# Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:57 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 3CCE |
| Title | : | Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535A |
| Authors | : | Blaha, G.; Gurel, G. |
| Deposited on | : | 2008-02-25 |
| Resolution | : | 2.75 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

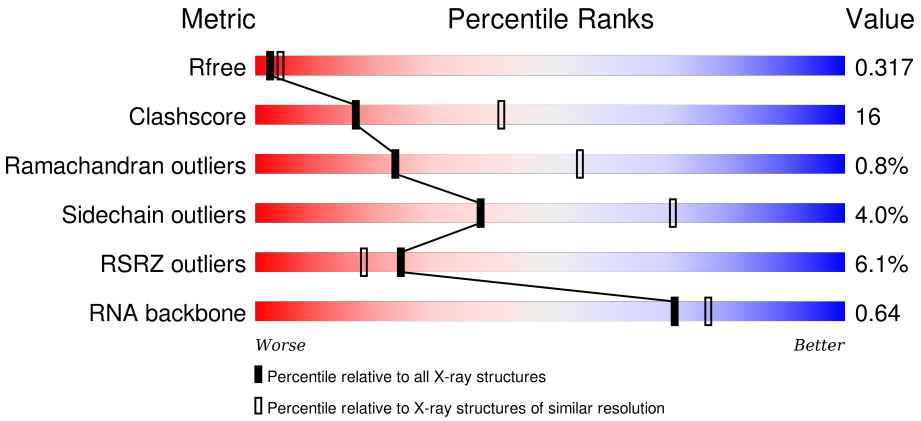
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 Å.

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



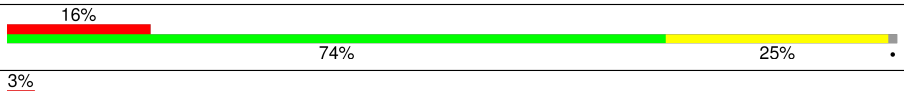
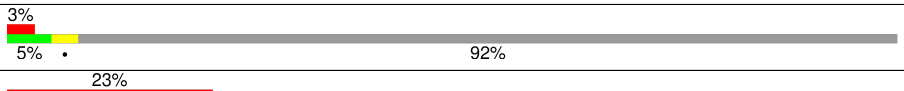
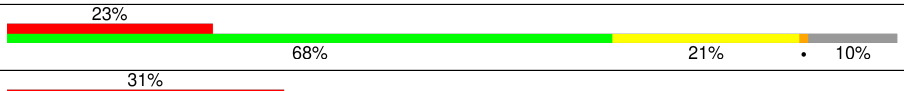
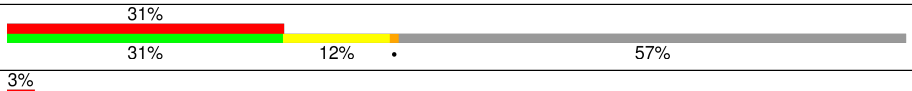
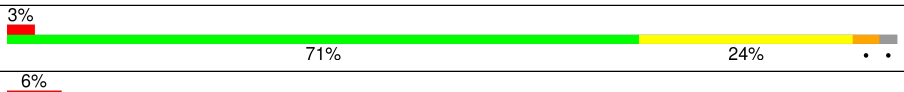
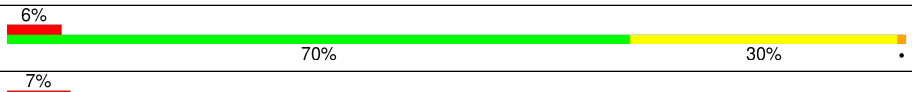
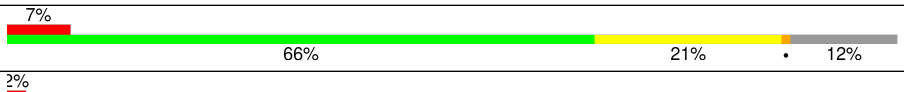
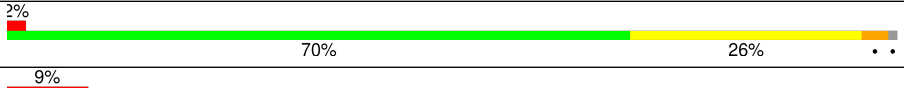
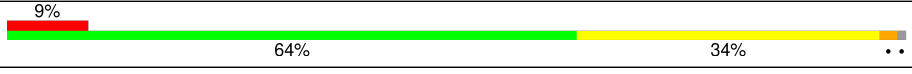
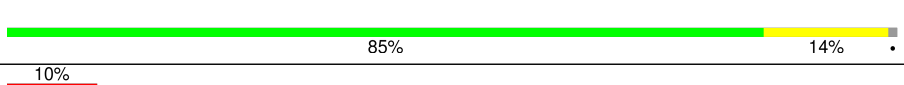
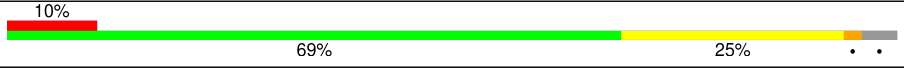
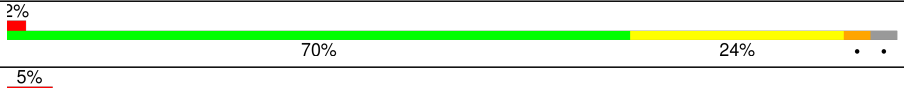
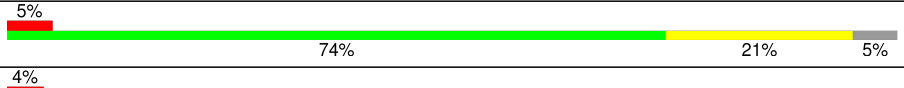
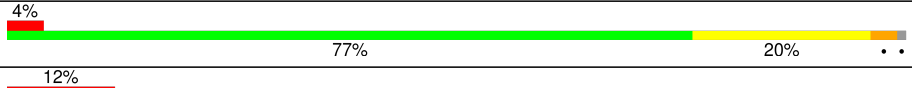
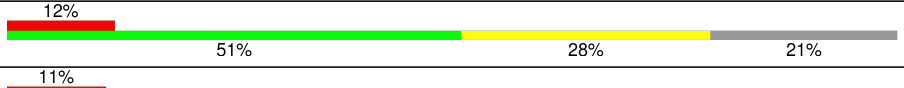
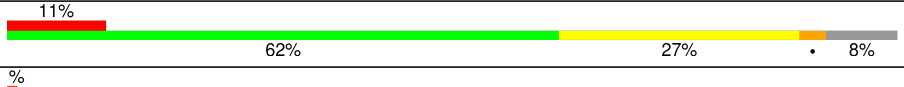
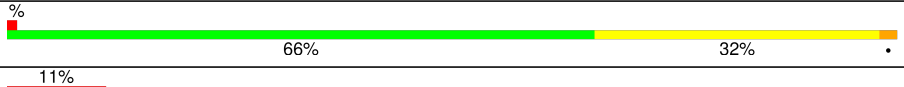
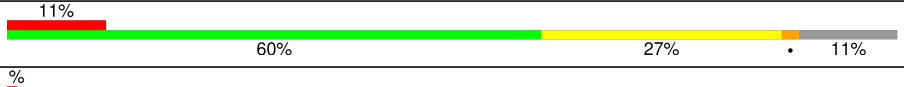
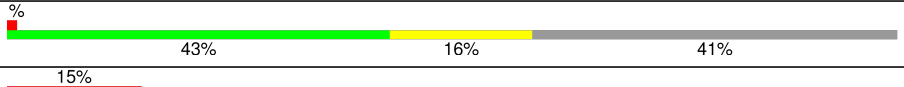
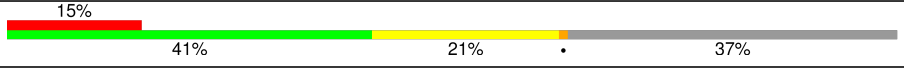
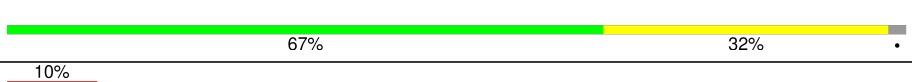
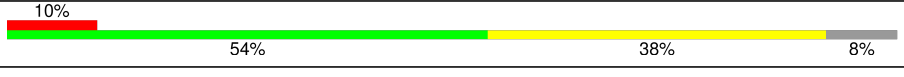

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 3340 (2.80-2.72) |
| Clashscore | 102246 | 3829 (2.80-2.72) |
| Ramachandran outliers | 100387 | 3767 (2.80-2.72) |
| Sidechain outliers | 100360 | 3770 (2.80-2.72) |
| RSRZ outliers | 91569 | 3352 (2.80-2.72) |
| RNA backbone | 2183 | 1006 (3.14-2.38) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 12% 65% 30% |
| 2 | B | 338 | 5% 62% 34% |
| 3 | C | 246 | 2% 67% 30% |
| 4 | D | 177 | 33% 41% 37% 21% |

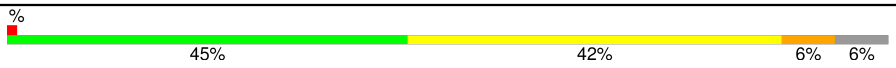
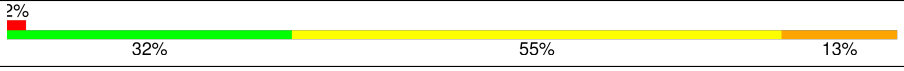
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | E | 178 |   |
| 6 | F | 120 |   |
| 7 | G | 348 |   |
| 8 | H | 177 |   |
| 9 | I | 162 |   |
| 10 | J | 145 |   |
| 11 | K | 132 |   |
| 12 | L | 165 |   |
| 13 | M | 196 |   |
| 14 | N | 187 |   |
| 15 | O | 116 |   |
| 16 | P | 149 |   |
| 17 | Q | 96 |   |
| 18 | R | 155 |   |
| 19 | S | 85 |   |
| 20 | T | 120 |   |
| 21 | U | 67 |   |
| 22 | V | 71 |   |
| 23 | W | 154 |   |
| 24 | X | 92 |   |
| 25 | Y | 241 |   |
| 26 | Z | 116 |   |
| 27 | 1 | 57 |   |
| 28 | 2 | 50 |   |
| 29 | 3 | 92 |   |

*Continued on next page...*

*Continued from previous page...*

| 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 |
|---|---|---|---|---|---|---|---|
| 32 | MG | 0 | 8008 | - | - | - | X |
| 32 | MG | 0 | 8015 | - | - | - | X |
| 32 | MG | 0 | 8062 | - | - | - | X |
| 32 | MG | 0 | 8075 | - | - | - | X |
| 32 | MG | 0 | 8079 | - | - | - | X |
| 32 | MG | A | 8051 | - | - | - | X |
| 33 | K | 0 | 8401 | - | - | - | X |
| 34 | NA | 0 | 8504 | - | - | - | X |
| 34 | NA | 0 | 8507 | - | - | - | X |
| 34 | NA | 0 | 8511 | - | - | - | X |
| 34 | NA | 0 | 8512 | - | - | - | X |
| 34 | NA | 0 | 8517 | - | - | - | X |
| 34 | NA | 0 | 8519 | - | - | - | X |
| 34 | NA | 0 | 8521 | - | - | - | X |
| 34 | NA | 0 | 8522 | - | - | - | X |
| 34 | NA | 0 | 8523 | - | - | - | X |
| 34 | NA | 0 | 8528 | - | - | - | X |
| 34 | NA | 0 | 8530 | - | - | - | X |
| 34 | NA | 0 | 8533 | - | - | - | X |
| 34 | NA | 0 | 8534 | - | - | - | X |
| 34 | NA | 0 | 8546 | - | - | - | X |
| 34 | NA | 0 | 8547 | - | - | - | X |
| 34 | NA | 0 | 8553 | - | - | - | X |
| 34 | NA | 0 | 8555 | - | - | - | X |
| 34 | NA | 0 | 8556 | - | - | - | X |
| 34 | NA | 0 | 8559 | - | - | - | X |
| 34 | NA | 0 | 8560 | - | - | - | X |
| 34 | NA | 0 | 8562 | - | - | - | X |
| 34 | NA | 0 | 8563 | - | - | - | X |
| 34 | NA | 0 | 8564 | - | - | - | X |
| 34 | NA | 0 | 8565 | - | - | - | X |
| 34 | NA | 0 | 8569 | - | - | - | X |
| 34 | NA | 0 | 8575 | - | - | - | X |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 34 | NA | Q | 8540 | - | - | - | X |
| 35 | CL | J | 8801 | - | - | X | - |
| 35 | CL | J | 8802 | - | - | X | - |
| 36 | SR | 0 | 8972 | - | - | - | X |
| 36 | SR | 0 | 8985 | - | - | - | X |
| 36 | SR | A | 8929 | - | - | - | X |
| 36 | SR | B | 8987 | - | - | - | X |

# 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99124 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 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1753 | 1072 | 352 | 324 | 5 | | | |

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

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

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

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

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

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

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

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

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

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

- 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 |
| | | | 59022 | 26350 | 10876 | 19051 | 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 | 0 | 86 | Total | Mg | 0 | 0 |
| | | | 86 | 86 | | |
| 32 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | A | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 32 | T | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 9 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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

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

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

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 34 | 0 | 67 | Total Na<br>67 67 | 0 | 0 |
| 34 | J | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | Q | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | C | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | R | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | 9 | 2 | Total Na<br>2 2 | 0 | 0 |
| 34 | S | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | M | 1 | Total Na<br>1 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 35 | 0 | 10 | Total Cl<br>10 10 | 0 | 0 |
| 35 | J | 3 | Total Cl<br>3 3 | 0 | 0 |
| 35 | Q | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | B | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | A | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | N | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | O | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | R | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | L | 1 | Total Cl<br>1 1 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 35 | 3 | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | M | 1 | Total Cl<br>1 1 | 0 | 0 |

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 36 | 0 | 92 | Total Sr<br>92 92 | 0 | 0 |
| 36 | 1 | 2 | Total Sr<br>2 2 | 0 | 0 |
| 36 | B | 2 | Total Sr<br>2 2 | 0 | 0 |
| 36 | 3 | 2 | Total Sr<br>2 2 | 0 | 0 |
| 36 | A | 3 | Total Sr<br>3 3 | 0 | 0 |
| 36 | R | 1 | Total Sr<br>1 1 | 0 | 0 |
| 36 | 9 | 4 | Total Sr<br>4 4 | 0 | 0 |
| 36 | S | 1 | Total Sr<br>1 1 | 0 | 0 |
| 36 | F | 1 | Total Sr<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 |
| 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 |
| 37 | U | 1 | Total Cd<br>1 1 | 0 | 0 |

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 38 | 0 | 5927 | Total O<br>5927 5927 | 0 | 0 |
| 38 | 9 | 144 | Total O<br>144 144 | 0 | 0 |
| 38 | A | 118 | Total O<br>118 118 | 0 | 0 |
| 38 | B | 144 | Total O<br>144 144 | 0 | 0 |
| 38 | C | 179 | Total O<br>179 179 | 0 | 0 |
| 38 | D | 46 | Total O<br>46 46 | 0 | 0 |
| 38 | E | 40 | Total O<br>40 40 | 0 | 0 |
| 38 | F | 27 | Total O<br>27 27 | 0 | 0 |
| 38 | G | 19 | Total O<br>19 19 | 0 | 0 |
| 38 | H | 68 | Total O<br>68 68 | 0 | 0 |
| 38 | I | 5 | Total O<br>5 5 | 0 | 0 |
| 38 | J | 55 | Total O<br>55 55 | 0 | 0 |
| 38 | K | 52 | Total O<br>52 52 | 0 | 0 |
| 38 | L | 84 | Total O<br>84 84 | 0 | 0 |
| 38 | M | 127 | Total O<br>127 127 | 0 | 0 |
| 38 | N | 63 | Total O<br>63 63 | 0 | 0 |
| 38 | O | 40 | Total O<br>40 40 | 0 | 0 |
| 38 | P | 61 | Total O<br>61 61 | 0 | 0 |
| 38 | Q | 43 | Total O<br>43 43 | 0 | 0 |
| 38 | R | 84 | Total O<br>84 84 | 0 | 0 |
| 38 | S | 33 | Total O<br>33 33 | 0 | 0 |
| 38 | T | 33 | Total O<br>33 33 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

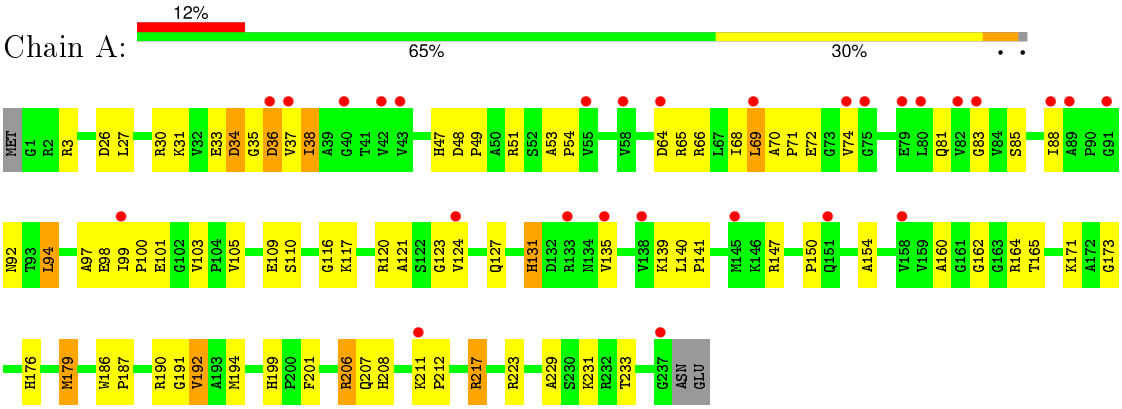
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 38 | U | 28 | Total O<br>28 28 | 0 | 0 |
| 38 | V | 14 | Total O<br>14 14 | 0 | 0 |
| 38 | W | 67 | Total O<br>67 67 | 0 | 0 |
| 38 | X | 30 | Total O<br>30 30 | 0 | 0 |
| 38 | Y | 100 | Total O<br>100 100 | 0 | 0 |
| 38 | Z | 32 | Total O<br>32 32 | 0 | 0 |
| 38 | 1 | 55 | Total O<br>55 55 | 0 | 0 |
| 38 | 2 | 42 | Total O<br>42 42 | 0 | 0 |
| 38 | 3 | 63 | Total O<br>63 63 | 0 | 0 |

# 3 Residue-property plots (i)

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

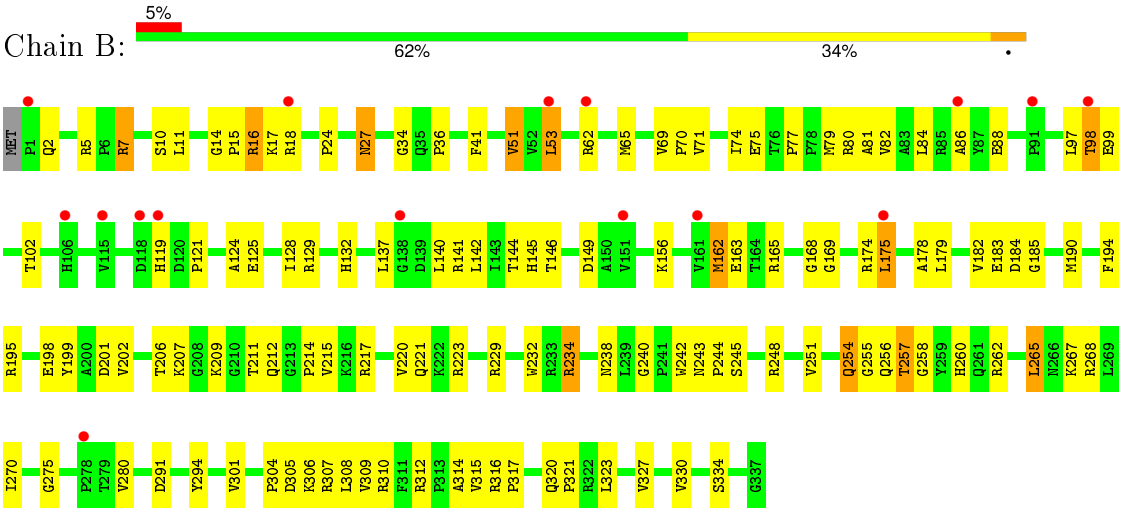
- Molecule 1: 50S ribosomal protein L2P

Chain A:



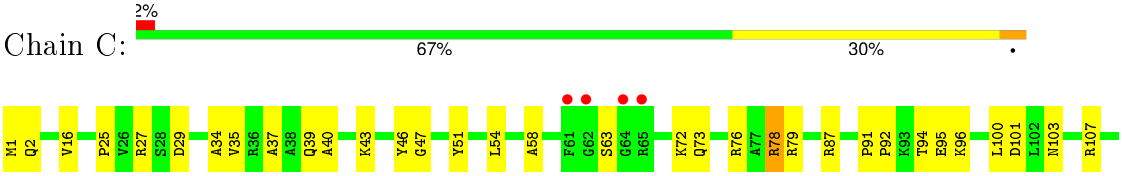

- Molecule 2: 50S ribosomal protein L3P

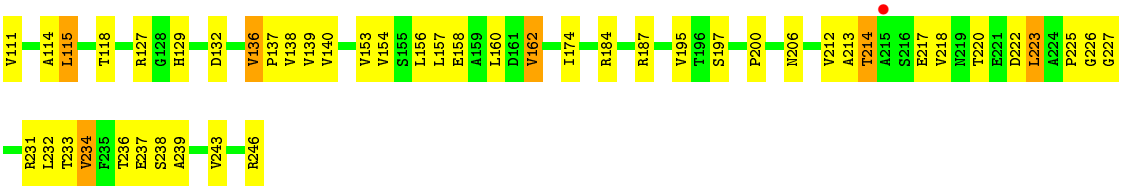
Chain B:



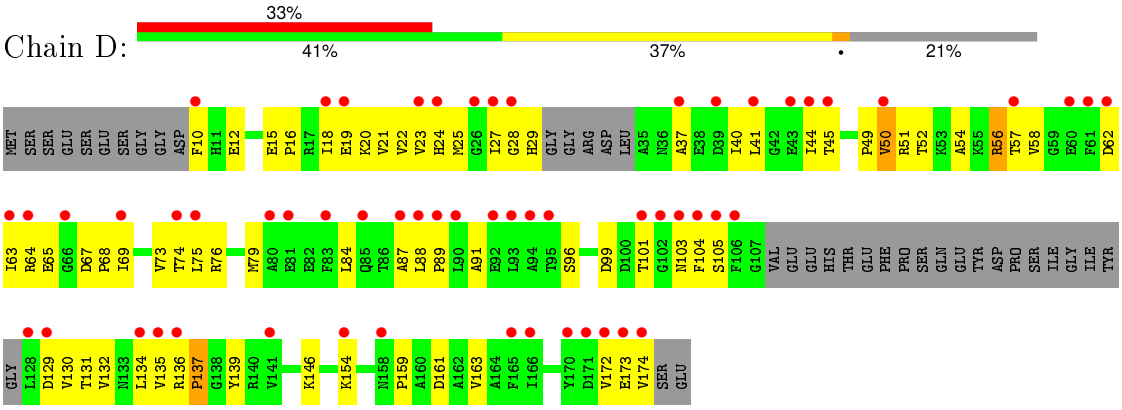

- Molecule 3: 50S ribosomal protein L4P

Chain C:

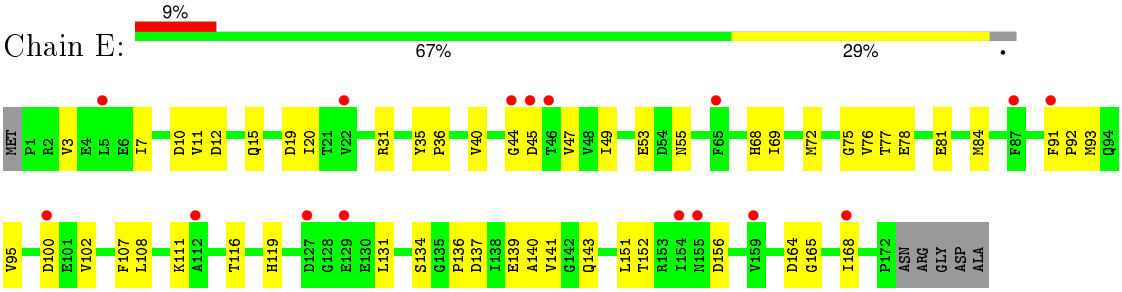




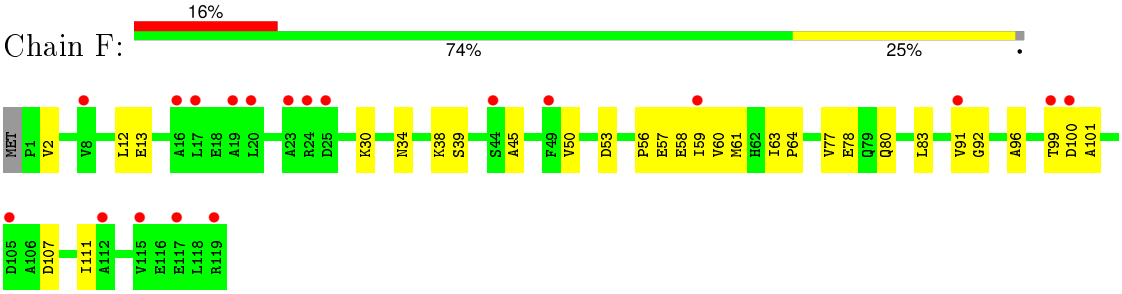

- Molecule 4: 50S ribosomal protein L5P



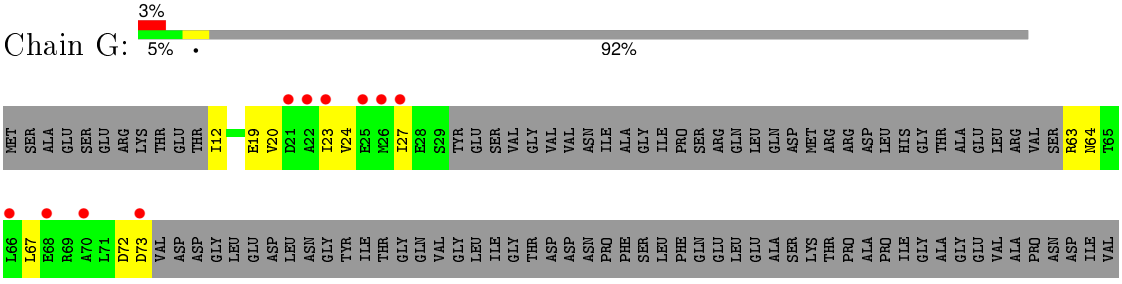

- Molecule 5: 50S ribosomal protein L6P

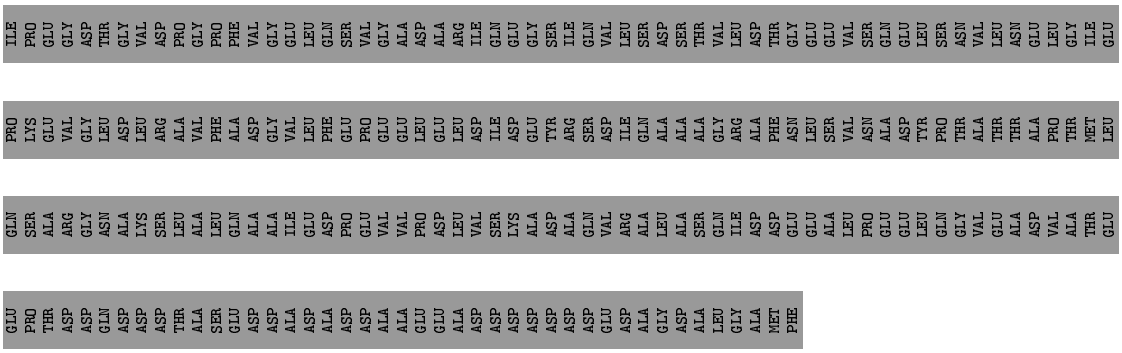



- Molecule 6: 50S ribosomal protein L7Ae



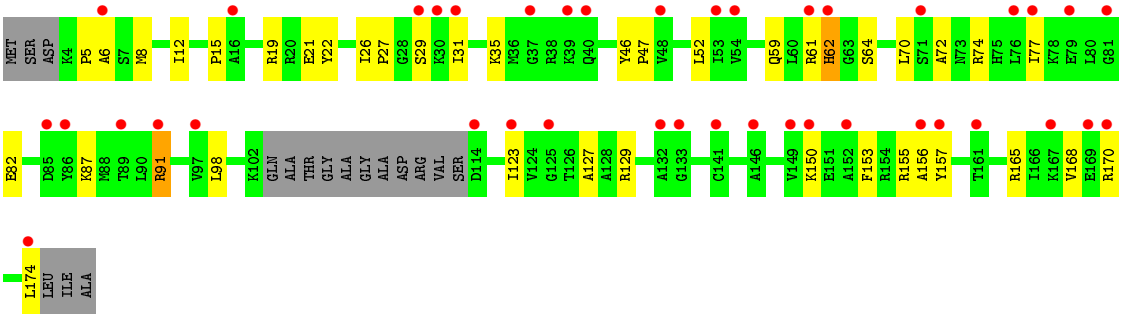

- Molecule 7: 50S ribosomal protein L10E





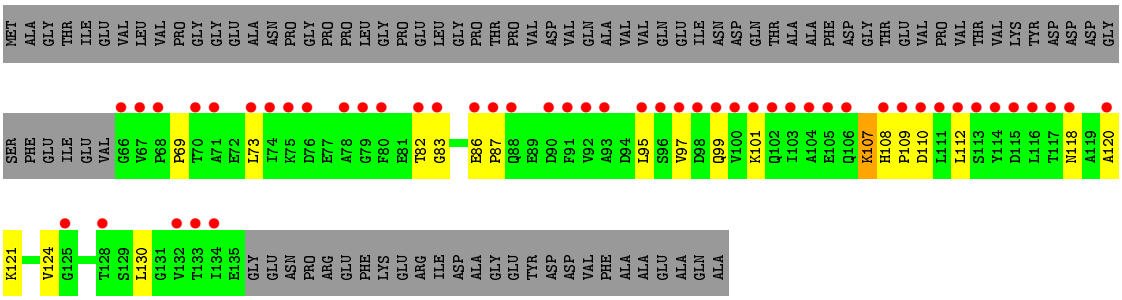
• Molecule 8: 50S ribosomal protein L10e

Chain H:

