U:C6 | 2.56 | 0.40 |
| 30:0:1327:G:C6 | 30:0:1331:G:C6 | 3.09 | 0.40 |
| 30:0:1656:A:H2' | 30:0:1657:A:O4' | 2.21 | 0.40 |
| 30:0:2765:C:H2' | 30:0:2766:A:C8 | 2.56 | 0.40 |
| 31:9:14:G:C8 | 31:9:14:G:C5' | 2.95 | 0.40 |
| 1:A:47:HIS:HA | 38:A:9024:HOH:O | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:139:GLU:OE2 | 30:0:2781:U:C1' | 2.68 | 0.40 |
| 5:E:166:VAL:HB | 38:E:6341:HOH:O | 2.19 | 0.40 |
| 7:G:19:GLU:O | 7:G:23:ILE:HG13 | 2.21 | 0.40 |
| 10:J:19:MET:HE3 | 10:J:132:LEU:HD11 | 2.03 | 0.40 |
| 10:J:127:ILE:HG22 | 33:J:8801:CL:CL | 2.58 | 0.40 |
| 11:K:74:VAL:HG12 | 11:K:75:ARG:HG3 | 2.02 | 0.40 |
| 12:L:73:VAL:HG23 | 12:L:74:THR:H | 1.86 | 0.40 |
| 16:P:7:LYS:HD3 | 16:P:21:VAL:HG22 | 2.03 | 0.40 |
| 17:Q:80:LYS:HG2 | 17:Q:82:LYS:HE3 | 2.02 | 0.40 |
| 23:W:4:LEU:HD23 | 23:W:4:LEU:HA | 1.88 | 0.40 |
| 27:1:28:HIS:CE1 | 27:1:31:LYS:HE2 | 2.56 | 0.40 |
| 30:0:245:C:N4 | 30:0:246:G:C6 | 2.89 | 0.40 |
| 30:0:559:U:C6 | 30:0:559:U:H3' | 2.57 | 0.40 |
| 30:0:1398:G:H2' | 30:0:1399:A:H8 | 1.85 | 0.40 |
| 30:0:1497:G:H4' | 30:0:1627:G:O2' | 2.21 | 0.40 |
| 30:0:1531:U:C2 | 30:0:1661:A:C2 | 3.10 | 0.40 |
| 30:0:1543:G:N1 | 30:0:1641:A:OP2 | 2.41 | 0.40 |
| 30:0:1576:G:H2' | 30:0:1577:U:H6 | 1.87 | 0.40 |
| 30:0:1577:U:O2' | 30:0:1578:C:H5' | 2.21 | 0.40 |
| 30:0:1589:G:C2 | 30:0:1605:G:N3 | 2.89 | 0.40 |
| 30:0:1626:A:H2' | 30:0:1627:G:O4' | 2.21 | 0.40 |
| 30:0:1947:G:N2 | 30:0:1966:U:C2 | 2.89 | 0.40 |
| 30:0:1972:U:O2' | 30:0:1973:A:H5" | 2.22 | 0.40 |
| 30:0:2319:C:H2' | 30:0:2320:U:H5' | 2.03 | 0.40 |
| 30:0:2526:C:H3' | 30:0:2526:C:H6 | 1.86 | 0.40 |
| 2:B:148:PRO:HD2 | 38:B:9047:HOH:O | 2.21 | 0.40 |
| 3:C:168:ARG:NH2 | 3:C:190:ALA:O | 2.55 | 0.40 |
| 9:I:78:ALA:HB1 | 9:I:93:ALA:CB | 2.51 | 0.40 |
| 9:I:120:ALA:O | 9:I:124:VAL:HG23 | 2.21 | 0.40 |
| 10:J:57:TYR:O | 10:J:61:VAL:HG23 | 2.21 | 0.40 |
| 12:L:117:GLU:HG2 | 38:L:9025:HOH:O | 2.20 | 0.40 |
| 13:M:64:ARG:HD2 | 38:M:8879:HOH:O | 2.21 | 0.40 |
| 13:M:74:LYS:O | 13:M:88:VAL:HG22 | 2.21 | 0.40 |
| 26:Z:65:ASN:CB | 26:Z:84:CYS:SG | 3.08 | 0.40 |
| 30:0:372:A:H2' | 30:0:373:G:H8 | 1.86 | 0.40 |
| 30:0:464:G:HO2' | 30:0:465:U:P | 2.44 | 0.40 |
| 30:0:611:U:O5' | 30:0:611:U:H6 | 2.05 | 0.40 |
| 30:0:727:G:N2 | 30:0:728:C:H1' | 2.36 | 0.40 |
| 30:0:1074:G:H4' | 30:0:1260:G:C6 | 2.57 | 0.40 |
| 30:0:1333:U:H2' | 30:0:1334:C:H6 | 1.86 | 0.40 |
| 30:0:1461:U:H1' | 38:0:7457:HOH:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1749:U:O2 | 30:0:1751:G:C8 | 2.75 | 0.40 |
| 30:0:1926:G:H2' | 30:0:1927:A:H8 | 1.86 | 0.40 |
| 30:0:2867:G:H2' | 30:0:2868:C:H6 | 1.86 | 0.40 |
| 31:9:2:U:OP2 | 31:9:2:U:H4' | 2.22 | 0.40 |
| 1:A:105:VAL:HG13 | 1:A:155:THR:O | 2.21 | 0.40 |
| 2:B:294:TYR:HE2 | 38:B:9123:HOH:O | 2.03 | 0.40 |
| 8:H:8:MET:SD | 30:0:2494:G:H4' | 2.61 | 0.40 |
| 8:H:91:ARG:O | 30:0:1003:U:H4' | 2.22 | 0.40 |
| 12:L:56:LYS:NZ | 38:L:9036:HOH:O | 2.54 | 0.40 |
| 12:L:67:ARG:O | 12:L:71:GLU:HG3 | 2.22 | 0.40 |
| 14:N:58:LEU:HD12 | 14:N:58:LEU:H | 1.85 | 0.40 |
| 16:P:89:ASN:HB3 | 16:P:92:GLU:HB2 | 2.03 | 0.40 |
| 24:X:39:LYS:HE2 | 30:0:2834:G:OP1 | 2.22 | 0.40 |
| 25:Y:210:GLY:N | 30:0:1313:A:H5" | 2.36 | 0.40 |
| 30:0:113:A:OP2 | 30:0:114:A:H2' | 2.21 | 0.40 |
| 30:0:1936:C:H2' | 30:0:1937:U:C6 | 2.56 | 0.40 |
| 30:0:1982:C:H2' | 30:0:1983:C:O4' | 2.21 | 0.40 |
| 30:0:2248:C:H2' | 30:0:2249:G:C8 | 2.54 | 0.40 |
| 30:0:2803:C:H2' | 30:0:2804:C:H6 | 1.86 | 0.40 |
| 30:0:2826:G:C6 | 30:0:2913:A:C6 | 3.10 | 0.40 |
| 31:9:27:C:C4 | 31:9:28:U:C5 | 3.09 | 0.40 |
| 1:A:88:ILE:O | 1:A:88:ILE:HG22 | 2.20 | 0.40 |
| 1:A:164:ARG:NH2 | 30:0:1877:G:OP1 | 2.53 | 0.40 |
| 2:B:10:SER:O | 2:B:16:ARG:NH1 | 2.45 | 0.40 |
| 13:M:34:GLU:HB3 | 13:M:38:GLU:HG3 | 2.02 | 0.40 |
| 16:P:59:ARG:HD3 | 38:0:6252:HOH:O | 2.22 | 0.40 |
| 20:T:21:LYS:HA | 20:T:24:ARG:HD2 | 2.04 | 0.40 |
| 23:W:139:GLY:O | 23:W:141:HIS:HD2 | 2.04 | 0.40 |
| 30:0:506:G:N2 | 30:0:509:A:H5' | 2.31 | 0.40 |
| 30:0:724:G:O2' | 30:0:725:C:H5' | 2.21 | 0.40 |
| 30:0:763:C:O2' | 30:0:764:C:H5' | 2.21 | 0.40 |
| 30:0:1130:U:H4' | 38:0:6109:HOH:O | 2.21 | 0.40 |
| 30:0:1135:G:O2' | 30:0:1136:U:H5' | 2.22 | 0.40 |
| 30:0:1163:G:C2 | 30:0:1184:C:N3 | 2.89 | 0.40 |
| 30:0:1191:A:H3' | 30:0:1191:A:C8 | 2.56 | 0.40 |
| 30:0:1397:C:O2' | 30:0:1398:G:H5' | 2.22 | 0.40 |
| 30:0:1589:G:H5' | 38:0:6843:HOH:O | 2.20 | 0.40 |
| 30:0:1815:A:H4' | 30:0:2751:C:O4' | 2.22 | 0.40 |
| 30:0:2295:G:N3 | 30:0:2361:A:H2 | 2.17 | 0.40 |
| 30:0:2321:A:H1' | 30:0:2322:U:H3' | 2.04 | 0.40 |
| 30:0:2694:A:C6 | 30:0:2702:A:C8 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2803:C:C4 | 30:0:2804:C:C5 | 3.10 | 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 |
|---|---|---|---|---|---|---|
| 1 | A | 235/240 (98%) | 202 (86%) | 27 (12%) | 6 (3%) | 5 24 |
| 2 | B | 335/338 (99%) | 309 (92%) | 17 (5%) | 9 (3%) | 5 23 |
| 3 | C | 244/246 (99%) | 222 (91%) | 20 (8%) | 2 (1%) | 19 53 |
| 4 | D | 134/177 (76%) | 110 (82%) | 20 (15%) | 4 (3%) | 4 20 |
| 5 | E | 170/178 (96%) | 157 (92%) | 12 (7%) | 1 (1%) | 25 60 |
| 6 | F | 117/120 (98%) | 106 (91%) | 7 (6%) | 4 (3%) | 3 17 |
| 7 | G | 25/348 (7%) | 24 (96%) | 1 (4%) | 0 | 100 100 |
| 8 | H | 156/177 (88%) | 144 (92%) | 10 (6%) | 2 (1%) | 12 41 |
| 9 | I | 68/162 (42%) | 52 (76%) | 12 (18%) | 4 (6%) | 1 7 |
| 10 | J | 140/145 (97%) | 131 (94%) | 8 (6%) | 1 (1%) | 22 56 |
| 11 | K | 130/132 (98%) | 121 (93%) | 8 (6%) | 1 (1%) | 19 53 |
| 12 | L | 141/165 (86%) | 120 (85%) | 21 (15%) | 0 | 100 100 |
| 13 | M | 192/196 (98%) | 179 (93%) | 9 (5%) | 4 (2%) | 7 29 |
| 14 | N | 184/187 (98%) | 163 (89%) | 17 (9%) | 4 (2%) | 6 28 |
| 15 | O | 113/116 (97%) | 107 (95%) | 6 (5%) | 0 | 100 100 |
| 16 | P | 141/149 (95%) | 133 (94%) | 8 (6%) | 0 | 100 100 |
| 17 | Q | 93/96 (97%) | 85 (91%) | 7 (8%) | 1 (1%) | 14 46 |
| 18 | R | 148/155 (96%) | 140 (95%) | 7 (5%) | 1 (1%) | 22 56 |
| 19 | S | 79/85 (93%) | 74 (94%) | 5 (6%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 20 | T | 117/120 (98%) | 107 (92%) | 8 (7%) | 2 (2%) | 9 34 |
| 21 | U | 51/67 (76%) | 42 (82%) | 8 (16%) | 1 (2%) | 7 30 |
| 22 | V | 63/71 (89%) | 58 (92%) | 5 (8%) | 0 | 100 100 |
| 23 | W | 152/154 (99%) | 140 (92%) | 10 (7%) | 2 (1%) | 12 41 |
| 24 | X | 80/92 (87%) | 74 (92%) | 4 (5%) | 2 (2%) | 5 25 |
| 25 | Y | 140/241 (58%) | 137 (98%) | 3 (2%) | 0 | 100 100 |
| 26 | Z | 71/116 (61%) | 58 (82%) | 8 (11%) | 5 (7%) | 1 4 |
| 27 | 1 | 54/57 (95%) | 51 (94%) | 3 (6%) | 0 | 100 100 |
| 28 | 2 | 42/50 (84%) | 39 (93%) | 2 (5%) | 1 (2%) | 6 26 |
| 29 | 3 | 90/92 (98%) | 74 (82%) | 13 (14%) | 3 (3%) | 4 18 |
| All | All | 3705/4472 (83%) | 3359 (91%) | 286 (8%) | 60 (2%) | 9 36 |

All (60) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 34 | ASP |
| 1 | A | 37 | VAL |
| 1 | A | 74 | VAL |
| 4 | D | 65 | GLU |
| 4 | D | 137 | PRO |
| 8 | H | 19 | ARG |
| 11 | K | 127 | ALA |
| 13 | M | 82 | ARG |
| 14 | N | 154 | LEU |
| 14 | N | 183 | ASP |
| 14 | N | 184 | ILE |
| 26 | Z | 105 | ARG |
| 29 | 3 | 64 | LYS |
| 2 | B | 306 | LYS |
| 6 | F | 61 | MET |
| 6 | F | 101 | ALA |
| 13 | M | 71 | SER |
| 21 | U | 51 | TRP |
| 24 | X | 70 | ILE |
| 26 | Z | 70 | ARG |
| 2 | B | 184 | ASP |
| 3 | C | 8 | LEU |
| 5 | E | 44 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | F | 27 | GLY |
| 9 | I | 83 | GLY |
| 20 | T | 44 | ALA |
| 23 | W | 36 | PRO |
| 23 | W | 49 | ASN |
| 24 | X | 87 | ALA |
| 26 | Z | 67 | GLY |
| 29 | 3 | 46 | ILE |
| 2 | B | 2 | GLN |
| 2 | B | 107 | SER |
| 4 | D | 56 | ARG |
| 9 | I | 106 | GLN |
| 13 | M | 86 | GLN |
| 20 | T | 46 | ASP |
| 26 | Z | 83 | TYR |
| 28 | 2 | 37 | HIS |
| 1 | A | 52 | SER |
| 1 | A | 119 | ALA |
| 2 | B | 206 | THR |
| 3 | C | 79 | ARG |
| 10 | J | 65 | ASN |
| 13 | M | 79 | ALA |
| 18 | R | 114 | VAL |
| 29 | 3 | 56 | PRO |
| 2 | B | 63 | GLU |
| 6 | F | 104 | ALA |
| 8 | H | 171 | GLY |
| 14 | N | 164 | ASP |
| 4 | D | 27 | ILE |
| 17 | Q | 48 | PRO |
| 2 | B | 34 | GLY |
| 2 | B | 169 | GLY |
| 26 | Z | 64 | PRO |
| 2 | B | 185 | GLY |
| 9 | I | 108 | HIS |
| 9 | I | 131 | GLY |
| 1 | A | 42 | VAL |

### 5.3.2 Protein sidechains (i)

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 | |
|---|---|---|---|---|---|---|
| 1 | A | 179/182 (98%) | 171 (96%) | 8 (4%) | 27 | 61 |
| 2 | B | 282/283 (100%) | 264 (94%) | 18 (6%) | 17 | 47 |
| 3 | C | 193/193 (100%) | 182 (94%) | 11 (6%) | 20 | 52 |
| 4 | D | 117/148 (79%) | 110 (94%) | 7 (6%) | 19 | 50 |
| 5 | E | 152/156 (97%) | 148 (97%) | 4 (3%) | 46 | 75 |
| 6 | F | 93/94 (99%) | 93 (100%) | 0 | 100 | 100 |
| 7 | G | 27/282 (10%) | 26 (96%) | 1 (4%) | 34 | 66 |
| 8 | H | 134/145 (92%) | 126 (94%) | 8 (6%) | 19 | 50 |
| 9 | I | 58/130 (45%) | 56 (97%) | 2 (3%) | 37 | 69 |
| 10 | J | 118/121 (98%) | 113 (96%) | 5 (4%) | 30 | 63 |
| 11 | K | 106/106 (100%) | 104 (98%) | 2 (2%) | 57 | 81 |
| 12 | L | 113/127 (89%) | 108 (96%) | 5 (4%) | 28 | 62 |
| 13 | M | 158/160 (99%) | 148 (94%) | 10 (6%) | 18 | 48 |
| 14 | N | 149/150 (99%) | 144 (97%) | 5 (3%) | 37 | 69 |
| 15 | O | 93/94 (99%) | 92 (99%) | 1 (1%) | 73 | 89 |
| 16 | P | 113/117 (97%) | 107 (95%) | 6 (5%) | 22 | 55 |
| 17 | Q | 79/80 (99%) | 78 (99%) | 1 (1%) | 69 | 87 |
| 18 | R | 117/122 (96%) | 114 (97%) | 3 (3%) | 46 | 75 |
| 19 | S | 71/74 (96%) | 70 (99%) | 1 (1%) | 67 | 86 |
| 20 | T | 105/106 (99%) | 99 (94%) | 6 (6%) | 20 | 52 |
| 21 | U | 44/53 (83%) | 41 (93%) | 3 (7%) | 16 | 45 |
| 22 | V | 51/57 (90%) | 49 (96%) | 2 (4%) | 32 | 65 |
| 23 | W | 130/130 (100%) | 124 (95%) | 6 (5%) | 27 | 60 |
| 24 | X | 66/74 (89%) | 61 (92%) | 5 (8%) | 13 | 39 |
| 25 | Y | 120/196 (61%) | 115 (96%) | 5 (4%) | 30 | 63 |
| 26 | Z | 60/94 (64%) | 57 (95%) | 3 (5%) | 24 | 57 |
| 27 | 1 | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 28 | 2 | 42/46 (91%) | 41 (98%) | 1 (2%) | 49 | 77 |
| 29 | 3 | 79/79 (100%) | 76 (96%) | 3 (4%) | 33 | 66 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| All | All | 3095/3646 (85%) | 2963 (96%) | 132 (4%) | 29 62 |

All (132) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3 | ARG |
| 1 | A | 94 | LEU |
| 1 | A | 131 | HIS |
| 1 | A | 153 | ARG |
| 1 | A | 179 | MET |
| 1 | A | 192 | VAL |
| 1 | A | 206 | ARG |
| 1 | A | 217 | ARG |
| 2 | B | 7 | ARG |
| 2 | B | 11 | LEU |
| 2 | B | 27 | ASN |
| 2 | B | 71 | VAL |
| 2 | B | 97 | LEU |
| 2 | B | 98 | THR |
| 2 | B | 132 | HIS |
| 2 | B | 162 | MET |
| 2 | B | 191 | ASN |
| 2 | B | 192 | ASP |
| 2 | B | 195 | ARG |
| 2 | B | 238 | ASN |
| 2 | B | 248 | ARG |
| 2 | B | 251 | VAL |
| 2 | B | 254 | GLN |
| 2 | B | 265 | LEU |
| 2 | B | 277 | GLU |
| 2 | B | 307 | ARG |
| 3 | C | 2 | GLN |
| 3 | C | 76 | ARG |
| 3 | C | 88 | SER |
| 3 | C | 136 | VAL |
| 3 | C | 187 | ARG |
| 3 | C | 202 | THR |
| 3 | C | 223 | LEU |
| 3 | C | 234 | VAL |
| 3 | C | 236 | THR |
| 3 | C | 237 | GLU |
| 3 | C | 243 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 19 | GLU |
| 4 | D | 24 | HIS |
| 4 | D | 29 | HIS |
| 4 | D | 50 | VAL |
| 4 | D | 61 | PHE |
| 4 | D | 149 | ARG |
| 4 | D | 161 | ASP |
| 5 | E | 7 | ILE |
| 5 | E | 68 | HIS |
| 5 | E | 126 | ILE |
| 5 | E | 155 | ASN |
| 7 | G | 73 | ASP |
| 8 | H | 21 | GLU |
| 8 | H | 33 | GLN |
| 8 | H | 45 | ASP |
| 8 | H | 61 | ARG |
| 8 | H | 62 | HIS |
| 8 | H | 87 | LYS |
| 8 | H | 91 | ARG |
| 8 | H | 157 | TYR |
| 9 | I | 114 | TYR |
| 9 | I | 115 | ASP |
| 10 | J | 46 | ILE |
| 10 | J | 52 | GLN |
| 10 | J | 74 | ARG |
| 10 | J | 107 | ASN |
| 10 | J | 130 | VAL |
| 11 | K | 10 | GLN |
| 11 | K | 55 | VAL |
| 12 | L | 35 | ARG |
| 12 | L | 99 | GLU |
| 12 | L | 101 | ASP |
| 12 | L | 104 | ASP |
| 12 | L | 114 | VAL |
| 13 | M | 10 | ASP |
| 13 | M | 46 | LEU |
| 13 | M | 68 | ARG |
| 13 | M | 73 | ARG |
| 13 | M | 82 | ARG |
| 13 | M | 86 | GLN |
| 13 | M | 93 | ARG |
| 13 | M | 99 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | M | 116 | ASN |
| 13 | M | 125 | ARG |
| 14 | N | 5 | ARG |
| 14 | N | 17 | ARG |
| 14 | N | 49 | THR |
| 14 | N | 56 | ASP |
| 14 | N | 80 | SER |
| 15 | O | 3 | THR |
| 16 | P | 21 | VAL |
| 16 | P | 79 | SER |
| 16 | P | 91 | LYS |
| 16 | P | 94 | TRP |
| 16 | P | 98 | ILE |
| 16 | P | 120 | ARG |
| 17 | Q | 16 | ASN |
| 18 | R | 13 | THR |
| 18 | R | 39 | THR |
| 18 | R | 143 | VAL |
| 19 | S | 30 | ASP |
| 20 | T | 5 | ASP |
| 20 | T | 39 | ASN |
| 20 | T | 73 | HIS |
| 20 | T | 96 | VAL |
| 20 | T | 115 | GLU |
| 20 | T | 117 | ASP |
| 21 | U | 25 | ASP |
| 21 | U | 52 | THR |
| 21 | U | 53 | ASP |
| 22 | V | 12 | THR |
| 22 | V | 65 | ASP |
| 23 | W | 1 | MET |
| 23 | W | 4 | LEU |
| 23 | W | 35 | VAL |
| 23 | W | 88 | THR |
| 23 | W | 125 | HIS |
| 23 | W | 146 | ILE |
| 24 | X | 27 | ASP |
| 24 | X | 46 | ASP |
| 24 | X | 52 | PRO |
| 24 | X | 72 | VAL |
| 24 | X | 79 | GLU |
| 25 | Y | 154 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | Y | 189 | ASN |
| 25 | Y | 203 | VAL |
| 25 | Y | 223 | ASP |
| 25 | Y | 235 | GLU |
| 26 | Z | 37 | ARG |
| 26 | Z | 70 | ARG |
| 26 | Z | 88 | PHE |
| 28 | 2 | 18 | ASN |
| 29 | 3 | 30 | GLN |
| 29 | 3 | 56 | PRO |
| 29 | 3 | 65 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 47 | HIS |
| 1 | A | 199 | HIS |
| 2 | B | 27 | ASN |
| 2 | B | 145 | HIS |
| 2 | B | 221 | GLN |
| 2 | B | 238 | ASN |
| 2 | B | 256 | GLN |
| 2 | B | 260 | HIS |
| 2 | B | 320 | GLN |
| 3 | C | 2 | GLN |
| 3 | C | 73 | GLN |
| 3 | C | 103 | ASN |
| 3 | C | 129 | HIS |
| 4 | D | 103 | ASN |
| 5 | E | 55 | ASN |
| 5 | E | 90 | HIS |
| 5 | E | 143 | GLN |
| 5 | E | 150 | GLN |
| 7 | G | 64 | ASN |
| 8 | H | 59 | GLN |
| 9 | I | 99 | GLN |
| 9 | I | 106 | GLN |
| 10 | J | 52 | GLN |
| 10 | J | 107 | ASN |
| 10 | J | 126 | ASN |
| 11 | K | 10 | GLN |
| 11 | K | 44 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | K | 67 | GLN |
| 12 | L | 18 | HIS |
| 12 | L | 41 | HIS |
| 12 | L | 116 | HIS |
| 13 | M | 24 | GLN |
| 13 | M | 29 | GLN |
| 13 | M | 170 | ASN |
| 14 | N | 40 | ASN |
| 14 | N | 53 | ASN |
| 14 | N | 93 | GLN |
| 14 | N | 107 | ASN |
| 14 | N | 132 | ASN |
| 16 | P | 50 | GLN |
| 16 | P | 66 | GLN |
| 16 | P | 73 | HIS |
| 16 | P | 88 | GLN |
| 16 | P | 118 | GLN |
| 17 | Q | 16 | ASN |
| 17 | Q | 27 | GLN |
| 17 | Q | 40 | HIS |
| 18 | R | 61 | GLN |
| 18 | R | 94 | ASN |
| 18 | R | 98 | ASN |
| 18 | R | 117 | HIS |
| 18 | R | 123 | GLN |
| 19 | S | 7 | HIS |
| 19 | S | 44 | GLN |
| 19 | S | 53 | ASN |
| 20 | T | 39 | ASN |
| 21 | U | 38 | ASN |
| 21 | U | 39 | ASN |
| 22 | V | 34 | GLN |
| 22 | V | 60 | GLN |
| 23 | W | 2 | HIS |
| 23 | W | 12 | ASN |
| 23 | W | 28 | HIS |
| 23 | W | 110 | GLN |
| 23 | W | 119 | HIS |
| 23 | W | 141 | HIS |
| 24 | X | 23 | HIS |
| 25 | Y | 134 | HIS |
| 25 | Y | 149 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | Y | 189 | ASN |
| 26 | Z | 80 | GLN |
| 27 | 1 | 8 | GLN |
| 27 | 1 | 16 | HIS |
| 27 | 1 | 28 | HIS |
| 28 | 2 | 18 | ASN |
| 28 | 2 | 41 | HIS |
| 28 | 2 | 45 | ASN |
| 29 | 3 | 30 | GLN |
| 29 | 3 | 48 | ASN |
| 29 | 3 | 91 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 30 | 0 | 2745/2923 (93%) | 250 (9%) | 21 (0%) |
| 31 | 9 | 121/122 (99%) | 19 (15%) | 2 (1%) |
| All | All | 2866/3045 (94%) | 269 (9%) | 23 (0%) |