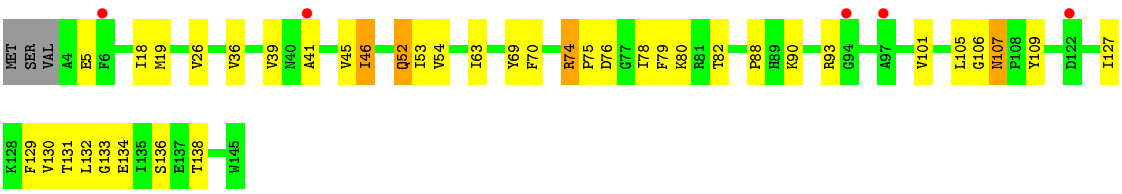
• Molecule 9: 50S ribosomal protein L11P

Chain I:

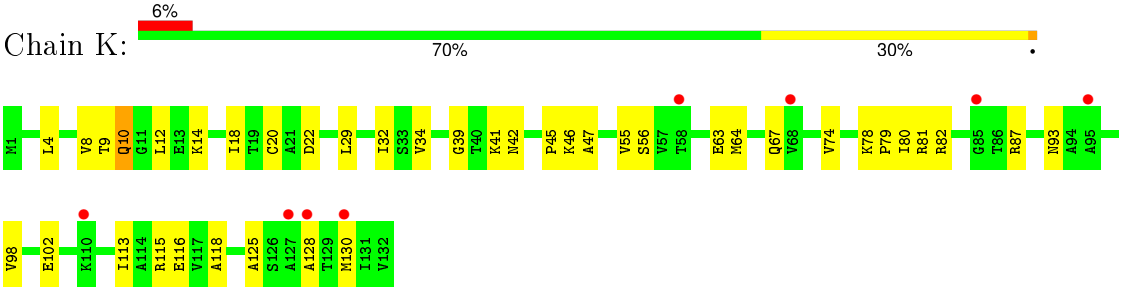
• Molecule 10: 50S ribosomal protein L13P

Chain J:

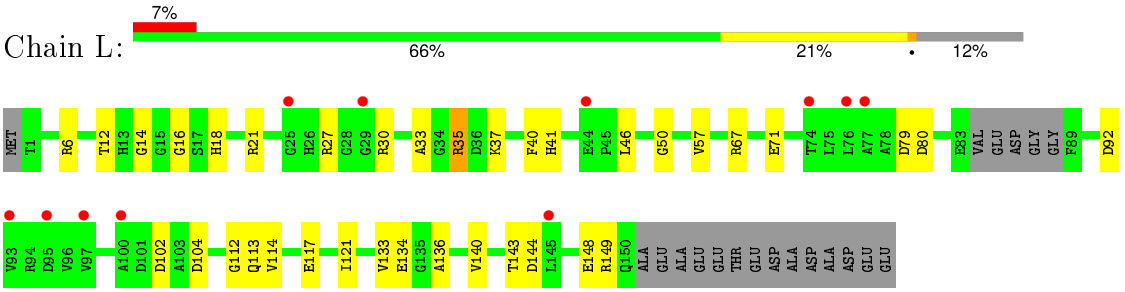
• Molecule 11: 50S ribosomal protein L14P

Chain K:



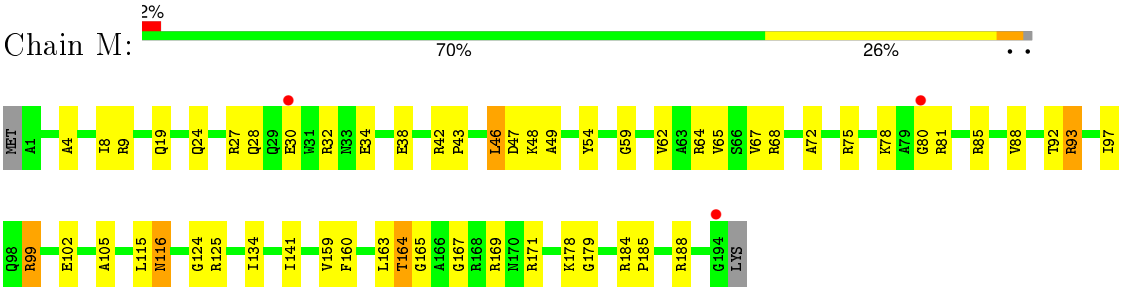

• Molecule 12: 50S ribosomal protein L15P

Chain L:



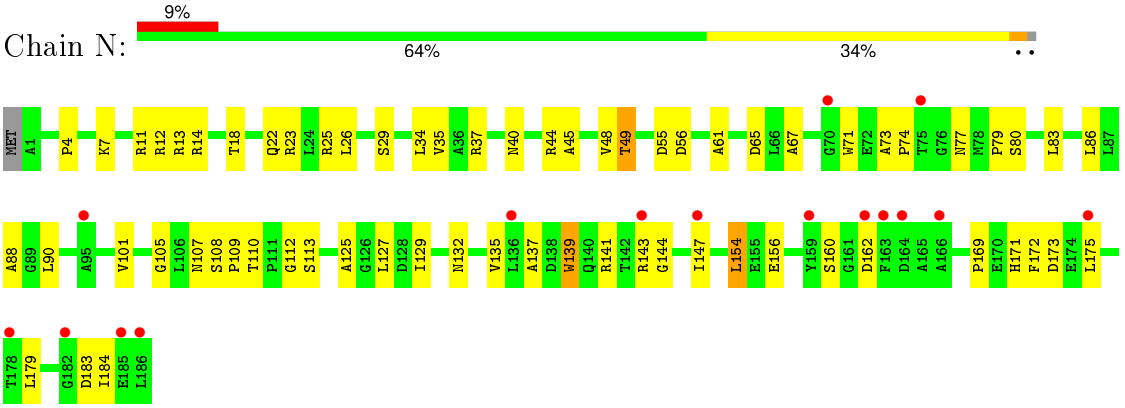

• Molecule 13: 50S ribosomal protein L15e

Chain M:



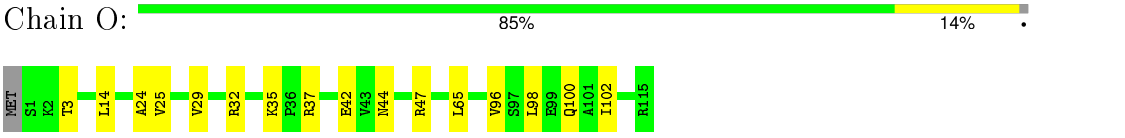

• Molecule 14: 50S ribosomal protein L18P

Chain N:



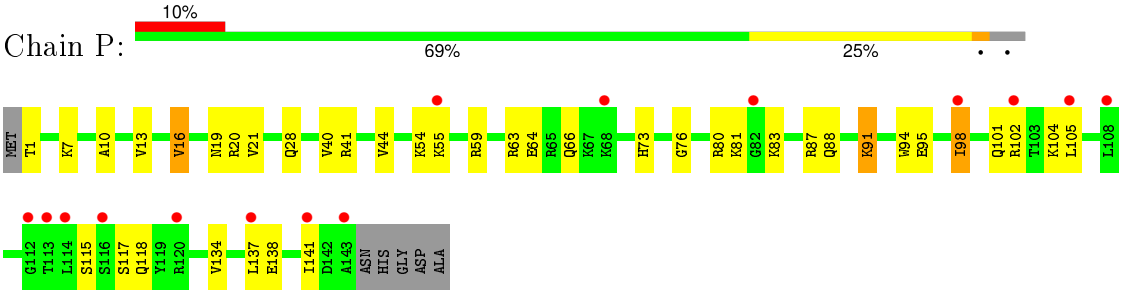

• Molecule 15: 50S ribosomal protein L18e

Chain O:



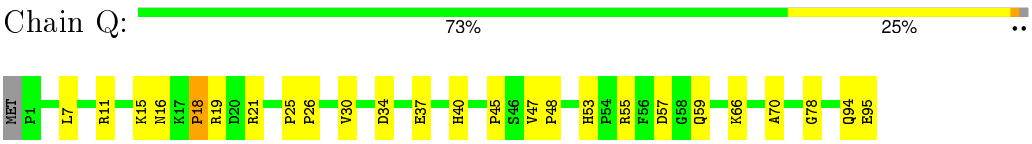
• Molecule 16: 50S ribosomal protein L19e

Chain P:



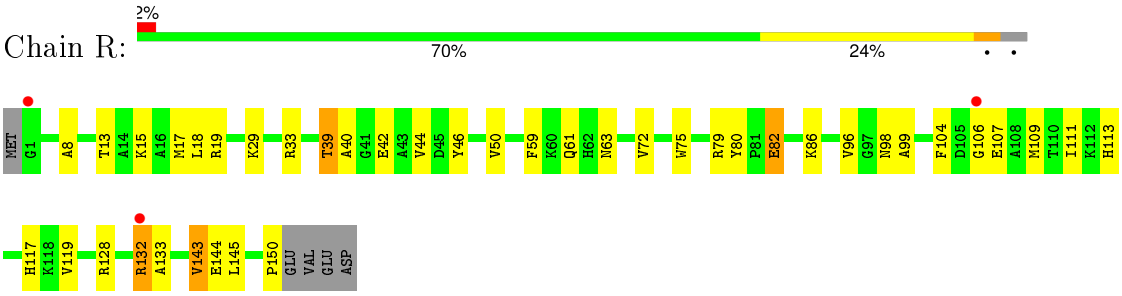

• Molecule 17: 50S ribosomal protein L21e

Chain Q:



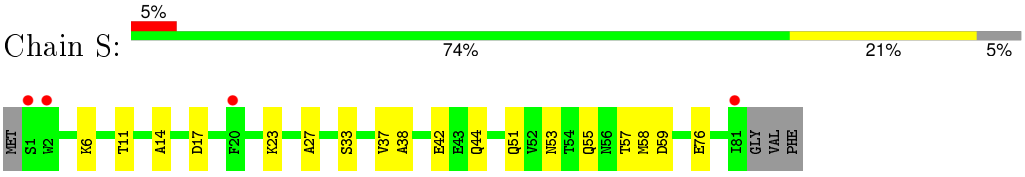

• Molecule 18: 50S ribosomal protein L22P

Chain R:



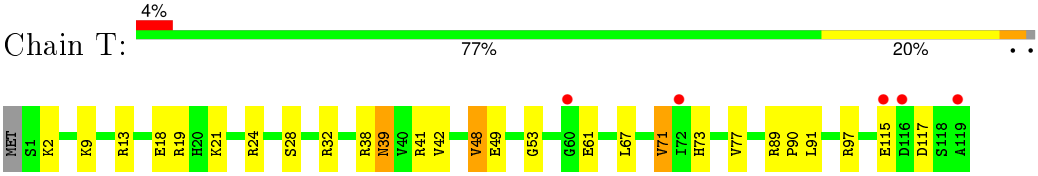

• Molecule 19: 50S ribosomal protein L23P

Chain S:



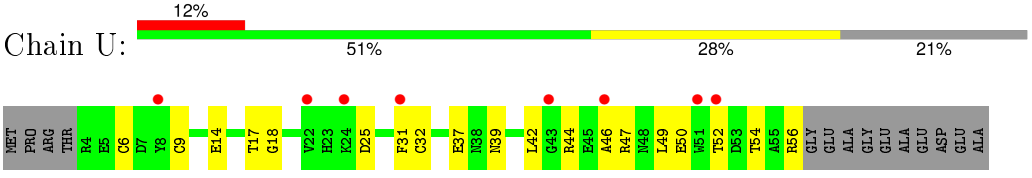

• Molecule 20: 50S ribosomal protein L24P

Chain T:



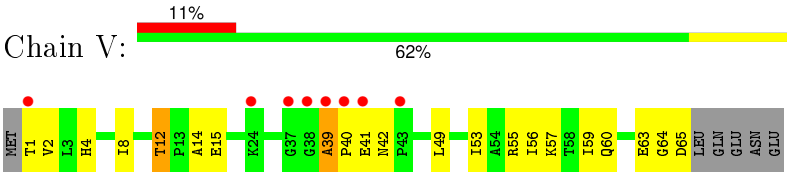

• Molecule 21: 50S ribosomal protein L24e

Chain U:



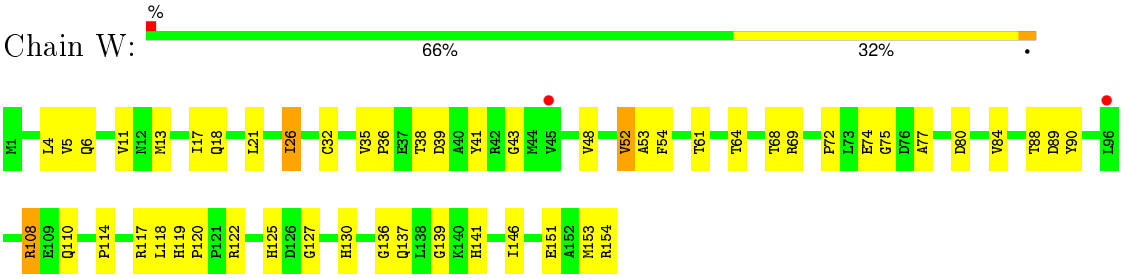

• Molecule 22: 50S ribosomal protein L29P

Chain V:



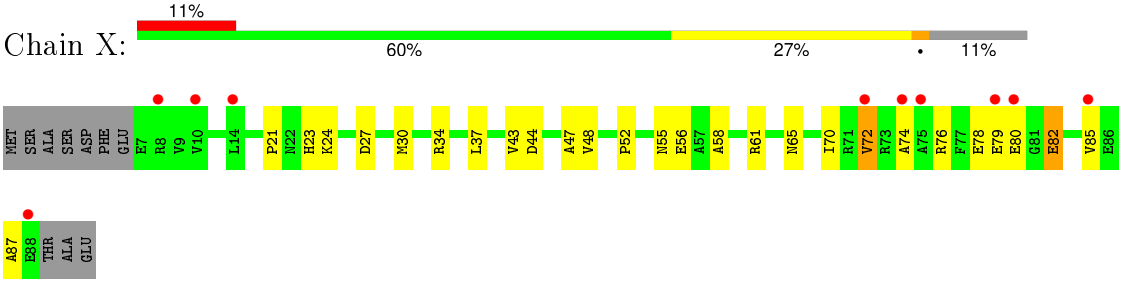

• Molecule 23: 50S ribosomal protein L30P

Chain W:



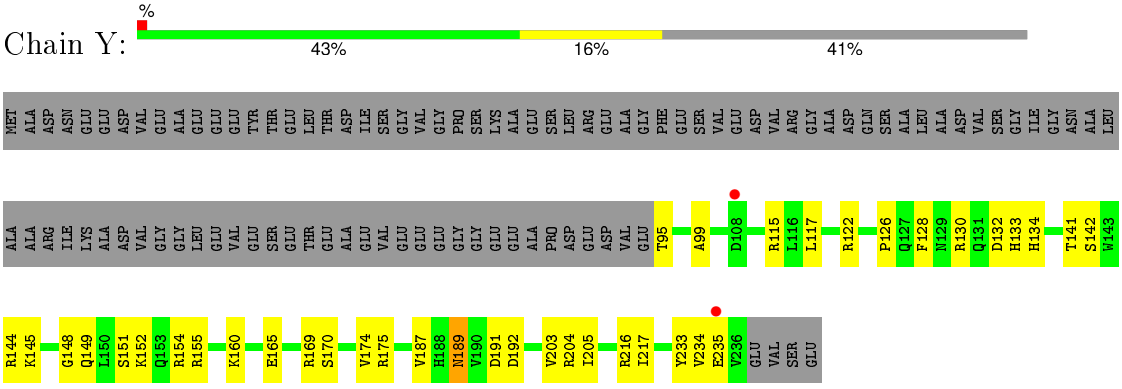

• Molecule 24: 50S ribosomal protein L31e

Chain X:



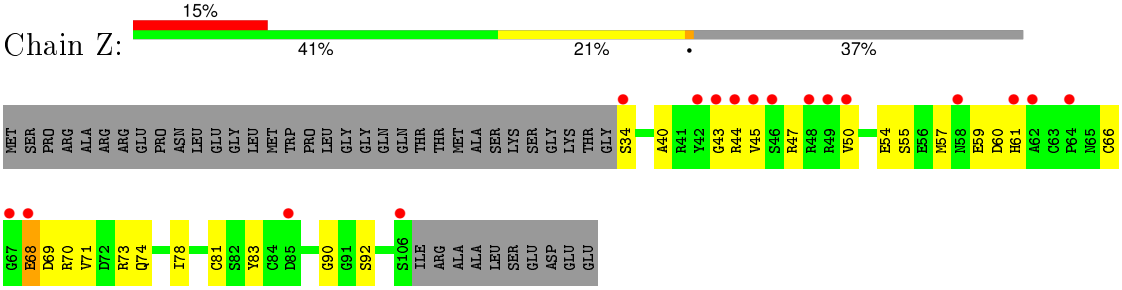

• Molecule 25: 50S ribosomal protein L32e

Chain Y:



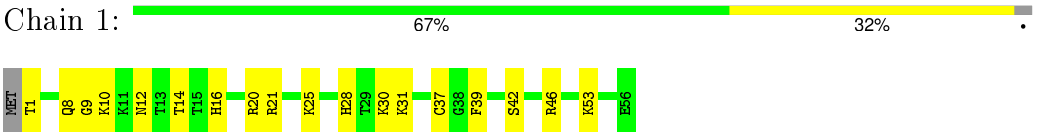

• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



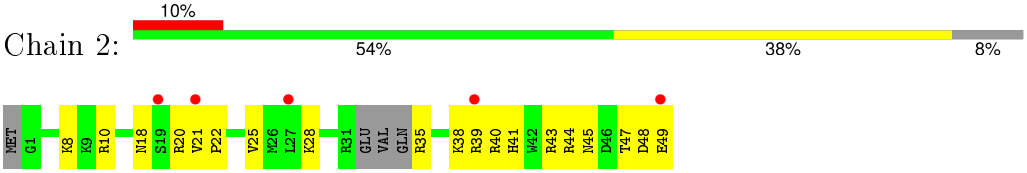

• Molecule 27: 50S ribosomal protein L37e

Chain 1:



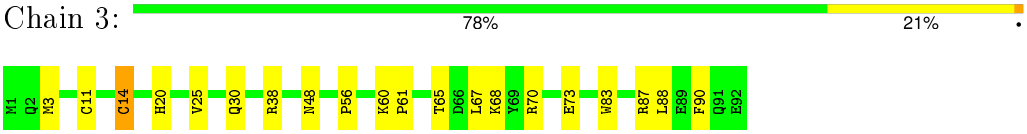

• Molecule 28: 50S ribosomal protein L39e

Chain 2:



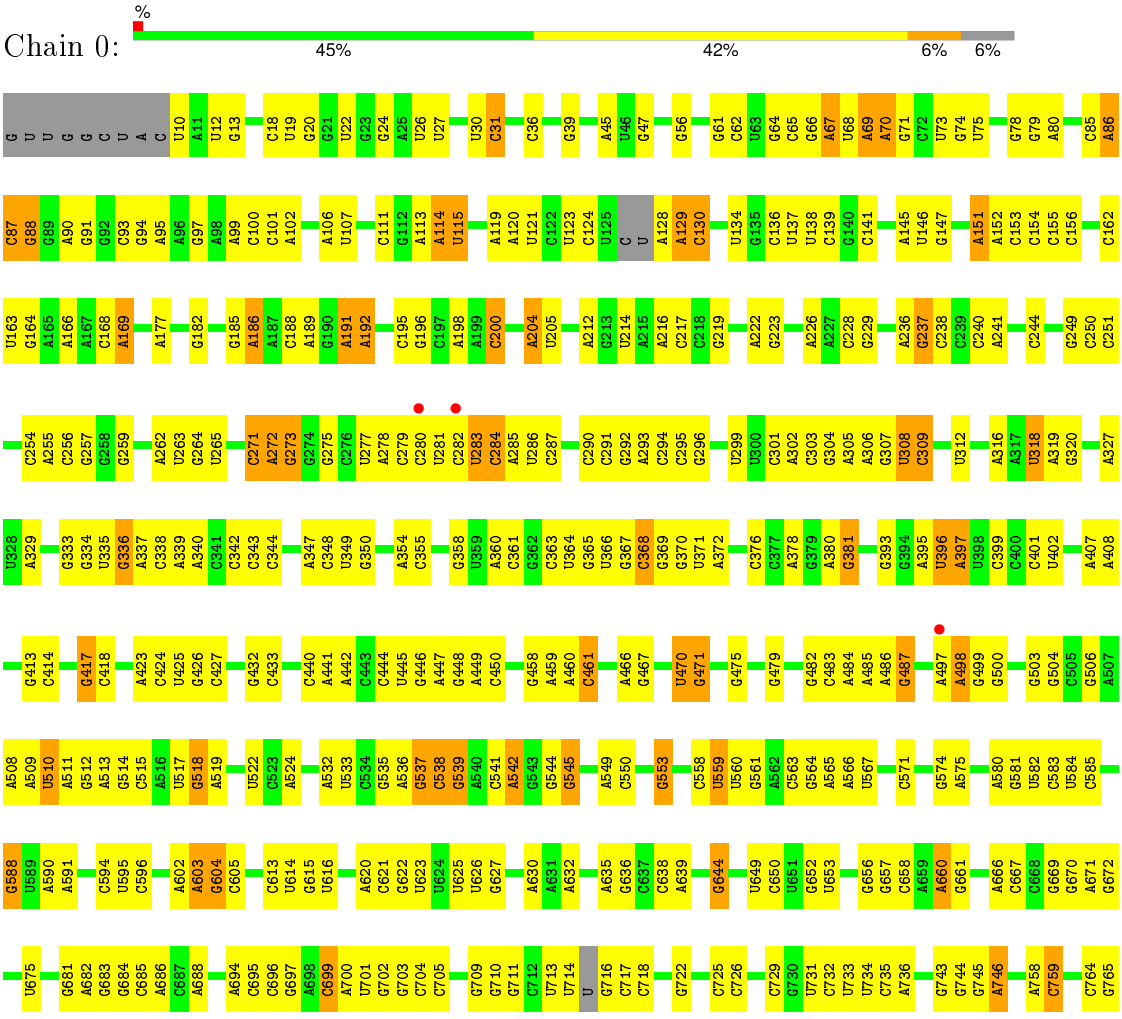

• Molecule 29: 50S ribosomal protein L44E

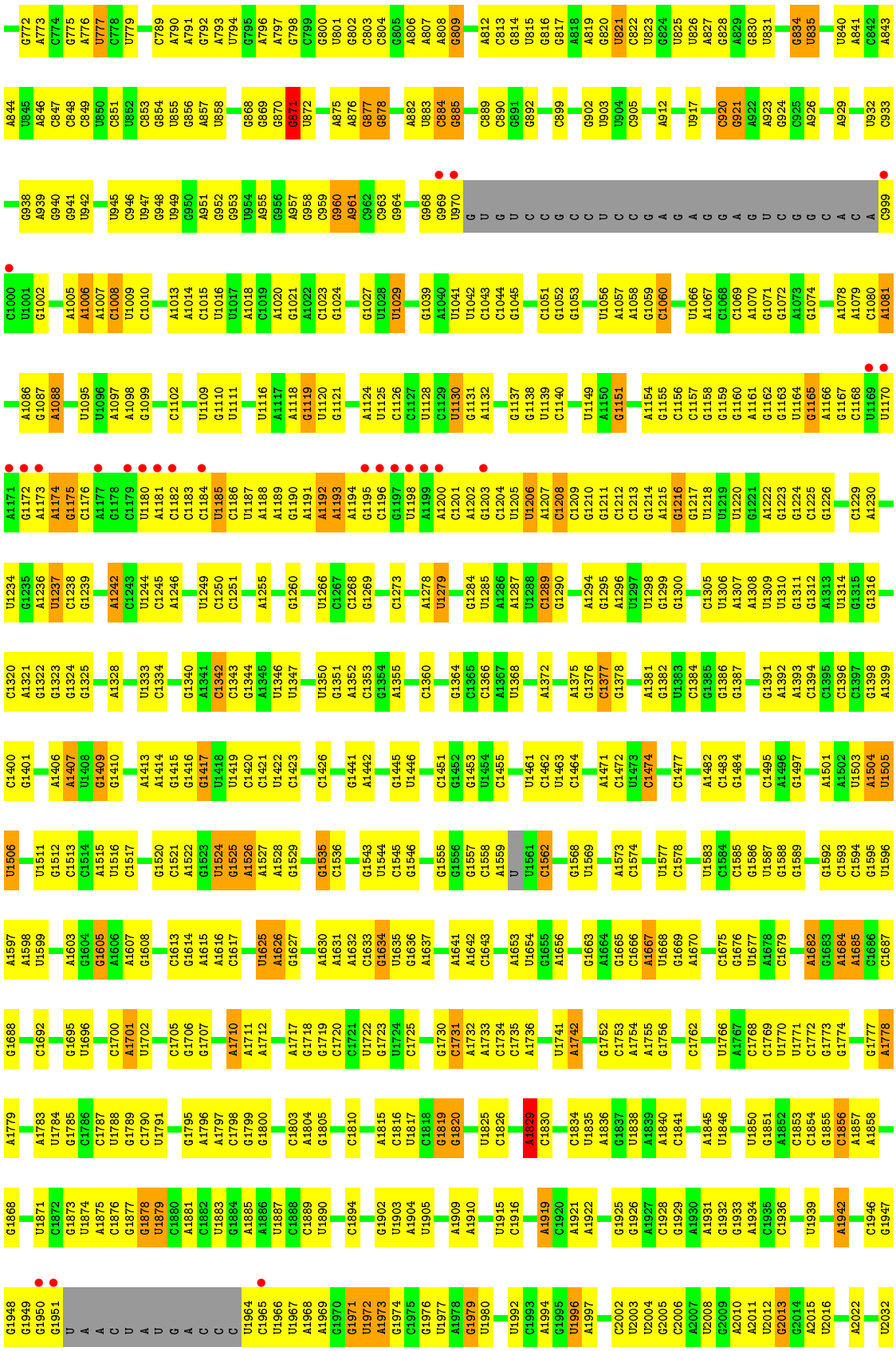
Chain 3:

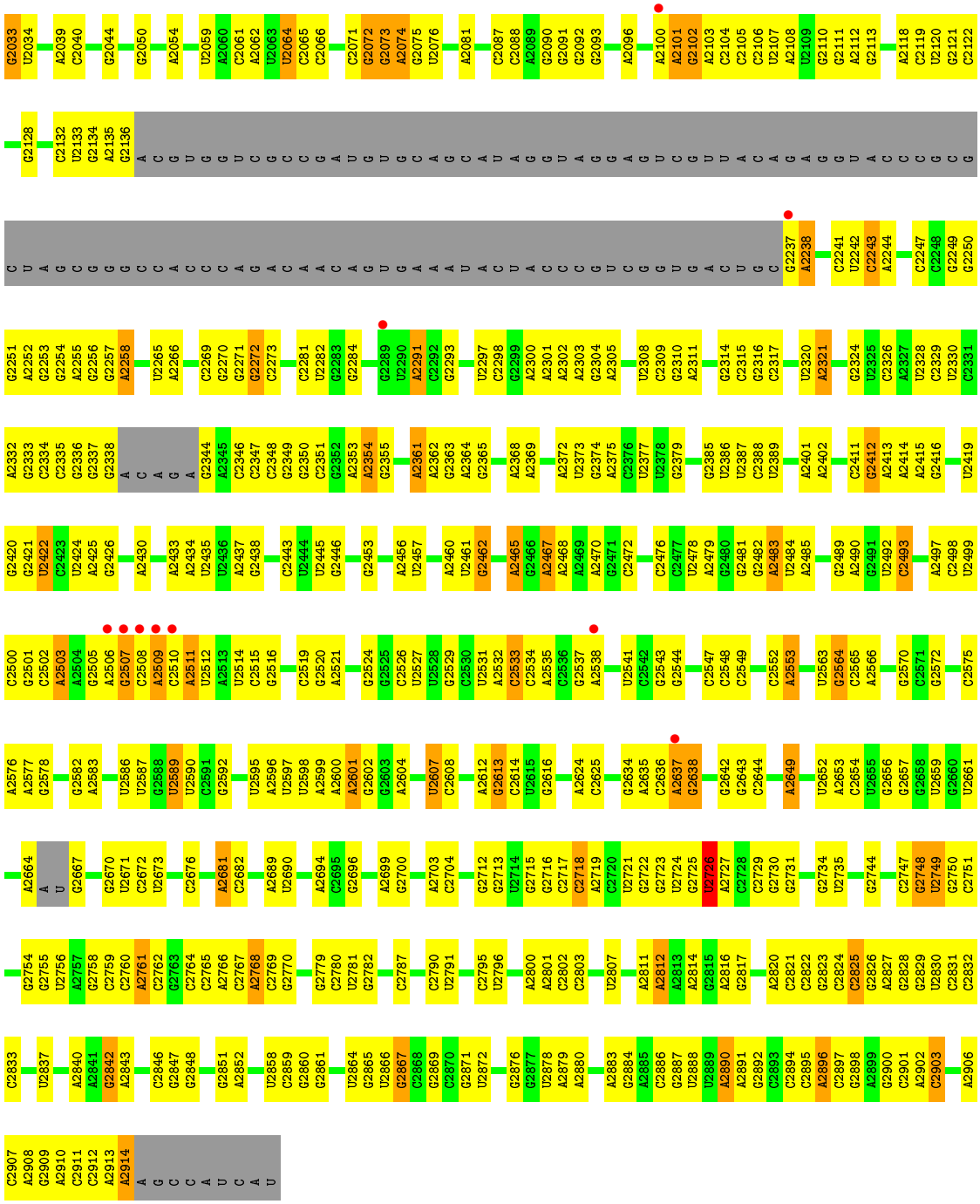



• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

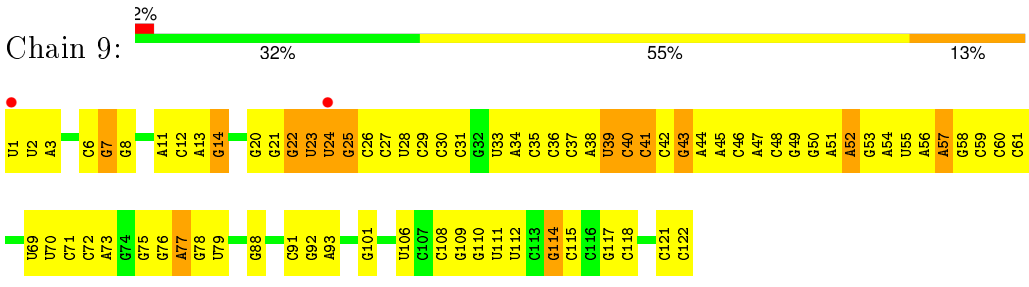






• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 212.83Å 299.90Å 576.01Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.33 – 2.75<br>85.81 – 2.41 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 81.3 (49.33-2.75)<br>81.1 (85.81-2.41) | Depositor<br>EDS |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.00 (at 2.40Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, $R_{free}$ | 0.183 , 0.232<br>0.312 , 0.317 | Depositor<br>DCC |
| $R_{free}$ test set | 2536 reflections (0.67%) | DCC |
| Wilson B-factor (Å$^2$) | 45.6 | Xtriage |
| Anisotropy | 0.228 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 78.9 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Outliers | 0 of 667164 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.83 | EDS |
| Total number of atoms | 99124 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 52.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.34 | 0/1786 | 0.65 | 0/2408 |
| 2 | B | 0.33 | 0/2690 | 0.64 | 0/3652 |
| 3 | C | 0.36 | 0/1885 | 0.65 | 0/2552 |
| 4 | D | 0.33 | 0/1111 | 0.55 | 0/1498 |
| 5 | E | 0.33 | 0/1382 | 0.56 | 0/1880 |
| 6 | F | 0.34 | 0/901 | 0.57 | 0/1224 |
| 7 | G | 0.30 | 0/241 | 0.50 | 0/324 |
| 8 | H | 0.35 | 0/1302 | 0.61 | 0/1743 |
| 9 | I | 0.30 | 0/526 | 0.50 | 0/716 |
| 10 | J | 0.34 | 0/1136 | 0.59 | 0/1530 |
| 11 | K | 0.35 | 0/1004 | 0.66 | 0/1351 |
| 12 | L | 0.31 | 0/1130 | 0.64 | 0/1509 |
| 13 | M | 0.34 | 0/1582 | 0.63 | 0/2116 |
| 14 | N | 0.30 | 0/1474 | 0.62 | 0/1999 |
| 15 | O | 0.34 | 0/874 | 0.60 | 0/1181 |
| 16 | P | 0.32 | 0/1147 | 0.53 | 0/1528 |
| 17 | Q | 0.34 | 0/749 | 0.65 | 0/1005 |
| 18 | R | 0.35 | 0/1172 | 0.64 | 0/1578 |
| 19 | S | 0.35 | 0/648 | 0.59 | 0/875 |
| 20 | T | 0.33 | 0/958 | 0.62 | 0/1289 |
| 21 | U | 0.34 | 0/417 | 0.57 | 0/562 |
| 22 | V | 0.31 | 0/502 | 0.49 | 0/675 |
| 23 | W | 0.34 | 0/1219 | 0.61 | 0/1655 |
| 24 | X | 0.34 | 0/664 | 0.60 | 0/895 |
| 25 | Y | 0.36 | 0/1146 | 0.62 | 0/1536 |
| 26 | Z | 0.36 | 0/584 | 0.58 | 0/781 |
| 27 | 1 | 0.40 | 0/438 | 0.63 | 0/578 |
| 28 | 2 | 0.34 | 0/401 | 0.60 | 0/529 |
| 29 | 3 | 0.36 | 0/771 | 0.59 | 0/1024 |
| 30 | 0 | 0.37 | 0/65960 | 0.68 | 6/102872 (0.0%) |
| 31 | 9 | 0.32 | 0/2904 | 0.67 | 1/4526 (0.0%) |
| All | All | 0.36 | 0/98704 | 0.66 | 7/147591 (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 |
|---|---|---|---|
| 23 | W | 0 | 1 |
| 30 | 0 | 0 | 26 |
| All | All | 0 | 27 |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 0 | 1819 | G | C5'-C4'-C3' | 6.12 | 125.79 | 116.00 |
| 30 | 0 | 871 | G | C5'-C4'-O4' | -6.04 | 101.86 | 109.10 |
| 30 | 0 | 1504 | A | C1'-O4'-C4' | -5.84 | 105.22 | 109.90 |
| 30 | 0 | 1504 | A | N9-C1'-C2' | 5.53 | 121.18 | 114.00 |
| 30 | 0 | 841 | A | C1'-O4'-C4' | -5.34 | 105.63 | 109.90 |
| 30 | 0 | 2726 | U | N1-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 31 | 9 | 39 | U | N1-C1'-C2' | 5.25 | 120.82 | 114.00 |

There are no chirality outliers.

All (27) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 30 | 0 | 1039 | G | Sidechain |
| 30 | 0 | 1078 | A | Sidechain |
| 30 | 0 | 1340 | G | Sidechain |
| 30 | 0 | 1417 | G | Sidechain |
| 30 | 0 | 1445 | G | Sidechain |
| 30 | 0 | 1653 | A | Sidechain |
| 30 | 0 | 1777 | G | Sidechain |
| 30 | 0 | 1829 | A | Sidechain |
| 30 | 0 | 1877 | G | Sidechain |
| 30 | 0 | 1878 | G | Sidechain |
| 30 | 0 | 1972 | U | Sidechain |
| 30 | 0 | 2076 | U | Sidechain |
| 30 | 0 | 22 | U | Sidechain |
| 30 | 0 | 2412 | G | Sidechain |
| 30 | 0 | 2465 | A | Sidechain |
| 30 | 0 | 2493 | C | Sidechain |
| 30 | 0 | 2503 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 30 | 0 | 2552 | C | Sidechain |
| 30 | 0 | 26 | U | Sidechain |
| 30 | 0 | 2607 | U | Sidechain |
| 30 | 0 | 2842 | G | Sidechain |
| 30 | 0 | 396 | U | Sidechain |
| 30 | 0 | 458 | G | Sidechain |
| 30 | 0 | 470 | U | Sidechain |
| 30 | 0 | 471 | G | Sidechain |
| 30 | 0 | 518 | G | 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 | 80 | 0 |
| 2 | B | 2625 | 0 | 2533 | 110 | 0 |
| 3 | C | 1860 | 0 | 1813 | 73 | 0 |
| 4 | D | 1094 | 0 | 1085 | 56 | 0 |
| 5 | E | 1357 | 0 | 1266 | 42 | 0 |
| 6 | F | 890 | 0 | 843 | 23 | 0 |
| 7 | G | 240 | 0 | 231 | 7 | 0 |
| 8 | H | 1282 | 0 | 1292 | 33 | 0 |
| 9 | I | 519 | 0 | 500 | 24 | 0 |
| 10 | J | 1120 | 0 | 1098 | 36 | 0 |
| 11 | K | 994 | 0 | 1027 | 37 | 0 |
| 12 | L | 1118 | 0 | 1076 | 30 | 0 |
| 13 | M | 1558 | 0 | 1573 | 48 | 0 |
| 14 | N | 1445 | 0 | 1401 | 61 | 0 |
| 15 | O | 865 | 0 | 873 | 22 | 0 |
| 16 | P | 1136 | 0 | 1123 | 36 | 0 |
| 17 | Q | 735 | 0 | 729 | 20 | 0 |
| 18 | R | 1149 | 0 | 1122 | 33 | 0 |
| 19 | S | 641 | 0 | 605 | 13 | 0 |
| 20 | T | 950 | 0 | 924 | 21 | 0 |
| 21 | U | 410 | 0 | 364 | 16 | 0 |
| 22 | V | 499 | 0 | 511 | 16 | 0 |
| 23 | W | 1196 | 0 | 1137 | 58 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 24 | X | 654 | 0 | 653 | 21 | 0 |
| 25 | Y | 1130 | 0 | 1133 | 41 | 0 |
| 26 | Z | 573 | 0 | 531 | 18 | 0 |
| 27 | 1 | 431 | 0 | 426 | 25 | 0 |
| 28 | 2 | 396 | 0 | 413 | 21 | 0 |
| 29 | 3 | 755 | 0 | 729 | 15 | 0 |
| 30 | 0 | 59022 | 0 | 29809 | 1550 | 0 |
| 31 | 9 | 2599 | 0 | 1325 | 114 | 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 | 2 | 0 | 0 | 0 | 0 |
| 34 | 0 | 67 | 0 | 0 | 0 | 0 |
| 34 | 9 | 2 | 0 | 0 | 0 | 0 |
| 34 | C | 1 | 0 | 0 | 0 | 0 |
| 34 | J | 1 | 0 | 0 | 0 | 0 |
| 34 | M | 1 | 0 | 0 | 0 | 0 |
| 34 | Q | 1 | 0 | 0 | 0 | 0 |
| 34 | R | 1 | 0 | 0 | 0 | 0 |
| 34 | S | 1 | 0 | 0 | 0 | 0 |
| 35 | 0 | 10 | 0 | 0 | 1 | 0 |
| 35 | 3 | 1 | 0 | 0 | 0 | 0 |
| 35 | A | 1 | 0 | 0 | 0 | 0 |
| 35 | B | 1 | 0 | 0 | 0 | 0 |
| 35 | J | 3 | 0 | 0 | 5 | 0 |
| 35 | L | 1 | 0 | 0 | 0 | 0 |
| 35 | M | 1 | 0 | 0 | 0 | 0 |
| 35 | N | 1 | 0 | 0 | 1 | 0 |
| 35 | O | 1 | 0 | 0 | 0 | 0 |
| 35 | Q | 1 | 0 | 0 | 0 | 0 |
| 35 | R | 1 | 0 | 0 | 0 | 0 |
| 36 | 0 | 92 | 0 | 0 | 0 | 0 |
| 36 | 1 | 2 | 0 | 0 | 0 | 0 |
| 36 | 3 | 2 | 0 | 0 | 0 | 0 |
| 36 | 9 | 4 | 0 | 0 | 0 | 0 |
| 36 | A | 3 | 0 | 0 | 0 | 0 |
| 36 | B | 2 | 0 | 0 | 0 | 0 |
| 36 | F | 1 | 0 | 0 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 36 | R | 1 | 0 | 0 | 0 | 0 |
| 36 | S | 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 | 5927 | 0 | 0 | 235 | 0 |
| 38 | 1 | 55 | 0 | 0 | 3 | 0 |
| 38 | 2 | 42 | 0 | 0 | 3 | 0 |
| 38 | 3 | 63 | 0 | 0 | 3 | 0 |
| 38 | 9 | 144 | 0 | 0 | 10 | 0 |
| 38 | A | 118 | 0 | 0 | 7 | 0 |
| 38 | B | 144 | 0 | 0 | 11 | 0 |
| 38 | C | 179 | 0 | 0 | 19 | 0 |
| 38 | D | 46 | 0 | 0 | 4 | 0 |
| 38 | E | 40 | 0 | 0 | 2 | 0 |
| 38 | F | 27 | 0 | 0 | 1 | 0 |
| 38 | G | 19 | 0 | 0 | 0 | 0 |
| 38 | H | 68 | 0 | 0 | 5 | 0 |
| 38 | I | 5 | 0 | 0 | 1 | 0 |
| 38 | J | 55 | 0 | 0 | 2 | 0 |
| 38 | K | 52 | 0 | 0 | 2 | 0 |
| 38 | L | 84 | 0 | 0 | 10 | 0 |
| 38 | M | 127 | 0 | 0 | 5 | 0 |
| 38 | N | 63 | 0 | 0 | 4 | 0 |
| 38 | O | 40 | 0 | 0 | 2 | 0 |
| 38 | P | 61 | 0 | 0 | 1 | 0 |
| 38 | Q | 43 | 0 | 0 | 1 | 0 |
| 38 | R | 84 | 0 | 0 | 5 | 0 |
| 38 | S | 33 | 0 | 0 | 2 | 0 |
| 38 | T | 33 | 0 | 0 | 2 | 0 |
| 38 | U | 28 | 0 | 0 | 2 | 0 |
| 38 | V | 14 | 0 | 0 | 1 | 0 |
| 38 | W | 67 | 0 | 0 | 5 | 0 |
| 38 | X | 30 | 0 | 0 | 0 | 0 |
| 38 | Y | 100 | 0 | 0 | 10 | 0 |
| 38 | Z | 32 | 0 | 0 | 0 | 0 |
| All | All | 99124 | 0 | 59911 | 2446 | 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 16.