All (269) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 31 | C |
| 30 | 0 | 67 | A |
| 30 | 0 | 69 | A |
| 30 | 0 | 70 | A |
| 30 | 0 | 71 | G |
| 30 | 0 | 86 | A |
| 30 | 0 | 87 | C |
| 30 | 0 | 88 | G |
| 30 | 0 | 114 | A |
| 30 | 0 | 115 | U |
| 30 | 0 | 120 | A |
| 30 | 0 | 130 | C |
| 30 | 0 | 141 | C |
| 30 | 0 | 151 | A |
| 30 | 0 | 166 | A |
| 30 | 0 | 185 | G |
| 30 | 0 | 186 | A |
| 30 | 0 | 191 | A |
| 30 | 0 | 192 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 198 | A |
| 30 | 0 | 200 | C |
| 30 | 0 | 219 | G |
| 30 | 0 | 237 | G |
| 30 | 0 | 271 | C |
| 30 | 0 | 272 | A |
| 30 | 0 | 273 | G |
| 30 | 0 | 283 | U |
| 30 | 0 | 284 | C |
| 30 | 0 | 308 | U |
| 30 | 0 | 309 | C |
| 30 | 0 | 318 | U |
| 30 | 0 | 336 | G |
| 30 | 0 | 337 | A |
| 30 | 0 | 358 | G |
| 30 | 0 | 381 | G |
| 30 | 0 | 397 | A |
| 30 | 0 | 409 | U |
| 30 | 0 | 417 | G |
| 30 | 0 | 461 | C |
| 30 | 0 | 473 | A |
| 30 | 0 | 487 | G |
| 30 | 0 | 498 | A |
| 30 | 0 | 510 | U |
| 30 | 0 | 511 | A |
| 30 | 0 | 514 | G |
| 30 | 0 | 537 | G |
| 30 | 0 | 538 | C |
| 30 | 0 | 539 | G |
| 30 | 0 | 542 | A |
| 30 | 0 | 545 | G |
| 30 | 0 | 553 | G |
| 30 | 0 | 559 | U |
| 30 | 0 | 581 | G |
| 30 | 0 | 588 | G |
| 30 | 0 | 604 | G |
| 30 | 0 | 620 | A |
| 30 | 0 | 632 | A |
| 30 | 0 | 644 | G |
| 30 | 0 | 660 | A |
| 30 | 0 | 688 | A |
| 30 | 0 | 699 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 701 | U |
| 30 | 0 | 759 | C |
| 30 | 0 | 777 | U |
| 30 | 0 | 809 | G |
| 30 | 0 | 821 | U |
| 30 | 0 | 835 | U |
| 30 | 0 | 840 | U |
| 30 | 0 | 846 | A |
| 30 | 0 | 857 | A |
| 30 | 0 | 858 | U |
| 30 | 0 | 868 | G |
| 30 | 0 | 869 | G |
| 30 | 0 | 872 | U |
| 30 | 0 | 875 | A |
| 30 | 0 | 877 | G |
| 30 | 0 | 878 | G |
| 30 | 0 | 882 | A |
| 30 | 0 | 884 | C |
| 30 | 0 | 885 | G |
| 30 | 0 | 898 | G |
| 30 | 0 | 905 | C |
| 30 | 0 | 920 | C |
| 30 | 0 | 921 | G |
| 30 | 0 | 923 | A |
| 30 | 0 | 953 | G |
| 30 | 0 | 960 | G |
| 30 | 0 | 961 | A |
| 30 | 0 | 1006 | A |
| 30 | 0 | 1008 | C |
| 30 | 0 | 1029 | U |
| 30 | 0 | 1045 | G |
| 30 | 0 | 1059 | G |
| 30 | 0 | 1060 | C |
| 30 | 0 | 1072 | G |
| 30 | 0 | 1081 | A |
| 30 | 0 | 1088 | A |
| 30 | 0 | 1109 | U |
| 30 | 0 | 1110 | G |
| 30 | 0 | 1119 | G |
| 30 | 0 | 1130 | U |
| 30 | 0 | 1137 | G |
| 30 | 0 | 1151 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 1164 | U |
| 30 | 0 | 1165 | G |
| 30 | 0 | 1166 | A |
| 30 | 0 | 1174 | A |
| 30 | 0 | 1175 | G |
| 30 | 0 | 1185 | U |
| 30 | 0 | 1192 | A |
| 30 | 0 | 1193 | A |
| 30 | 0 | 1205 | U |
| 30 | 0 | 1206 | U |
| 30 | 0 | 1216 | G |
| 30 | 0 | 1234 | U |
| 30 | 0 | 1238 | C |
| 30 | 0 | 1239 | G |
| 30 | 0 | 1242 | A |
| 30 | 0 | 1279 | U |
| 30 | 0 | 1289 | C |
| 30 | 0 | 1331 | G |
| 30 | 0 | 1342 | C |
| 30 | 0 | 1353 | C |
| 30 | 0 | 1360 | C |
| 30 | 0 | 1377 | C |
| 30 | 0 | 1378 | G |
| 30 | 0 | 1407 | A |
| 30 | 0 | 1474 | C |
| 30 | 0 | 1485 | A |
| 30 | 0 | 1488 | U |
| 30 | 0 | 1505 | U |
| 30 | 0 | 1506 | U |
| 30 | 0 | 1524 | U |
| 30 | 0 | 1525 | G |
| 30 | 0 | 1526 | A |
| 30 | 0 | 1528 | A |
| 30 | 0 | 1559 | A |
| 30 | 0 | 1562 | C |
| 30 | 0 | 1592 | G |
| 30 | 0 | 1625 | U |
| 30 | 0 | 1626 | A |
| 30 | 0 | 1634 | G |
| 30 | 0 | 1656 | A |
| 30 | 0 | 1667 | A |
| 30 | 0 | 1682 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 1684 | A |
| 30 | 0 | 1685 | A |
| 30 | 0 | 1692 | C |
| 30 | 0 | 1701 | A |
| 30 | 0 | 1710 | A |
| 30 | 0 | 1722 | U |
| 30 | 0 | 1723 | G |
| 30 | 0 | 1725 | C |
| 30 | 0 | 1730 | G |
| 30 | 0 | 1731 | C |
| 30 | 0 | 1732 | A |
| 30 | 0 | 1752 | G |
| 30 | 0 | 1778 | A |
| 30 | 0 | 1779 | A |
| 30 | 0 | 1798 | C |
| 30 | 0 | 1819 | G |
| 30 | 0 | 1820 | G |
| 30 | 0 | 1829 | A |
| 30 | 0 | 1856 | C |
| 30 | 0 | 1879 | U |
| 30 | 0 | 1919 | A |
| 30 | 0 | 1942 | A |
| 30 | 0 | 1968 | A |
| 30 | 0 | 1971 | G |
| 30 | 0 | 1973 | A |
| 30 | 0 | 1978 | A |
| 30 | 0 | 1979 | G |
| 30 | 0 | 1996 | U |
| 30 | 0 | 2006 | C |
| 30 | 0 | 2008 | U |
| 30 | 0 | 2011 | A |
| 30 | 0 | 2012 | U |
| 30 | 0 | 2013 | G |
| 30 | 0 | 2033 | G |
| 30 | 0 | 2034 | U |
| 30 | 0 | 2064 | U |
| 30 | 0 | 2072 | G |
| 30 | 0 | 2073 | G |
| 30 | 0 | 2074 | A |
| 30 | 0 | 2096 | A |
| 30 | 0 | 2101 | A |
| 30 | 0 | 2102 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 2103 | A |
| 30 | 0 | 2110 | G |
| 30 | 0 | 2243 | C |
| 30 | 0 | 2258 | A |
| 30 | 0 | 2271 | G |
| 30 | 0 | 2272 | G |
| 30 | 0 | 2291 | A |
| 30 | 0 | 2317 | C |
| 30 | 0 | 2321 | A |
| 30 | 0 | 2322 | U |
| 30 | 0 | 2354 | A |
| 30 | 0 | 2361 | A |
| 30 | 0 | 2369 | A |
| 30 | 0 | 2422 | U |
| 30 | 0 | 2462 | G |
| 30 | 0 | 2469 | A |
| 30 | 0 | 2476 | C |
| 30 | 0 | 2483 | A |
| 30 | 0 | 2507 | G |
| 30 | 0 | 2509 | A |
| 30 | 0 | 2511 | A |
| 30 | 0 | 2513 | A |
| 30 | 0 | 2533 | C |
| 30 | 0 | 2537 | G |
| 30 | 0 | 2541 | U |
| 30 | 0 | 2553 | A |
| 30 | 0 | 2564 | G |
| 30 | 0 | 2570 | G |
| 30 | 0 | 2589 | U |
| 30 | 0 | 2601 | A |
| 30 | 0 | 2602 | G |
| 30 | 0 | 2608 | C |
| 30 | 0 | 2613 | G |
| 30 | 0 | 2634 | G |
| 30 | 0 | 2637 | A |
| 30 | 0 | 2638 | G |
| 30 | 0 | 2649 | A |
| 30 | 0 | 2664 | A |
| 30 | 0 | 2676 | C |
| 30 | 0 | 2681 | A |
| 30 | 0 | 2682 | C |
| 30 | 0 | 2718 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 2719 | A |
| 30 | 0 | 2726 | U |
| 30 | 0 | 2747 | C |
| 30 | 0 | 2748 | G |
| 30 | 0 | 2749 | U |
| 30 | 0 | 2750 | G |
| 30 | 0 | 2762 | C |
| 30 | 0 | 2768 | A |
| 30 | 0 | 2792 | A |
| 30 | 0 | 2800 | A |
| 30 | 0 | 2811 | A |
| 30 | 0 | 2812 | A |
| 30 | 0 | 2825 | C |
| 30 | 0 | 2867 | G |
| 30 | 0 | 2876 | G |
| 30 | 0 | 2890 | A |
| 30 | 0 | 2896 | A |
| 30 | 0 | 2903 | C |
| 30 | 0 | 2906 | A |
| 30 | 0 | 2912 | C |
| 30 | 0 | 2914 | A |
| 31 | 9 | 2 | U |
| 31 | 9 | 7 | G |
| 31 | 9 | 14 | G |
| 31 | 9 | 22 | G |
| 31 | 9 | 23 | U |
| 31 | 9 | 24 | U |
| 31 | 9 | 25 | G |
| 31 | 9 | 34 | A |
| 31 | 9 | 39 | U |
| 31 | 9 | 40 | C |
| 31 | 9 | 41 | C |
| 31 | 9 | 43 | G |
| 31 | 9 | 44 | A |
| 31 | 9 | 52 | A |
| 31 | 9 | 57 | A |
| 31 | 9 | 66 | G |
| 31 | 9 | 77 | A |
| 31 | 9 | 114 | G |
| 31 | 9 | 122 | C |

All (23) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 69 | A |
| 30 | 0 | 129 | A |
| 30 | 0 | 396 | U |
| 30 | 0 | 603 | A |
| 30 | 0 | 644 | G |
| 30 | 0 | 834 | G |
| 30 | 0 | 857 | A |
| 30 | 0 | 871 | G |
| 30 | 0 | 877 | G |
| 30 | 0 | 1237 | U |
| 30 | 0 | 1352 | A |
| 30 | 0 | 1377 | C |
| 30 | 0 | 1474 | C |
| 30 | 0 | 1506 | U |
| 30 | 0 | 2011 | A |
| 30 | 0 | 2321 | A |
| 30 | 0 | 2467 | A |
| 30 | 0 | 2526 | C |
| 30 | 0 | 2718 | C |
| 30 | 0 | 2726 | U |
| 30 | 0 | 2791 | U |
| 31 | 9 | 43 | G |
| 31 | 9 | 65 | A |

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

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 | $\#\|Z\| > 2$ |
| 30 | 1MA | 0 | 628 | 30,35 | 16,25,26 | 1.39 | 3 (18%) | 18,37,40 | 1.19 | 2 (11%) |
| 30 | PSU | 0 | 2621 | 30 | 18,21,22 | 1.41 | 2 (11%) | 22,30,33 | 1.30 | 3 (13%) |
| 30 | OMU | 0 | 2587 | 30 | 19,22,23 | 0.38 | 0 | 26,31,34 | 0.41 | 0 |
| 30 | UR3 | 0 | 2619 | 30 | 19,22,23 | 0.47 | 0 | 26,32,35 | 0.62 | 1 (3%) |
| 30 | OMG | 0 | 2588 | 30 | 18,26,27 | 1.09 | 3 (16%) | 19,38,41 | 0.74 | 1 (5%) |

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 |
|---|---|---|---|---|---|---|---|
| 30 | 1MA | 0 | 628 | 30,35 | - | 0/3/25/26 | 0/3/3/3 |
| 30 | PSU | 0 | 2621 | 30 | - | 0/7/25/26 | 0/2/2/2 |
| 30 | OMU | 0 | 2587 | 30 | - | 0/9/27/28 | 0/2/2/2 |
| 30 | UR3 | 0 | 2619 | 30 | - | 0/7/25/26 | 0/2/2/2 |
| 30 | OMG | 0 | 2588 | 30 | - | 0/5/27/28 | 0/3/3/3 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 0 | 2621 | PSU | C2-N1 | 4.51 | 1.42 | 1.36 |
| 30 | 0 | 628 | 1MA | C2-N3 | 3.73 | 1.33 | 1.29 |
| 30 | 0 | 2588 | OMG | C5-C6 | -2.91 | 1.41 | 1.47 |
| 30 | 0 | 628 | 1MA | C6-N6 | 2.57 | 1.34 | 1.27 |
| 30 | 0 | 2621 | PSU | C6-C5 | 2.56 | 1.38 | 1.35 |
| 30 | 0 | 2588 | OMG | C8-N7 | -2.48 | 1.30 | 1.35 |
| 30 | 0 | 628 | 1MA | C8-N7 | -2.05 | 1.31 | 1.35 |
| 30 | 0 | 2588 | OMG | C5-C4 | -2.03 | 1.37 | 1.43 |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 0 | 2621 | PSU | C6-C5-C4 | 3.45 | 120.61 | 118.20 |
| 30 | 0 | 2621 | PSU | C6-N1-C2 | -2.90 | 119.72 | 122.68 |
| 30 | 0 | 2621 | PSU | O2-C2-N1 | 2.78 | 125.86 | 122.79 |
| 30 | 0 | 628 | 1MA | N1-C2-N3 | 2.75 | 129.23 | 126.02 |
| 30 | 0 | 628 | 1MA | C5-C6-N1 | 2.58 | 117.75 | 113.90 |
| 30 | 0 | 2619 | UR3 | C4-N3-C2 | 2.48 | 126.90 | 124.56 |
| 30 | 0 | 2588 | OMG | O6-C6-C5 | 2.20 | 128.67 | 124.37 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 30 | 0 | 2621 | PSU | 1 | 0 |
| 30 | 0 | 2587 | OMU | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 30 | 0 | 2588 | OMG | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 305 ligands modelled in this entry, 305 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, $95^{th}$ 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 | A | 237/240 (98%) | -0.14 | 8 (3%) 45 29 | 36, 71, 108, 128 | 0 |
| 2 | B | 337/338 (99%) | -0.45 | 0 100 100 | 38, 67, 98, 112 | 0 |
| 3 | C | 246/246 (100%) | -0.38 | 0 100 100 | 32, 56, 80, 91 | 0 |
| 4 | D | 140/177 (79%) | 1.53 | 52 (37%) 0 0 | 89, 121, 144, 151 | 0 |
| 5 | E | 172/178 (96%) | -0.07 | 4 (2%) 60 43 | 57, 83, 104, 113 | 0 |
| 6 | F | 119/120 (99%) | 0.50 | 15 (12%) 3 2 | 64, 88, 121, 131 | 0 |
| 7 | G | 29/348 (8%) | 1.11 | 4 (13%) 2 1 | 92, 107, 116, 118 | 0 |
| 8 | H | 160/177 (90%) | 0.89 | 31 (19%) 1 0 | 65, 89, 118, 127 | 0 |
| 9 | I | 70/162 (43%) | 3.64 | 50 (71%) 0 0 | 145, 162, 177, 179 | 0 |
| 10 | J | 142/145 (97%) | -0.38 | 1 (0%) 87 76 | 47, 63, 86, 105 | 0 |
| 11 | K | 132/132 (100%) | -0.38 | 0 100 100 | 45, 63, 91, 100 | 0 |
| 12 | L | 145/165 (87%) | 0.55 | 21 (14%) 2 1 | 41, 88, 131, 140 | 0 |
| 13 | M | 194/196 (98%) | 0.25 | 20 (10%) 6 4 | 37, 53, 115, 122 | 0 |
| 14 | N | 186/187 (99%) | 0.65 | 26 (13%) 2 1 | 70, 90, 134, 139 | 0 |
| 15 | O | 115/116 (99%) | -0.37 | 0 100 100 | 46, 64, 81, 87 | 0 |
| 16 | P | 143/149 (95%) | -0.30 | 0 100 100 | 48, 67, 85, 96 | 0 |
| 17 | Q | 95/96 (98%) | -0.17 | 1 (1%) 80 65 | 57, 69, 89, 97 | 0 |
| 18 | R | 150/155 (96%) | -0.50 | 0 100 100 | 39, 56, 79, 95 | 0 |
| 19 | S | 81/85 (95%) | -0.28 | 2 (2%) 57 40 | 52, 70, 89, 104 | 0 |
| 20 | T | 119/120 (99%) | -0.03 | 5 (4%) 36 23 | 48, 67, 95, 125 | 0 |
| 21 | U | 53/67 (79%) | 4.50 | 50 (94%) 0 0 | 112, 125, 131, 134 | 0 |
| 22 | V | 65/71 (91%) | 0.92 | 12 (18%) 1 0 | 51, 83, 131, 135 | 0 |
| 23 | W | 154/154 (100%) | -0.34 | 1 (0%) 89 78 | 45, 62, 79, 92 | 0 |
| 24 | X | 82/92 (89%) | 0.03 | 4 (4%) 29 18 | 54, 72, 95, 109 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 25 | Y | 142/241 (58%) | -0.60 | 0 100 100 | 30, 53, 78, 97 | 0 |
| 26 | Z | 73/116 (62%) | 7.40 | 59 (80%) 0 0 | 111, 130, 139, 142 | 0 |
| 27 | 1 | 56/57 (98%) | -0.51 | 0 100 100 | 30, 39, 47, 65 | 0 |
| 28 | 2 | 46/50 (92%) | -0.22 | 3 (6%) 18 11 | 39, 72, 104, 110 | 0 |
| 29 | 3 | 92/92 (100%) | 8.50 | 91 (98%) 0 0 | 123, 135, 142, 148 | 0 |
| 30 | 0 | 2749/2923 (94%) | -0.63 | 10 (0%) 92 84 | 25, 58, 106, 183 | 0 |
| 31 | 9 | 122/122 (100%) | -0.81 | 2 (1%) 72 55 | 51, 90, 111, 159 | 0 |
| All | All | 6646/7517 (88%) | -0.00 | 472 (7%) 16 9 | 25, 66, 129, 183 | 0 |

All (472) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 26 | Z | 58 | ASN | 25.7 |
| 29 | 3 | 39 | GLN | 21.9 |
| 29 | 3 | 41 | GLU | 19.7 |
| 29 | 3 | 47 | GLY | 18.8 |
| 29 | 3 | 35 | TRP | 18.8 |
| 26 | Z | 35 | SER | 18.6 |
| 26 | Z | 55 | SER | 18.4 |
| 29 | 3 | 32 | GLY | 18.0 |
| 26 | Z | 46 | SER | 17.8 |
| 26 | Z | 36 | GLY | 17.3 |
| 13 | M | 87 | GLY | 17.0 |
| 29 | 3 | 44 | SER | 16.6 |
| 29 | 3 | 42 | ARG | 15.8 |
| 29 | 3 | 45 | GLY | 15.7 |
| 29 | 3 | 36 | ILE | 15.5 |
| 29 | 3 | 48 | ASN | 15.4 |
| 26 | Z | 50 | VAL | 15.4 |
| 26 | Z | 39 | GLY | 15.1 |
| 26 | Z | 56 | GLU | 14.9 |
| 26 | Z | 38 | PHE | 14.7 |
| 26 | Z | 34 | SER | 14.7 |
| 29 | 3 | 43 | ASN | 14.5 |
| 26 | Z | 43 | GLY | 14.3 |
| 26 | Z | 59 | GLU | 14.0 |
| 29 | 3 | 33 | MET | 13.9 |
| 29 | 3 | 38 | ARG | 13.8 |
| 29 | 3 | 40 | ARG | 13.5 |
| 26 | Z | 69 | ASP | 13.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 29 | 3 | 82 | GLY | 13.1 |
| 26 | Z | 82 | SER | 12.7 |
| 29 | 3 | 11 | CYS | 12.7 |
| 13 | M | 80 | GLY | 12.6 |
| 26 | Z | 42 | TYR | 12.6 |
| 29 | 3 | 37 | ASP | 12.3 |
| 29 | 3 | 34 | LYS | 12.3 |
| 26 | Z | 44 | ARG | 12.0 |
| 29 | 3 | 62 | THR | 11.9 |
| 26 | Z | 57 | MET | 11.7 |
| 29 | 3 | 56 | PRO | 11.7 |
| 29 | 3 | 15 | ASN | 11.4 |
| 26 | Z | 45 | VAL | 11.3 |
| 29 | 3 | 57 | GLY | 11.1 |
| 26 | Z | 54 | GLU | 11.0 |
| 29 | 3 | 20 | HIS | 10.8 |
| 26 | Z | 68 | GLU | 10.6 |
| 29 | 3 | 59 | ASP | 10.5 |
| 29 | 3 | 81 | GLU | 10.5 |
| 29 | 3 | 55 | VAL | 10.4 |
| 29 | 3 | 31 | THR | 10.1 |
| 26 | Z | 53 | ILE | 10.1 |
| 29 | 3 | 51 | LYS | 10.0 |
| 9 | I | 70 | THR | 9.9 |
| 9 | I | 104 | ALA | 9.6 |
| 29 | 3 | 83 | TRP | 9.6 |
| 9 | I | 74 | ILE | 9.6 |
| 29 | 3 | 30 | GLN | 9.4 |
| 29 | 3 | 10 | TYR | 9.3 |
| 29 | 3 | 71 | CYS | 9.2 |
| 13 | M | 83 | SER | 9.2 |
| 29 | 3 | 53 | SER | 9.0 |
| 21 | U | 40 | ALA | 9.0 |
| 13 | M | 89 | THR | 8.9 |
| 29 | 3 | 18 | GLN | 8.8 |
| 29 | 3 | 27 | SER | 8.8 |
| 13 | M | 90 | ARG | 8.8 |
| 29 | 3 | 14 | CYS | 8.7 |
| 26 | Z | 49 | ARG | 8.6 |
| 29 | 3 | 19 | GLU | 8.4 |
| 26 | Z | 77 | GLY | 8.4 |
| 29 | 3 | 78 | HIS | 8.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 21 | U | 9 | CYS | 8.3 |
| 26 | Z | 78 | ILE | 8.3 |
| 26 | Z | 71 | VAL | 8.2 |
| 21 | U | 31 | PHE | 8.2 |
| 26 | Z | 60 | ASP | 8.0 |
| 29 | 3 | 13 | HIS | 8.0 |
| 21 | U | 43 | GLY | 8.0 |
| 9 | I | 128 | THR | 8.0 |
| 29 | 3 | 80 | ARG | 7.9 |
| 29 | 3 | 61 | PRO | 7.8 |
| 26 | Z | 48 | ARG | 7.8 |
| 29 | 3 | 16 | GLU | 7.7 |
| 29 | 3 | 9 | THR | 7.7 |
| 29 | 3 | 12 | PRO | 7.7 |
| 26 | Z | 81 | CYS | 7.7 |
| 13 | M | 82 | ARG | 7.7 |
| 21 | U | 36 | CYS | 7.6 |
| 29 | 3 | 46 | ILE | 7.6 |
| 29 | 3 | 1 | MET | 7.6 |
| 21 | U | 38 | ASN | 7.5 |
| 21 | U | 52 | THR | 7.5 |
| 29 | 3 | 58 | GLY | 7.5 |
| 26 | Z | 37 | ARG | 7.4 |
| 29 | 3 | 17 | HIS | 7.3 |
| 9 | I | 106 | GLN | 7.3 |
| 9 | I | 66 | GLY | 7.3 |
| 21 | U | 54 | THR | 7.2 |
| 29 | 3 | 8 | ASN | 7.1 |
| 4 | D | 57 | THR | 7.1 |
| 26 | Z | 52 | GLU | 7.0 |
| 26 | Z | 61 | HIS | 7.0 |
| 26 | Z | 79 | TRP | 7.0 |
| 29 | 3 | 69 | TYR | 7.0 |
| 22 | V | 39 | ALA | 7.0 |
| 22 | V | 1 | THR | 7.0 |
| 21 | U | 51 | TRP | 6.9 |
| 21 | U | 41 | ASP | 6.9 |
| 29 | 3 | 91 | GLN | 6.9 |
| 9 | I | 71 | ALA | 6.8 |
| 29 | 3 | 77 | ALA | 6.7 |
| 29 | 3 | 52 | PHE | 6.7 |
| 26 | Z | 67 | GLY | 6.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 29 | 3 | 22 | VAL | 6.7 |
| 13 | M | 70 | GLY | 6.7 |
| 29 | 3 | 74 | CYS | 6.7 |
| 21 | U | 46 | ALA | 6.6 |
| 12 | L | 60 | GLU | 6.6 |
| 26 | Z | 62 | ALA | 6.5 |
| 13 | M | 81 | ARG | 6.4 |
| 26 | Z | 63 | CYS | 6.4 |
| 26 | Z | 47 | ARG | 6.4 |
| 29 | 3 | 28 | GLY | 6.3 |
| 9 | I | 113 | SER | 6.3 |
| 29 | 3 | 29 | ARG | 6.2 |
| 14 | N | 166 | ALA | 6.2 |
| 26 | Z | 51 | ALA | 6.2 |
| 9 | I | 103 | ILE | 6.1 |
| 9 | I | 97 | VAL | 6.1 |
| 13 | M | 74 | LYS | 6.0 |
| 29 | 3 | 49 | ASP | 6.0 |
| 26 | Z | 40 | ALA | 6.0 |
| 4 | D | 69 | ILE | 5.9 |