All (2446) 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) |
|---|---|---|---|
| 14:N:37:ARG:NH1 | 31:9:6:C:H5" | 1.60 | 1.15 |
| 30:0:1160:G:C5' | 30:0:1161:A:H5' | 1.78 | 1.11 |
| 13:M:171:ARG:HD3 | 30:0:156:C:H5" | 1.32 | 1.11 |
| 30:0:871:G:H8 | 30:0:871:G:H5' | 1.12 | 1.11 |
| 30:0:871:G:C8 | 30:0:871:G:H5' | 1.84 | 1.11 |
| 30:0:2717:C:H2' | 30:0:2718:C:H5" | 1.33 | 1.10 |
| 30:0:2291:A:C8 | 30:0:2309:C:H5' | 1.87 | 1.09 |
| 30:0:1160:G:H5' | 30:0:1161:A:C5' | 1.82 | 1.08 |
| 30:0:381:G:H5" | 38:0:4322:HOH:O | 1.54 | 1.07 |
| 31:9:56:A:H2' | 31:9:57:A:H5" | 1.38 | 1.05 |
| 30:0:2502:C:H2' | 30:0:2503:A:H5' | 1.33 | 1.05 |
| 30:0:2502:C:C2' | 30:0:2503:A:H5' | 1.89 | 1.01 |
| 10:J:82:THR:HG23 | 30:0:1242:A:H5' | 1.39 | 1.01 |
| 30:0:1209:C:H2' | 30:0:1210:G:H8 | 1.19 | 1.01 |
| 31:9:76:G:H3' | 31:9:77:A:H5" | 1.39 | 1.01 |
| 30:0:282:C:H1' | 30:0:368:C:N4 | 1.77 | 1.00 |
| 30:0:2717:C:C2' | 30:0:2718:C:H5" | 1.91 | 0.99 |
| 22:V:1:THR:HB | 30:0:93:C:H5" | 1.42 | 0.99 |
| 16:P:115:SER:H | 16:P:118:GLN:HE21 | 1.08 | 0.99 |
| 30:0:2812:A:H2 | 30:0:2814:A:H62 | 1.07 | 0.98 |
| 30:0:1118:A:H3' | 30:0:1118:A:H8 | 1.28 | 0.98 |
| 30:0:1372:A:H3' | 38:0:7202:HOH:O | 1.64 | 0.98 |
| 15:O:3:THR:HG22 | 30:0:656:G:H5' | 1.45 | 0.97 |
| 30:0:1116:U:H3 | 30:0:1246:A:H62 | 1.11 | 0.96 |
| 8:H:59:GLN:HE21 | 8:H:129:ARG:HE | 1.12 | 0.95 |
| 30:0:2908:A:H2' | 30:0:2909:G:O4' | 1.66 | 0.95 |
| 30:0:545:G:H8 | 30:0:545:G:H5' | 1.30 | 0.95 |
| 30:0:542:A:H5' | 30:0:542:A:H8 | 1.32 | 0.95 |
| 30:0:1160:G:H5' | 30:0:1161:A:H5' | 0.96 | 0.94 |
| 30:0:1666:C:O2' | 30:0:1667:A:H5" | 1.67 | 0.94 |
| 11:K:10:GLN:H | 11:K:10:GLN:HE21 | 1.15 | 0.93 |
| 30:0:2769:C:C2' | 30:0:2770:G:H5' | 1.98 | 0.93 |
| 30:0:2497:A:H1' | 30:0:2526:C:N4 | 1.84 | 0.93 |
| 30:0:1603:A:H5' | 30:0:1605:G:O4' | 1.68 | 0.92 |
| 30:0:1118:A:H3' | 30:0:1118:A:C8 | 2.04 | 0.92 |
| 30:0:1701:A:H4' | 30:0:1702:U:H5" | 1.49 | 0.92 |
| 31:9:14:G:H5' | 31:9:14:G:H8 | 1.36 | 0.91 |
| 30:0:1205:U:H2' | 30:0:1206:U:H5" | 1.52 | 0.91 |
| 30:0:960:G:H3' | 30:0:960:G:N3 | 1.85 | 0.91 |
| 30:0:2812:A:H1' | 38:0:5804:HOH:O | 1.71 | 0.91 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:143:GLN:HE21 | 30:0:2780:C:H1' | 1.34 | 0.91 |
| 30:0:871:G:C5' | 30:0:871:G:H8 | 1.85 | 0.90 |
| 31:9:3:A:N6 | 31:9:22:G:H1' | 1.86 | 0.90 |
| 30:0:870:G:H2' | 30:0:871:G:H5" | 1.53 | 0.90 |
| 30:0:282:C:O2' | 30:0:283:U:H5' | 1.71 | 0.90 |
| 2:B:212:GLN:HB2 | 2:B:257:THR:HG21 | 1.54 | 0.89 |
| 30:0:1679:C:H5' | 38:0:9328:HOH:O | 1.72 | 0.89 |
| 24:X:37:LEU:HD13 | 24:X:85:VAL:HG21 | 1.55 | 0.89 |
| 30:0:182:G:H5' | 38:0:5169:HOH:O | 1.72 | 0.88 |
| 30:0:1474:C:H6 | 30:0:1474:C:H5' | 1.36 | 0.88 |
| 30:0:2524:G:N2 | 30:0:2526:C:H41 | 1.71 | 0.88 |
| 30:0:1119:G:N2 | 30:0:1246:A:C2 | 2.42 | 0.88 |
| 30:0:1666:C:H2' | 30:0:1667:A:H5' | 1.55 | 0.87 |
| 30:0:2769:C:H2' | 30:0:2770:G:H5' | 1.55 | 0.87 |
| 30:0:2508:C:H2' | 38:0:6774:HOH:O | 1.72 | 0.87 |
| 30:0:1118:A:H62 | 30:0:1244:U:H3 | 1.23 | 0.87 |
| 8:H:59:GLN:NE2 | 8:H:129:ARG:HE | 1.71 | 0.87 |
| 31:9:56:A:C2' | 31:9:57:A:H5" | 2.05 | 0.87 |
| 30:0:2506:A:HO2' | 30:0:2507:G:H8 | 1.16 | 0.87 |
| 30:0:2637:A:H5' | 38:0:9279:HOH:O | 1.74 | 0.86 |
| 30:0:1278:A:H4' | 30:0:1279:U:C4 | 2.10 | 0.86 |
| 15:O:3:THR:CG2 | 30:0:656:G:H5' | 2.05 | 0.86 |
| 30:0:1130:U:H5' | 38:0:7684:HOH:O | 1.75 | 0.86 |
| 30:0:541:C:C2' | 30:0:542:A:H5" | 2.05 | 0.86 |
| 2:B:238:ASN:HD22 | 2:B:240:GLY:H | 1.22 | 0.85 |
| 23:W:88:THR:HB | 38:W:6679:HOH:O | 1.75 | 0.85 |
| 30:0:558:C:C2' | 30:0:559:U:H5" | 2.06 | 0.85 |
| 31:9:49:G:H5" | 38:9:9088:HOH:O | 1.75 | 0.85 |
| 30:0:1116:U:HO2' | 30:0:1118:A:H2 | 0.86 | 0.85 |
| 30:0:1119:G:H22 | 30:0:1246:A:H2 | 1.19 | 0.85 |
| 30:0:2884:G:H5' | 38:0:4133:HOH:O | 1.76 | 0.84 |
| 30:0:506:G:H22 | 30:0:509:A:C5' | 1.89 | 0.84 |
| 31:9:54:A:O2' | 31:9:55:U:H5' | 1.77 | 0.84 |
| 30:0:1451:C:H5' | 30:0:1505:U:C5 | 2.12 | 0.84 |
| 23:W:137:GLN:HE21 | 23:W:141:HIS:HE1 | 1.21 | 0.84 |
| 23:W:88:THR:HG22 | 23:W:89:ASP:H | 1.41 | 0.83 |
| 30:0:2586:U:H3 | 30:0:2592:G:H22 | 1.23 | 0.83 |
| 30:0:1183:C:H2' | 38:0:6259:HOH:O | 1.77 | 0.83 |
| 30:0:558:C:O2' | 30:0:559:U:H5" | 1.79 | 0.83 |
| 30:0:877:G:H5' | 30:0:878:G:OP1 | 1.79 | 0.82 |
| 30:0:282:C:H1' | 30:0:368:C:H41 | 1.41 | 0.82 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1209:C:H2' | 30:0:1210:G:C8 | 2.10 | 0.82 |
| 31:9:92:G:H2' | 31:9:93:A:C8 | 2.14 | 0.82 |
| 15:O:32:ARG:HE | 15:O:35:LYS:HD2 | 1.43 | 0.82 |
| 30:0:2524:G:H21 | 30:0:2526:C:H41 | 1.23 | 0.82 |
| 11:K:39:GLY:HA2 | 38:0:5233:HOH:O | 1.79 | 0.82 |
| 4:D:154:LYS:HD2 | 4:D:154:LYS:H | 1.42 | 0.82 |
| 30:0:1835:U:H5 | 30:0:1840:A:N7 | 1.76 | 0.82 |
| 30:0:2896:A:H5" | 38:0:6114:HOH:O | 1.78 | 0.82 |
| 30:0:855:U:H5" | 38:0:3639:HOH:O | 1.80 | 0.82 |
| 1:A:223:ARG:HH12 | 30:0:2270:G:H4' | 1.44 | 0.82 |
| 30:0:559:U:H5' | 30:0:559:U:H6 | 1.45 | 0.81 |
| 30:0:1741:U:H5' | 30:0:1742:A:OP1 | 1.80 | 0.81 |
| 10:J:75:PRO:HG2 | 10:J:105:LEU:HD21 | 1.61 | 0.81 |
| 30:0:2748:G:H2' | 38:0:7557:HOH:O | 1.78 | 0.81 |
| 23:W:88:THR:HG23 | 23:W:110:GLN:HB3 | 1.62 | 0.81 |
| 30:0:1527:A:H1' | 30:0:1528:A:C8 | 2.16 | 0.81 |
| 30:0:2529:G:H3' | 38:0:7196:HOH:O | 1.80 | 0.81 |
| 30:0:506:G:H22 | 30:0:509:A:H5" | 1.45 | 0.81 |
| 22:V:12:THR:HG22 | 22:V:15:GLU:HG3 | 1.61 | 0.81 |
| 17:Q:15:LYS:HD3 | 30:0:2364:A:H5" | 1.62 | 0.80 |
| 30:0:2497:A:H1' | 30:0:2526:C:H42 | 1.46 | 0.80 |
| 30:0:541:C:H2' | 30:0:542:A:C5' | 2.11 | 0.80 |
| 22:V:1:THR:HG23 | 22:V:2:VAL:H | 1.47 | 0.80 |
| 11:K:29:LEU:HB3 | 11:K:55:VAL:HG11 | 1.63 | 0.80 |
| 27:1:25:LYS:HD2 | 28:2:49:GLU:H | 1.47 | 0.80 |
| 30:0:545:G:H5' | 30:0:545:G:C8 | 2.15 | 0.80 |
| 30:0:2505:G:O2' | 30:0:2506:A:H5' | 1.82 | 0.80 |
| 16:P:117:SER:HB3 | 30:0:1593:C:OP1 | 1.82 | 0.80 |
| 30:0:541:C:H2' | 30:0:542:A:H5" | 1.64 | 0.79 |
| 30:0:2506:A:O2' | 30:0:2507:G:H8 | 1.65 | 0.79 |
| 30:0:2570:G:H5" | 38:0:4925:HOH:O | 1.82 | 0.79 |
| 3:C:115:LEU:HD13 | 3:C:223:LEU:HD21 | 1.63 | 0.79 |
| 23:W:4:LEU:HD23 | 23:W:54:PHE:HB3 | 1.64 | 0.79 |
| 14:N:37:ARG:HH11 | 31:9:6:C:H5" | 1.44 | 0.79 |
| 31:9:20:G:H3' | 38:9:9054:HOH:O | 1.82 | 0.79 |
| 30:0:1878:G:H1' | 38:0:6135:HOH:O | 1.81 | 0.79 |
| 14:N:83:LEU:HD13 | 14:N:175:LEU:HD23 | 1.65 | 0.79 |
| 30:0:1165:G:H21 | 30:0:1173:A:H5" | 1.48 | 0.78 |
| 30:0:2604:A:H5' | 38:0:5805:HOH:O | 1.83 | 0.78 |
| 2:B:206:THR:HG21 | 30:0:2716:G:H5" | 1.65 | 0.78 |
| 30:0:1856:C:H5' | 30:0:1858:A:O4' | 1.83 | 0.78 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:567:U:H5” | 38:0:6420:HOH:O | 1.83 | 0.78 |
| 30:0:1206:U:H5’ | 30:0:1206:U:H6 | 1.47 | 0.78 |
| 13:M:99:ARG:HD2 | 13:M:167:GLY:HA2 | 1.66 | 0.78 |
| 30:0:2635:A:O2’ | 30:0:2636:C:H5’ | 1.83 | 0.78 |
| 30:0:2769:C:H2’ | 30:0:2770:G:C5’ | 2.14 | 0.78 |
| 14:N:37:ARG:HH12 | 31:9:6:C:H5” | 1.49 | 0.78 |
| 10:J:52:GLN:NE2 | 30:0:1119:G:H2’ | 1.99 | 0.78 |
| 13:M:164:THR:HG22 | 13:M:167:GLY:H | 1.46 | 0.77 |
| 30:0:69:A:H5’ | 30:0:69:A:H8 | 1.49 | 0.77 |
| 30:0:254:C:H2’ | 30:0:254:C:O2 | 1.84 | 0.77 |
| 30:0:2565:C:H4’ | 38:0:4847:HOH:O | 1.84 | 0.77 |
| 30:0:2563:U:H2’ | 30:0:2565:C:O5’ | 1.85 | 0.77 |
| 1:A:199:HIS:HD2 | 1:A:201:PHE:H | 1.31 | 0.77 |
| 30:0:1205:U:H2’ | 30:0:1206:U:C5’ | 2.13 | 0.77 |
| 16:P:115:SER:H | 16:P:118:GLN:NE2 | 1.83 | 0.77 |
| 30:0:711:G:H1’ | 38:0:7109:HOH:O | 1.84 | 0.77 |
| 30:0:1300:G:H1’ | 38:0:4697:HOH:O | 1.84 | 0.77 |
| 16:P:88:GLN:NE2 | 30:0:1800:G:H1’ | 1.98 | 0.77 |
| 3:C:127:ARG:NH2 | 3:C:225:PRO:HG2 | 1.99 | 0.77 |
| 30:0:1205:U:C2’ | 30:0:1206:U:H5” | 2.15 | 0.76 |
| 30:0:2812:A:H2 | 30:0:2814:A:N6 | 1.83 | 0.76 |
| 30:0:1973:A:H8 | 30:0:1973:A:H5’ | 1.49 | 0.76 |
| 29:3:25:VAL:HG22 | 29:3:68:LYS:HG3 | 1.67 | 0.76 |
| 30:0:1184:C:H1’ | 38:0:7483:HOH:O | 1.85 | 0.76 |
| 30:0:536:A:H3’ | 38:0:5057:HOH:O | 1.86 | 0.76 |
| 30:0:1342:C:C2’ | 30:0:1343:C:H5’ | 2.14 | 0.76 |
| 31:9:14:G:H5’ | 31:9:14:G:C8 | 2.18 | 0.76 |
| 30:0:2587:OMU:H5 | 38:0:7502:HOH:O | 1.85 | 0.76 |
| 30:0:1979:G:H2’ | 38:0:3302:HOH:O | 1.85 | 0.76 |
| 30:0:1641:A:H2’ | 30:0:1642:A:H5’ | 1.67 | 0.76 |
| 30:0:1185:U:H2’ | 30:0:1186:C:H6 | 1.50 | 0.76 |
| 30:0:69:A:H5’ | 30:0:69:A:C8 | 2.21 | 0.76 |
| 30:0:1701:A:H5” | 30:0:1702:U:H3’ | 1.68 | 0.75 |
| 30:0:1474:C:C6 | 30:0:1474:C:H5’ | 2.20 | 0.75 |
| 30:0:396:U:H1’ | 38:0:7643:HOH:O | 1.86 | 0.75 |
| 26:Z:44:ARG:HH21 | 30:0:1771:U:H5’ | 1.52 | 0.75 |
| 18:R:8:ALA:HB1 | 18:R:13:THR:HG21 | 1.69 | 0.75 |
| 22:V:39:ALA:H | 22:V:40:PRO:HD2 | 1.51 | 0.75 |
| 23:W:6:GLN:HB2 | 23:W:26:ILE:HD12 | 1.69 | 0.75 |
| 30:0:1182:C:H1’ | 30:0:1192:A:H8 | 1.51 | 0.75 |
| 1:A:223:ARG:NH1 | 30:0:2270:G:H4’ | 2.02 | 0.75 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:282:C:O2 | 30:0:282:C:H2' | 1.85 | 0.75 |
| 30:0:31:C:H2' | 38:0:7701:HOH:O | 1.86 | 0.75 |
| 30:0:2498:C:O2' | 30:0:2499:U:H5' | 1.87 | 0.75 |
| 30:0:1455:C:H3' | 38:0:7887:HOH:O | 1.86 | 0.74 |
| 20:T:24:ARG:HH21 | 20:T:39:ASN:HD22 | 1.34 | 0.74 |
| 30:0:1919:A:H4' | 38:0:4863:HOH:O | 1.86 | 0.74 |
| 30:0:2426:G:H1' | 38:0:6107:HOH:O | 1.87 | 0.74 |
| 30:0:1118:A:C8 | 30:0:1118:A:C3' | 2.69 | 0.74 |
| 14:N:144:GLY:O | 14:N:147:ILE:HG22 | 1.88 | 0.74 |
| 13:M:134:ILE:HG23 | 13:M:141:ILE:HD13 | 1.69 | 0.74 |
| 30:0:2456:A:H1' | 38:0:6611:HOH:O | 1.87 | 0.74 |
| 10:J:131:THR:HB | 10:J:134:GLU:HG3 | 1.70 | 0.74 |
| 31:9:54:A:H2 | 38:9:9061:HOH:O | 1.70 | 0.74 |
| 30:0:582:U:H2' | 30:0:583:C:H6 | 1.53 | 0.74 |
| 14:N:113:SER:HB2 | 38:N:8854:HOH:O | 1.88 | 0.74 |
| 10:J:82:THR:CG2 | 30:0:1242:A:H5' | 2.16 | 0.73 |
| 30:0:2073:G:H5" | 38:0:3832:HOH:O | 1.88 | 0.73 |
| 30:0:564:G:H1' | 38:0:6328:HOH:O | 1.86 | 0.73 |
| 30:0:1634:G:H3' | 38:0:3900:HOH:O | 1.87 | 0.73 |
| 23:W:80:ASP:O | 23:W:84:VAL:HG23 | 1.88 | 0.73 |
| 17:Q:95:GLU:HA | 30:0:949:U:H4' | 1.71 | 0.73 |
| 18:R:39:THR:HG22 | 18:R:42:GLU:H | 1.53 | 0.73 |
| 30:0:2004:U:H4' | 38:0:5318:HOH:O | 1.87 | 0.73 |
| 30:0:2851:G:O2' | 30:0:2852:A:H5' | 1.89 | 0.73 |
| 30:0:542:A:H5' | 30:0:542:A:C8 | 2.21 | 0.73 |
| 28:2:43:ARG:HH22 | 30:0:1684:A:H1' | 1.53 | 0.73 |
| 30:0:1615:A:H4' | 38:0:5899:HOH:O | 1.88 | 0.73 |
| 21:U:47:ARG:HG3 | 38:U:4381:HOH:O | 1.89 | 0.73 |
| 10:J:127:ILE:HG22 | 35:J:8801:CL:CL | 2.24 | 0.73 |
| 30:0:2524:G:H21 | 30:0:2526:C:N4 | 1.85 | 0.73 |
| 30:0:854:G:H5" | 38:0:3639:HOH:O | 1.88 | 0.73 |
| 30:0:603:A:H5" | 30:0:604:G:OP1 | 1.88 | 0.73 |
| 2:B:18:ARG:HE | 2:B:256:GLN:HE21 | 1.35 | 0.73 |
| 30:0:1060:C:H6 | 30:0:1060:C:H5' | 1.53 | 0.73 |
| 30:0:558:C:H2' | 30:0:559:U:C5' | 2.19 | 0.73 |
| 9:I:73:LEU:HD12 | 9:I:107:LYS:NZ | 2.04 | 0.73 |
| 30:0:318:U:H5' | 30:0:339:A:C2 | 2.24 | 0.73 |
| 30:0:1157:C:H2' | 30:0:1158:G:H8 | 1.53 | 0.73 |
| 10:J:18:ILE:HD13 | 30:0:1244:U:OP1 | 1.89 | 0.73 |
| 30:0:2769:C:O2' | 30:0:2770:G:H5' | 1.89 | 0.73 |
| 30:0:2420:G:O2' | 30:0:2421:G:H5' | 1.88 | 0.73 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:78:ARG:HG3 | 3:C:78:ARG:HH11 | 1.54 | 0.73 |
| 30:0:1213:C:O2' | 30:0:1214:G:H5' | 1.89 | 0.73 |
| 3:C:139:VAL:HG13 | 38:C:8654:HOH:O | 1.87 | 0.73 |
| 31:9:55:U:H4' | 31:9:56:A:C8 | 2.24 | 0.73 |
| 30:0:1119:G:N2 | 30:0:1246:A:H2 | 1.84 | 0.73 |
| 30:0:871:G:C8 | 30:0:871:G:C5' | 2.63 | 0.72 |
| 30:0:1666:C:H2' | 30:0:1667:A:C5' | 2.19 | 0.72 |
| 30:0:214:U:H5' | 38:0:6153:HOH:O | 1.88 | 0.72 |
| 31:9:75:G:H1 | 31:9:106:U:H3 | 1.37 | 0.72 |
| 30:0:848:C:H5' | 38:0:7287:HOH:O | 1.89 | 0.72 |
| 30:0:1942:A:H3' | 38:0:7363:HOH:O | 1.88 | 0.72 |
| 30:0:1942:A:H5' | 38:0:7363:HOH:O | 1.88 | 0.72 |
| 3:C:1:MET:HG2 | 3:C:2:GLN:H | 1.52 | 0.72 |
| 30:0:2010:A:H2' | 38:0:5975:HOH:O | 1.90 | 0.72 |
| 23:W:84:VAL:HG12 | 38:W:6679:HOH:O | 1.89 | 0.72 |
| 23:W:21:LEU:HD21 | 23:W:48:VAL:HG11 | 1.72 | 0.72 |
| 30:0:1528:A:H2' | 30:0:1529:G:O4' | 1.88 | 0.72 |
| 30:0:1595:G:O2' | 30:0:1596:U:H5' | 1.89 | 0.72 |
| 30:0:1964:U:O2 | 30:0:1964:U:H2' | 1.88 | 0.72 |
| 30:0:2787:C:H5 | 38:0:4647:HOH:O | 1.72 | 0.72 |
| 30:0:1603:A:H5" | 30:0:1605:G:H5' | 1.72 | 0.72 |
| 30:0:1834:C:H2' | 30:0:1840:A:N6 | 2.04 | 0.72 |
| 2:B:258:GLY:H | 2:B:260:HIS:CE1 | 2.08 | 0.72 |
| 25:Y:216:ARG:HD3 | 38:Y:8139:HOH:O | 1.90 | 0.72 |
| 30:0:12:U:H2' | 30:0:13:G:H5' | 1.72 | 0.71 |
| 30:0:2481:G:H5" | 38:0:4556:HOH:O | 1.89 | 0.71 |
| 30:0:272:A:H5' | 30:0:273:G:OP2 | 1.89 | 0.71 |
| 30:0:969:G:H1 | 30:0:999:C:H42 | 1.38 | 0.71 |
| 30:0:363:C:H1' | 38:0:5292:HOH:O | 1.90 | 0.71 |
| 13:M:102:GLU:OE1 | 13:M:164:THR:HG21 | 1.88 | 0.71 |
| 30:0:603:A:H1' | 30:0:605:C:C2 | 2.25 | 0.71 |
| 22:V:1:THR:CB | 30:0:93:C:H5" | 2.17 | 0.71 |
| 30:0:2768:A:H2' | 30:0:2769:C:O4' | 1.90 | 0.71 |
| 30:0:2748:G:H1' | 38:0:7912:HOH:O | 1.91 | 0.71 |
| 19:S:51:GLN:HE21 | 19:S:53:ASN:HD21 | 1.38 | 0.71 |
| 30:0:2533:C:H5' | 30:0:2533:C:H6 | 1.54 | 0.71 |
| 1:A:47:HIS:HD2 | 30:0:1654:U:H2' | 1.56 | 0.71 |
| 14:N:141:ARG:HH12 | 31:9:35:C:H2' | 1.56 | 0.71 |
| 30:0:1701:A:H5' | 38:0:6302:HOH:O | 1.89 | 0.71 |
| 3:C:162:VAL:HG22 | 3:C:232:LEU:HD21 | 1.73 | 0.71 |
| 30:0:870:G:C2' | 30:0:871:G:H5" | 2.20 | 0.71 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:172:VAL:HG12 | 4:D:173:GLU:H | 1.55 | 0.71 |
| 1:A:72:GLU:HG3 | 26:Z:90:GLY:HA2 | 1.72 | 0.70 |
| 2:B:195:ARG:HG2 | 2:B:323:LEU:HD22 | 1.72 | 0.70 |
| 31:9:7:G:H5' | 38:9:9098:HOH:O | 1.91 | 0.70 |
| 30:0:2243:C:H5" | 38:0:3756:HOH:O | 1.91 | 0.70 |
| 1:A:192:VAL:CG1 | 1:A:207:GLN:HB3 | 2.21 | 0.70 |
| 5:E:81:GLU:HG2 | 5:E:134:SER:HB3 | 1.73 | 0.70 |
| 30:0:560:U:H2' | 30:0:561:G:H8 | 1.56 | 0.70 |
| 3:C:140:VAL:HB | 38:C:8657:HOH:O | 1.91 | 0.70 |
| 30:0:2502:C:H2' | 30:0:2503:A:C5' | 2.17 | 0.70 |
| 30:0:960:G:C3' | 30:0:960:G:N3 | 2.54 | 0.70 |
| 10:J:70:PHE:CE1 | 30:0:2676:C:H4' | 2.26 | 0.70 |
| 30:0:2453:G:H3' | 38:0:5935:HOH:O | 1.91 | 0.70 |
| 23:W:72:PRO:HG2 | 23:W:77:ALA:HB3 | 1.73 | 0.70 |
| 30:0:1116:U:O2' | 30:0:1118:A:H2 | 1.69 | 0.70 |
| 23:W:6:GLN:HB2 | 23:W:26:ILE:CD1 | 2.21 | 0.70 |
| 30:0:1666:C:C2' | 30:0:1667:A:C5' | 2.70 | 0.70 |
| 31:9:3:A:H61 | 31:9:22:G:H1' | 1.56 | 0.70 |
| 14:N:40:ASN:ND2 | 31:9:28:U:H5" | 2.06 | 0.70 |
| 30:0:2005:G:H3' | 30:0:2005:G:OP2 | 1.91 | 0.70 |
| 30:0:2578:G:H5' | 30:0:2578:G:H8 | 1.56 | 0.69 |
| 30:0:1377:C:H6 | 30:0:1377:C:H5' | 1.57 | 0.69 |
| 30:0:2372:A:H2' | 30:0:2373:U:C6 | 2.27 | 0.69 |
| 2:B:201:ASP:HB2 | 2:B:312:ARG:HD2 | 1.75 | 0.69 |
| 30:0:2717:C:H2' | 30:0:2718:C:C5' | 2.18 | 0.69 |
| 30:0:1701:A:H4' | 30:0:1702:U:C5' | 2.19 | 0.69 |
| 31:9:13:A:O2' | 31:9:14:G:H5" | 1.92 | 0.69 |
| 30:0:2073:G:OP2 | 30:0:2490:A:H5' | 1.93 | 0.69 |
| 30:0:401:C:H2' | 30:0:402:U:C6 | 2.27 | 0.69 |
| 30:0:613:C:H2' | 30:0:614:U:H6 | 1.57 | 0.69 |
| 30:0:441:A:H1' | 30:0:442:A:N7 | 2.08 | 0.69 |
| 9:I:110:ASP:O | 30:0:1163:G:H5' | 1.91 | 0.69 |
| 31:9:36:C:C5 | 31:9:37:C:C5 | 2.80 | 0.69 |
| 29:3:70:ARG:HD3 | 38:3:9059:HOH:O | 1.90 | 0.69 |
| 30:0:1441:G:O2' | 30:0:1442:A:H5' | 1.92 | 0.69 |
| 4:D:135:VAL:HG21 | 4:D:139:TYR:CD1 | 2.27 | 0.69 |
| 30:0:625:U:H5" | 30:0:1044:C:N4 | 2.08 | 0.69 |
| 14:N:49:THR:HG22 | 14:N:56:ASP:HB2 | 1.75 | 0.69 |
| 30:0:1667:A:H8 | 30:0:1667:A:H5' | 1.57 | 0.69 |
| 30:0:1477:C:H5' | 30:0:1868:G:C5' | 2.22 | 0.69 |
| 28:2:41:HIS:H | 28:2:45:ASN:HD22 | 1.39 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:271:C:H41 | 30:0:378:A:H2 | 1.36 | 0.69 |
| 11:K:74:VAL:HG11 | 11:K:113:ILE:HG12 | 1.74 | 0.69 |
| 30:0:249:G:O2' | 30:0:250:C:H5' | 1.93 | 0.69 |
| 11:K:98:VAL:HG13 | 11:K:102:GLU:HA | 1.74 | 0.69 |
| 30:0:544:G:H2' | 30:0:545:G:H5" | 1.75 | 0.68 |
| 26:Z:70:ARG:HD3 | 26:Z:83:TYR:HB2 | 1.74 | 0.68 |
| 30:0:2535:A:H2 | 38:0:4805:HOH:O | 1.75 | 0.68 |
| 31:9:29:C:H2' | 31:9:30:C:H5' | 1.75 | 0.68 |
| 30:0:2616:G:H1' | 38:0:9426:HOH:O | 1.93 | 0.68 |
| 30:0:1204:C:H2' | 30:0:1205:U:O4' | 1.92 | 0.68 |
| 30:0:816:G:C6 | 30:0:817:G:N1 | 2.61 | 0.68 |
| 30:0:1730:G:H5' | 30:0:1731:C:C5 | 2.28 | 0.68 |
| 30:0:1819:G:H2' | 30:0:1820:G:H4' | 1.73 | 0.68 |
| 26:Z:66:CYS:SG | 26:Z:68:GLU:HB2 | 2.33 | 0.68 |
| 1:A:100:PRO:HG2 | 1:A:103:VAL:HG21 | 1.73 | 0.68 |
| 13:M:178:LYS:HB2 | 38:0:6895:HOH:O | 1.92 | 0.68 |
| 6:F:63:ILE:HB | 6:F:64:PRO:HD3 | 1.74 | 0.68 |
| 30:0:2768:A:O2' | 30:0:2769:C:H5' | 1.94 | 0.68 |
| 30:0:1201:C:H2' | 30:0:1202:A:H5' | 1.75 | 0.68 |
| 30:0:1342:C:H2' | 30:0:1343:C:H5' | 1.76 | 0.68 |
| 15:O:47:ARG:HG3 | 15:O:47:ARG:HH11 | 1.58 | 0.68 |
| 30:0:2812:A:C2 | 30:0:2814:A:N6 | 2.58 | 0.68 |
| 14:N:48:VAL:CG1 | 14:N:55:ASP:HB3 | 2.24 | 0.67 |
| 11:K:87:ARG:HG3 | 30:0:2721:U:H4' | 1.76 | 0.67 |
| 30:0:1183:C:N4 | 30:0:1184:C:H41 | 1.92 | 0.67 |
| 30:0:1191:A:H2' | 30:0:1193:A:H5' | 1.76 | 0.67 |
| 30:0:2534:C:H1' | 38:0:3501:HOH:O | 1.95 | 0.67 |
| 30:0:2659:U:H5" | 38:0:4130:HOH:O | 1.95 | 0.67 |
| 31:9:24:U:H3' | 31:9:25:G:H5' | 1.77 | 0.67 |
| 30:0:1422:U:H2' | 30:0:1423:C:C6 | 2.29 | 0.67 |
| 8:H:6:ALA:HA | 8:H:61:ARG:HH12 | 1.59 | 0.67 |
| 2:B:207:LYS:HG3 | 30:0:2717:C:OP1 | 1.95 | 0.67 |
| 1:A:199:HIS:CD2 | 1:A:201:PHE:H | 2.12 | 0.67 |
| 30:0:308:U:H5' | 30:0:309:C:OP1 | 1.93 | 0.67 |
| 30:0:2703:A:H2' | 30:0:2704:C:H6 | 1.60 | 0.66 |
| 30:0:1165:G:H21 | 30:0:1173:A:C5' | 2.08 | 0.66 |
| 11:K:74:VAL:CG1 | 11:K:113:ILE:HG12 | 2.25 | 0.66 |
| 30:0:2485:A:H3' | 38:0:4900:HOH:O | 1.95 | 0.66 |
| 2:B:41:PHE:CD1 | 2:B:79:MET:HE2 | 2.31 | 0.66 |
| 30:0:1185:U:H2' | 30:0:1186:C:C6 | 2.28 | 0.66 |
| 30:0:1603:A:C5' | 30:0:1605:G:H5' | 2.25 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:559:U:H5' | 30:0:559:U:C6 | 2.29 | 0.66 |
| 18:R:99:ALA:HB1 | 18:R:109:MET:HE1 | 1.77 | 0.66 |
| 30:0:1857:A:H5" | 38:0:6720:HOH:O | 1.94 | 0.66 |
| 27:1:1:THR:HA | 38:1:8959:HOH:O | 1.94 | 0.66 |
| 31:9:49:G:O2' | 31:9:50:G:H5' | 1.96 | 0.66 |
| 23:W:21:LEU:HD21 | 23:W:48:VAL:CG1 | 2.26 | 0.66 |
| 30:0:1477:C:H5' | 30:0:1868:G:H5' | 1.77 | 0.66 |
| 30:0:280:C:H2' | 30:0:281:U:O4' | 1.96 | 0.66 |
| 30:0:281:U:H2' | 30:0:282:C:O4' | 1.94 | 0.66 |
| 30:0:582:U:H2' | 30:0:583:C:C6 | 2.31 | 0.66 |