| 29 | 3 | 92 | GLU | 5.9 |
| 29 | 3 | 66 | ASP | 5.9 |
| 13 | M | 78 | LYS | 5.8 |
| 26 | Z | 65 | ASN | 5.8 |
| 21 | U | 30 | HIS | 5.8 |
| 9 | I | 132 | VAL | 5.7 |
| 4 | D | 18 | ILE | 5.7 |
| 9 | I | 100 | VAL | 5.7 |
| 29 | 3 | 90 | PHE | 5.7 |
| 21 | U | 12 | ASP | 5.7 |
| 21 | U | 19 | THR | 5.7 |
| 26 | Z | 74 | GLN | 5.6 |
| 29 | 3 | 84 | ARG | 5.6 |
| 26 | Z | 66 | CYS | 5.6 |
| 29 | 3 | 76 | LYS | 5.5 |
| 29 | 3 | 3 | MET | 5.5 |
| 21 | U | 53 | ASP | 5.5 |
| 4 | D | 63 | ILE | 5.5 |
| 26 | Z | 93 | TYR | 5.5 |
| 21 | U | 33 | SER | 5.5 |
| 9 | I | 111 | LEU | 5.4 |
| 21 | U | 42 | LEU | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 26 | Z | 76 | THR | 5.4 |
| 26 | Z | 88 | PHE | 5.3 |
| 29 | 3 | 68 | LYS | 5.3 |
| 26 | Z | 41 | ARG | 5.3 |
| 26 | Z | 70 | ARG | 5.3 |
| 4 | D | 135 | VAL | 5.3 |
| 9 | I | 117 | THR | 5.3 |
| 21 | U | 29 | THR | 5.3 |
| 9 | I | 73 | LEU | 5.2 |
| 29 | 3 | 60 | LYS | 5.2 |
| 9 | I | 109 | PRO | 5.2 |
| 21 | U | 24 | LYS | 5.2 |
| 31 | 9 | 1 | U | 5.2 |
| 29 | 3 | 88 | LEU | 5.1 |
| 29 | 3 | 7 | PHE | 5.1 |
| 9 | I | 102 | GLN | 5.1 |
| 19 | S | 81 | ILE | 5.1 |
| 29 | 3 | 85 | ALA | 5.1 |
| 13 | M | 86 | GLN | 5.1 |
| 4 | D | 75 | LEU | 5.0 |
| 29 | 3 | 86 | GLY | 5.0 |
| 26 | Z | 89 | THR | 5.0 |
| 21 | U | 55 | ALA | 5.0 |
| 29 | 3 | 5 | ARG | 5.0 |
| 14 | N | 179 | LEU | 5.0 |
| 29 | 3 | 4 | PRO | 5.0 |
| 29 | 3 | 23 | GLU | 5.0 |
| 21 | U | 32 | CYS | 5.0 |
| 26 | Z | 85 | ASP | 5.0 |
| 13 | M | 79 | ALA | 4.9 |
| 9 | I | 72 | GLU | 4.9 |
| 26 | Z | 80 | GLN | 4.9 |
| 13 | M | 71 | SER | 4.9 |
| 22 | V | 43 | PRO | 4.8 |
| 21 | U | 39 | ASN | 4.8 |
| 29 | 3 | 6 | ARG | 4.8 |
| 9 | I | 108 | HIS | 4.8 |
| 29 | 3 | 25 | VAL | 4.8 |
| 29 | 3 | 70 | ARG | 4.8 |
| 20 | T | 119 | ALA | 4.8 |
| 4 | D | 27 | ILE | 4.7 |
| 29 | 3 | 2 | GLN | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 29 | 3 | 50 | GLY | 4.7 |
| 21 | U | 45 | GLU | 4.7 |
| 9 | I | 105 | GLU | 4.7 |
| 21 | U | 47 | ARG | 4.7 |
| 9 | I | 116 | LEU | 4.6 |
| 21 | U | 11 | THR | 4.6 |
| 29 | 3 | 72 | GLY | 4.6 |
| 4 | D | 25 | MET | 4.5 |
| 21 | U | 48 | ASN | 4.5 |
| 29 | 3 | 54 | LYS | 4.5 |
| 9 | I | 118 | ASN | 4.5 |
| 21 | U | 25 | ASP | 4.5 |
| 22 | V | 38 | GLY | 4.5 |
| 29 | 3 | 64 | LYS | 4.5 |
| 9 | I | 78 | ALA | 4.5 |
| 9 | I | 110 | ASP | 4.5 |
| 4 | D | 40 | ILE | 4.4 |
| 13 | M | 76 | ARG | 4.4 |
| 4 | D | 166 | ILE | 4.4 |
| 21 | U | 28 | THR | 4.4 |
| 4 | D | 90 | LEU | 4.4 |
| 21 | U | 6 | CYS | 4.4 |
| 29 | 3 | 75 | GLY | 4.4 |
| 21 | U | 8 | TYR | 4.3 |
| 26 | Z | 92 | SER | 4.3 |
| 29 | 3 | 89 | GLU | 4.3 |
| 22 | V | 40 | PRO | 4.3 |
| 21 | U | 13 | ILE | 4.3 |
| 22 | V | 37 | GLY | 4.2 |
| 9 | I | 69 | PRO | 4.2 |
| 29 | 3 | 65 | THR | 4.2 |
| 29 | 3 | 67 | LEU | 4.2 |
| 26 | Z | 86 | TYR | 4.2 |
| 29 | 3 | 73 | GLU | 4.1 |
| 12 | L | 106 | VAL | 4.1 |
| 7 | G | 27 | ILE | 4.1 |
| 21 | U | 4 | ARG | 4.1 |
| 29 | 3 | 21 | GLU | 4.1 |
| 9 | I | 94 | ASP | 4.1 |
| 26 | Z | 83 | TYR | 4.1 |
| 9 | I | 67 | VAL | 4.1 |
| 21 | U | 23 | HIS | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | D | 88 | LEU | 4.1 |
| 21 | U | 10 | GLY | 4.0 |
| 13 | M | 75 | ARG | 4.0 |
| 13 | M | 73 | ARG | 4.0 |
| 4 | D | 26 | GLY | 4.0 |
| 13 | M | 88 | VAL | 4.0 |
| 26 | Z | 72 | ASP | 3.9 |
| 24 | X | 10 | VAL | 3.9 |
| 4 | D | 84 | LEU | 3.8 |
| 30 | 0 | 970 | U | 3.8 |
| 22 | V | 44 | GLY | 3.8 |
| 4 | D | 134 | LEU | 3.8 |
| 9 | I | 93 | ALA | 3.8 |
| 8 | H | 84 | GLY | 3.8 |
| 29 | 3 | 87 | ARG | 3.8 |
| 9 | I | 98 | ASP | 3.7 |
| 4 | D | 87 | ALA | 3.7 |
| 8 | H | 39 | LYS | 3.7 |
| 9 | I | 112 | LEU | 3.7 |
| 4 | D | 44 | ILE | 3.7 |
| 7 | G | 23 | ILE | 3.7 |
| 1 | A | 237 | GLY | 3.7 |
| 9 | I | 91 | PHE | 3.7 |
| 9 | I | 75 | LYS | 3.6 |
| 8 | H | 82 | GLU | 3.6 |
| 21 | U | 37 | GLU | 3.6 |
| 29 | 3 | 24 | LYS | 3.6 |
| 12 | L | 105 | TYR | 3.6 |
| 9 | I | 80 | PHE | 3.6 |
| 9 | I | 92 | VAL | 3.6 |
| 21 | U | 5 | GLU | 3.6 |
| 6 | F | 17 | LEU | 3.6 |
| 30 | 0 | 735 | C | 3.6 |
| 6 | F | 75 | ILE | 3.6 |
| 9 | I | 119 | ALA | 3.5 |
| 1 | A | 64 | ASP | 3.5 |
| 8 | H | 40 | GLN | 3.5 |
| 8 | H | 66 | GLU | 3.5 |
| 29 | 3 | 26 | ARG | 3.5 |
| 9 | I | 95 | LEU | 3.5 |
| 12 | L | 48 | LYS | 3.5 |
| 6 | F | 106 | ALA | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 26 | Z | 103 | VAL | 3.5 |
| 4 | D | 11 | HIS | 3.4 |
| 26 | Z | 73 | ARG | 3.4 |
| 8 | H | 133 | GLY | 3.4 |
| 8 | H | 77 | ILE | 3.4 |
| 29 | 3 | 63 | LYS | 3.4 |
| 30 | 0 | 1198 | U | 3.4 |
| 9 | I | 82 | THR | 3.4 |
| 12 | L | 120 | LEU | 3.4 |
| 4 | D | 130 | VAL | 3.4 |
| 9 | I | 68 | PRO | 3.3 |
| 8 | H | 86 | TYR | 3.3 |
| 13 | M | 77 | HIS | 3.2 |
| 22 | V | 2 | VAL | 3.2 |
| 4 | D | 41 | LEU | 3.2 |
| 4 | D | 129 | ASP | 3.2 |
| 9 | I | 88 | GLN | 3.2 |
| 4 | D | 157 | LEU | 3.2 |
| 1 | A | 37 | VAL | 3.2 |
| 28 | 2 | 49 | GLU | 3.2 |
| 8 | H | 69 | ARG | 3.2 |
| 9 | I | 83 | GLY | 3.1 |
| 4 | D | 93 | LEU | 3.1 |
| 4 | D | 128 | LEU | 3.1 |
| 26 | Z | 84 | CYS | 3.1 |
| 28 | 2 | 48 | ASP | 3.1 |
| 8 | H | 81 | GLY | 3.1 |
| 9 | I | 76 | ASP | 3.1 |
| 9 | I | 127 | CYS | 3.1 |
| 8 | H | 36 | MET | 3.1 |
| 13 | M | 84 | LYS | 3.1 |
| 8 | H | 35 | LYS | 3.0 |
| 9 | I | 124 | VAL | 3.0 |
| 1 | A | 65 | ARG | 3.0 |
| 4 | D | 165 | PHE | 3.0 |
| 30 | 0 | 1172 | G | 3.0 |
| 4 | D | 104 | PHE | 3.0 |
| 30 | 0 | 1177 | A | 3.0 |
| 8 | H | 38 | ARG | 3.0 |
| 12 | L | 123 | ASP | 3.0 |
| 9 | I | 121 | LYS | 3.0 |
| 14 | N | 155 | GLU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | D | 10 | PHE | 2.9 |
| 8 | H | 76 | LEU | 2.9 |
| 14 | N | 78 | MET | 2.9 |
| 21 | U | 22 | VAL | 2.9 |
| 12 | L | 96 | VAL | 2.9 |
| 4 | D | 16 | PRO | 2.9 |
| 8 | H | 149 | VAL | 2.9 |
| 6 | F | 99 | THR | 2.9 |
| 6 | F | 49 | PHE | 2.9 |
| 4 | D | 17 | ARG | 2.9 |
| 4 | D | 92 | GLU | 2.8 |
| 30 | 0 | 1199 | A | 2.8 |
| 8 | H | 89 | THR | 2.8 |
| 8 | H | 88 | MET | 2.8 |
| 12 | L | 79 | ASP | 2.8 |
| 9 | I | 101 | LYS | 2.8 |
| 4 | D | 67 | ASP | 2.8 |
| 4 | D | 58 | VAL | 2.8 |
| 12 | L | 142 | LEU | 2.7 |
| 14 | N | 178 | THR | 2.7 |
| 21 | U | 44 | ARG | 2.7 |
| 6 | F | 108 | VAL | 2.7 |
| 14 | N | 142 | THR | 2.7 |
| 14 | N | 95 | ALA | 2.7 |
| 4 | D | 70 | GLY | 2.7 |
| 21 | U | 20 | MET | 2.7 |
| 14 | N | 159 | TYR | 2.7 |
| 4 | D | 23 | VAL | 2.7 |
| 22 | V | 41 | GLU | 2.7 |
| 24 | X | 88 | GLU | 2.7 |
| 24 | X | 71 | ARG | 2.7 |
| 8 | H | 141 | CYS | 2.6 |
| 4 | D | 56 | ARG | 2.6 |
| 12 | L | 125 | PHE | 2.6 |
| 6 | F | 44 | SER | 2.6 |
| 21 | U | 49 | LEU | 2.6 |
| 22 | V | 3 | LEU | 2.6 |
| 14 | N | 145 | ALA | 2.6 |
| 4 | D | 83 | PHE | 2.6 |
| 21 | U | 21 | PHE | 2.6 |
| 14 | N | 97 | VAL | 2.6 |
| 22 | V | 8 | ILE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 12 | L | 80 | ASP | 2.6 |
| 14 | N | 185 | GLU | 2.6 |
| 21 | U | 56 | ARG | 2.6 |
| 6 | F | 119 | ARG | 2.6 |
| 4 | D | 80 | ALA | 2.6 |
| 6 | F | 20 | LEU | 2.6 |
| 8 | H | 31 | ILE | 2.5 |
| 4 | D | 106 | PHE | 2.5 |
| 12 | L | 130 | ARG | 2.5 |
| 12 | L | 124 | ASP | 2.5 |
| 5 | E | 5 | LEU | 2.5 |
| 12 | L | 91 | VAL | 2.5 |
| 9 | I | 79 | GLY | 2.5 |
| 9 | I | 122 | GLU | 2.5 |
| 21 | U | 35 | LYS | 2.5 |
| 22 | V | 36 | ALA | 2.5 |
| 4 | D | 28 | GLY | 2.5 |
| 4 | D | 89 | PRO | 2.5 |
| 9 | I | 123 | VAL | 2.5 |
| 26 | Z | 104 | ARG | 2.5 |
| 19 | S | 45 | TYR | 2.5 |
| 12 | L | 76 | LEU | 2.5 |
| 4 | D | 73 | VAL | 2.4 |
| 20 | T | 116 | ASP | 2.4 |
| 6 | F | 19 | ALA | 2.4 |
| 4 | D | 51 | ARG | 2.4 |
| 14 | N | 83 | LEU | 2.4 |
| 12 | L | 114 | VAL | 2.4 |
| 14 | N | 180 | LEU | 2.4 |
| 4 | D | 101 | THR | 2.4 |
| 14 | N | 181 | ASP | 2.4 |
| 8 | H | 126 | THR | 2.4 |
| 12 | L | 89 | PHE | 2.4 |
| 14 | N | 75 | THR | 2.4 |
| 7 | G | 63 | ARG | 2.4 |
| 20 | T | 42 | VAL | 2.4 |
| 8 | H | 145 | ASP | 2.4 |
| 14 | N | 84 | THR | 2.4 |
| 6 | F | 28 | ALA | 2.4 |
| 8 | H | 73 | ASN | 2.4 |
| 12 | L | 75 | LEU | 2.4 |
| 12 | L | 118 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | G | 25 | GLU | 2.3 |
| 9 | I | 99 | GLN | 2.3 |
| 4 | D | 171 | ASP | 2.3 |
| 8 | H | 85 | ASP | 2.3 |
| 4 | D | 61 | PHE | 2.3 |
| 13 | M | 72 | ALA | 2.3 |
| 30 | 0 | 1170 | U | 2.3 |
| 5 | E | 118 | ILE | 2.3 |
| 8 | H | 79 | GLU | 2.3 |
| 8 | H | 98 | LEU | 2.3 |
| 10 | J | 70 | PHE | 2.3 |
| 6 | F | 37 | THR | 2.3 |
| 26 | Z | 64 | PRO | 2.3 |
| 14 | N | 153 | GLN | 2.3 |
| 1 | A | 52 | SER | 2.3 |
| 4 | D | 64 | ARG | 2.3 |
| 31 | 9 | 24 | U | 2.3 |
| 14 | N | 92 | ALA | 2.3 |
| 30 | 0 | 1163 | G | 2.3 |
| 8 | H | 132 | ALA | 2.2 |
| 9 | I | 120 | ALA | 2.2 |
| 4 | D | 172 | VAL | 2.2 |
| 20 | T | 118 | SER | 2.2 |
| 14 | N | 156 | GLU | 2.2 |
| 12 | L | 62 | ALA | 2.2 |
| 1 | A | 145 | MET | 2.2 |
| 30 | 0 | 282 | C | 2.2 |
| 5 | E | 100 | ASP | 2.2 |
| 5 | E | 87 | PHE | 2.2 |
| 14 | N | 172 | PHE | 2.2 |
| 23 | W | 45 | VAL | 2.2 |
| 4 | D | 19 | GLU | 2.2 |
| 6 | F | 97 | ALA | 2.2 |
| 8 | H | 169 | GLU | 2.2 |
| 14 | N | 81 | ALA | 2.2 |
| 14 | N | 163 | PHE | 2.2 |
| 4 | D | 24 | HIS | 2.2 |
| 4 | D | 62 | ASP | 2.1 |
| 4 | D | 158 | ASN | 2.1 |
| 8 | H | 29 | SER | 2.1 |
| 28 | 2 | 39 | ARG | 2.1 |
| 14 | N | 182 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 21 | U | 27 | ALA | 2.1 |
| 21 | U | 15 | PRO | 2.1 |
| 17 | Q | 20 | ASP | 2.1 |
| 6 | F | 16 | ALA | 2.1 |
| 4 | D | 43 | GLU | 2.1 |
| 20 | T | 112 | LEU | 2.1 |
| 21 | U | 18 | GLY | 2.1 |
| 6 | F | 115 | VAL | 2.1 |
| 14 | N | 149 | GLU | 2.1 |
| 24 | X | 7 | GLU | 2.1 |
| 21 | U | 26 | GLY | 2.1 |
| 1 | A | 133 | ARG | 2.1 |
| 21 | U | 50 | GLU | 2.1 |
| 30 | 0 | 1000 | C | 2.1 |
| 14 | N | 69 | TYR | 2.1 |
| 26 | Z | 96 | GLU | 2.1 |
| 21 | U | 7 | ASP | 2.0 |
| 12 | L | 141 | GLU | 2.0 |
| 21 | U | 14 | GLU | 2.0 |
| 8 | H | 74 | ARG | 2.0 |
| 8 | H | 64 | SER | 2.0 |
| 8 | H | 68 | SER | 2.0 |
| 1 | A | 82 | VAL | 2.0 |
| 14 | N | 7 | LYS | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 30 | 1MA | 0 | 628 | 23/24 | 0.98 | 0.14 | 38,44,47,47 | 0 |
| 30 | OMU | 0 | 2587 | 21/22 | 0.98 | 0.11 | 43,47,50,51 | 0 |
| 30 | OMG | 0 | 2588 | 24/25 | 0.98 | 0.12 | 41,43,46,50 | 0 |
| 30 | UR3 | 0 | 2619 | 21/22 | 0.98 | 0.13 | 47,49,51,54 | 0 |
| 30 | PSU | 0 | 2621 | 20/21 | 0.98 | 0.18 | 39,41,53,53 | 0 |

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 33 | CL | 3 | 8804 | 1/1 | 0.25 | 0.20 | 128,128,128,128 | 0 |
| 35 | NA | 0 | 8528 | 1/1 | 0.51 | 0.67 | 76,76,76,76 | 0 |
| 34 | SR | 0 | 8979 | 1/1 | 0.53 | 0.19 | 196,196,196,196 | 0 |
| 34 | SR | 0 | 9006 | 1/1 | 0.57 | 0.98 | 200,200,200,200 | 0 |
| 35 | NA | J | 8538 | 1/1 | 0.58 | 0.15 | 78,78,78,78 | 0 |
| 32 | MG | 0 | 8040 | 1/1 | 0.59 | 0.39 | 86,86,86,86 | 0 |
| 35 | NA | 0 | 8563 | 1/1 | 0.59 | 0.12 | 117,117,117,117 | 0 |
| 34 | SR | 0 | 8988 | 1/1 | 0.61 | 0.08 | 173,173,173,173 | 0 |
| 35 | NA | 0 | 8570 | 1/1 | 0.66 | 0.09 | 61,61,61,61 | 0 |
| 35 | NA | 0 | 8511 | 1/1 | 0.67 | 0.08 | 81,81,81,81 | 0 |
| 34 | SR | 0 | 8991 | 1/1 | 0.67 | 0.08 | 180,180,180,180 | 0 |
| 34 | SR | 0 | 8982 | 1/1 | 0.68 | 1.93 | 200,200,200,200 | 0 |
| 34 | SR | 0 | 9004 | 1/1 | 0.71 | 0.84 | 200,200,200,200 | 0 |
| 35 | NA | 0 | 8506 | 1/1 | 0.72 | 0.20 | 83,83,83,83 | 0 |
| 34 | SR | 0 | 9001 | 1/1 | 0.75 | 0.13 | 177,177,177,177 | 0 |
| 32 | MG | A | 8051 | 1/1 | 0.76 | 0.25 | 94,94,94,94 | 0 |
| 35 | NA | 0 | 8525 | 1/1 | 0.77 | 0.16 | 75,75,75,75 | 0 |
| 35 | NA | B | 8552 | 1/1 | 0.78 | 0.28 | 89,89,89,89 | 0 |
| 37 | CD | Z | 8703 | 1/1 | 0.78 | 0.46 | 200,200,200,200 | 0 |
| 37 | CD | 3 | 8704 | 1/1 | 0.78 | 0.66 | 200,200,200,200 | 0 |
| 34 | SR | 0 | 8977 | 1/1 | 0.80 | 0.07 | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8089 | 1/1 | 0.80 | 0.25 | 65,65,65,65 | 0 |
| 34 | SR | 0 | 8938 | 1/1 | 0.80 | 0.08 | 183,183,183,183 | 0 |
| 34 | SR | 0 | 8959 | 1/1 | 0.80 | 0.27 | 200,200,200,200 | 0 |
| 34 | SR | 0 | 9007 | 1/1 | 0.80 | 1.77 | 200,200,200,200 | 0 |
| 34 | SR | 0 | 9002 | 1/1 | 0.82 | 0.12 | 193,193,193,193 | 0 |
| 35 | NA | 0 | 8535 | 1/1 | 0.83 | 0.29 | 67,67,67,67 | 0 |
| 35 | NA | 0 | 8562 | 1/1 | 0.83 | 0.97 | 82,82,82,82 | 0 |
| 32 | MG | 0 | 8071 | 1/1 | 0.84 | 0.12 | 60,60,60,60 | 0 |
| 34 | SR | 0 | 8962 | 1/1 | 0.84 | 0.09 | 172,172,172,172 | 0 |
| 35 | NA | 0 | 8509 | 1/1 | 0.84 | 0.13 | 69,69,69,69 | 0 |
| 34 | SR | 3 | 8999 | 1/1 | 0.84 | 0.28 | 187,187,187,187 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 34 | SR | 0 | 8992 | 1/1 | 0.84 | 0.23 | 159,159,159,159 | 0 |
| 33 | CL | J | 8801 | 1/1 | 0.84 | 0.12 | 95,95,95,95 | 0 |
| 35 | NA | 0 | 8502 | 1/1 | 0.85 | 0.12 | 69,69,69,69 | 0 |
| 34 | SR | 0 | 8951 | 1/1 | 0.85 | 0.10 | 155,155,155,155 | 0 |
| 35 | NA | H | 8518 | 1/1 | 0.85 | 0.42 | 91,91,91,91 | 0 |
| 32 | MG | 0 | 8075 | 1/1 | 0.85 | 0.05 | 55,55,55,55 | 0 |
| 34 | SR | 0 | 8985 | 1/1 | 0.86 | 0.06 | 164,164,164,164 | 0 |
| 35 | NA | Q | 8540 | 1/1 | 0.86 | 0.11 | 79,79,79,79 | 0 |
| 34 | SR | 0 | 8928 | 1/1 | 0.86 | 0.04 | 137,137,137,137 | 0 |
| 34 | SR | 0 | 8953 | 1/1 | 0.86 | 0.55 | 200,200,200,200 | 0 |
| 34 | SR | 0 | 8957 | 1/1 | 0.86 | 0.34 | 200,200,200,200 | 0 |
| 34 | SR | 0 | 8994 | 1/1 | 0.86 | 0.48 | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8081 | 1/1 | 0.86 | 0.17 | 88,88,88,88 | 0 |
| 34 | SR | 0 | 8919 | 1/1 | 0.87 | 0.09 | 168,168,168,168 | 0 |
| 35 | NA | 0 | 8555 | 1/1 | 0.87 | 0.42 | 52,52,52,52 | 0 |
| 35 | NA | 0 | 8560 | 1/1 | 0.87 | 0.56 | 118,118,118,118 | 0 |
| 34 | SR | 9 | 8980 | 1/1 | 0.87 | 0.15 | 183,183,183,183 | 0 |
| 35 | NA | 0 | 8545 | 1/1 | 0.88 | 0.80 | 58,58,58,58 | 0 |
| 35 | NA | 0 | 8548 | 1/1 | 0.88 | 0.12 | 56,56,56,56 | 0 |
| 34 | SR | 0 | 8989 | 1/1 | 0.88 | 0.20 | 178,178,178,178 | 0 |
| 32 | MG | 0 | 8056 | 1/1 | 0.89 | 0.06 | 57,57,57,57 | 0 |
| 34 | SR | 9 | 9003 | 1/1 | 0.89 | 0.10 | 187,187,187,187 | 0 |
| 34 | SR | 0 | 8993 | 1/1 | 0.89 | 0.08 | 167,167,167,167 | 0 |
| 35 | NA | 0 | 8508 | 1/1 | 0.89 | 0.47 | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8067 | 1/1 | 0.89 | 0.11 | 35,35,35,35 | 0 |
| 32 | MG | 9 | 8074 | 1/1 | 0.89 | 0.07 | 87,87,87,87 | 0 |
| 34 | SR | 3 | 8932 | 1/1 | 0.90 | 0.23 | 178,178,178,178 | 0 |
| 35 | NA | 0 | 8551 | 1/1 | 0.90 | 0.46 | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8080 | 1/1 | 0.90 | 0.75 | 83,83,83,83 | 0 |
| 34 | SR | 0 | 8944 | 1/1 | 0.90 | 0.07 | 172,172,172,172 | 0 |
| 32 | MG | 0 | 8030 | 1/1 | 0.90 | 0.47 | 90,90,90,90 | 0 |
| 34 | SR | 0 | 8975 | 1/1 | 0.90 | 0.14 | 149,149,149,149 | 0 |
| 35 | NA | 0 | 8536 | 1/1 | 0.90 | 0.17 | 64,64,64,64 | 0 |
| 35 | NA | 0 | 8544 | 1/1 | 0.90 | 0.19 | 79,79,79,79 | 0 |
| 34 | SR | 0 | 8976 | 1/1 | 0.90 | 0.29 | 193,193,193,193 | 0 |
| 35 | NA | 0 | 8522 | 1/1 | 0.91 | 0.14 | 82,82,82,82 | 0 |
| 35 | NA | 0 | 8565 | 1/1 | 0.91 | 1.10 | 78,78,78,78 | 0 |
| 34 | SR | 0 | 8983 | 1/1 | 0.91 | 0.33 | 197,197,197,197 | 0 |
| 35 | NA | 9 | 8543 | 1/1 | 0.91 | 0.21 | 61,61,61,61 | 0 |
| 36 | K | 0 | 8401 | 1/1 | 0.91 | 0.63 | 139,139,139,139 | 0 |
| 34 | SR | 0 | 8946 | 1/1 | 0.91 | 0.20 | 137,137,137,137 | 0 |
| 34 | SR | 0 | 8954 | 1/1 | 0.91 | 0.12 | 108,108,108,108 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 34 | SR | L | 8969 | 1/1 | 0.92 | 0.29 | 200,200,200,200 | 0 |