| 30:0:2509:A:H2' | 30:0:2510:C:O4' | 1.96 | 0.65 |
| 30:0:506:G:H22 | 30:0:509:A:H5' | 1.61 | 0.65 |
| 1:A:192:VAL:HG12 | 38:A:9055:HOH:O | 1.96 | 0.65 |
| 30:0:1855:G:H4' | 30:0:1856:C:O5' | 1.96 | 0.65 |
| 30:0:969:G:H1 | 30:0:999:C:N4 | 1.94 | 0.65 |
| 1:A:94:LEU:HG | 1:A:99:ILE:HD11 | 1.77 | 0.65 |
| 30:0:625:U:H5' | 38:0:3191:HOH:O | 1.96 | 0.65 |
| 3:C:118:THR:O | 3:C:136:VAL:HG13 | 1.96 | 0.65 |
| 30:0:1157:C:H2' | 30:0:1158:G:C8 | 2.31 | 0.65 |
| 30:0:1189:A:H3' | 38:0:7692:HOH:O | 1.95 | 0.65 |
| 30:0:1211:G:H2' | 30:0:1212:C:H6 | 1.61 | 0.65 |
| 30:0:1687:C:H3' | 38:0:9459:HOH:O | 1.94 | 0.65 |
| 1:A:36:ASP:HB2 | 1:A:85:SER:H | 1.60 | 0.65 |
| 30:0:1186:C:H42 | 30:0:1190:G:H22 | 1.44 | 0.65 |
| 8:H:168:VAL:HG13 | 38:H:212:HOH:O | 1.95 | 0.65 |
| 18:R:117:HIS:HD2 | 30:0:20:G:H21 | 1.45 | 0.65 |
| 22:V:55:ARG:O | 22:V:59:ILE:HG12 | 1.97 | 0.65 |
| 6:F:30:LYS:HE2 | 6:F:99:THR:HG21 | 1.79 | 0.65 |
| 30:0:714:U:H4' | 38:0:5753:HOH:O | 1.95 | 0.65 |
| 30:0:2672:C:H1' | 38:0:6699:HOH:O | 1.96 | 0.65 |
| 31:9:20:G:O2' | 31:9:21:G:H5' | 1.97 | 0.65 |
| 30:0:1834:C:H2' | 30:0:1840:A:H62 | 1.61 | 0.65 |
| 30:0:2004:U:O5' | 30:0:2004:U:H6 | 1.80 | 0.65 |
| 11:K:63:GLU:HB2 | 38:K:6344:HOH:O | 1.97 | 0.65 |
| 6:F:77:VAL:HG21 | 6:F:83:LEU:HD13 | 1.77 | 0.65 |
| 8:H:29:SER:HA | 8:H:62:HIS:HD2 | 1.61 | 0.65 |
| 30:0:2781:U:H2' | 30:0:2782:G:H5' | 1.77 | 0.65 |
| 1:A:51:ARG:HB2 | 38:A:9068:HOH:O | 1.97 | 0.65 |
| 30:0:558:C:C2' | 30:0:559:U:C5' | 2.75 | 0.64 |
| 30:0:1632:A:H2' | 30:0:1633:C:H5' | 1.79 | 0.64 |
| 30:0:558:C:H2' | 30:0:559:U:H5" | 1.76 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1058:A:H2' | 30:0:1060:C:H5" | 1.79 | 0.64 |
| 4:D:25:MET:SD | 4:D:40:ILE:HD11 | 2.36 | 0.64 |
| 30:0:380:A:H2' | 38:0:7242:HOH:O | 1.96 | 0.64 |
| 30:0:1666:C:C2' | 30:0:1667:A:H5" | 2.27 | 0.64 |
| 30:0:1342:C:O2' | 30:0:1343:C:H5' | 1.98 | 0.64 |
| 30:0:272:A:H3' | 38:0:7547:HOH:O | 1.96 | 0.64 |
| 31:9:1:U:H4' | 31:9:3:A:OP1 | 1.97 | 0.64 |
| 30:0:595:U:H2' | 30:0:596:C:H6 | 1.63 | 0.64 |
| 11:K:14:LYS:HB2 | 11:K:45:PRO:HG2 | 1.80 | 0.64 |
| 30:0:2894:C:O2' | 30:0:2895:C:H5' | 1.97 | 0.64 |
| 25:Y:169:ARG:HD2 | 30:0:1328:A:OP1 | 1.97 | 0.64 |
| 12:L:41:HIS:HD2 | 30:0:926:A:O2' | 1.79 | 0.64 |
| 18:R:128:ARG:NH2 | 30:0:2054:A:N3 | 2.45 | 0.64 |
| 30:0:2361:A:H5" | 38:0:9009:HOH:O | 1.97 | 0.64 |
| 31:9:64:C:C2' | 31:9:65:A:H5' | 2.27 | 0.64 |
| 30:0:1175:G:H1' | 30:0:1193:A:C8 | 2.32 | 0.64 |
| 30:0:2824:C:H5" | 30:0:2825:C:H5' | 1.79 | 0.64 |
| 30:0:1116:U:H3 | 30:0:1246:A:N6 | 1.89 | 0.64 |
| 18:R:18:LEU:HB2 | 18:R:143:VAL:HG13 | 1.79 | 0.64 |
| 30:0:2781:U:C2' | 30:0:2782:G:H5' | 2.28 | 0.64 |
| 30:0:1398:G:O2' | 30:0:1399:A:H5' | 1.98 | 0.64 |
| 15:O:42:GLU:HB2 | 38:O:2176:HOH:O | 1.97 | 0.64 |
| 5:E:100:ASP:HB2 | 38:E:2789:HOH:O | 1.97 | 0.64 |
| 30:0:1180:U:O2' | 30:0:1181:A:H5' | 1.98 | 0.63 |
| 30:0:544:G:C2' | 30:0:545:G:H5" | 2.28 | 0.63 |
| 30:0:541:C:C2' | 30:0:542:A:C5' | 2.74 | 0.63 |
| 28:2:41:HIS:HD2 | 28:2:44:ARG:H | 1.44 | 0.63 |
| 20:T:61:GLU:HG2 | 38:T:3851:HOH:O | 1.97 | 0.63 |
| 30:0:2510:C:H42 | 30:0:2564:G:H22 | 1.47 | 0.63 |
| 8:H:72:ALA:HB2 | 8:H:156:ALA:HB2 | 1.80 | 0.63 |
| 30:0:1307:A:H2' | 30:0:1308:A:C8 | 2.33 | 0.63 |
| 24:X:74:ALA:HB2 | 24:X:85:VAL:HG13 | 1.80 | 0.63 |
| 30:0:1165:G:H4' | 30:0:1174:A:O2' | 1.98 | 0.63 |
| 30:0:1634:G:H2' | 30:0:1635:U:H6 | 1.63 | 0.63 |
| 30:0:2335:C:H2' | 30:0:2336:G:H8 | 1.64 | 0.63 |
| 2:B:320:GLN:HE21 | 2:B:321:PRO:HD2 | 1.62 | 0.63 |
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:CB | 2.28 | 0.63 |
| 5:E:93:MET:HE1 | 5:E:165:GLY:H | 1.61 | 0.63 |
| 31:9:56:A:C3' | 31:9:57:A:H5" | 2.29 | 0.63 |
| 30:0:281:U:O2' | 30:0:282:C:H5' | 1.99 | 0.63 |
| 23:W:13:MET:HE1 | 23:W:18:GLN:HA | 1.80 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:214:THR:HG23 | 38:C:8640:HOH:O | 1.96 | 0.63 |
| 30:0:316:A:N3 | 30:0:336:G:O2' | 2.30 | 0.63 |
| 30:0:236:A:H4' | 30:0:237:G:H5' | 1.81 | 0.63 |
| 27:1:25:LYS:HD2 | 28:2:49:GLU:N | 2.13 | 0.63 |
| 30:0:1878:G:C1' | 38:0:6135:HOH:O | 2.43 | 0.63 |
| 30:0:74:G:H2' | 30:0:75:U:C6 | 2.34 | 0.63 |
| 14:N:37:ARG:NH1 | 31:9:6:C:C5' | 2.52 | 0.63 |
| 3:C:27:ARG:NH2 | 30:0:657:G:OP1 | 2.31 | 0.63 |
| 30:0:2717:C:O2' | 30:0:2718:C:H5" | 1.97 | 0.63 |
| 30:0:541:C:H2' | 30:0:542:A:H5' | 1.80 | 0.63 |
| 30:0:1278:A:H4' | 30:0:1279:U:N3 | 2.13 | 0.63 |
| 30:0:1377:C:H5' | 30:0:1377:C:C6 | 2.34 | 0.63 |
| 6:F:91:VAL:HG12 | 6:F:92:GLY:N | 2.13 | 0.63 |
| 31:9:33:U:H2' | 38:9:9065:HOH:O | 1.98 | 0.63 |
| 3:C:218:VAL:HG12 | 38:C:8628:HOH:O | 1.99 | 0.63 |
| 18:R:99:ALA:HB1 | 18:R:109:MET:CE | 2.29 | 0.62 |
| 30:0:694:A:H2' | 30:0:695:C:H5' | 1.80 | 0.62 |
| 30:0:285:A:H2' | 30:0:286:U:O4' | 1.98 | 0.62 |
| 14:N:7:LYS:HE3 | 17:Q:21:ARG:O | 1.99 | 0.62 |
| 31:9:64:C:H2' | 31:9:65:A:H5' | 1.81 | 0.62 |
| 30:0:2071:C:H5' | 38:0:9532:HOH:O | 1.99 | 0.62 |
| 30:0:533:U:H3' | 38:0:3754:HOH:O | 1.98 | 0.62 |
| 25:Y:115:ARG:HH21 | 30:0:1266:U:H4' | 1.64 | 0.62 |
| 30:0:2670:G:O2' | 30:0:2671:U:H5' | 1.99 | 0.62 |
| 3:C:236:THR:HG22 | 3:C:239:ALA:HB2 | 1.80 | 0.62 |
| 30:0:2414:A:H2' | 30:0:2415:A:C8 | 2.34 | 0.62 |
| 30:0:2320:U:H4' | 30:0:2321:A:O4' | 1.99 | 0.62 |
| 3:C:236:THR:HG22 | 3:C:239:ALA:CB | 2.30 | 0.62 |
| 30:0:200:C:H2' | 38:0:3449:HOH:O | 2.00 | 0.62 |
| 3:C:2:GLN:HB3 | 38:C:8587:HOH:O | 1.98 | 0.62 |
| 30:0:1398:G:H2' | 30:0:1399:A:C8 | 2.34 | 0.62 |
| 30:0:920:C:H4' | 30:0:921:G:C2 | 2.34 | 0.62 |
| 5:E:49:ILE:HD11 | 5:E:69:ILE:HD12 | 1.82 | 0.62 |
| 1:A:191:GLY:HA2 | 1:A:194:MET:HE3 | 1.81 | 0.62 |
| 2:B:179:LEU:O | 2:B:183:GLU:HG2 | 2.00 | 0.62 |
| 2:B:262:ARG:HG3 | 30:0:2716:G:H5' | 1.82 | 0.62 |
| 30:0:2512:U:H4' | 30:0:2514:U:O4 | 1.99 | 0.62 |
| 27:1:10:LYS:HG3 | 38:1:8981:HOH:O | 2.00 | 0.62 |
| 30:0:162:C:H2' | 30:0:163:U:H5' | 1.80 | 0.62 |
| 2:B:162:MET:HG3 | 2:B:310:ARG:HD3 | 1.82 | 0.61 |
| 31:9:55:U:H4' | 31:9:56:A:H8 | 1.62 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:HB2 | 1.82 | 0.61 |
| 30:0:1524:U:H5" | 30:0:1524:U:H6 | 1.63 | 0.61 |
| 30:0:585:C:H5" | 38:0:4883:HOH:O | 1.99 | 0.61 |
| 30:0:1132:A:N6 | 30:0:1229:C:H2' | 2.16 | 0.61 |
| 30:0:2900:G:H2' | 30:0:2901:C:O4' | 1.99 | 0.61 |
| 30:0:1654:U:H5" | 38:0:7439:HOH:O | 1.99 | 0.61 |
| 30:0:1838:U:H3' | 38:0:5538:HOH:O | 1.98 | 0.61 |
| 5:E:20:ILE:HD11 | 5:E:40:VAL:HG11 | 1.83 | 0.61 |
| 30:0:137:U:H2' | 30:0:139:C:C5 | 2.35 | 0.61 |
| 38:C:8669:HOH:O | 30:0:2100:A:H5' | 1.99 | 0.61 |
| 30:0:2507:G:H2' | 30:0:2510:C:N4 | 2.15 | 0.61 |
| 9:I:108:HIS:H | 9:I:109:PRO:HD2 | 1.66 | 0.61 |
| 2:B:307:ARG:HH11 | 2:B:307:ARG:HG3 | 1.66 | 0.61 |
| 30:0:1350:U:H4' | 38:0:5132:HOH:O | 2.00 | 0.61 |
| 30:0:1603:A:H5' | 30:0:1605:G:C4' | 2.30 | 0.61 |
| 30:0:1972:U:H2' | 30:0:1973:A:H5" | 1.83 | 0.61 |
| 1:A:211:LYS:HB2 | 38:A:9083:HOH:O | 2.00 | 0.61 |
| 30:0:2064:U:H5' | 30:0:2652:U:H4' | 1.82 | 0.61 |
| 30:0:2908:A:O5' | 30:0:2908:A:H8 | 1.83 | 0.61 |
| 12:L:18:HIS:HD2 | 30:0:902:G:N7 | 1.99 | 0.61 |
| 2:B:212:GLN:HB2 | 2:B:257:THR:CG2 | 2.28 | 0.61 |
| 30:0:1835:U:C5 | 30:0:1840:A:N7 | 2.65 | 0.61 |
| 29:3:48:ASN:HD21 | 30:0:2468:A:H61 | 1.48 | 0.61 |
| 12:L:133:VAL:HA | 38:L:8873:HOH:O | 2.00 | 0.61 |
| 3:C:127:ARG:HD3 | 3:C:129:HIS:HE1 | 1.65 | 0.61 |
| 3:C:37:ALA:HA | 3:C:100:LEU:HD12 | 1.82 | 0.61 |
| 30:0:1226:G:H5' | 38:0:4541:HOH:O | 1.99 | 0.61 |
| 2:B:145:HIS:HD2 | 2:B:146:THR:O | 1.83 | 0.61 |
| 12:L:6:ARG:HD3 | 30:0:1299:G:O6 | 2.00 | 0.61 |
| 23:W:4:LEU:HD22 | 23:W:52:VAL:HG21 | 1.83 | 0.61 |
| 25:Y:132:ASP:OD2 | 30:0:621:C:H5' | 2.00 | 0.61 |
| 21:U:17:THR:HG22 | 21:U:18:GLY:N | 2.16 | 0.61 |
| 25:Y:235:GLU:H | 25:Y:235:GLU:CD | 2.04 | 0.60 |
| 2:B:74:ILE:HD13 | 2:B:309:VAL:HG21 | 1.82 | 0.60 |
| 2:B:304:PRO:HD2 | 2:B:307:ARG:NE | 2.16 | 0.60 |
| 26:Z:60:ASP:HB3 | 26:Z:69:ASP:HB3 | 1.83 | 0.60 |
| 3:C:95:GLU:HG3 | 38:C:8682:HOH:O | 2.00 | 0.60 |
| 30:0:1181:A:C2' | 30:0:1182:C:H5' | 2.32 | 0.60 |
| 30:0:1741:U:O2' | 30:0:2723:G:H4' | 2.01 | 0.60 |
| 30:0:401:C:H2' | 30:0:402:U:H6 | 1.64 | 0.60 |
| 30:0:1819:G:H5' | 38:0:4725:HOH:O | 2.00 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:2:40:ARG:HD2 | 28:2:47:THR:HG22 | 1.83 | 0.60 |
| 3:C:76:ARG:HG2 | 3:C:78:ARG:NH1 | 2.15 | 0.60 |
| 30:0:1819:G:H2' | 30:0:1820:G:C5' | 2.31 | 0.60 |
| 21:U:52:THR:HG22 | 21:U:54:THR:H | 1.66 | 0.60 |
| 30:0:10:U:C4 | 30:0:532:A:N7 | 2.70 | 0.60 |
| 20:T:24:ARG:HH21 | 20:T:39:ASN:ND2 | 1.98 | 0.60 |
| 30:0:595:U:H2' | 30:0:596:C:C6 | 2.37 | 0.60 |
| 18:R:128:ARG:NH2 | 30:0:2054:A:C2 | 2.70 | 0.60 |
| 30:0:1587:U:H2' | 30:0:1588:G:O4' | 2.02 | 0.60 |
| 30:0:447:A:O2' | 30:0:448:G:H5' | 2.01 | 0.60 |
| 8:H:155:ARG:NH1 | 30:0:2503:A:H5" | 2.17 | 0.60 |
| 30:0:558:C:H2' | 30:0:559:U:H5' | 1.83 | 0.60 |
| 30:0:2372:A:H2' | 30:0:2373:U:H6 | 1.66 | 0.60 |
| 30:0:847:C:H4' | 38:0:3759:HOH:O | 1.99 | 0.60 |
| 10:J:19:MET:HE1 | 10:J:132:LEU:HD21 | 1.83 | 0.60 |
| 29:3:73:GLU:HB3 | 38:3:9049:HOH:O | 2.01 | 0.60 |
| 10:J:26:VAL:HG13 | 10:J:36:VAL:HG11 | 1.82 | 0.60 |
| 30:0:541:C:O2' | 30:0:542:A:H5" | 2.02 | 0.60 |
| 30:0:1202:A:C2' | 30:0:1203:G:H5' | 2.32 | 0.60 |
| 30:0:396:U:O2' | 30:0:418:C:H4' | 2.02 | 0.60 |
| 8:H:6:ALA:HA | 8:H:61:ARG:NH1 | 2.17 | 0.60 |
| 30:0:407:A:H2' | 30:0:408:A:C8 | 2.37 | 0.60 |
| 29:3:67:LEU:HD11 | 29:3:88:LEU:HD21 | 1.82 | 0.60 |
| 30:0:2281:C:C2' | 30:0:2282:U:H5' | 2.32 | 0.60 |
| 30:0:282:C:O2' | 30:0:283:U:C5' | 2.49 | 0.60 |
| 30:0:1583:U:H1' | 38:0:9989:HOH:O | 2.02 | 0.60 |
| 23:W:21:LEU:HD22 | 23:W:26:ILE:CD1 | 2.32 | 0.60 |
| 3:C:238:SER:HB2 | 38:C:8577:HOH:O | 2.01 | 0.60 |
| 21:U:46:ALA:HB1 | 21:U:52:THR:HG21 | 1.83 | 0.60 |
| 30:0:130:C:H2' | 38:0:3166:HOH:O | 2.02 | 0.60 |
| 13:M:179:GLY:O | 30:0:399:C:H5' | 2.02 | 0.60 |
| 30:0:807:A:O2' | 30:0:808:A:H5' | 2.01 | 0.60 |
| 13:M:163:LEU:HD21 | 30:0:188:C:H5" | 1.84 | 0.60 |
| 9:I:86:GLU:HG2 | 30:0:1180:U:H4' | 1.83 | 0.59 |
| 7:G:12:ILE:HG23 | 38:0:5471:HOH:O | 2.02 | 0.59 |
| 13:M:164:THR:HG23 | 13:M:165:GLY:N | 2.17 | 0.59 |
| 31:9:47:A:C2 | 31:9:48:C:C2 | 2.89 | 0.59 |
| 11:K:98:VAL:CG1 | 11:K:102:GLU:HA | 2.32 | 0.59 |
| 30:0:1676:G:O2' | 30:0:1677:U:H5' | 2.03 | 0.59 |
| 19:S:55:GLN:NE2 | 30:0:1446:U:H2' | 2.18 | 0.59 |
| 30:0:1172:G:H5" | 38:0:7275:HOH:O | 2.01 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1206:U:H2' | 30:0:1207:A:O4' | 2.01 | 0.59 |
| 2:B:18:ARG:HG3 | 2:B:256:GLN:HG3 | 1.82 | 0.59 |
| 2:B:51:VAL:HG23 | 2:B:330:VAL:HG22 | 1.83 | 0.59 |
| 30:0:2135:A:O2' | 30:0:2136:G:H5' | 2.03 | 0.59 |
| 11:K:32:ILE:HD11 | 11:K:56:SER:HB3 | 1.84 | 0.59 |
| 30:0:1165:G:N2 | 30:0:1173:A:H5" | 2.15 | 0.59 |
| 30:0:2826:G:C6 | 30:0:2913:A:N6 | 2.70 | 0.59 |
| 5:E:68:HIS:O | 5:E:72:MET:HG3 | 2.01 | 0.59 |
| 10:J:45:VAL:HG23 | 10:J:130:VAL:O | 2.00 | 0.59 |
| 4:D:105:SER:OG | 30:0:2338:G:H1' | 2.03 | 0.59 |
| 4:D:65:GLU:HA | 38:D:6752:HOH:O | 2.02 | 0.59 |
| 13:M:164:THR:HG22 | 13:M:167:GLY:N | 2.16 | 0.59 |
| 30:0:2505:G:C2' | 30:0:2506:A:H5' | 2.32 | 0.59 |
| 31:9:92:G:H2' | 31:9:93:A:H8 | 1.67 | 0.59 |
| 30:0:1524:U:C5' | 30:0:1524:U:H6 | 2.16 | 0.59 |
| 30:0:1766:U:O2 | 30:0:1778:A:H5' | 2.01 | 0.59 |
| 1:A:186:TRP:CG | 1:A:187:PRO:HA | 2.38 | 0.59 |
| 25:Y:126:PRO:HG2 | 25:Y:128:PHE:CE1 | 2.37 | 0.59 |
| 30:0:2748:G:H5' | 38:0:7557:HOH:O | 2.02 | 0.59 |
| 30:0:1165:G:N2 | 30:0:1173:A:C5' | 2.66 | 0.59 |
| 13:M:125:ARG:HD2 | 38:M:8893:HOH:O | 2.02 | 0.59 |
| 14:N:34:LEU:HD22 | 14:N:129:ILE:HD13 | 1.83 | 0.59 |
| 30:0:1042:U:O2' | 30:0:1043:C:H5' | 2.02 | 0.59 |
| 30:0:424:C:H2' | 30:0:425:U:C6 | 2.38 | 0.59 |
| 3:C:16:VAL:HG21 | 38:C:8634:HOH:O | 2.02 | 0.59 |
| 30:0:482:G:H4' | 30:0:508:A:N1 | 2.18 | 0.59 |
| 10:J:63:ILE:HD11 | 30:0:1236:A:C8 | 2.38 | 0.59 |
| 30:0:522:U:O2' | 30:0:1366:C:H5' | 2.02 | 0.59 |
| 30:0:1641:A:C2' | 30:0:1642:A:H5' | 2.32 | 0.59 |
| 30:0:853:C:H3' | 38:0:4563:HOH:O | 2.03 | 0.59 |
| 30:0:1511:U:O2' | 30:0:1512:G:H5' | 2.03 | 0.59 |
| 30:0:2374:G:H2' | 30:0:2375:A:C8 | 2.37 | 0.59 |
| 30:0:1973:A:H5' | 30:0:1973:A:C8 | 2.36 | 0.59 |
| 16:P:10:ALA:HA | 16:P:13:VAL:HG12 | 1.85 | 0.59 |
| 28:2:39:ARG:HG2 | 38:2:3143:HOH:O | 2.03 | 0.59 |
| 30:0:1790:C:H2' | 30:0:1791:U:H6 | 1.67 | 0.59 |
| 30:0:255:A:H2' | 30:0:256:C:C6 | 2.38 | 0.59 |
| 30:0:2324:G:N2 | 30:0:2377:U:H1' | 2.17 | 0.59 |
| 30:0:368:C:H2' | 30:0:369:G:H5' | 1.84 | 0.58 |
| 10:J:52:GLN:HE22 | 30:0:1119:G:H2' | 1.67 | 0.58 |
| 27:1:9:GLY:HA2 | 30:0:1687:C:O2 | 2.02 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:36:ASP:O | 1:A:38:ILE:N | 2.36 | 0.58 |
| 30:0:1321:A:H2' | 30:0:1322:G:C8 | 2.38 | 0.58 |
| 30:0:1196:C:N4 | 30:0:1204:C:H42 | 2.01 | 0.58 |
| 30:0:2467:A:O2' | 30:0:2468:A:H2' | 2.02 | 0.58 |
| 30:0:123:U:H5' | 38:0:6671:HOH:O | 2.03 | 0.58 |
| 8:H:15:PRO:HG3 | 30:0:1053:G:OP1 | 2.02 | 0.58 |
| 30:0:1904:A:H2' | 30:0:1905:U:O4' | 2.03 | 0.58 |
| 1:A:94:LEU:HG | 1:A:99:ILE:CD1 | 2.33 | 0.58 |
| 30:0:2335:C:H2' | 30:0:2336:G:C8 | 2.38 | 0.58 |
| 17:Q:21:ARG:HH12 | 30:0:2353:A:H1' | 1.67 | 0.58 |
| 30:0:10:U:C4 | 30:0:532:A:C8 | 2.91 | 0.58 |
| 3:C:79:ARG:O | 3:C:87:ARG:HG2 | 2.03 | 0.58 |
| 30:0:1182:C:C1' | 30:0:1192:A:H8 | 2.16 | 0.58 |
| 28:2:41:HIS:HB3 | 28:2:44:ARG:HB2 | 1.84 | 0.58 |
| 30:0:1170:U:H2' | 30:0:1172:G:OP2 | 2.02 | 0.58 |
| 30:0:2878:U:H2' | 30:0:2879:A:O4' | 2.02 | 0.58 |
| 30:0:1948:G:H2' | 30:0:1949:G:C8 | 2.39 | 0.58 |
| 11:K:4:LEU:HD22 | 11:K:116:GLU:HB3 | 1.85 | 0.58 |
| 30:0:2281:C:H2' | 30:0:2282:U:H5' | 1.85 | 0.58 |
| 3:C:78:ARG:HG3 | 3:C:78:ARG:NH1 | 2.15 | 0.58 |
| 30:0:960:G:H8 | 38:0:5987:HOH:O | 1.85 | 0.58 |
| 30:0:2852:A:H5" | 38:0:5246:HOH:O | 2.03 | 0.58 |
| 8:H:174:LEU:HD21 | 30:0:1220:U:H4' | 1.85 | 0.58 |
| 1:A:121:ALA:O | 1:A:124:VAL:HG22 | 2.03 | 0.58 |
| 9:I:112:LEU:CD1 | 30:0:1162:G:H1' | 2.34 | 0.58 |
| 30:0:2768:A:H5" | 38:0:4434:HOH:O | 2.03 | 0.58 |
| 3:C:76:ARG:HG2 | 3:C:78:ARG:HH12 | 1.69 | 0.58 |
| 3:C:237:GLU:HG3 | 38:C:8634:HOH:O | 2.04 | 0.58 |
| 12:L:14:GLY:O | 30:0:1295:G:H5" | 2.03 | 0.58 |
| 30:0:440:C:H2' | 30:0:441:A:C8 | 2.39 | 0.58 |
| 31:9:37:C:H2' | 31:9:38:A:H8 | 1.68 | 0.58 |
| 30:0:1819:G:H2' | 30:0:1820:G:C4' | 2.34 | 0.58 |
| 25:Y:141:THR:HG23 | 38:Y:8158:HOH:O | 2.03 | 0.58 |
| 24:X:23:HIS:HE1 | 30:0:2044:G:OP1 | 1.86 | 0.58 |
| 22:V:64:GLY:O | 22:V:65:ASP:HB2 | 2.04 | 0.58 |
| 14:N:71:TRP:CE3 | 14:N:175:LEU:HD22 | 2.38 | 0.58 |
| 13:M:134:ILE:CG2 | 13:M:141:ILE:HD13 | 2.34 | 0.58 |
| 30:0:681:G:N3 | 30:0:681:G:H5' | 2.19 | 0.58 |
| 30:0:2820:A:H2' | 30:0:2821:C:C6 | 2.38 | 0.58 |
| 30:0:2643:G:H5" | 38:0:3933:HOH:O | 2.03 | 0.58 |
| 14:N:141:ARG:NH1 | 31:9:35:C:H2' | 2.18 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:W:68:THR:HG23 | 23:W:69:ARG:HG2 | 1.86 | 0.58 |
| 11:K:20:CYS:HB2 | 11:K:29:LEU:HG | 1.86 | 0.57 |
| 30:0:1947:G:H2' | 30:0:1948:G:H8 | 1.69 | 0.57 |
| 30:0:2760:C:H5" | 38:0:5337:HOH:O | 2.03 | 0.57 |
| 19:S:76:GLU:HB3 | 38:S:8992:HOH:O | 2.04 | 0.57 |
| 30:0:249:G:N2 | 30:0:250:C:C2 | 2.72 | 0.57 |
| 30:0:1730:G:C5' | 30:0:1731:C:C6 | 2.86 | 0.57 |
| 28:2:38:LYS:HE3 | 38:0:4231:HOH:O | 2.04 | 0.57 |
| 2:B:27:ASN:H | 2:B:27:ASN:HD22 | 1.51 | 0.57 |
| 24:X:47:ALA:HB1 | 24:X:82:GLU:HB3 | 1.86 | 0.57 |
| 27:1:16:HIS:HD2 | 30:0:470:U:O2' | 1.86 | 0.57 |
| 3:C:174:ILE:HD11 | 30:0:338:C:H4' | 1.85 | 0.57 |
| 2:B:238:ASN:HD22 | 2:B:240:GLY:N | 1.97 | 0.57 |
| 6:F:91:VAL:HG12 | 6:F:92:GLY:H | 1.68 | 0.57 |
| 30:0:1191:A:C2 | 30:0:1207:A:C2 | 2.93 | 0.57 |
| 31:9:76:G:C3' | 31:9:77:A:H5" | 2.25 | 0.57 |
| 3:C:129:HIS:CE1 | 3:C:231:ARG:HA | 2.38 | 0.57 |
| 30:0:2003:U:HO2' | 30:0:2004:U:H5 | 1.52 | 0.57 |
| 30:0:1965:C:O2' | 30:0:1966:U:H5' | 2.04 | 0.57 |
| 30:0:395:A:H5" | 38:0:3928:HOH:O | 2.05 | 0.57 |
| 30:0:2254:G:O2' | 30:0:2255:A:H5' | 2.04 | 0.57 |
| 30:0:2532:A:H2 | 38:0:7579:HOH:O | 1.87 | 0.57 |
| 30:0:360:A:H2' | 30:0:361:C:O4' | 2.04 | 0.57 |
| 30:0:185:G:H4' | 30:0:186:A:OP1 | 2.04 | 0.57 |
| 31:9:23:U:O2' | 31:9:24:U:H4' | 2.05 | 0.57 |
| 31:9:3:A:C8 | 31:9:26:C:C2 | 2.93 | 0.57 |
| 38:O:7674:HOH:O | 30:0:653:U:H5" | 2.05 | 0.57 |
| 13:M:188:ARG:HD3 | 30:0:155:C:OP2 | 2.03 | 0.57 |
| 30:0:602:A:O2' | 30:0:605:C:H4' | 2.04 | 0.57 |
| 30:0:1524:U:OP1 | 30:0:1524:U:H4' | 2.05 | 0.57 |
| 21:U:14:GLU:O | 21:U:17:THR:HB | 2.05 | 0.57 |
| 30:0:65:C:O2' | 30:0:66:G:H5' | 2.03 | 0.57 |
| 28:2:35:ARG:HB2 | 38:2:2691:HOH:O | 2.05 | 0.57 |
| 30:0:119:A:H2' | 30:0:120:A:H5" | 1.86 | 0.57 |
| 2:B:244:PRO:HB3 | 30:0:1234:U:N3 | 2.19 | 0.57 |
| 30:0:2314:G:C2' | 30:0:2315:C:H5' | 2.34 | 0.57 |
| 30:0:1116:U:O2' | 30:0:1118:A:C2 | 2.50 | 0.57 |
| 9:I:73:LEU:HD12 | 9:I:107:LYS:HZ2 | 1.67 | 0.57 |
| 30:0:1333:U:H2' | 30:0:1334:C:C6 | 2.40 | 0.57 |
| 30:0:2282:U:H4' | 30:0:2309:C:C5 | 2.39 | 0.57 |
| 30:0:2507:G:H2' | 30:0:2510:C:H42 | 1.70 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:R:39:THR:HG23 | 18:R:107:GLU:O | 2.05 | 0.57 |
| 1:A:192:VAL:HG13 | 1:A:207:GLN:HB3 | 1.87 | 0.57 |
| 5:E:93:MET:HE1 | 5:E:165:GLY:N | 2.19 | 0.57 |
| 30:0:1515:A:H2' | 30:0:1516:U:C6 | 2.40 | 0.57 |
| 14:N:13:ARG:NH1 | 30:0:2368:A:C6 | 2.72 | 0.57 |
| 13:M:30:GLU:O | 13:M:34:GLU:HG3 | 2.04 | 0.57 |
| 30:0:711:G:C2 | 30:0:718:C:C2 | 2.92 | 0.57 |
| 8:H:98:LEU:HD11 | 8:H:127:ALA:HB2 | 1.86 | 0.57 |
| 30:0:291:C:H2' | 30:0:292:G:O4' | 2.05 | 0.57 |
| 30:0:1351:G:H1' | 38:0:4693:HOH:O | 2.04 | 0.57 |
| 30:0:1189:A:O2' | 30:0:1208:C:H2' | 2.05 | 0.56 |
| 30:0:2831:C:O2' | 30:0:2832:C:H5' | 2.05 | 0.56 |
| 30:0:2533:C:C6 | 30:0:2533:C:H5' | 2.38 | 0.56 |
| 23:W:13:MET:CE | 23:W:18:GLN:HA | 2.35 | 0.56 |
| 3:C:174:ILE:CD1 | 30:0:338:C:H4' | 2.35 | 0.56 |
| 30:0:2897:C:O2' | 30:0:2898:G:H5' | 2.05 | 0.56 |
| 16:P:59:ARG:O | 16:P:63:ARG:HG3 | 2.05 | 0.56 |
| 30:0:538:C:H5" | 30:0:539:G:C8 | 2.40 | 0.56 |
| 30:0:1504:A:H4' | 30:0:1506:U:C5 | 2.40 | 0.56 |
| 5:E:116:THR:HG22 | 5:E:151:LEU:HD22 | 1.87 | 0.56 |
| 30:0:432:G:O2' | 30:0:433:C:H5' | 2.05 | 0.56 |
| 11:K:118:ALA:HA | 11:K:125:ALA:HB2 | 1.85 | 0.56 |
| 26:Z:81:CYS:SG | 26:Z:83:TYR:HB3 | 2.45 | 0.56 |
| 19:S:11:THR:H | 19:S:14:ALA:HB3 | 1.69 | 0.56 |
| 1:A:105:VAL:CG1 | 1:A:154:ALA:HB1 | 2.35 | 0.56 |
| 2:B:294:TYR:HE2 | 38:B:9116:HOH:O | 1.88 | 0.56 |
| 23:W:5:VAL:HG11 | 23:W:153:MET:CE | 2.35 | 0.56 |
| 15:O:14:LEU:HD23 | 15:O:102:ILE:HD11 | 1.88 | 0.56 |
| 19:S:57:THR:HG23 | 38:S:8980:HOH:O | 2.05 | 0.56 |
| 30:0:812:A:H2' | 30:0:813:C:C6 | 2.40 | 0.56 |
| 30:0:2781:U:H2' | 30:0:2782:G:C5' | 2.35 | 0.56 |
| 30:0:1634:G:H2' | 30:0:1635:U:C6 | 2.41 | 0.56 |
| 14:N:139:TRP:HA | 14:N:139:TRP:CE3 | 2.40 | 0.56 |
| 30:0:2297:U:H1' | 38:0:5188:HOH:O | 2.04 | 0.56 |
| 30:0:851:C:O2 | 30:0:2022:A:H2 | 1.87 | 0.56 |
| 30:0:2282:U:H4' | 30:0:2309:C:H5 | 1.71 | 0.56 |
| 30:0:483:C:C4 | 30:0:484:A:C6 | 2.94 | 0.56 |
| 30:0:484:A:N1 | 30:0:506:G:H4' | 2.21 | 0.56 |
| 30:0:2300:A:H4' | 30:0:2301:A:O5' | 2.05 | 0.56 |
| 25:Y:130:ARG:HB2 | 25:Y:142:SER:O | 2.05 | 0.56 |
| 30:0:2472:C:O2' | 30:0:2634:G:H4' | 2.04 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1189:A:H1' | 30:0:1209:C:O4' | 2.05 | 0.56 |
| 8:H:59:GLN:HE21 | 8:H:129:ARG:NE | 1.94 | 0.56 |
| 24:X:72:VAL:HG22 | 24:X:85:VAL:HG12 | 1.86 | 0.56 |
| 31:9:35:C:H5" | 38:9:9075:HOH:O | 2.06 | 0.56 |
| 2:B:7:ARG:HG2 | 2:B:7:ARG:HH11 | 1.70 | 0.56 |
| 4:D:56:ARG:NH2 | 30:0:2332:A:H5' | 2.21 | 0.56 |
| 8:H:22:TYR:CZ | 30:0:1007:A:H2' | 2.41 | 0.56 |
| 13:M:24:GLN:NE2 | 13:M:27:ARG:HH11 | 2.04 | 0.56 |
| 4:D:159:PRO:O | 4:D:163:VAL:HG23 | 2.06 | 0.56 |
| 30:0:1130:U:H2' | 30:0:1131:G:O4' | 2.06 | 0.56 |
| 30:0:559:U:C5 | 30:0:560:U:C5 | 2.94 | 0.56 |
| 30:0:2482:G:H5' | 38:0:5036:HOH:O | 2.05 | 0.56 |
| 1:A:47:HIS:CD2 | 30:0:1654:U:H2' | 2.37 | 0.56 |
| 30:0:282:C:C2' | 30:0:282:C:O2 | 2.54 | 0.56 |
| 2:B:162:MET:HE2 | 2:B:310:ARG:HD3 | 1.87 | 0.56 |
| 22:V:42:ASN:HB3 | 38:V:7247:HOH:O | 2.06 | 0.56 |
| 18:R:29:LYS:HB3 | 38:R:8936:HOH:O | 2.06 | 0.56 |
| 30:0:151:A:C2 | 30:0:152:A:C2 | 2.94 | 0.56 |
| 30:0:2831:C:C2' | 30:0:2832:C:H5' | 2.36 | 0.56 |
| 30:0:1772:C:H5' | 30:0:1773:G:C5 | 2.41 | 0.56 |
| 4:D:103:ASN:ND2 | 4:D:134:LEU:H | 2.04 | 0.56 |
| 10:J:74:ARG:HB3 | 10:J:74:ARG:HH11 | 1.70 | 0.56 |
| 15:O:32:ARG:HH21 | 15:O:35:LYS:NZ | 2.04 | 0.55 |
| 38:M:8868:HOH:O | 30:0:2244:A:H1' | 2.06 | 0.55 |
| 2:B:156:LYS:HD3 | 38:0:3870:HOH:O | 2.05 | 0.55 |
| 31:9:49:G:H2' | 31:9:50:G:O4' | 2.05 | 0.55 |
| 30:0:1787:C:H4' | 30:0:2883:A:O4' | 2.06 | 0.55 |
| 14:N:61:ALA:HB3 | 14:N:88:ALA:HB2 | 1.88 | 0.55 |
| 3:C:47:GLY:HA2 | 3:C:92:PRO:HB2 | 1.87 | 0.55 |
| 30:0:1426:C:H2' | 38:0:9598:HOH:O | 2.06 | 0.55 |
| 30:0:1545:C:H2' | 30:0:1546:G:O4' | 2.06 | 0.55 |
| 30:0:553:G:O4' | 30:0:1325:G:H5' | 2.06 | 0.55 |
| 14:N:37:ARG:HH11 | 31:9:6:C:C5' | 2.15 | 0.55 |
| 30:0:1972:U:C2' | 30:0:1973:A:H5" | 2.36 | 0.55 |
| 11:K:45:PRO:HB2 | 38:0:7387:HOH:O | 2.06 | 0.55 |
| 12:L:136:ALA:HB3 | 38:L:8873:HOH:O | 2.05 | 0.55 |
| 30:0:2886:C:O2' | 30:0:2887:G:H5' | 2.07 | 0.55 |
| 14:N:80:SER:HB2 | 38:N:8833:HOH:O | 2.05 | 0.55 |
| 2:B:265:LEU:HD21 | 2:B:316:ARG:HD3 | 1.88 | 0.55 |
| 2:B:211:THR:HG23 | 30:0:2840:A:OP1 | 2.06 | 0.55 |
| 30:0:1191:A:C2' | 30:0:1193:A:H5' | 2.37 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:960:G:N3 | 30:0:960:G:C2' | 2.69 | 0.55 |
| 21:U:39:ASN:ND2 | 21:U:44:ARG:HH11 | 2.04 | 0.55 |
| 29:3:3:MET:O | 29:3:90:PHE:HA | 2.06 | 0.55 |
| 30:0:1202:A:H2' | 30:0:1203:G:C5' | 2.37 | 0.55 |
| 20:T:9:LYS:HD3 | 38:0:3761:HOH:O | 2.06 | 0.55 |
| 2:B:98:THR:HG22 | 30:0:2820:A:OP1 | 2.07 | 0.55 |
| 23:W:35:VAL:HG23 | 23:W:41:TYR:CD2 | 2.42 | 0.55 |
| 30:0:2599:A:H5" | 38:0:3384:HOH:O | 2.05 | 0.55 |
| 14:N:37:ARG:HD3 | 35:N:8807:CL:CL | 2.44 | 0.55 |
| 9:I:87:PRO:HG2 | 30:0:1181:A:H4' | 1.87 | 0.55 |
| 6:F:58:GLU:CD | 13:M:27:ARG:HH22 | 2.08 | 0.55 |
| 30:0:669:G:O2' | 30:0:670:G:H5' | 2.07 | 0.55 |
| 30:0:1120:U:H5' | 30:0:1121:G:OP2 | 2.07 | 0.55 |
| 14:N:12:ARG:HD3 | 14:N:18:THR:OG1 | 2.06 | 0.55 |
| 18:R:111:ILE:HG23 | 18:R:145:LEU:HD11 | 1.89 | 0.55 |
| 18:R:132:ARG:HG2 | 18:R:133:ALA:N | 2.21 | 0.55 |
| 4:D:173:GLU:HG3 | 4:D:174:VAL:H | 1.71 | 0.55 |
| 30:0:1790:C:H2' | 30:0:1791:U:C6 | 2.41 | 0.55 |
| 18:R:98:ASN:HD21 | 30:0:500:G:H21 | 1.54 | 0.55 |
| 27:1:21:ARG:HD2 | 27:1:37:CYS:SG | 2.47 | 0.55 |
| 15:O:25:VAL:CG1 | 30:0:710:G:H5' | 2.36 | 0.55 |
| 2:B:86:ALA:HA | 38:B:9045:HOH:O | 2.05 | 0.55 |
| 30:0:1972:U:H2' | 30:0:1973:A:C5' | 2.37 | 0.55 |
| 3:C:236:THR:HA | 38:C:8657:HOH:O | 2.07 | 0.55 |
| 10:J:69:TYR:CE1 | 30:0:2081:A:H4' | 2.42 | 0.55 |
| 25:Y:117:LEU:HA | 25:Y:174:VAL:HG11 | 1.88 | 0.55 |
| 18:R:59:PHE:O | 18:R:63:ASN:HB3 | 2.06 | 0.55 |
| 2:B:267:LYS:HE2 | 38:B:8994:HOH:O | 2.06 | 0.55 |
| 31:9:24:U:H3' | 31:9:25:G:C5' | 2.35 | 0.55 |
| 30:0:2514:U:OP1 | 30:0:2572:G:H1' | 2.06 | 0.55 |
| 30:0:2297:U:H2' | 30:0:2298:C:H6 | 1.71 | 0.55 |
| 4:D:103:ASN:HD22 | 4:D:134:LEU:H | 1.54 | 0.55 |
| 30:0:1544:U:O2' | 30:0:1545:C:H5' | 2.05 | 0.55 |
| 15:O:96:VAL:HG13 | 15:O:100:GLN:HB2 | 1.89 | 0.55 |
| 30:0:794:U:H3 | 30:0:819:A:H61 | 1.54 | 0.55 |
| 30:0:512:G:O3' | 30:0:513:A:H8 | 1.89 | 0.55 |
| 30:0:1706:G:C6 | 30:0:1707:G:C6 | 2.95 | 0.55 |
| 13:M:46:LEU:HG | 38:M:8921:HOH:O | 2.06 | 0.55 |
| 13:M:65:VAL:HG21 | 13:M:105:ALA:HB2 | 1.89 | 0.55 |
| 23:W:154:ARG:NH1 | 30:0:588:G:O6 | 2.40 | 0.55 |
| 30:0:2851:G:C2' | 30:0:2852:A:H5' | 2.37 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1504:A:H5' | 38:0:4423:HOH:O | 2.06 | 0.54 |
| 30:0:88:G:H5' | 30:0:88:G:H8 | 1.72 | 0.54 |
| 30:0:713:U:O5' | 30:0:713:U:H6 | 1.90 | 0.54 |
| 6:F:96:ALA:HA | 38:F:3111:HOH:O | 2.06 | 0.54 |
| 30:0:1915:U:O2' | 30:0:1916:C:H5' | 2.06 | 0.54 |
| 30:0:1202:A:H2' | 30:0:1203:G:O4' | 2.08 | 0.54 |
| 30:0:2790:C:HO2' | 30:0:2791:U:H6 | 1.54 | 0.54 |
| 4:D:131:THR:HG21 | 30:0:2348:C:H1' | 1.89 | 0.54 |
| 30:0:515:C:H5" | 38:0:5660:HOH:O | 2.06 | 0.54 |
| 30:0:1160:G:H2' | 38:0:5647:HOH:O | 2.07 | 0.54 |
| 23:W:137:GLN:HE21 | 23:W:141:HIS:CE1 | 2.13 | 0.54 |
| 30:0:1202:A:O2' | 30:0:1203:G:H5' | 2.07 | 0.54 |
| 1:A:190:ARG:NH2 | 1:A:207:GLN:OE1 | 2.40 | 0.54 |
| 30:0:1903:U:O2' | 30:0:1904:A:N7 | 2.40 | 0.54 |
| 30:0:644:G:N3 | 30:0:644:G:H5' | 2.22 | 0.54 |
| 23:W:88:THR:HG23 | 23:W:110:GLN:HE21 | 1.72 | 0.54 |
| 30:0:1730:G:H5" | 30:0:1731:C:H6 | 1.71 | 0.54 |
| 10:J:127:ILE:CG2 | 35:J:8801:CL:CL | 2.91 | 0.54 |
| 2:B:119:HIS:O | 2:B:121:PRO:HD3 | 2.07 | 0.54 |
| 20:T:38:ARG:NH1 | 38:T:6217:HOH:O | 2.41 | 0.54 |
| 21:U:9:CYS:HA | 21:U:52:THR:HG23 | 1.90 | 0.54 |
| 30:0:2326:C:H4' | 30:0:2412:G:H4' | 1.89 | 0.54 |
| 30:0:1521:C:H2' | 30:0:1522:A:H8 | 1.72 | 0.54 |
| 27:1:20:ARG:HG2 | 30:0:111:C:O2' | 2.08 | 0.54 |
| 14:N:4:PRO:HG3 | 31:9:69:U:OP1 | 2.07 | 0.54 |
| 27:1:25:LYS:CD | 28:2:49:GLU:H | 2.18 | 0.54 |
| 2:B:162:MET:HE1 | 2:B:308:LEU:HD21 | 1.89 | 0.54 |
| 2:B:51:VAL:HG13 | 2:B:53:LEU:HD13 | 1.90 | 0.54 |
| 30:0:2314:G:H2' | 30:0:2315:C:H5' | 1.90 | 0.54 |
| 30:0:553:G:H5' | 38:0:3505:HOH:O | 2.08 | 0.54 |
| 30:0:1406:A:H5' | 30:0:1407:A:C8 | 2.42 | 0.54 |
| 19:S:17:ASP:HB3 | 19:S:23:LYS:HB2 | 1.90 | 0.54 |
| 15:O:37:ARG:HD2 | 30:0:656:G:OP2 | 2.08 | 0.54 |
| 30:0:1041:U:H2' | 30:0:1042:U:H5' | 1.89 | 0.54 |
| 12:L:46:LEU:O | 30:0:2430:A:H4' | 2.07 | 0.54 |
| 30:0:1559:A:H4' | 38:0:5879:HOH:O | 2.08 | 0.54 |
| 9:I:118:ASN:HB3 | 30:0:1185:U:H5" | 1.88 | 0.54 |
| 30:0:2421:G:H2' | 38:0:4085:HOH:O | 2.07 | 0.54 |
| 30:0:920:C:H5" | 30:0:921:G:O5' | 2.08 | 0.54 |
| 30:0:1573:A:H2' | 30:0:1574:C:O4' | 2.08 | 0.54 |
| 30:0:2329:C:O2' | 30:0:2330:U:H5' | 2.08 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:64:ARG:HD3 | 4:D:67:ASP:HB3 | 1.90 | 0.54 |
| 19:S:33:SER:O | 19:S:37:VAL:HG23 | 2.08 | 0.54 |
| 30:0:1193:A:C2 | 30:0:1194:A:N6 | 2.76 | 0.54 |
| 2:B:212:GLN:HA | 30:0:1733:A:H4' | 1.89 | 0.54 |
| 23:W:21:LEU:HD22 | 23:W:26:ILE:HD13 | 1.89 | 0.54 |
| 30:0:1165:G:O3' | 30:0:1174:A:H4' | 2.08 | 0.54 |
| 30:0:812:A:H1' | 38:0:3964:HOH:O | 2.08 | 0.54 |
| 17:Q:25:PRO:HB2 | 38:9:9079:HOH:O | 2.07 | 0.54 |
| 30:0:2460:A:C2 | 30:0:2461:U:C2 | 2.95 | 0.54 |
| 1:A:101:GLU:OE2 | 1:A:131:HIS:HB2 | 2.08 | 0.54 |
| 30:0:1544:U:H2' | 30:0:1545:C:H6 | 1.72 | 0.53 |
| 30:0:1495:C:H1' | 30:0:1573:A:H1' | 1.90 | 0.53 |
| 25:Y:151:SER:HB3 | 25:Y:154:ARG:CB | 2.38 | 0.53 |
| 16:P:76:GLY:HA3 | 30:0:1785:G:OP1 | 2.08 | 0.53 |
| 2:B:84:LEU:HD23 | 2:B:142:LEU:HD23 | 1.91 | 0.53 |
| 30:0:822:C:H2' | 30:0:823:U:H6 | 1.73 | 0.53 |
| 30:0:2134:G:N2 | 30:0:2242:U:C2 | 2.76 | 0.53 |
| 24:X:76:ARG:HH11 | 24:X:76:ARG:HG3 | 1.71 | 0.53 |
| 22:V:57:LYS:HA | 22:V:60:GLN:HE21 | 1.72 | 0.53 |
| 30:0:1803:C:H2' | 30:0:1804:A:C8 | 2.43 | 0.53 |
| 31:9:54:A:C2' | 31:9:55:U:H5' | 2.38 | 0.53 |
| 30:0:2510:C:H5' | 30:0:2511:A:OP2 | 2.08 | 0.53 |
| 8:H:35:LYS:HE3 | 30:0:968:G:H1' | 1.88 | 0.53 |
| 4:D:27:ILE:HB | 4:D:69:ILE:O | 2.08 | 0.53 |
| 30:0:963:C:H2' | 30:0:964:G:C8 | 2.43 | 0.53 |
| 30:0:2667:G:H1' | 30:0:2914:A:N3 | 2.24 | 0.53 |
| 26:Z:61:HIS:HB2 | 26:Z:71:VAL:HB | 1.90 | 0.53 |
| 30:0:1289:C:O2' | 30:0:1290:G:H5' | 2.09 | 0.53 |
| 9:I:69:PRO:HA | 30:0:1164:U:OP1 | 2.09 | 0.53 |
| 25:Y:187:VAL:HB | 38:Y:8140:HOH:O | 2.08 | 0.53 |
| 30:0:2241:C:O2' | 30:0:2242:U:H5' | 2.09 | 0.53 |
| 30:0:1118:A:N6 | 30:0:1244:U:H3 | 1.99 | 0.53 |
| 31:9:29:C:C2' | 31:9:30:C:H5' | 2.38 | 0.53 |
| 16:P:13:VAL:HG21 | 16:P:41:ARG:HG2 | 1.89 | 0.53 |
| 30:0:821:U:O2' | 30:0:822:C:H5' | 2.08 | 0.53 |
| 30:0:2251:G:H2' | 30:0:2252:A:C8 | 2.43 | 0.53 |
| 30:0:349:U:H2' | 30:0:350:G:O4' | 2.09 | 0.53 |
| 1:A:51:ARG:NH1 | 1:A:120:ARG:O | 2.39 | 0.53 |
| 30:0:1632:A:C2' | 30:0:1633:C:H5' | 2.39 | 0.53 |
| 6:F:91:VAL:HG11 | 30:0:262:A:OP2 | 2.09 | 0.53 |
| 2:B:53:LEU:HD11 | 2:B:327:VAL:HG22 | 1.89 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:184:ARG:NH2 | 30:0:450:C:OP1 | 2.29 | 0.53 |
| 10:J:76:ASP:HA | 38:J:8865:HOH:O | 2.09 | 0.53 |
| 2:B:141:ARG:HD2 | 2:B:163:GLU:OE2 | 2.09 | 0.53 |
| 30:0:635:A:H2' | 30:0:636:G:H5" | 1.90 | 0.53 |
| 30:0:1909:A:N1 | 30:0:2128:G:H1' | 2.24 | 0.53 |
| 14:N:35:VAL:HG12 | 14:N:37:ARG:HG2 | 1.91 | 0.53 |
| 30:0:1166:A:C6 | 30:0:1167:G:C6 | 2.97 | 0.53 |
| 2:B:312:ARG:HD3 | 2:B:315:VAL:HG13 | 1.90 | 0.53 |
| 25:Y:151:SER:HB3 | 25:Y:154:ARG:HB2 | 1.90 | 0.53 |
| 5:E:107:PHE:CE1 | 5:E:152:THR:HB | 2.43 | 0.53 |
| 30:0:574:G:O2' | 30:0:575:A:H5' | 2.09 | 0.53 |
| 30:0:222:A:H2' | 30:0:223:G:O4' | 2.08 | 0.53 |
| 8:H:26:ILE:HA | 8:H:123:ILE:HG21 | 1.89 | 0.53 |
| 12:L:67:ARG:HB2 | 12:L:112:GLY:HA3 | 1.90 | 0.53 |
| 27:1:12:ASN:O | 30:0:1415:G:H5' | 2.08 | 0.53 |
| 30:0:559:U:C5' | 30:0:559:U:H6 | 2.19 | 0.53 |
| 30:0:2073:G:C6 | 30:0:2489:G:H4' | 2.44 | 0.53 |
| 30:0:2065:C:O2' | 30:0:2066:C:H5' | 2.09 | 0.53 |
| 14:N:25:ARG:HG2 | 30:0:2416:G:O2' | 2.09 | 0.53 |
| 14:N:132:ASN:O | 14:N:135:VAL:HG12 | 2.09 | 0.53 |
| 30:0:128:A:O2' | 30:0:129:A:H5' | 2.09 | 0.53 |
| 10:J:107:ASN:HD22 | 10:J:109:TYR:H | 1.57 | 0.53 |
| 30:0:2111:G:H1' | 38:0:9051:HOH:O | 2.08 | 0.53 |
| 30:0:2769:C:H2' | 30:0:2770:G:O4' | 2.09 | 0.53 |
| 5:E:139:GLU:OE2 | 30:0:2781:U:H1' | 2.09 | 0.53 |
| 30:0:441:A:H8 | 30:0:441:A:O5' | 1.92 | 0.53 |
| 30:0:290:C:O2' | 30:0:291:C:H5' | 2.09 | 0.53 |
| 14:N:139:TRP:HA | 14:N:139:TRP:HE3 | 1.74 | 0.53 |
| 6:F:34:ASN:HA | 13:M:4:ALA:HB2 | 1.91 | 0.53 |
| 30:0:1181:A:H2' | 30:0:1182:C:H5' | 1.90 | 0.52 |
| 31:9:3:A:H1' | 38:9:9037:HOH:O | 2.09 | 0.52 |
| 30:0:1594:C:O2' | 30:0:1595:G:H5' | 2.09 | 0.52 |
| 30:0:24:G:N2 | 30:0:518:G:H1' | 2.24 | 0.52 |
| 30:0:1625:U:H5" | 38:0:6037:HOH:O | 2.09 | 0.52 |
| 5:E:143:GLN:NE2 | 30:0:2780:C:H1' | 2.13 | 0.52 |
| 30:0:615:G:H2' | 30:0:616:U:C6 | 2.44 | 0.52 |
| 30:0:1733:A:C6 | 30:0:1734:C:C2 | 2.98 | 0.52 |
| 30:0:2500:C:O2' | 30:0:2501:G:H5' | 2.08 | 0.52 |
| 14:N:48:VAL:HG11 | 14:N:55:ASP:HB3 | 1.90 | 0.52 |
| 30:0:204:A:H2' | 30:0:205:U:H5' | 1.90 | 0.52 |
| 4:D:57:THR:HG23 | 4:D:63:ILE:HA | 1.91 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:58:VAL:HB | 4:D:62:ASP:HB3 | 1.89 | 0.52 |
| 30:0:90:A:H2' | 30:0:91:G:O4' | 2.08 | 0.52 |
| 30:0:1419:U:H2' | 30:0:1685:A:C2 | 2.44 | 0.52 |
| 31:9:59:C:H2' | 31:9:60:C:C6 | 2.43 | 0.52 |
| 30:0:1181:A:H1' | 38:0:7132:HOH:O | 2.09 | 0.52 |
| 1:A:223:ARG:HB2 | 30:0:2272:G:H5' | 1.90 | 0.52 |
| 28:2:49:GLU:HB2 | 38:2:719:HOH:O | 2.10 | 0.52 |
| 23:W:48:VAL:HG12 | 23:W:52:VAL:HB | 1.90 | 0.52 |
| 35:0:8813:CL:CL | 38:0:4697:HOH:O | 2.56 | 0.52 |
| 38:L:8841:HOH:O | 30:0:2453:G:H5" | 2.09 | 0.52 |
| 15:O:47:ARG:HG3 | 15:O:47:ARG:NH1 | 2.25 | 0.52 |
| 4:D:28:GLY:HA2 | 4:D:69:ILE:HG23 | 1.91 | 0.52 |
| 5:E:91:PHE:CE1 | 30:0:2694:A:H4' | 2.43 | 0.52 |
| 30:0:2598:U:O2 | 30:0:2600:A:H8 | 1.92 | 0.52 |
| 30:0:1216:G:O2' | 30:0:1217:G:H5' | 2.10 | 0.52 |
| 30:0:1461:U:H2' | 30:0:1462:C:C6 | 2.44 | 0.52 |
| 30:0:1161:A:C6 | 30:0:1162:G:N7 | 2.77 | 0.52 |
| 30:0:1189:A:H1' | 30:0:1209:C:C1' | 2.40 | 0.52 |
| 8:H:6:ALA:HB3 | 30:0:2521:A:OP2 | 2.09 | 0.52 |
| 30:0:1588:G:C6 | 30:0:1589:G:N1 | 2.77 | 0.52 |
| 30:0:1482:A:O2' | 30:0:1483:C:H5' | 2.10 | 0.52 |
| 25:Y:99:ALA:HB2 | 25:Y:233:TYR:CE2 | 2.44 | 0.52 |
| 2:B:305:ASP:O | 2:B:306:LYS:HB2 | 2.10 | 0.52 |
| 30:0:899:C:H5' | 38:0:3209:HOH:O | 2.09 | 0.52 |
| 16:P:134:VAL:O | 16:P:137:LEU:HB3 | 2.10 | 0.52 |
| 26:Z:74:GLN:HB2 | 26:Z:78:ILE:HG22 | 1.90 | 0.52 |
| 1:A:206:ARG:HD3 | 38:0:4620:HOH:O | 2.08 | 0.52 |
| 30:0:1196:C:H42 | 30:0:1204:C:H42 | 1.58 | 0.52 |
| 31:9:91:C:H2' | 31:9:92:G:O4' | 2.10 | 0.52 |
| 30:0:1202:A:H2' | 30:0:1203:G:H5' | 1.90 | 0.52 |
| 30:0:1871:U:O4' | 30:0:1873:G:C8 | 2.63 | 0.52 |
| 2:B:17:LYS:O | 2:B:260:HIS:HD2 | 1.91 | 0.52 |
| 30:0:1309:U:O2' | 30:0:1310:U:H5' | 2.09 | 0.52 |
| 17:Q:19:ARG:HH21 | 31:9:11:A:P | 2.33 | 0.52 |
| 25:Y:169:ARG:HD3 | 30:0:1328:A:C8 | 2.44 | 0.52 |
| 16:P:91:LYS:O | 16:P:95:GLU:HG3 | 2.08 | 0.52 |
| 3:C:63:SER:OG | 30:0:2101:A:H2' | 2.09 | 0.52 |
| 21:U:6:CYS:HB2 | 21:U:32:CYS:HB3 | 1.90 | 0.52 |
| 14:N:67:ALA:HA | 14:N:71:TRP:HB3 | 1.92 | 0.52 |
| 11:K:113:ILE:HD12 | 11:K:128:ALA:HB2 | 1.92 | 0.52 |
| 30:0:136:C:H2' | 30:0:137:U:O4' | 2.09 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:T:38:ARG:HH21 | 30:0:306:A:P | 2.33 | 0.52 |
| 30:0:2866:U:C2 | 30:0:2891:A:C8 | 2.98 | 0.52 |
| 30:0:2273:C:H5" | 38:0:4515:HOH:O | 2.10 | 0.52 |
| 31:9:108:C:H2' | 31:9:109:G:C8 | 2.45 | 0.52 |
| 30:0:1029:U:O2' | 30:0:1273:C:OP1 | 2.25 | 0.52 |
| 23:W:117:ARG:HD3 | 30:0:1287:A:O4' | 2.10 | 0.52 |
| 11:K:10:GLN:H | 11:K:10:GLN:NE2 | 1.96 | 0.52 |
| 30:0:2032:U:O2' | 30:0:2033:G:H5" | 2.09 | 0.52 |
| 9:I:73:LEU:HD12 | 9:I:107:LYS:HZ1 | 1.73 | 0.52 |
| 30:0:1964:U:C2' | 30:0:1964:U:O2 | 2.58 | 0.52 |
| 3:C:217:GLU:HG3 | 30:0:672:G:O6 | 2.10 | 0.52 |
| 18:R:33:ARG:NH1 | 38:R:8947:HOH:O | 2.42 | 0.52 |
| 11:K:18:ILE:HG22 | 11:K:93:ASN:HB2 | 1.92 | 0.52 |
| 30:0:2112:A:H2' | 30:0:2113:G:C8 | 2.45 | 0.52 |
| 9:I:112:LEU:HD12 | 30:0:1162:G:H1' | 1.92 | 0.51 |
| 30:0:2827:A:H2' | 30:0:2828:G:O4' | 2.10 | 0.51 |
| 30:0:407:A:H8 | 38:0:4468:HOH:O | 1.93 | 0.51 |
| 30:0:1333:U:H2' | 30:0:1334:C:H6 | 1.75 | 0.51 |
| 30:0:152:A:H2' | 30:0:153:C:C6 | 2.45 | 0.51 |
| 22:V:56:ILE:O | 22:V:60:GLN:HG3 | 2.09 | 0.51 |
| 31:9:59:C:H6 | 31:9:59:C:O5' | 1.92 | 0.51 |
| 30:0:951:A:C2' | 30:0:952:G:H5' | 2.39 | 0.51 |
| 8:H:70:LEU:O | 8:H:74:ARG:HB2 | 2.09 | 0.51 |
| 30:0:2636:C:H3' | 38:0:9279:HOH:O | 2.09 | 0.51 |
| 30:0:876:A:N3 | 30:0:876:A:H2' | 2.23 | 0.51 |
| 30:0:792:G:O2' | 30:0:793:A:H5' | 2.11 | 0.51 |
| 31:9:58:G:H1' | 38:9:9067:HOH:O | 2.09 | 0.51 |
| 10:J:54:VAL:HG11 | 10:J:138:THR:HG21 | 1.92 | 0.51 |
| 30:0:638:C:H2' | 30:0:639:A:C8 | 2.46 | 0.51 |
| 31:9:42:C:H5' | 31:9:43:G:OP2 | 2.10 | 0.51 |
| 30:0:1163:G:H2' | 30:0:1164:U:C5 | 2.44 | 0.51 |
| 30:0:2896:A:N3 | 30:0:2896:A:H2' | 2.25 | 0.51 |
| 30:0:154:C:H2' | 30:0:155:C:H6 | 1.76 | 0.51 |
| 30:0:821:U:H2' | 30:0:822:C:H6 | 1.75 | 0.51 |
| 24:X:21:PRO:HG2 | 24:X:24:LYS:HD3 | 1.91 | 0.51 |
| 30:0:1279:U:O2 | 30:0:1279:U:H2' | 2.09 | 0.51 |
| 22:V:12:THR:HG23 | 22:V:14:ALA:H | 1.74 | 0.51 |
| 30:0:603:A:H4' | 30:0:605:C:C6 | 2.46 | 0.51 |
| 30:0:255:A:H2' | 30:0:256:C:H6 | 1.74 | 0.51 |
| 30:0:1755:A:H2' | 30:0:1756:G:O4' | 2.11 | 0.51 |
| 2:B:125:GLU:O | 2:B:129:ARG:HG3 | 2.10 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1137:G:H1' | 38:0:3884:HOH:O | 2.09 | 0.51 |
| 30:0:2724:U:H2' | 30:0:2725:G:O4' | 2.10 | 0.51 |
| 2:B:254:GLN:HG2 | 2:B:255:GLY:N | 2.25 | 0.51 |
| 30:0:1525:G:H5' | 30:0:1526:A:OP2 | 2.11 | 0.51 |
| 30:0:2566:A:C2 | 30:0:2696:G:O4' | 2.63 | 0.51 |
| 30:0:2478:U:O2' | 30:0:2479:A:H5' | 2.10 | 0.51 |
| 30:0:1081:A:H5" | 38:0:3158:HOH:O | 2.10 | 0.51 |
| 5:E:84:MET:HG2 | 5:E:168:ILE:HA | 1.93 | 0.51 |
| 30:0:877:G:C2 | 30:0:885:G:O4' | 2.63 | 0.51 |
| 30:0:1524:U:H5" | 30:0:1524:U:C6 | 2.46 | 0.51 |
| 23:W:43:GLY:HA3 | 30:0:945:U:O2' | 2.11 | 0.51 |
| 30:0:684:G:H2' | 30:0:685:C:C6 | 2.46 | 0.51 |
| 2:B:248:ARG:O | 2:B:251:VAL:HG22 | 2.11 | 0.51 |
| 30:0:2758:G:H2' | 30:0:2759:C:C6 | 2.46 | 0.51 |
| 31:9:54:A:HO2' | 31:9:55:U:H5' | 1.75 | 0.51 |
| 23:W:88:THR:HG22 | 23:W:89:ASP:N | 2.18 | 0.51 |
| 31:9:31:C:C2 | 31:9:50:G:C2 | 2.99 | 0.51 |
| 30:0:2823:G:H4' | 30:0:2827:A:O4' | 2.11 | 0.51 |
| 24:X:43:VAL:HG12 | 24:X:44:ASP:N | 2.26 | 0.51 |
| 3:C:111:VAL:HB | 38:C:8519:HOH:O | 2.11 | 0.51 |
| 6:F:39:SER:HB3 | 6:F:45:ALA:HB2 | 1.91 | 0.51 |
| 3:C:43:LYS:HG2 | 30:0:449:A:N7 | 2.26 | 0.51 |
| 1:A:33:GLU:CD | 1:A:33:GLU:H | 2.14 | 0.51 |
| 1:A:69:LEU:HB3 | 38:A:9039:HOH:O | 2.11 | 0.51 |
| 30:0:1185:U:H5' | 38:0:7483:HOH:O | 2.09 | 0.51 |
| 30:0:2830:U:O2' | 30:0:2831:C:H5' | 2.11 | 0.51 |
| 25:Y:189:ASN:HA | 25:Y:217:ILE:HD11 | 1.93 | 0.51 |
| 30:0:10:U:C6 | 30:0:10:U:H3' | 2.46 | 0.51 |
| 4:D:99:ASP:HB3 | 4:D:103:ASN:HB2 | 1.90 | 0.51 |
| 30:0:821:U:H2' | 30:0:822:C:C6 | 2.46 | 0.51 |
| 30:0:2344:G:N3 | 30:0:2344:G:H2' | 2.26 | 0.51 |
| 30:0:955:A:C2 | 30:0:1013:A:C4 | 2.99 | 0.51 |
| 30:0:958:G:O2' | 30:0:959:C:H5' | 2.10 | 0.51 |
| 12:L:148:GLU:HA | 38:L:8872:HOH:O | 2.10 | 0.51 |