| 33 | CL | O | 8808 | 1/1 | 0.92 | 0.17 | 86,86,86,86 | 0 |
| 35 | NA | 0 | 8566 | 1/1 | 0.92 | 0.30 | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8031 | 1/1 | 0.92 | 0.39 | 83,83,83,83 | 0 |
| 33 | CL | 0 | 8805 | 1/1 | 0.92 | 0.17 | 98,98,98,98 | 0 |
| 36 | K | M | 8402 | 1/1 | 0.92 | 0.19 | 87,87,87,87 | 0 |
| 34 | SR | 0 | 8971 | 1/1 | 0.92 | 0.06 | 192,192,192,192 | 0 |
| 34 | SR | H | 8972 | 1/1 | 0.92 | 0.10 | 164,164,164,164 | 0 |
| 34 | SR | 0 | 8996 | 1/1 | 0.92 | 0.52 | 200,200,200,200 | 0 |
| 35 | NA | 0 | 8542 | 1/1 | 0.93 | 0.53 | 58,58,58,58 | 0 |
| 33 | CL | B | 8819 | 1/1 | 0.93 | 0.22 | 69,69,69,69 | 0 |
| 34 | SR | 0 | 8997 | 1/1 | 0.93 | 0.15 | 189,189,189,189 | 0 |
| 35 | NA | 0 | 8547 | 1/1 | 0.93 | 0.99 | 67,67,67,67 | 0 |
| 35 | NA | S | 8510 | 1/1 | 0.93 | 0.03 | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8063 | 1/1 | 0.93 | 0.30 | 116,116,116,116 | 0 |
| 35 | NA | 0 | 8553 | 1/1 | 0.93 | 0.28 | 89,89,89,89 | 0 |
| 33 | CL | J | 8802 | 1/1 | 0.93 | 0.06 | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8053 | 1/1 | 0.93 | 0.05 | 63,63,63,63 | 0 |
| 34 | SR | 0 | 8915 | 1/1 | 0.93 | 0.08 | 126,126,126,126 | 0 |
| 32 | MG | 0 | 8059 | 1/1 | 0.93 | 0.09 | 51,51,51,51 | 0 |
| 35 | NA | 0 | 8521 | 1/1 | 0.93 | 0.45 | 64,64,64,64 | 0 |
| 34 | SR | 9 | 8978 | 1/1 | 0.93 | 0.06 | 157,157,157,157 | 0 |
| 35 | NA | 0 | 8567 | 1/1 | 0.93 | 0.25 | 78,78,78,78 | 0 |
| 32 | MG | 0 | 8061 | 1/1 | 0.93 | 0.17 | 36,36,36,36 | 0 |
| 35 | NA | 0 | 8526 | 1/1 | 0.93 | 0.15 | 46,46,46,46 | 0 |
| 33 | CL | 0 | 8815 | 1/1 | 0.93 | 0.22 | 89,89,89,89 | 0 |
| 35 | NA | 0 | 8530 | 1/1 | 0.93 | 0.44 | 74,74,74,74 | 0 |
| 34 | SR | A | 8930 | 1/1 | 0.93 | 0.15 | 142,142,142,142 | 0 |
| 34 | SR | B | 8987 | 1/1 | 0.93 | 0.62 | 200,200,200,200 | 0 |
| 35 | NA | 0 | 8550 | 1/1 | 0.94 | 0.26 | 71,71,71,71 | 0 |
| 32 | MG | 0 | 8006 | 1/1 | 0.94 | 0.12 | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8019 | 1/1 | 0.94 | 0.19 | 29,29,29,29 | 0 |
| 34 | SR | 0 | 8917 | 1/1 | 0.94 | 0.16 | 114,114,114,114 | 0 |
| 35 | NA | 0 | 8557 | 1/1 | 0.94 | 0.06 | 65,65,65,65 | 0 |
| 35 | NA | 0 | 8558 | 1/1 | 0.94 | 0.20 | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8082 | 1/1 | 0.94 | 0.23 | 76,76,76,76 | 0 |
| 35 | NA | 0 | 8527 | 1/1 | 0.94 | 0.28 | 72,72,72,72 | 0 |
| 34 | SR | 0 | 8968 | 1/1 | 0.94 | 0.06 | 177,177,177,177 | 0 |
| 34 | SR | 0 | 8922 | 1/1 | 0.94 | 0.17 | 168,168,168,168 | 0 |
| 32 | MG | 0 | 8044 | 1/1 | 0.94 | 0.05 | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8066 | 1/1 | 0.94 | 0.18 | 69,69,69,69 | 0 |
| 35 | NA | 0 | 8568 | 1/1 | 0.94 | 0.33 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 35 | NA | 0 | 8569 | 1/1 | 0.94 | 0.18 | 50,50,50,50 | 0 |
| 34 | SR | 0 | 8939 | 1/1 | 0.94 | 0.04 | 144,144,144,144 | 0 |
| 35 | NA | 0 | 8571 | 1/1 | 0.94 | 0.12 | 79,79,79,79 | 0 |
| 35 | NA | 0 | 8573 | 1/1 | 0.94 | 0.13 | 73,73,73,73 | 0 |
| 32 | MG | 0 | 8028 | 1/1 | 0.94 | 0.17 | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8055 | 1/1 | 0.94 | 0.06 | 62,62,62,62 | 0 |
| 35 | NA | 0 | 8546 | 1/1 | 0.94 | 0.74 | 94,94,94,94 | 0 |
| 32 | MG | A | 8050 | 1/1 | 0.94 | 0.05 | 64,64,64,64 | 0 |
| 33 | CL | N | 8807 | 1/1 | 0.94 | 0.22 | 87,87,87,87 | 0 |
| 32 | MG | 0 | 8060 | 1/1 | 0.95 | 0.06 | 53,53,53,53 | 0 |
| 34 | SR | 0 | 8947 | 1/1 | 0.95 | 0.26 | 200,200,200,200 | 0 |
| 32 | MG | Y | 8086 | 1/1 | 0.95 | 0.07 | 50,50,50,50 | 0 |
| 34 | SR | S | 8961 | 1/1 | 0.95 | 0.09 | 128,128,128,128 | 0 |
| 32 | MG | 0 | 8020 | 1/1 | 0.95 | 0.16 | 41,41,41,41 | 0 |
| 34 | SR | 0 | 8956 | 1/1 | 0.95 | 0.12 | 169,169,169,169 | 0 |
| 32 | MG | 0 | 8021 | 1/1 | 0.95 | 0.09 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8083 | 1/1 | 0.95 | 0.10 | 55,55,55,55 | 0 |
| 35 | NA | 0 | 8519 | 1/1 | 0.95 | 0.15 | 52,52,52,52 | 0 |
| 33 | CL | Y | 8820 | 1/1 | 0.95 | 0.07 | 52,52,52,52 | 0 |
| 34 | SR | 0 | 9000 | 1/1 | 0.95 | 0.07 | 183,183,183,183 | 0 |
| 35 | NA | 0 | 8564 | 1/1 | 0.95 | 0.43 | 69,69,69,69 | 0 |
| 34 | SR | 0 | 8963 | 1/1 | 0.95 | 0.06 | 133,133,133,133 | 0 |
| 34 | SR | 0 | 8965 | 1/1 | 0.95 | 0.06 | 134,134,134,134 | 0 |
| 32 | MG | 0 | 8036 | 1/1 | 0.95 | 0.10 | 48,48,48,48 | 0 |
| 34 | SR | 0 | 8920 | 1/1 | 0.95 | 0.05 | 127,127,127,127 | 0 |
| 32 | MG | 0 | 8090 | 1/1 | 0.95 | 0.17 | 97,97,97,97 | 0 |
| 35 | NA | 0 | 8533 | 1/1 | 0.95 | 0.09 | 70,70,70,70 | 0 |
| 32 | MG | 0 | 8091 | 1/1 | 0.95 | 0.11 | 56,56,56,56 | 0 |
| 34 | SR | A | 8929 | 1/1 | 0.95 | 0.11 | 139,139,139,139 | 0 |
| 35 | NA | 0 | 8574 | 1/1 | 0.95 | 0.58 | 60,60,60,60 | 0 |
| 35 | NA | 0 | 8537 | 1/1 | 0.95 | 0.15 | 50,50,50,50 | 0 |
| 35 | NA | 9 | 8572 | 1/1 | 0.95 | 0.27 | 88,88,88,88 | 0 |
| 32 | MG | 0 | 8092 | 1/1 | 0.95 | 0.08 | 76,76,76,76 | 0 |
| 34 | SR | 0 | 8943 | 1/1 | 0.95 | 0.13 | 84,84,84,84 | 0 |
| 37 | CD | U | 8701 | 1/1 | 0.95 | 0.45 | 200,200,200,200 | 0 |
| 35 | NA | C | 8503 | 1/1 | 0.95 | 0.17 | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8026 | 1/1 | 0.95 | 0.08 | 50,50,50,50 | 0 |
| 34 | SR | B | 8950 | 1/1 | 0.96 | 0.16 | 130,130,130,130 | 0 |
| 34 | SR | 0 | 8941 | 1/1 | 0.96 | 0.11 | 114,114,114,114 | 0 |
| 32 | MG | 0 | 8068 | 1/1 | 0.96 | 0.09 | 56,56,56,56 | 0 |
| 32 | MG | 0 | 8085 | 1/1 | 0.96 | 0.17 | 76,76,76,76 | 0 |
| 33 | CL | J | 8821 | 1/1 | 0.96 | 0.10 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 33 | CL | L | 8810 | 1/1 | 0.96 | 0.05 | 64,64,64,64 | 0 |
| 32 | MG | 0 | 8087 | 1/1 | 0.96 | 0.09 | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8033 | 1/1 | 0.96 | 0.06 | 63,63,63,63 | 0 |
| 34 | SR | 0 | 8908 | 1/1 | 0.96 | 0.11 | 85,85,85,85 | 0 |
| 35 | NA | 0 | 8513 | 1/1 | 0.96 | 0.41 | 68,68,68,68 | 0 |
| 35 | NA | 0 | 8561 | 1/1 | 0.96 | 0.31 | 65,65,65,65 | 0 |
| 35 | NA | 0 | 8514 | 1/1 | 0.96 | 0.29 | 55,55,55,55 | 0 |
| 35 | NA | 0 | 8515 | 1/1 | 0.96 | 0.15 | 32,32,32,32 | 0 |
| 35 | NA | 0 | 8517 | 1/1 | 0.96 | 0.09 | 38,38,38,38 | 0 |
| 34 | SR | 0 | 8955 | 1/1 | 0.96 | 0.07 | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8073 | 1/1 | 0.96 | 0.07 | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8010 | 1/1 | 0.96 | 0.13 | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8064 | 1/1 | 0.96 | 0.18 | 45,45,45,45 | 0 |
| 34 | SR | 0 | 8960 | 1/1 | 0.96 | 0.02 | 151,151,151,151 | 0 |
| 32 | MG | 0 | 8093 | 1/1 | 0.96 | 0.06 | 36,36,36,36 | 0 |
| 33 | CL | 0 | 8816 | 1/1 | 0.96 | 0.43 | 85,85,85,85 | 0 |
| 35 | NA | 0 | 8529 | 1/1 | 0.96 | 0.11 | 48,48,48,48 | 0 |
| 34 | SR | 0 | 8927 | 1/1 | 0.96 | 0.06 | 181,181,181,181 | 0 |
| 34 | SR | 0 | 8966 | 1/1 | 0.96 | 0.09 | 105,105,105,105 | 0 |
| 34 | SR | 0 | 8967 | 1/1 | 0.96 | 0.04 | 131,131,131,131 | 0 |
| 32 | MG | 0 | 8052 | 1/1 | 0.96 | 0.09 | 44,44,44,44 | 0 |
| 34 | SR | 0 | 8970 | 1/1 | 0.96 | 0.05 | 125,125,125,125 | 0 |
| 34 | SR | 0 | 8933 | 1/1 | 0.96 | 0.04 | 135,135,135,135 | 0 |
| 34 | SR | 0 | 8937 | 1/1 | 0.96 | 0.15 | 113,113,113,113 | 0 |
| 32 | MG | 0 | 8039 | 1/1 | 0.96 | 0.19 | 84,84,84,84 | 0 |
| 32 | MG | 0 | 8003 | 1/1 | 0.97 | 0.17 | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8062 | 1/1 | 0.97 | 0.17 | 56,56,56,56 | 0 |
| 32 | MG | 0 | 8077 | 1/1 | 0.97 | 0.08 | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8079 | 1/1 | 0.97 | 0.20 | 66,66,66,66 | 0 |
| 35 | NA | M | 8539 | 1/1 | 0.97 | 0.14 | 42,42,42,42 | 0 |
| 34 | SR | 0 | 8942 | 1/1 | 0.97 | 0.09 | 124,124,124,124 | 0 |
| 33 | CL | 0 | 8814 | 1/1 | 0.97 | 0.16 | 79,79,79,79 | 0 |