| 11:K:10:GLN:N | 11:K:10:GLN:HE21 | 1.97 | 0.51 |
| 30:0:2768:A:N3 | 30:0:2768:A:H3' | 2.26 | 0.51 |
| 10:J:45:VAL:HG21 | 10:J:129:PHE:CD1 | 2.45 | 0.51 |
| 30:0:1245:C:O5' | 30:0:1245:C:H6 | 1.93 | 0.51 |
| 16:P:40:VAL:O | 16:P:44:VAL:HG23 | 2.11 | 0.51 |
| 30:0:2638:G:H1' | 38:0:4596:HOH:O | 2.11 | 0.51 |
| 2:B:5:ARG:NH1 | 30:0:2547:C:OP2 | 2.44 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:407:A:H5' | 38:0:6041:HOH:O | 2.11 | 0.51 |
| 1:A:179:MET:HG2 | 1:A:186:TRP:CB | 2.41 | 0.51 |
| 19:S:57:THR:HG22 | 19:S:58:MET:N | 2.26 | 0.51 |
| 25:Y:204:ARG:HH22 | 30:0:553:G:P | 2.33 | 0.51 |
| 30:0:1614:G:H2' | 38:0:4642:HOH:O | 2.10 | 0.51 |
| 30:0:2102:G:H5' | 30:0:2538:A:C2 | 2.45 | 0.51 |
| 30:0:1118:A:C8 | 30:0:1119:G:H5" | 2.46 | 0.51 |
| 30:0:1667:A:C8 | 30:0:1667:A:H5' | 2.44 | 0.51 |
| 2:B:190:MET:HE2 | 2:B:194:PHE:CD1 | 2.46 | 0.51 |
| 30:0:18:C:H2' | 30:0:19:U:C6 | 2.46 | 0.51 |
| 2:B:36:PRO:HA | 2:B:168:GLY:HA3 | 1.93 | 0.51 |
| 26:Z:57:MET:SD | 26:Z:73:ARG:HD2 | 2.51 | 0.51 |
| 30:0:877:G:C5' | 30:0:878:G:OP1 | 2.55 | 0.50 |
| 30:0:1857:A:N6 | 30:0:2247:C:H1' | 2.26 | 0.50 |
| 2:B:140:LEU:HD12 | 2:B:174:ARG:HG3 | 1.91 | 0.50 |
| 6:F:38:LYS:HE3 | 30:0:244:C:OP2 | 2.11 | 0.50 |
| 14:N:169:PRO:O | 14:N:172:PHE:HB3 | 2.11 | 0.50 |
| 30:0:2858:U:H2' | 30:0:2859:C:C6 | 2.46 | 0.50 |
| 2:B:221:GLN:HE22 | 11:K:42:ASN:HD22 | 1.59 | 0.50 |
| 30:0:2347:C:H2' | 30:0:2348:C:H6 | 1.76 | 0.50 |
| 2:B:36:PRO:HG3 | 2:B:169:GLY:H | 1.75 | 0.50 |
| 30:0:2681:A:H8 | 38:0:5592:HOH:O | 1.92 | 0.50 |
| 31:9:52:A:H2' | 31:9:53:G:O4' | 2.10 | 0.50 |
| 30:0:1829:A:C2' | 30:0:1830:C:H5' | 2.40 | 0.50 |
| 30:0:1829:A:H2' | 30:0:1830:C:H5' | 1.94 | 0.50 |
| 30:0:1284:G:O2' | 30:0:1285:U:H5' | 2.11 | 0.50 |
| 38:I:5331:HOH:O | 30:0:1164:U:H5 | 1.94 | 0.50 |
| 30:0:1194:A:N1 | 30:0:1195:G:C6 | 2.79 | 0.50 |
| 30:0:2505:G:H8 | 38:0:5653:HOH:O | 1.94 | 0.50 |
| 30:0:694:A:C2' | 30:0:695:C:H5' | 2.41 | 0.50 |
| 2:B:280:VAL:HG13 | 2:B:334:SER:HA | 1.93 | 0.50 |
| 30:0:1163:G:H2' | 30:0:1164:U:C6 | 2.45 | 0.50 |
| 30:0:1166:A:C6 | 30:0:1181:A:C2 | 2.99 | 0.50 |
| 4:D:69:ILE:HD12 | 30:0:2346:C:H5' | 1.93 | 0.50 |
| 30:0:2102:G:C2 | 30:0:2104:C:C4 | 3.00 | 0.50 |
| 14:N:143:ARG:HH21 | 14:N:169:PRO:HB2 | 1.75 | 0.50 |
| 30:0:1921:A:O2' | 30:0:1922:A:H5' | 2.12 | 0.50 |
| 2:B:62:ARG:HA | 2:B:65:MET:CE | 2.41 | 0.50 |
| 24:X:78:GLU:HG2 | 24:X:79:GLU:H | 1.75 | 0.50 |
| 1:A:109:GLU:HG2 | 1:A:116:GLY:H | 1.75 | 0.50 |
| 30:0:1190:G:N3 | 30:0:1190:G:H3' | 2.26 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2718:C:H6 | 30:0:2718:C:H5' | 1.77 | 0.50 |
| 30:0:1118:A:H8 | 30:0:1119:G:H5" | 1.77 | 0.50 |
| 30:0:920:C:H5' | 30:0:921:G:C4 | 2.46 | 0.50 |
| 30:0:255:A:O2' | 30:0:256:C:H5' | 2.12 | 0.50 |
| 30:0:1762:C:H4' | 38:0:4668:HOH:O | 2.11 | 0.50 |
| 30:0:2256:G:C2' | 30:0:2257:G:H5' | 2.42 | 0.50 |
| 17:Q:66:LYS:HB2 | 17:Q:70:ALA:O | 2.11 | 0.50 |
| 30:0:368:C:C2' | 30:0:369:G:H5' | 2.42 | 0.50 |
| 8:H:59:GLN:HG2 | 8:H:129:ARG:HG2 | 1.92 | 0.50 |
| 30:0:12:U:C2' | 30:0:13:G:H5' | 2.41 | 0.50 |
| 30:0:1819:G:C2' | 30:0:1820:G:H5' | 2.41 | 0.50 |
| 1:A:191:GLY:HA2 | 1:A:194:MET:CE | 2.41 | 0.50 |
| 10:J:74:ARG:O | 10:J:78:ILE:HG12 | 2.11 | 0.50 |
| 30:0:1521:C:C2 | 30:0:1522:A:C8 | 3.00 | 0.50 |
| 10:J:107:ASN:HD21 | 10:J:109:TYR:HB2 | 1.76 | 0.50 |
| 10:J:107:ASN:ND2 | 10:J:109:TYR:H | 2.09 | 0.50 |
| 30:0:2553:A:H2' | 30:0:2553:A:N3 | 2.26 | 0.50 |
| 1:A:212:PRO:HB2 | 38:0:4369:HOH:O | 2.12 | 0.50 |
| 30:0:2730:G:O2' | 30:0:2731:G:H5' | 2.11 | 0.50 |
| 9:I:82:THR:CG2 | 30:0:1168:C:H5" | 2.42 | 0.50 |
| 30:0:1131:G:C6 | 30:0:1230:A:C4 | 3.00 | 0.50 |
| 30:0:559:U:C3' | 30:0:559:U:C6 | 2.95 | 0.50 |
| 30:0:1522:A:C2 | 30:0:1665:G:C6 | 2.99 | 0.50 |
| 30:0:2729:C:O2' | 30:0:2730:G:H5' | 2.10 | 0.50 |
| 30:0:1205:U:C2' | 30:0:1206:U:C5' | 2.84 | 0.50 |
| 5:E:143:GLN:NE2 | 30:0:2779:G:H21 | 2.10 | 0.50 |
| 30:0:1406:A:H4' | 30:0:1407:A:H5" | 1.93 | 0.50 |
| 30:0:2597:U:H2' | 30:0:2598:U:H5' | 1.94 | 0.50 |
| 30:0:2445:U:H2' | 30:0:2446:G:C8 | 2.47 | 0.50 |
| 9:I:95:LEU:HD23 | 9:I:99:GLN:OE1 | 2.11 | 0.50 |
| 9:I:87:PRO:HD3 | 38:0:3242:HOH:O | 2.12 | 0.50 |
| 30:0:2291:A:N9 | 30:0:2309:C:H5' | 2.26 | 0.50 |
| 30:0:2909:G:H2' | 30:0:2910:A:H8 | 1.76 | 0.50 |
| 30:0:2756:U:H3 | 30:0:2896:A:H2 | 1.57 | 0.50 |
| 6:F:58:GLU:HA | 6:F:61:MET:HE2 | 1.94 | 0.50 |
| 30:0:204:A:C2' | 30:0:205:U:H5' | 2.41 | 0.50 |
| 13:M:28:GLN:O | 13:M:32:ARG:HG3 | 2.12 | 0.50 |
| 4:D:88:LEU:HB2 | 4:D:89:PRO:HD3 | 1.94 | 0.50 |
| 30:0:1209:C:C2 | 30:0:1210:G:C8 | 3.00 | 0.49 |
| 13:M:171:ARG:NH2 | 30:0:189:A:OP1 | 2.45 | 0.49 |
| 31:9:3:A:H2' | 38:9:9040:HOH:O | 2.11 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:67:A:H5" | 30:0:69:A:C8 | 2.47 | 0.49 |
| 1:A:199:HIS:HE1 | 30:0:1881:A:OP1 | 1.95 | 0.49 |
| 2:B:320:GLN:HE21 | 2:B:321:PRO:CD | 2.24 | 0.49 |
| 30:0:73:U:O2' | 30:0:74:G:H5' | 2.12 | 0.49 |
| 23:W:64:THR:O | 23:W:68:THR:HG22 | 2.11 | 0.49 |
| 30:0:1707:G:H1' | 30:0:1711:A:N6 | 2.26 | 0.49 |
| 14:N:77:ASN:OD1 | 14:N:79:PRO:HD2 | 2.12 | 0.49 |
| 30:0:941:G:C5 | 30:0:942:U:C4 | 3.00 | 0.49 |
| 26:Z:34:SER:HA | 30:0:797:A:H5' | 1.94 | 0.49 |
| 30:0:2712:G:H5' | 38:0:5233:HOH:O | 2.11 | 0.49 |
| 10:J:75:PRO:HG2 | 10:J:105:LEU:CD2 | 2.38 | 0.49 |
| 30:0:256:C:H2' | 30:0:257:G:O4' | 2.12 | 0.49 |
| 2:B:62:ARG:HA | 2:B:65:MET:HE2 | 1.93 | 0.49 |
| 30:0:2831:C:C2 | 30:0:2910:A:C2 | 3.00 | 0.49 |
| 30:0:1878:G:O2' | 30:0:1879:U:OP2 | 2.30 | 0.49 |
| 2:B:144:THR:HG22 | 2:B:145:HIS:N | 2.27 | 0.49 |
| 30:0:652:G:H8 | 38:0:3021:HOH:O | 1.95 | 0.49 |
| 6:F:58:GLU:HB3 | 13:M:8:ILE:HG23 | 1.93 | 0.49 |
| 3:C:107:ARG:O | 3:C:111:VAL:HG23 | 2.13 | 0.49 |
| 1:A:33:GLU:O | 1:A:34:ASP:HB2 | 2.12 | 0.49 |
| 30:0:946:C:O2' | 30:0:947:U:H5' | 2.12 | 0.49 |
| 27:1:28:HIS:HE1 | 30:0:776:A:OP1 | 1.94 | 0.49 |
| 30:0:333:G:O2' | 30:0:334:G:H5' | 2.13 | 0.49 |
| 30:0:702:G:C2 | 30:0:703:G:C8 | 3.00 | 0.49 |
| 10:J:88:PRO:HA | 35:J:8802:CL:CL | 2.49 | 0.49 |
| 11:K:34:VAL:HG21 | 11:K:46:LYS:O | 2.12 | 0.49 |
| 30:0:185:G:H4' | 30:0:186:A:H4' | 1.93 | 0.49 |
| 30:0:1909:A:H2' | 30:0:1910:A:C8 | 2.48 | 0.49 |
| 4:D:50:VAL:HG13 | 31:9:41:C:O4' | 2.12 | 0.49 |
| 16:P:81:LYS:HG2 | 38:0:9543:HOH:O | 2.12 | 0.49 |
| 30:0:1187:U:O2' | 30:0:1189:A:H2 | 1.95 | 0.49 |
| 30:0:2781:U:O2' | 30:0:2782:G:H5' | 2.12 | 0.49 |
| 30:0:711:G:N2 | 30:0:718:C:C2 | 2.80 | 0.49 |
| 30:0:2004:U:H5" | 30:0:2005:G:C8 | 2.47 | 0.49 |
| 30:0:1377:C:H1' | 38:0:9041:HOH:O | 2.12 | 0.49 |
| 27:1:16:HIS:HE1 | 30:0:775:G:OP1 | 1.95 | 0.49 |
| 30:0:947:U:H2' | 30:0:948:G:H8 | 1.77 | 0.49 |
| 30:0:1768:C:H2' | 30:0:1769:C:O4' | 2.13 | 0.49 |
| 16:P:7:LYS:HD3 | 16:P:21:VAL:CG2 | 2.41 | 0.49 |
| 4:D:51:ARG:HH11 | 4:D:68:PRO:HB3 | 1.76 | 0.49 |
| 30:0:95:A:H5" | 30:0:97:G:O4' | 2.13 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1607:A:C4 | 30:0:1608:G:C8 | 3.00 | 0.49 |
| 20:T:18:GLU:O | 20:T:21:LYS:HG2 | 2.11 | 0.49 |
| 30:0:363:C:H2' | 30:0:364:U:H6 | 1.77 | 0.49 |
| 5:E:47:VAL:HG11 | 5:E:69:ILE:HD13 | 1.94 | 0.49 |
| 2:B:162:MET:CE | 2:B:308:LEU:HD21 | 2.42 | 0.49 |
| 30:0:1588:G:C6 | 30:0:1589:G:C6 | 3.01 | 0.49 |
| 23:W:5:VAL:HG11 | 23:W:153:MET:HE3 | 1.94 | 0.49 |
| 18:R:29:LYS:HE2 | 30:0:524:A:C5' | 2.42 | 0.49 |
| 15:O:25:VAL:HG12 | 30:0:709:G:O3' | 2.13 | 0.49 |
| 30:0:2112:A:H2' | 30:0:2113:G:H8 | 1.77 | 0.49 |
| 30:0:951:A:O2' | 30:0:952:G:H5' | 2.13 | 0.49 |
| 30:0:1854:C:H2' | 30:0:1875:A:H61 | 1.78 | 0.49 |
| 11:K:130:MET:SD | 21:U:25:ASP:O | 2.70 | 0.49 |
| 30:0:734:U:O2' | 30:0:736:A:N7 | 2.44 | 0.49 |
| 30:0:1189:A:N7 | 30:0:1190:G:C8 | 2.81 | 0.49 |
| 10:J:70:PHE:CD1 | 30:0:2676:C:H4' | 2.46 | 0.49 |
| 30:0:1730:G:C5' | 30:0:1731:C:H6 | 2.25 | 0.49 |
| 30:0:1778:A:H2' | 30:0:1779:A:H5' | 1.94 | 0.49 |
| 30:0:952:G:N3 | 30:0:2302:A:H2' | 2.28 | 0.49 |
| 29:3:11:CYS:SG | 29:3:14:CYS:HB2 | 2.52 | 0.49 |
| 29:3:30:GLN:NE2 | 38:3:9043:HOH:O | 2.43 | 0.49 |
| 30:0:1568:G:C5 | 30:0:1569:U:C5 | 3.01 | 0.49 |
| 31:9:31:C:C2 | 31:9:50:G:N2 | 2.81 | 0.49 |
| 30:0:2498:C:C2' | 30:0:2499:U:H5' | 2.43 | 0.49 |
| 30:0:2481:G:C3' | 30:0:2482:G:H5" | 2.42 | 0.49 |
| 30:0:1730:G:H5' | 30:0:1731:C:H5 | 1.78 | 0.49 |
| 1:A:53:ALA:HB3 | 38:A:9068:HOH:O | 2.12 | 0.49 |
| 25:Y:149:GLN:O | 25:Y:154:ARG:NH1 | 2.46 | 0.49 |
| 2:B:142:LEU:HD21 | 2:B:178:ALA:HB1 | 1.94 | 0.49 |
| 31:9:73:A:N1 | 31:9:108:C:O2 | 2.45 | 0.49 |
| 30:0:1682:A:H5" | 38:0:9457:HOH:O | 2.13 | 0.49 |
| 30:0:1066:U:H2' | 30:0:1067:A:C8 | 2.47 | 0.49 |
| 30:0:2829:G:O2' | 30:0:2830:U:H5' | 2.13 | 0.49 |
| 10:J:131:THR:HG22 | 10:J:133:GLY:H | 1.78 | 0.49 |
| 20:T:97:ARG:NH2 | 30:0:309:C:OP1 | 2.46 | 0.49 |
| 25:Y:189:ASN:HD22 | 25:Y:192:ASP:H | 1.61 | 0.49 |
| 1:A:81:GLN:HB2 | 1:A:92:ASN:ND2 | 2.28 | 0.49 |
| 30:0:2890:A:H8 | 30:0:2890:A:H5" | 1.77 | 0.49 |
| 30:0:1783:A:O2' | 30:0:1784:U:H5' | 2.12 | 0.49 |
| 30:0:503:G:H2' | 30:0:504:G:H8 | 1.77 | 0.49 |
| 8:H:150:LYS:HA | 38:H:230:HOH:O | 2.13 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:Z:55:SER:O | 26:Z:59:GLU:HG3 | 2.12 | 0.49 |
| 30:0:2756:U:N3 | 30:0:2896:A:C2 | 2.75 | 0.49 |
| 30:0:2578:G:C8 | 30:0:2578:G:H5' | 2.43 | 0.49 |
| 1:A:48:ASP:HB3 | 38:A:9068:HOH:O | 2.13 | 0.49 |
| 30:0:1398:G:H2' | 30:0:1399:A:H8 | 1.75 | 0.49 |
| 1:A:211:LYS:HD2 | 38:A:9083:HOH:O | 2.13 | 0.49 |
| 30:0:2064:U:H5' | 30:0:2652:U:O3' | 2.13 | 0.49 |
| 30:0:1007:A:H1' | 38:0:3138:HOH:O | 2.12 | 0.49 |
| 25:Y:170:SER:OG | 25:Y:175:ARG:HG3 | 2.12 | 0.49 |
| 11:K:82:ARG:NH2 | 11:K:115:ARG:HG2 | 2.28 | 0.49 |
| 30:0:2847:G:O2' | 30:0:2848:G:H5' | 2.12 | 0.49 |
| 30:0:1816:C:H2' | 30:0:1817:U:O4' | 2.13 | 0.49 |
| 30:0:1180:U:H2' | 30:0:1181:A:O4' | 2.13 | 0.48 |
| 3:C:76:ARG:HD3 | 38:C:8570:HOH:O | 2.13 | 0.48 |
| 20:T:2:LYS:HG2 | 30:0:447:A:OP1 | 2.13 | 0.48 |
| 24:X:23:HIS:HD2 | 38:0:9959:HOH:O | 1.96 | 0.48 |
| 30:0:703:G:O2' | 30:0:704:C:H5' | 2.13 | 0.48 |
| 30:0:1016:U:O2' | 30:0:2303:A:N7 | 2.38 | 0.48 |
| 23:W:125:HIS:CE1 | 30:0:1097:A:H5" | 2.47 | 0.48 |
| 30:0:1497:G:H4' | 30:0:1627:G:O2' | 2.13 | 0.48 |
| 31:9:92:G:C6 | 31:9:93:A:C6 | 3.01 | 0.48 |
| 15:O:32:ARG:HD3 | 15:O:32:ARG:O | 2.13 | 0.48 |
| 30:0:814:G:H2' | 30:0:815:U:C6 | 2.48 | 0.48 |
| 30:0:69:A:H2' | 30:0:70:A:OP2 | 2.12 | 0.48 |
| 22:V:39:ALA:N | 22:V:40:PRO:HD2 | 2.25 | 0.48 |
| 30:0:613:C:H2' | 30:0:614:U:C6 | 2.44 | 0.48 |
| 12:L:18:HIS:HB2 | 30:0:903:U:O4 | 2.13 | 0.48 |
| 30:0:1676:G:H1' | 38:0:9434:HOH:O | 2.13 | 0.48 |
| 30:0:499:G:O2' | 30:0:500:G:H5' | 2.13 | 0.48 |
| 2:B:140:LEU:CD1 | 2:B:174:ARG:HG3 | 2.44 | 0.48 |
| 30:0:1323:G:H5' | 38:0:4709:HOH:O | 2.13 | 0.48 |
| 31:9:61:C:H2' | 31:9:62:A:H8 | 1.77 | 0.48 |
| 30:0:626:U:C4 | 30:0:627:G:C6 | 3.01 | 0.48 |
| 30:0:371:U:O2' | 30:0:372:A:H5' | 2.13 | 0.48 |
| 30:0:2510:C:H42 | 30:0:2564:G:N2 | 2.11 | 0.48 |
| 16:P:88:GLN:HE21 | 30:0:1800:G:H1' | 1.76 | 0.48 |
| 30:0:308:U:C4 | 30:0:342:C:H1' | 2.48 | 0.48 |
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:HB3 | 1.93 | 0.48 |
| 30:0:2353:A:H4' | 30:0:2354:A:O5' | 2.13 | 0.48 |
| 30:0:961:A:H4' | 38:0:6790:HOH:O | 2.13 | 0.48 |
| 25:Y:154:ARG:HH22 | 30:0:1071:G:H4' | 1.78 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:76:ARG:NE | 31:9:44:A:O4' | 2.46 | 0.48 |
| 30:0:2433:A:H2' | 30:0:2434:A:C8 | 2.48 | 0.48 |
| 24:X:30:MET:HG2 | 30:0:1384:C:H5' | 1.94 | 0.48 |
| 30:0:2831:C:H6 | 38:0:7228:HOH:O | 1.96 | 0.48 |
| 30:0:581:G:O2' | 30:0:582:U:H5' | 2.12 | 0.48 |
| 14:N:110:THR:HB | 14:N:113:SER:OG | 2.13 | 0.48 |
| 30:0:1377:C:H6 | 30:0:1377:C:C5' | 2.25 | 0.48 |
| 5:E:69:ILE:HA | 5:E:72:MET:CE | 2.44 | 0.48 |
| 31:9:39:U:H1' | 31:9:44:A:H61 | 1.78 | 0.48 |
| 17:Q:7:LEU:HD12 | 30:0:2424:U:H1' | 1.96 | 0.48 |
| 30:0:1087:G:H4' | 30:0:1088:A:OP1 | 2.12 | 0.48 |
| 30:0:466:A:H2' | 30:0:467:G:O4' | 2.13 | 0.48 |
| 30:0:1190:G:H2' | 38:0:4064:HOH:O | 2.13 | 0.48 |
| 13:M:99:ARG:HD2 | 13:M:167:GLY:CA | 2.41 | 0.48 |
| 30:0:2908:A:O2' | 30:0:2909:G:H5' | 2.13 | 0.48 |
| 30:0:2768:A:C2' | 30:0:2769:C:O4' | 2.61 | 0.48 |
| 1:A:140:LEU:HB3 | 1:A:141:PRO:HD2 | 1.94 | 0.48 |
| 27:1:1:THR:HB | 38:0:7157:HOH:O | 2.13 | 0.48 |
| 15:O:14:LEU:CD2 | 15:O:102:ILE:HD11 | 2.43 | 0.48 |
| 30:0:513:A:N3 | 38:0:3665:HOH:O | 2.35 | 0.48 |
| 30:0:2256:G:O2' | 30:0:2257:G:H5' | 2.14 | 0.48 |
| 2:B:223:ARG:HG3 | 2:B:232:TRP:O | 2.13 | 0.48 |
| 11:K:12:LEU:HB2 | 11:K:47:ALA:HB3 | 1.96 | 0.48 |
| 24:X:61:ARG:O | 30:0:2744:G:H5" | 2.14 | 0.48 |
| 31:9:71:C:H2' | 31:9:72:C:H6 | 1.79 | 0.48 |
| 30:0:790:A:H1' | 30:0:1710:A:H2' | 1.95 | 0.48 |
| 30:0:802:G:O2' | 30:0:803:C:H5' | 2.13 | 0.48 |
| 30:0:2754:G:C2' | 30:0:2755:G:H5' | 2.43 | 0.48 |
| 30:0:1343:C:H2' | 30:0:1344:G:O5' | 2.14 | 0.48 |
| 30:0:1520:G:H2' | 30:0:1521:C:C6 | 2.48 | 0.48 |
| 11:K:41:LYS:HA | 30:0:2582:G:O3' | 2.14 | 0.48 |
| 16:P:7:LYS:HD3 | 16:P:21:VAL:HG22 | 1.95 | 0.48 |
| 30:0:305:A:C5 | 30:0:329:A:C2 | 3.02 | 0.48 |
| 4:D:23:VAL:HG12 | 4:D:130:VAL:HG22 | 1.96 | 0.48 |
| 30:0:1311:G:C2 | 30:0:1312:G:C8 | 3.01 | 0.48 |
| 14:N:65:ASP:HB3 | 38:N:8821:HOH:O | 2.13 | 0.48 |
| 8:H:165:ARG:HB3 | 38:H:235:HOH:O | 2.13 | 0.48 |
| 11:K:55:VAL:HG12 | 11:K:56:SER:N | 2.28 | 0.48 |
| 23:W:21:LEU:HD13 | 23:W:26:ILE:HD11 | 1.95 | 0.48 |
| 30:0:1422:U:H2' | 30:0:1423:C:H6 | 1.76 | 0.48 |
| 8:H:61:ARG:HG3 | 8:H:61:ARG:HH11 | 1.78 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:246:ARG:NE | 38:C:8628:HOH:O | 2.43 | 0.48 |
| 21:U:17:THR:CG2 | 21:U:18:GLY:N | 2.77 | 0.48 |
| 27:1:28:HIS:HD2 | 27:1:30:LYS:H | 1.59 | 0.48 |
| 30:0:735:C:O5' | 30:0:735:C:H6 | 1.97 | 0.48 |
| 30:0:661:G:C5 | 30:0:686:A:C2 | 3.02 | 0.48 |
| 1:A:135:VAL:HG21 | 1:A:147:ARG:HB3 | 1.96 | 0.48 |
| 8:H:170:ARG:HD2 | 38:H:194:HOH:O | 2.13 | 0.48 |
| 12:L:117:GLU:HA | 38:L:8852:HOH:O | 2.13 | 0.48 |
| 30:0:1188:A:C5 | 30:0:1189:A:C2 | 3.01 | 0.48 |
| 30:0:1201:C:C2' | 30:0:1202:A:H5' | 2.42 | 0.48 |
| 30:0:285:A:N6 | 30:0:367:G:H1' | 2.28 | 0.48 |
| 5:E:72:MET:O | 5:E:76:VAL:HG22 | 2.14 | 0.48 |
| 30:0:1789:G:H2' | 30:0:1790:C:O5' | 2.13 | 0.48 |
| 12:L:143:THR:HG22 | 12:L:144:ASP:N | 2.28 | 0.48 |
| 11:K:9:THR:HA | 38:0:3293:HOH:O | 2.14 | 0.48 |
| 30:0:1976:G:O2' | 30:0:1977:U:H5' | 2.14 | 0.48 |
| 30:0:2090:G:H2' | 30:0:2091:G:C8 | 2.49 | 0.48 |
| 30:0:1159:G:H1 | 30:0:1208:C:H42 | 1.61 | 0.48 |
| 30:0:2635:A:C2' | 30:0:2636:C:H5' | 2.44 | 0.48 |
| 30:0:1543:G:N1 | 30:0:1641:A:OP2 | 2.34 | 0.48 |
| 30:0:2419:U:H5" | 30:0:2420:G:H5' | 1.95 | 0.48 |
| 30:0:675:U:H6 | 30:0:675:U:O5' | 1.97 | 0.48 |
| 9:I:97:VAL:HG12 | 9:I:101:LYS:HE3 | 1.94 | 0.48 |
| 6:F:53:ASP:OD1 | 6:F:80:GLN:HB2 | 2.14 | 0.48 |
| 30:0:2656:G:C2' | 30:0:2657:G:H5' | 2.44 | 0.48 |
| 30:0:732:C:O2' | 30:0:733:U:H5' | 2.13 | 0.48 |
| 13:M:171:ARG:CD | 30:0:156:C:H5" | 2.23 | 0.48 |
| 30:0:506:G:N2 | 30:0:509:A:H5" | 2.20 | 0.48 |
| 30:0:363:C:H2' | 30:0:364:U:C6 | 2.49 | 0.48 |
| 1:A:88:ILE:HD13 | 1:A:100:PRO:HD3 | 1.95 | 0.48 |
| 30:0:1506:U:H6 | 30:0:1506:U:H5' | 1.79 | 0.48 |
| 23:W:41:TYR:OH | 30:0:1024:G:H4' | 2.14 | 0.48 |
| 30:0:1613:C:H2' | 30:0:1614:G:O4' | 2.14 | 0.48 |
| 30:0:2858:U:H2' | 30:0:2859:C:H6 | 1.78 | 0.48 |
| 10:J:39:VAL:HG13 | 10:J:106:GLY:O | 2.13 | 0.48 |
| 20:T:77:VAL:HG11 | 20:T:91:LEU:HD11 | 1.95 | 0.48 |
| 30:0:2837:U:H2' | 38:0:6856:HOH:O | 2.14 | 0.48 |
| 30:0:1902:G:N2 | 30:0:1936:C:C2 | 2.82 | 0.48 |
| 38:C:8666:HOH:O | 30:0:656:G:H1' | 2.14 | 0.47 |
| 30:0:2769:C:C2' | 30:0:2770:G:C5' | 2.78 | 0.47 |
| 31:9:1:U:C4' | 31:9:3:A:OP1 | 2.62 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:250:C:H2' | 30:0:251:C:H6 | 1.79 | 0.47 |
| 30:0:1512:G:O2' | 30:0:1513:C:H5' | 2.14 | 0.47 |
| 14:N:4:PRO:HB2 | 30:0:1010:C:H4' | 1.94 | 0.47 |
| 30:0:947:U:O2' | 30:0:948:G:H5' | 2.14 | 0.47 |
| 30:0:2074:A:H1' | 38:0:9890:HOH:O | 2.14 | 0.47 |
| 13:M:64:ARG:HD2 | 38:M:8880:HOH:O | 2.14 | 0.47 |
| 30:0:814:G:H4' | 38:0:3141:HOH:O | 2.14 | 0.47 |
| 30:0:2672:C:H2' | 30:0:2673:U:H6 | 1.78 | 0.47 |
| 13:M:34:GLU:HB3 | 13:M:38:GLU:HG3 | 1.96 | 0.47 |
| 30:0:128:A:O2' | 30:0:129:A:C5' | 2.62 | 0.47 |
| 31:9:108:C:H2' | 31:9:109:G:H8 | 1.78 | 0.47 |
| 30:0:1562:C:O2 | 30:0:1562:C:H2' | 2.12 | 0.47 |
| 30:0:2493:C:O2 | 30:0:2493:C:H2' | 2.14 | 0.47 |
| 30:0:843:A:C2 | 30:0:846:A:C8 | 3.02 | 0.47 |
| 30:0:2869:G:H5' | 38:0:5510:HOH:O | 2.14 | 0.47 |
| 30:0:800:G:H2' | 30:0:801:U:C6 | 2.49 | 0.47 |
| 29:3:65:THR:HB | 29:3:83:TRP:H | 1.79 | 0.47 |
| 30:0:101:C:H2' | 30:0:102:A:C8 | 2.49 | 0.47 |
| 30:0:814:G:H2' | 30:0:815:U:H6 | 1.79 | 0.47 |
| 12:L:41:HIS:CD2 | 30:0:926:A:O2' | 2.65 | 0.47 |
| 9:I:108:HIS:N | 9:I:109:PRO:HD2 | 2.29 | 0.47 |
| 30:0:2134:G:H2' | 30:0:2135:A:H8 | 1.79 | 0.47 |
| 30:0:1321:A:H2' | 30:0:1322:G:H8 | 1.80 | 0.47 |
| 30:0:2253:G:H2' | 30:0:2254:G:H8 | 1.79 | 0.47 |
| 1:A:171:LYS:HB2 | 30:0:820:G:C6 | 2.49 | 0.47 |
| 29:3:11:CYS:HB2 | 29:3:20:HIS:CE1 | 2.49 | 0.47 |
| 30:0:2795:C:O2' | 30:0:2796:U:H5' | 2.15 | 0.47 |
| 9:I:120:ALA:O | 9:I:124:VAL:HG23 | 2.14 | 0.47 |
| 26:Z:45:VAL:HG23 | 30:0:1887:U:OP1 | 2.14 | 0.47 |
| 1:A:217:ARG:HG2 | 1:A:229:ALA:HB2 | 1.96 | 0.47 |
| 31:9:114:G:H2' | 31:9:115:C:C6 | 2.49 | 0.47 |
| 30:0:1268:C:H2' | 30:0:1269:G:H8 | 1.79 | 0.47 |
| 1:A:65:ARG:O | 1:A:66:ARG:HG3 | 2.15 | 0.47 |
| 30:0:1667:A:H2' | 30:0:1668:U:C6 | 2.49 | 0.47 |
| 5:E:143:GLN:HE21 | 30:0:2780:C:C1' | 2.15 | 0.47 |
| 30:0:1165:G:C4' | 30:0:1174:A:O2' | 2.60 | 0.47 |
| 3:C:197:SER:HB3 | 38:C:8577:HOH:O | 2.15 | 0.47 |
| 2:B:41:PHE:HB3 | 2:B:190:MET:HE1 | 1.96 | 0.47 |
| 1:A:171:LYS:HB2 | 30:0:820:G:C5 | 2.50 | 0.47 |
| 30:0:671:A:O2' | 30:0:672:G:H2' | 2.14 | 0.47 |
| 30:0:2256:G:H2' | 30:0:2257:G:C5' | 2.45 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1568:G:O2' | 30:0:1569:U:H5' | 2.14 | 0.47 |
| 30:0:660:A:H4' | 30:0:661:G:O5' | 2.14 | 0.47 |
| 3:C:58:ALA:HA | 3:C:73:GLN:HE21 | 1.79 | 0.47 |
| 30:0:834:G:H3' | 30:0:835:U:H4' | 1.95 | 0.47 |
| 4:D:41:LEU:HA | 4:D:44:ILE:HG22 | 1.96 | 0.47 |