| 32 | MG | B | 8042 | 1/1 | 0.97 | 0.07 | 69,69,69,69 | 0 |
| 32 | MG | 0 | 8041 | 1/1 | 0.97 | 0.16 | 36,36,36,36 | 0 |
| 33 | CL | 0 | 8822 | 1/1 | 0.97 | 0.42 | 88,88,88,88 | 0 |
| 32 | MG | 0 | 8065 | 1/1 | 0.97 | 0.06 | 42,42,42,42 | 0 |
| 34 | SR | 0 | 8974 | 1/1 | 0.97 | 0.06 | 166,166,166,166 | 0 |
| 32 | MG | 0 | 8002 | 1/1 | 0.97 | 0.10 | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8058 | 1/1 | 0.97 | 0.06 | 18,18,18,18 | 0 |
| 32 | MG | 0 | 8045 | 1/1 | 0.97 | 0.10 | 31,31,31,31 | 0 |
| 34 | SR | 0 | 8931 | 1/1 | 0.97 | 0.09 | 111,111,111,111 | 0 |
| 32 | MG | 0 | 8047 | 1/1 | 0.97 | 0.31 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 35 | NA | 0 | 8520 | 1/1 | 0.97 | 0.10 | 56,56,56,56 | 0 |
| 34 | SR | 0 | 8958 | 1/1 | 0.97 | 0.07 | 116,116,116,116 | 0 |
| 35 | NA | 0 | 8554 | 1/1 | 0.97 | 0.86 | 69,69,69,69 | 0 |
| 34 | SR | 0 | 8984 | 1/1 | 0.97 | 0.09 | 119,119,119,119 | 0 |
| 35 | NA | 0 | 8524 | 1/1 | 0.97 | 0.69 | 73,73,73,73 | 0 |
| 35 | NA | 0 | 8541 | 1/1 | 0.98 | 0.23 | 64,64,64,64 | 0 |
| 32 | MG | T | 8057 | 1/1 | 0.98 | 0.07 | 65,65,65,65 | 0 |
| 34 | SR | F | 9005 | 1/1 | 0.98 | 0.07 | 147,147,147,147 | 0 |
| 32 | MG | 0 | 8001 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8032 | 1/1 | 0.98 | 0.04 | 52,52,52,52 | 0 |
| 34 | SR | R | 8912 | 1/1 | 0.98 | 0.19 | 95,95,95,95 | 0 |
| 34 | SR | 0 | 8945 | 1/1 | 0.98 | 0.09 | 105,105,105,105 | 0 |
| 35 | NA | 0 | 8549 | 1/1 | 0.98 | 0.85 | 56,56,56,56 | 0 |
| 32 | MG | 0 | 8024 | 1/1 | 0.98 | 0.16 | 62,62,62,62 | 0 |
| 35 | NA | 0 | 8505 | 1/1 | 0.98 | 0.66 | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8035 | 1/1 | 0.98 | 0.10 | 66,66,66,66 | 0 |
| 34 | SR | 0 | 8949 | 1/1 | 0.98 | 0.15 | 117,117,117,117 | 0 |
| 34 | SR | 0 | 8986 | 1/1 | 0.98 | 1.04 | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8025 | 1/1 | 0.98 | 0.10 | 37,37,37,37 | 0 |
| 35 | NA | 0 | 8512 | 1/1 | 0.98 | 0.15 | 56,56,56,56 | 0 |
| 35 | NA | 0 | 8559 | 1/1 | 0.98 | 0.17 | 77,77,77,77 | 0 |
| 32 | MG | 0 | 8038 | 1/1 | 0.98 | 0.08 | 74,74,74,74 | 0 |
| 34 | SR | 0 | 8910 | 1/1 | 0.98 | 0.09 | 108,108,108,108 | 0 |
| 34 | SR | 0 | 8911 | 1/1 | 0.98 | 0.13 | 88,88,88,88 | 0 |
| 34 | SR | 0 | 8914 | 1/1 | 0.98 | 0.27 | 133,133,133,133 | 0 |
| 33 | CL | 0 | 8803 | 1/1 | 0.98 | 0.09 | 60,60,60,60 | 0 |
| 34 | SR | 0 | 8995 | 1/1 | 0.98 | 0.19 | 150,150,150,150 | 0 |
| 32 | MG | 0 | 8069 | 1/1 | 0.98 | 0.10 | 102,102,102,102 | 0 |
| 33 | CL | 0 | 8812 | 1/1 | 0.98 | 0.05 | 61,61,61,61 | 0 |
| 35 | NA | 0 | 8523 | 1/1 | 0.98 | 0.14 | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8012 | 1/1 | 0.98 | 0.16 | 25,25,25,25 | 0 |
| 32 | MG | 0 | 8072 | 1/1 | 0.98 | 0.06 | 59,59,59,59 | 0 |
| 34 | SR | 0 | 8926 | 1/1 | 0.98 | 0.14 | 122,122,122,122 | 0 |
| 32 | MG | 0 | 8027 | 1/1 | 0.98 | 0.12 | 47,47,47,47 | 0 |
| 33 | CL | 0 | 8817 | 1/1 | 0.98 | 0.14 | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8005 | 1/1 | 0.98 | 0.21 | 42,42,42,42 | 0 |
| 34 | SR | 0 | 9008 | 1/1 | 0.98 | 0.14 | 92,92,92,92 | 0 |
| 32 | MG | 0 | 8076 | 1/1 | 0.98 | 0.06 | 40,40,40,40 | 0 |
| 35 | NA | 0 | 8534 | 1/1 | 0.98 | 0.13 | 50,50,50,50 | 0 |
| 32 | MG | 0 | 8043 | 1/1 | 0.98 | 0.13 | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8078 | 1/1 | 0.98 | 0.26 | 65,65,65,65 | 0 |
| 34 | SR | 0 | 8973 | 1/1 | 0.98 | 0.16 | 146,146,146,146 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 32 | MG | 0 | 8017 | 1/1 | 0.99 | 0.17 | 40,40,40,40 | 0 |
| 34 | SR | 0 | 8990 | 1/1 | 0.99 | 0.14 | 137,137,137,137 | 0 |
| 34 | SR | 0 | 8940 | 1/1 | 0.99 | 0.09 | 93,93,93,93 | 0 |
| 33 | CL | A | 8809 | 1/1 | 0.99 | 0.15 | 104,104,104,104 | 0 |
| 32 | MG | 0 | 8018 | 1/1 | 0.99 | 0.24 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8007 | 1/1 | 0.99 | 0.18 | 36,36,36,36 | 0 |
| 35 | NA | 0 | 8531 | 1/1 | 0.99 | 0.06 | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8008 | 1/1 | 0.99 | 0.13 | 31,31,31,31 | 0 |
| 32 | MG | 0 | 8009 | 1/1 | 0.99 | 0.24 | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8037 | 1/1 | 0.99 | 0.21 | 77,77,77,77 | 0 |
| 34 | SR | 0 | 8998 | 1/1 | 0.99 | 0.18 | 178,178,178,178 | 0 |
| 34 | SR | 1 | 8913 | 1/1 | 0.99 | 0.06 | 95,95,95,95 | 0 |
| 34 | SR | 0 | 8948 | 1/1 | 0.99 | 0.10 | 115,115,115,115 | 0 |
| 33 | CL | M | 8818 | 1/1 | 0.99 | 0.05 | 49,49,49,49 | 0 |
| 32 | MG | 0 | 8022 | 1/1 | 0.99 | 0.20 | 33,33,33,33 | 0 |
| 34 | SR | 0 | 8901 | 1/1 | 0.99 | 0.18 | 66,66,66,66 | 0 |
| 34 | SR | 0 | 8902 | 1/1 | 0.99 | 0.15 | 68,68,68,68 | 0 |
| 34 | SR | 0 | 8905 | 1/1 | 0.99 | 0.25 | 72,72,72,72 | 0 |
| 34 | SR | 0 | 8907 | 1/1 | 0.99 | 0.13 | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8023 | 1/1 | 0.99 | 0.17 | 28,28,28,28 | 0 |
| 33 | CL | R | 8806 | 1/1 | 0.99 | 0.14 | 58,58,58,58 | 0 |
| 32 | MG | K | 8054 | 1/1 | 0.99 | 0.17 | 57,57,57,57 | 0 |
| 32 | MG | 0 | 8011 | 1/1 | 0.99 | 0.22 | 25,25,25,25 | 0 |
| 32 | MG | 0 | 8004 | 1/1 | 0.99 | 0.12 | 29,29,29,29 | 0 |
| 34 | SR | 0 | 8916 | 1/1 | 0.99 | 0.05 | 105,105,105,105 | 0 |
| 35 | NA | 0 | 8556 | 1/1 | 0.99 | 0.80 | 71,71,71,71 | 0 |
| 34 | SR | 0 | 8964 | 1/1 | 0.99 | 0.12 | 134,134,134,134 | 0 |
| 32 | MG | 0 | 8084 | 1/1 | 0.99 | 0.14 | 35,35,35,35 | 0 |
| 35 | NA | R | 8532 | 1/1 | 0.99 | 0.11 | 50,50,50,50 | 0 |
| 34 | SR | 0 | 8918 | 1/1 | 0.99 | 0.12 | 85,85,85,85 | 0 |
| 35 | NA | 0 | 8501 | 1/1 | 0.99 | 0.16 | 39,39,39,39 | 0 |
| 33 | CL | 0 | 8811 | 1/1 | 0.99 | 0.20 | 81,81,81,81 | 0 |
| 32 | MG | 0 | 8013 | 1/1 | 0.99 | 0.06 | 28,28,28,28 | 0 |
| 34 | SR | 0 | 8921 | 1/1 | 0.99 | 0.13 | 83,83,83,83 | 0 |
| 35 | NA | 0 | 8507 | 1/1 | 0.99 | 0.24 | 43,43,43,43 | 0 |
| 33 | CL | 0 | 8813 | 1/1 | 0.99 | 0.07 | 60,60,60,60 | 0 |
| 34 | SR | 0 | 8924 | 1/1 | 0.99 | 0.20 | 124,124,124,124 | 0 |
| 34 | SR | 0 | 8925 | 1/1 | 0.99 | 0.13 | 98,98,98,98 | 0 |
| 32 | MG | 0 | 8014 | 1/1 | 0.99 | 0.17 | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8088 | 1/1 | 0.99 | 0.10 | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8046 | 1/1 | 0.99 | 0.10 | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8016 | 1/1 | 0.99 | 0.17 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 35 | NA | 0 | 8516 | 1/1 | 0.99 | 0.19 | 39,39,39,39 | 0 |
| 35 | NA | 0 | 8575 | 1/1 | 0.99 | 0.23 | 103,103,103,103 | 0 |
| 34 | SR | 0 | 8981 | 1/1 | 0.99 | 0.13 | 161,161,161,161 | 0 |
| 32 | MG | 0 | 8048 | 1/1 | 0.99 | 0.24 | 29,29,29,29 | 0 |
| 34 | SR | 0 | 8934 | 1/1 | 0.99 | 0.13 | 133,133,133,133 | 0 |
| 34 | SR | 0 | 8935 | 1/1 | 0.99 | 0.11 | 103,103,103,103 | 0 |
| 37 | CD | O | 8705 | 1/1 | 0.99 | 0.08 | 100,100,100,100 | 0 |
| 34 | SR | 0 | 8936 | 1/1 | 0.99 | 0.11 | 95,95,95,95 | 0 |
| 32 | MG | 0 | 8070 | 1/1 | 0.99 | 0.17 | 66,66,66,66 | 0 |
| 32 | MG | 0 | 8049 | 1/1 | 0.99 | 0.23 | 64,64,64,64 | 0 |
| 32 | MG | 0 | 8015 | 1/1 | 1.00 | 0.13 | 45,45,45,45 | 0 |
| 34 | SR | 0 | 8909 | 1/1 | 1.00 | 0.14 | 93,93,93,93 | 0 |
| 34 | SR | 1 | 8952 | 1/1 | 1.00 | 0.15 | 90,90,90,90 | 0 |
| 34 | SR | 0 | 8903 | 1/1 | 1.00 | 0.19 | 57,57,57,57 | 0 |
| 34 | SR | 0 | 8904 | 1/1 | 1.00 | 0.20 | 57,57,57,57 | 0 |
| 34 | SR | 0 | 8923 | 1/1 | 1.00 | 0.13 | 109,109,109,109 | 0 |
| 32 | MG | 0 | 8029 | 1/1 | 1.00 | 0.13 | 59,59,59,59 | 0 |
| 34 | SR | 0 | 8906 | 1/1 | 1.00 | 0.21 | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8034 | 1/1 | 1.00 | 0.07 | 50,50,50,50 | 0 |
| 37 | CD | 1 | 8702 | 1/1 | 1.00 | 0.10 | 61,61,61,61 | 0 |
| 35 | NA | 0 | 8504 | 1/1 | 1.00 | 0.12 | 40,40,40,40 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.