| 26:Z:43:GLY:O | 26:Z:47:ARG:HG2 | 2.14 | 0.47 |
| 30:0:1187:U:H2' | 38:0:6916:HOH:O | 2.15 | 0.47 |
| 30:0:69:A:H8 | 30:0:69:A:C5' | 2.21 | 0.47 |
| 30:0:2826:G:C6 | 30:0:2913:A:C6 | 3.02 | 0.47 |
| 2:B:229:ARG:NH2 | 30:0:1753:C:O2 | 2.45 | 0.47 |
| 30:0:1126:C:H6 | 30:0:1126:C:O5' | 1.97 | 0.47 |
| 5:E:108:LEU:HD11 | 5:E:164:ASP:HB2 | 1.96 | 0.47 |
| 30:0:2105:C:O2' | 30:0:2284:G:N2 | 2.48 | 0.47 |
| 12:L:92:ASP:HA | 12:L:121:ILE:HB | 1.96 | 0.47 |
| 8:H:5:PRO:HD2 | 8:H:8:MET:SD | 2.55 | 0.47 |
| 30:0:1166:A:H1' | 30:0:1192:A:C2 | 2.50 | 0.47 |
| 30:0:559:U:H3' | 30:0:559:U:C6 | 2.50 | 0.47 |
| 3:C:114:ALA:HB1 | 3:C:223:LEU:HB3 | 1.96 | 0.47 |
| 12:L:134:GLU:HG3 | 38:L:8856:HOH:O | 2.15 | 0.47 |
| 1:A:186:TRP:CD1 | 1:A:187:PRO:HA | 2.49 | 0.47 |
| 30:0:423:A:C5 | 30:0:424:C:C5 | 3.02 | 0.47 |
| 14:N:61:ALA:CB | 14:N:88:ALA:HB2 | 2.44 | 0.47 |
| 5:E:91:PHE:HE1 | 30:0:2694:A:H4' | 1.78 | 0.47 |
| 30:0:1014:A:H5" | 31:9:101:G:O2' | 2.14 | 0.47 |
| 31:9:39:U:C2' | 31:9:40:C:OP1 | 2.63 | 0.47 |
| 30:0:1126:C:HO2' | 30:0:1128:U:H6 | 1.60 | 0.47 |
| 30:0:2411:C:H4' | 38:0:4964:HOH:O | 2.13 | 0.47 |
| 8:H:64:SER:OG | 30:0:2520:G:H5' | 2.13 | 0.47 |
| 30:0:2265:U:H2' | 30:0:2266:A:C8 | 2.49 | 0.47 |
| 12:L:35:ARG:O | 12:L:40:PHE:HA | 2.15 | 0.47 |
| 30:0:1883:U:H5" | 30:0:2013:G:OP2 | 2.14 | 0.47 |
| 3:C:34:ALA:HB3 | 3:C:220:THR:HG21 | 1.97 | 0.47 |
| 13:M:99:ARG:CD | 13:M:167:GLY:HA2 | 2.41 | 0.47 |
| 30:0:2831:C:H2' | 30:0:2832:C:C5' | 2.45 | 0.47 |
| 30:0:1477:C:C5' | 30:0:1868:G:H5" | 2.44 | 0.47 |
| 30:0:1730:G:H5' | 30:0:1731:C:C6 | 2.48 | 0.47 |
| 1:A:36:ASP:HA | 1:A:83:GLY:HA3 | 1.97 | 0.47 |
| 4:D:37:ALA:O | 4:D:40:ILE:HG12 | 2.14 | 0.47 |
| 30:0:36:C:C2 | 30:0:447:A:C2 | 3.03 | 0.47 |
| 30:0:1948:G:H2' | 30:0:1949:G:H8 | 1.79 | 0.47 |
| 24:X:43:VAL:HG11 | 24:X:82:GLU:HA | 1.95 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2531:U:O2' | 30:0:2532:A:H5' | 2.14 | 0.47 |
| 12:L:71:GLU:HG2 | 30:0:700:A:C2 | 2.49 | 0.47 |
| 30:0:1391:G:H2' | 30:0:1392:A:H5' | 1.97 | 0.47 |
| 30:0:304:G:H1' | 30:0:347:A:N6 | 2.29 | 0.47 |
| 18:R:82:GLU:O | 18:R:86:LYS:HG3 | 2.13 | 0.47 |
| 13:M:124:GLY:HA3 | 30:0:2132:C:H1' | 1.96 | 0.47 |
| 25:Y:155:ARG:NH1 | 38:Y:8128:HOH:O | 2.48 | 0.47 |
| 30:0:1471:A:H5' | 38:0:3197:HOH:O | 2.15 | 0.47 |
| 3:C:154:VAL:O | 3:C:158:GLU:HG3 | 2.15 | 0.47 |
| 6:F:50:VAL:HG13 | 6:F:60:VAL:HG11 | 1.96 | 0.47 |
| 30:0:1182:C:C1' | 30:0:1192:A:C8 | 2.97 | 0.47 |
| 30:0:2829:G:C2 | 30:0:2912:C:C2 | 3.03 | 0.47 |
| 12:L:133:VAL:HB | 38:L:8856:HOH:O | 2.15 | 0.47 |
| 30:0:151:A:H2' | 30:0:152:A:O4' | 2.14 | 0.47 |
| 30:0:2891:A:N3 | 30:0:2891:A:H2' | 2.29 | 0.47 |
| 1:A:27:LEU:HD12 | 1:A:69:LEU:HD22 | 1.95 | 0.47 |
| 14:N:11:ARG:HG3 | 14:N:14:ARG:NH1 | 2.30 | 0.47 |
| 30:0:2871:G:H2' | 30:0:2872:U:C6 | 2.50 | 0.47 |
| 16:P:54:LYS:HB2 | 30:0:1717:A:H5" | 1.95 | 0.47 |
| 30:0:960:G:H3' | 30:0:960:G:C4 | 2.47 | 0.47 |
| 30:0:560:U:H2' | 30:0:561:G:C8 | 2.44 | 0.47 |
| 12:L:50:GLY:C | 30:0:2453:G:H4' | 2.35 | 0.47 |
| 27:1:28:HIS:CD2 | 27:1:31:LYS:HG3 | 2.50 | 0.47 |
| 30:0:485:A:N3 | 30:0:487:G:H5" | 2.29 | 0.47 |
| 27:1:46:ARG:HA | 38:0:3028:HOH:O | 2.15 | 0.47 |
| 30:0:2087:C:O2' | 30:0:2088:C:H5' | 2.15 | 0.47 |
| 2:B:199:TYR:HE2 | 2:B:268:ARG:HB2 | 1.79 | 0.47 |
| 30:0:1205:U:H2' | 30:0:1206:U:H5' | 1.96 | 0.47 |
| 30:0:2831:C:H2' | 30:0:2832:C:H5' | 1.97 | 0.47 |
| 30:0:1789:G:C2' | 30:0:1790:C:O5' | 2.63 | 0.47 |
| 30:0:2326:C:H4' | 30:0:2412:G:C4' | 2.44 | 0.47 |
| 30:0:1788:U:C2 | 30:0:1805:G:N2 | 2.83 | 0.47 |
| 14:N:86:LEU:O | 14:N:90:LEU:HG | 2.14 | 0.46 |
| 30:0:254:C:C2' | 30:0:254:C:O2 | 2.54 | 0.46 |
| 30:0:2072:G:C6 | 30:0:2533:C:H1' | 2.50 | 0.46 |
| 30:0:1947:G:N2 | 30:0:1966:U:O2 | 2.48 | 0.46 |
| 24:X:43:VAL:HG22 | 24:X:76:ARG:NH1 | 2.29 | 0.46 |
| 30:0:820:G:O2' | 30:0:856:G:H4' | 2.14 | 0.46 |
| 30:0:2256:G:H2' | 30:0:2257:G:H5' | 1.97 | 0.46 |
| 30:0:2833:C:H1' | 30:0:2848:G:N2 | 2.30 | 0.46 |
| 14:N:11:ARG:NH1 | 31:9:8:G:O6 | 2.48 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:314:ALA:HB3 | 2:B:317:PRO:HG3 | 1.97 | 0.46 |
| 23:W:61:THR:HG23 | 23:W:151:GLU:HG3 | 1.97 | 0.46 |
| 30:0:825:U:H5" | 30:0:826:U:OP1 | 2.15 | 0.46 |
| 30:0:2911:C:O2' | 30:0:2912:C:H5' | 2.15 | 0.46 |
| 14:N:86:LEU:HD12 | 14:N:125:ALA:HB2 | 1.97 | 0.46 |
| 30:0:1174:A:C5 | 30:0:1201:C:H4' | 2.50 | 0.46 |
| 30:0:1771:U:O2' | 30:0:1773:G:N7 | 2.46 | 0.46 |
| 1:A:233:THR:HB | 30:0:1942:A:H5" | 1.98 | 0.46 |
| 14:N:141:ARG:HH21 | 31:9:48:C:H4' | 1.79 | 0.46 |
| 30:0:2825:C:H4' | 30:0:2826:G:O5' | 2.15 | 0.46 |
| 30:0:920:C:H4' | 30:0:921:G:N2 | 2.30 | 0.46 |
| 30:0:10:U:C6 | 30:0:10:U:C3' | 2.98 | 0.46 |
| 30:0:1706:G:C5 | 30:0:1707:G:C6 | 3.03 | 0.46 |
| 24:X:30:MET:HE1 | 24:X:58:ALA:HB3 | 1.97 | 0.46 |
| 30:0:2106:C:H1' | 30:0:2484:U:C2 | 2.49 | 0.46 |
| 30:0:2092:G:H2' | 30:0:2613:G:OP1 | 2.15 | 0.46 |
| 28:2:28:LYS:O | 30:0:87:C:H2' | 2.15 | 0.46 |
| 3:C:200:PRO:HB3 | 3:C:212:VAL:HG23 | 1.97 | 0.46 |
| 30:0:789:C:H5' | 38:0:6228:HOH:O | 2.15 | 0.46 |
| 3:C:35:VAL:HG21 | 3:C:227:GLY:HA2 | 1.96 | 0.46 |
| 13:M:43:PRO:HG3 | 13:M:62:VAL:HG21 | 1.98 | 0.46 |
| 30:0:2577:A:H8 | 38:0:9606:HOH:O | 1.98 | 0.46 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:HG23 | 1.97 | 0.46 |
| 30:0:544:G:C3' | 30:0:545:G:H5" | 2.45 | 0.46 |
| 31:9:3:A:H2 | 31:9:21:G:N3 | 2.14 | 0.46 |
| 30:0:1596:U:H2' | 30:0:1598:A:OP2 | 2.14 | 0.46 |
| 30:0:1634:G:C4 | 30:0:1635:U:C5 | 3.03 | 0.46 |
| 1:A:211:LYS:HD3 | 38:0:6884:HOH:O | 2.15 | 0.46 |
| 30:0:2598:U:O2 | 30:0:2600:A:C8 | 2.68 | 0.46 |
| 25:Y:99:ALA:HB2 | 25:Y:233:TYR:CZ | 2.50 | 0.46 |
| 30:0:2871:G:H2' | 30:0:2872:U:H6 | 1.79 | 0.46 |
| 30:0:1400:C:O2' | 30:0:1401:G:H5' | 2.15 | 0.46 |
| 30:0:277:U:O2' | 30:0:278:A:H5' | 2.15 | 0.46 |
| 30:0:1557:G:O2' | 30:0:1558:C:H5' | 2.15 | 0.46 |
| 31:9:27:C:H2' | 31:9:28:U:O4' | 2.16 | 0.46 |
| 30:0:1878:G:C4' | 38:0:6135:HOH:O | 2.64 | 0.46 |
| 30:0:2482:G:H4' | 30:0:2483:A:C5' | 2.45 | 0.46 |
| 2:B:41:PHE:CZ | 2:B:79:MET:HG3 | 2.50 | 0.46 |
| 15:O:25:VAL:HG12 | 30:0:709:G:O2' | 2.16 | 0.46 |
| 30:0:876:A:N3 | 30:0:876:A:C2' | 2.79 | 0.46 |
| 30:0:2105:C:H2' | 30:0:2106:C:C6 | 2.50 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2284:G:H1' | 38:0:9576:HOH:O | 2.15 | 0.46 |
| 30:0:1200:A:H3' | 38:0:5769:HOH:O | 2.15 | 0.46 |
| 30:0:2802:C:H2' | 30:0:2803:C:C6 | 2.50 | 0.46 |
| 1:A:123:GLY:HA3 | 1:A:162:GLY:HA2 | 1.96 | 0.46 |
| 13:M:80:GLY:O | 13:M:81:ARG:HD2 | 2.14 | 0.46 |
| 30:0:354:A:H2' | 30:0:355:C:H6 | 1.80 | 0.46 |
| 30:0:1102:C:H5 | 38:0:3497:HOH:O | 1.98 | 0.46 |
| 3:C:127:ARG:HD3 | 3:C:129:HIS:CE1 | 2.48 | 0.46 |
| 2:B:243:ASN:HA | 2:B:244:PRO:C | 2.35 | 0.46 |
| 30:0:1515:A:H2' | 30:0:1516:U:H6 | 1.80 | 0.46 |
| 30:0:590:A:H2' | 30:0:591:A:H5' | 1.97 | 0.46 |
| 14:N:11:ARG:HD3 | 31:9:114:G:O6 | 2.15 | 0.46 |
| 30:0:1125:U:H3' | 30:0:1126:C:C6 | 2.51 | 0.46 |
| 21:U:49:LEU:HG | 38:U:3805:HOH:O | 2.15 | 0.46 |
| 16:P:101:GLN:HG3 | 38:0:3511:HOH:O | 2.15 | 0.46 |
| 30:0:228:C:H2' | 30:0:229:G:H5' | 1.96 | 0.46 |
| 29:3:61:PRO:HG3 | 30:0:2462:G:O6 | 2.16 | 0.46 |
| 30:0:343:C:O2' | 30:0:344:C:H5' | 2.15 | 0.46 |
| 30:0:716:G:C6 | 30:0:717:C:N4 | 2.83 | 0.46 |
| 30:0:445:U:H2' | 30:0:446:G:H8 | 1.81 | 0.46 |
| 30:0:1175:G:N7 | 30:0:1176:C:N3 | 2.63 | 0.46 |
| 30:0:241:A:C2 | 30:0:378:A:H4' | 2.51 | 0.46 |
| 30:0:2703:A:H2' | 30:0:2704:C:C6 | 2.46 | 0.46 |
| 16:P:59:ARG:HH22 | 16:P:66:GLN:NE2 | 2.12 | 0.46 |
| 30:0:1067:A:H5' | 38:0:4351:HOH:O | 2.15 | 0.46 |
| 30:0:2613:G:O2' | 30:0:2614:C:H5' | 2.15 | 0.46 |
| 30:0:1420:C:H2' | 30:0:1420:C:O2 | 2.15 | 0.46 |
| 31:9:12:C:H5' | 31:9:70:U:O4' | 2.15 | 0.46 |
| 14:N:112:GLY:HA2 | 14:N:137:ALA:HB2 | 1.96 | 0.46 |
| 2:B:214:PRO:HD2 | 38:0:9081:HOH:O | 2.15 | 0.46 |
| 30:0:1616:A:H5" | 30:0:1617:C:OP1 | 2.16 | 0.46 |
| 30:0:1346:U:H2' | 30:0:1347:U:C6 | 2.51 | 0.46 |
| 17:Q:53:HIS:CD2 | 30:0:2389:U:H4' | 2.50 | 0.46 |
| 5:E:11:VAL:HG12 | 5:E:12:ASP:N | 2.31 | 0.46 |
| 9:I:130:LEU:HA | 38:0:7420:HOH:O | 2.15 | 0.46 |
| 14:N:175:LEU:O | 14:N:179:LEU:HG | 2.15 | 0.46 |
| 3:C:1:MET:CG | 3:C:2:GLN:H | 2.26 | 0.46 |
| 30:0:138:U:OP2 | 30:0:139:C:C5 | 2.69 | 0.46 |
| 2:B:307:ARG:HG3 | 2:B:307:ARG:NH1 | 2.30 | 0.46 |
| 30:0:2840:A:H3' | 38:0:7661:HOH:O | 2.15 | 0.46 |
| 4:D:64:ARG:HB3 | 4:D:67:ASP:OD2 | 2.15 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2346:C:O5' | 30:0:2346:C:H6 | 1.98 | 0.46 |
| 30:0:1617:C:C4 | 30:0:1643:C:H4' | 2.50 | 0.46 |
| 2:B:202:VAL:HG11 | 2:B:301:VAL:HG13 | 1.98 | 0.46 |
| 1:A:71:PRO:HD2 | 1:A:74:VAL:HG21 | 1.98 | 0.46 |
| 30:0:2061:C:C2' | 30:0:2062:A:H5' | 2.46 | 0.46 |
| 16:P:64:GLU:HG3 | 38:P:166:HOH:O | 2.15 | 0.46 |
| 30:0:2093:G:H5" | 38:0:9483:HOH:O | 2.15 | 0.46 |
| 30:0:889:C:H2' | 30:0:890:C:C6 | 2.51 | 0.46 |
| 1:A:127:GLN:HB3 | 1:A:139:LYS:HB3 | 1.98 | 0.46 |
| 30:0:2401:A:H2' | 30:0:2402:A:C8 | 2.51 | 0.46 |
| 30:0:370:G:O2' | 30:0:371:U:H5' | 2.15 | 0.46 |
| 30:0:2908:A:C2' | 30:0:2909:G:H5' | 2.46 | 0.46 |
| 30:0:1741:U:C4 | 30:0:2033:G:C8 | 3.04 | 0.46 |
| 30:0:1202:A:C8 | 30:0:1203:G:C8 | 3.04 | 0.46 |
| 31:9:34:A:H2' | 31:9:35:C:O4' | 2.16 | 0.46 |
| 5:E:3:VAL:HG22 | 5:E:49:ILE:HB | 1.97 | 0.46 |
| 30:0:510:U:O5' | 30:0:510:U:H6 | 1.99 | 0.46 |
| 3:C:103:ASN:HB3 | 38:0:9117:HOH:O | 2.16 | 0.46 |
| 4:D:20:LYS:HA | 4:D:75:LEU:O | 2.15 | 0.46 |
| 30:0:729:C:C2 | 30:0:743:G:C2 | 3.04 | 0.46 |
| 30:0:1463:U:H2' | 30:0:1464:C:C6 | 2.51 | 0.46 |
| 1:A:110:SER:HB2 | 1:A:117:LYS:HG3 | 1.98 | 0.46 |
| 30:0:1873:G:H2' | 30:0:1874:U:H5' | 1.98 | 0.46 |
| 30:0:1845:A:O2' | 30:0:1846:U:H5' | 2.15 | 0.46 |
| 30:0:162:C:C2' | 30:0:163:U:H5' | 2.45 | 0.46 |
| 30:0:1453:G:C2 | 30:0:1675:C:C2 | 3.04 | 0.46 |
| 4:D:56:ARG:HH22 | 30:0:2332:A:H5' | 1.79 | 0.46 |
| 17:Q:25:PRO:HA | 17:Q:26:PRO:HD3 | 1.81 | 0.46 |
| 1:A:206:ARG:O | 1:A:208:HIS:HD2 | 1.98 | 0.46 |
| 30:0:1309:U:C2' | 30:0:1310:U:H5' | 2.46 | 0.46 |
| 30:0:1008:C:O2' | 30:0:1009:U:H5' | 2.16 | 0.46 |
| 30:0:417:G:P | 38:0:7436:HOH:O | 2.73 | 0.46 |
| 16:P:80:ARG:HG2 | 16:P:87:ARG:CZ | 2.46 | 0.46 |
| 30:0:39:G:N2 | 30:0:444:C:C2 | 2.84 | 0.46 |
| 5:E:137:ASP:O | 5:E:141:VAL:HG23 | 2.16 | 0.46 |
| 6:F:13:GLU:OE2 | 6:F:78:GLU:HG2 | 2.15 | 0.46 |
| 30:0:2764:C:O2' | 30:0:2765:C:H5' | 2.16 | 0.46 |
| 30:0:932:U:H2' | 30:0:933:C:C6 | 2.51 | 0.46 |
| 30:0:1700:C:H5" | 30:0:1701:A:OP2 | 2.15 | 0.46 |
| 31:9:3:A:OP2 | 31:9:25:G:N2 | 2.48 | 0.46 |
| 30:0:560:U:C2 | 30:0:561:G:C8 | 3.04 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:567:U:C5' | 38:0:5300:HOH:O | 2.63 | 0.46 |
| 30:0:1838:U:C4 | 30:0:2644:C:N4 | 2.84 | 0.46 |
| 23:W:118:LEU:HD12 | 23:W:153:MET:HE3 | 1.97 | 0.46 |
| 24:X:56:GLU:HG2 | 30:0:1400:C:H4' | 1.98 | 0.46 |
| 30:0:1156:C:O5' | 30:0:1156:C:H6 | 1.99 | 0.46 |
| 30:0:2103:A:N3 | 30:0:2103:A:H2' | 2.30 | 0.46 |
| 27:1:42:SER:HB2 | 38:1:8957:HOH:O | 2.16 | 0.46 |
| 25:Y:165:GLU:HB3 | 38:Y:8163:HOH:O | 2.16 | 0.46 |
| 2:B:102:THR:HG23 | 2:B:182:VAL:HG12 | 1.98 | 0.46 |
| 3:C:156:LEU:O | 3:C:160:LEU:HG | 2.16 | 0.46 |
| 4:D:91:ALA:HB1 | 38:D:5198:HOH:O | 2.15 | 0.46 |
| 30:0:1535:G:H2' | 30:0:1536:C:C6 | 2.50 | 0.46 |
| 30:0:238:C:H4' | 30:0:287:C:OP1 | 2.16 | 0.46 |
| 30:0:369:G:C2 | 30:0:370:G:C8 | 3.04 | 0.45 |
| 30:0:2526:C:H2' | 30:0:2527:U:H5' | 1.98 | 0.45 |
| 1:A:190:ARG:NH1 | 30:0:1845:A:OP2 | 2.47 | 0.45 |
| 30:0:1675:C:O2' | 30:0:1676:G:H5' | 2.16 | 0.45 |
| 31:9:52:A:O2' | 31:9:53:G:H5' | 2.16 | 0.45 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:CG2 | 2.46 | 0.45 |
| 30:0:1393:A:H2' | 30:0:1394:C:C6 | 2.51 | 0.45 |
| 21:U:42:LEU:HD22 | 30:0:1810:C:H1' | 1.98 | 0.45 |
| 30:0:630:A:H5' | 38:0:9367:HOH:O | 2.16 | 0.45 |
| 30:0:1735:C:H2' | 30:0:1736:A:C8 | 2.50 | 0.45 |
| 30:0:1741:U:H3' | 38:0:9774:HOH:O | 2.16 | 0.45 |
| 30:0:1973:A:H2' | 30:0:1974:G:O4' | 2.15 | 0.45 |
| 30:0:536:A:N1 | 30:0:2075:G:O2' | 2.44 | 0.45 |
| 30:0:2499:U:H2' | 30:0:2500:C:C6 | 2.51 | 0.45 |
| 31:9:37:C:H2' | 31:9:38:A:C8 | 2.48 | 0.45 |
| 11:K:34:VAL:HB | 38:0:7387:HOH:O | 2.15 | 0.45 |
| 30:0:137:U:OP1 | 30:0:259:G:O2' | 2.34 | 0.45 |
| 30:0:797:A:H2' | 30:0:798:G:O4' | 2.16 | 0.45 |
| 30:0:735:C:H2' | 30:0:736:A:H5' | 1.99 | 0.45 |
| 30:0:340:A:O5' | 30:0:340:A:C8 | 2.69 | 0.45 |
| 30:0:80:A:C2 | 30:0:94:G:N3 | 2.85 | 0.45 |
| 30:0:1501:A:H4' | 38:0:5614:HOH:O | 2.15 | 0.45 |
| 30:0:1636:G:O2' | 30:0:1637:A:H5' | 2.16 | 0.45 |
| 4:D:15:GLU:HA | 4:D:16:PRO:HD3 | 1.78 | 0.45 |
| 30:0:2883:A:H2' | 30:0:2884:G:O4' | 2.17 | 0.45 |
| 30:0:806:A:H2' | 30:0:807:A:O4' | 2.17 | 0.45 |
| 30:0:2121:G:O2' | 30:0:2122:C:H5' | 2.16 | 0.45 |
| 30:0:497:A:H2' | 30:0:498:A:C5' | 2.46 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2435:U:H1' | 38:0:5442:HOH:O | 2.16 | 0.45 |
| 38:Y:8136:HOH:O | 30:0:1316:G:H5" | 2.15 | 0.45 |
| 17:Q:45:PRO:O | 30:0:2365:G:H4' | 2.16 | 0.45 |
| 2:B:14:GLY:HA2 | 2:B:15:PRO:C | 2.37 | 0.45 |
| 30:0:1160:G:O2' | 30:0:1190:G:H1' | 2.17 | 0.45 |
| 30:0:2909:G:H2' | 30:0:2910:A:C8 | 2.51 | 0.45 |
| 3:C:127:ARG:CZ | 3:C:225:PRO:HG2 | 2.45 | 0.45 |
| 30:0:364:U:H2' | 30:0:365:G:C8 | 2.51 | 0.45 |
| 30:0:1477:C:C5' | 30:0:1868:G:C5' | 2.93 | 0.45 |
| 30:0:1730:G:H5" | 30:0:1731:C:C6 | 2.51 | 0.45 |
| 30:0:1041:U:C2' | 30:0:1042:U:H5' | 2.47 | 0.45 |
| 16:P:105:LEU:HD21 | 16:P:137:LEU:HD11 | 1.99 | 0.45 |
| 30:0:883:U:C2' | 30:0:883:U:O2 | 2.64 | 0.45 |
| 10:J:46:ILE:HD11 | 10:J:53:ILE:HG23 | 1.97 | 0.45 |
| 5:E:119:HIS:O | 5:E:140:ALA:HB1 | 2.17 | 0.45 |
| 20:T:41:ARG:HH11 | 20:T:41:ARG:HG2 | 1.82 | 0.45 |
| 30:0:1163:G:N2 | 38:0:4740:HOH:O | 2.49 | 0.45 |
| 30:0:281:U:H5 | 38:0:7610:HOH:O | 2.00 | 0.45 |
| 30:0:282:C:C2' | 30:0:283:U:H5' | 2.46 | 0.45 |
| 5:E:143:GLN:NE2 | 30:0:2780:C:C1' | 2.79 | 0.45 |
| 31:9:3:A:C8 | 31:9:26:C:O2 | 2.69 | 0.45 |
| 31:9:3:A:H8 | 31:9:26:C:O2 | 1.99 | 0.45 |
| 22:V:39:ALA:C | 22:V:41:GLU:H | 2.20 | 0.45 |
| 30:0:2499:U:H2' | 30:0:2500:C:H6 | 1.81 | 0.45 |
| 5:E:69:ILE:HA | 5:E:72:MET:HE2 | 1.99 | 0.45 |
| 30:0:2064:U:H2' | 30:0:2065:C:H6 | 1.81 | 0.45 |
| 19:S:57:THR:HG22 | 19:S:59:ASP:H | 1.80 | 0.45 |
| 2:B:141:ARG:HG2 | 2:B:165:ARG:HA | 1.98 | 0.45 |
| 1:A:231:LYS:HG3 | 30:0:1853:C:OP1 | 2.17 | 0.45 |
| 12:L:33:ALA:HB3 | 38:L:8892:HOH:O | 2.17 | 0.45 |
| 4:D:22:VAL:HG22 | 4:D:74:THR:HG22 | 1.97 | 0.45 |
| 4:D:104:PHE:CE2 | 4:D:132:VAL:HB | 2.52 | 0.45 |
| 30:0:2308:U:C5 | 30:0:2310:G:C8 | 3.05 | 0.45 |
| 2:B:262:ARG:HD2 | 30:0:2715:G:O2' | 2.17 | 0.45 |
| 30:0:2908:A:H2' | 30:0:2909:G:C4' | 2.45 | 0.45 |
| 30:0:2421:G:H3' | 30:0:2422:U:C5' | 2.47 | 0.45 |
| 3:C:236:THR:HG21 | 38:C:8577:HOH:O | 2.17 | 0.45 |
| 30:0:1903:U:O2' | 30:0:1904:A:C8 | 2.69 | 0.45 |
| 30:0:1120:U:H5" | 30:0:1120:U:C6 | 2.52 | 0.45 |
| 30:0:1521:C:H2' | 30:0:1522:A:C8 | 2.50 | 0.45 |
| 14:N:4:PRO:HD2 | 38:0:6790:HOH:O | 2.17 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:9:39:U:H3' | 31:9:40:C:H5" | 1.99 | 0.45 |
| 30:0:1098:A:H2' | 30:0:1099:G:O4' | 2.17 | 0.45 |
| 12:L:12:THR:HG21 | 12:L:16:GLY:O | 2.17 | 0.45 |
| 30:0:2515:C:H2' | 30:0:2516:G:O4' | 2.16 | 0.45 |
| 30:0:1149:U:C5 | 30:0:1215:A:C5 | 3.04 | 0.45 |
| 30:0:134:U:C2 | 30:0:145:A:C2 | 3.05 | 0.45 |
| 30:0:517:U:H1' | 38:0:7592:HOH:O | 2.16 | 0.45 |
| 30:0:1992:U:H2' | 30:0:1994:A:OP2 | 2.17 | 0.45 |
| 30:0:1815:A:H4' | 30:0:2751:C:O4' | 2.17 | 0.45 |
| 30:0:1175:G:C1' | 30:0:1193:A:C8 | 2.98 | 0.45 |
| 30:0:1196:C:H42 | 30:0:1204:C:N4 | 2.14 | 0.45 |
| 30:0:283:U:H5 | 30:0:284:C:N3 | 2.13 | 0.45 |
| 2:B:234:ARG:NH2 | 30:0:2039:A:OP2 | 2.50 | 0.45 |
| 30:0:1165:G:N2 | 30:0:1173:A:H5' | 2.32 | 0.45 |
| 30:0:1773:G:N2 | 30:0:1774:G:C8 | 2.84 | 0.45 |
| 30:0:581:G:H5' | 38:0:7694:HOH:O | 2.16 | 0.45 |
| 30:0:2004:U:H6 | 30:0:2004:U:P | 2.40 | 0.45 |
| 31:9:63:C:O2' | 31:9:64:C:H5' | 2.17 | 0.45 |
| 3:C:54:LEU:HD23 | 3:C:79:ARG:HG3 | 1.99 | 0.45 |
| 19:S:57:THR:CG2 | 19:S:58:MET:N | 2.79 | 0.45 |
| 30:0:61:G:C6 | 30:0:62:C:C4 | 3.05 | 0.45 |
| 2:B:69:VAL:HA | 2:B:70:PRO:HD3 | 1.82 | 0.45 |
| 22:V:49:LEU:O | 22:V:53:ILE:HG13 | 2.17 | 0.45 |
| 30:0:1249:U:H2' | 30:0:1250:C:C6 | 2.51 | 0.45 |
| 30:0:1996:U:O2' | 30:0:1997:A:H5' | 2.16 | 0.45 |
| 4:D:10:PHE:HA | 38:D:7345:HOH:O | 2.15 | 0.45 |
| 30:0:31:C:H4' | 38:0:7442:HOH:O | 2.17 | 0.45 |
| 30:0:168:C:O2' | 30:0:169:A:H5' | 2.16 | 0.45 |
| 2:B:81:ALA:HB1 | 2:B:142:LEU:HD13 | 1.99 | 0.45 |
| 1:A:206:ARG:HH11 | 1:A:206:ARG:HG3 | 1.82 | 0.45 |
| 26:Z:34:SER:HB3 | 30:0:797:A:H4' | 1.99 | 0.45 |
| 4:D:75:LEU:HD22 | 4:D:79:MET:HB3 | 1.98 | 0.45 |
| 25:Y:144:ARG:NE | 38:Y:8181:HOH:O | 2.49 | 0.45 |
| 30:0:844:A:C6 | 30:0:882:A:C5 | 3.05 | 0.45 |
| 14:N:171:HIS:CE1 | 38:N:8861:HOH:O | 2.69 | 0.45 |
| 30:0:2583:A:H5' | 38:0:9803:HOH:O | 2.17 | 0.45 |
| 30:0:559:U:H2' | 30:0:560:U:O4' | 2.17 | 0.45 |
| 23:W:52:VAL:HG22 | 23:W:53:ALA:H | 1.82 | 0.45 |
| 30:0:2072:G:H3' | 30:0:2073:G:C5' | 2.47 | 0.45 |
| 30:0:968:G:H2' | 30:0:969:G:H8 | 1.82 | 0.45 |
| 1:A:35:GLY:O | 1:A:36:ASP:HB3 | 2.16 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:M:24:GLN:HE22 | 13:M:27:ARG:HH11 | 1.64 | 0.45 |
| 30:0:553:G:H3' | 38:0:4084:HOH:O | 2.15 | 0.45 |
| 2:B:211:THR:HG21 | 38:0:7472:HOH:O | 2.17 | 0.45 |
| 30:0:1711:A:O2' | 30:0:1712:A:H5' | 2.16 | 0.45 |
| 2:B:5:ARG:NH2 | 30:0:2548:C:OP2 | 2.50 | 0.45 |
| 14:N:109:PRO:HB3 | 30:0:2413:A:N7 | 2.32 | 0.45 |
| 30:0:240:C:O2 | 30:0:240:C:H2' | 2.17 | 0.45 |
| 30:0:1577:U:O2' | 30:0:1578:C:H5' | 2.17 | 0.45 |
| 18:R:15:LYS:HE3 | 38:R:8982:HOH:O | 2.16 | 0.45 |
| 3:C:72:LYS:HE3 | 38:C:8505:HOH:O | 2.17 | 0.45 |
| 11:K:64:MET:HA | 11:K:67:GLN:HE21 | 1.81 | 0.45 |
| 6:F:2:VAL:HG22 | 6:F:57:GLU:OE1 | 2.17 | 0.45 |
| 23:W:130:HIS:O | 23:W:136:GLY:HA3 | 2.17 | 0.45 |
| 1:A:54:PRO:HG2 | 1:A:160:ALA:HB3 | 1.99 | 0.45 |
| 30:0:1825:U:O2' | 30:0:1826:C:H5' | 2.16 | 0.45 |
| 30:0:960:G:C3' | 30:0:960:G:C4 | 3.00 | 0.45 |
| 2:B:217:ARG:HG3 | 2:B:257:THR:HB | 1.99 | 0.45 |
| 30:0:68:U:O2' | 30:0:69:A:H5" | 2.17 | 0.45 |
| 30:0:2361:A:C5' | 38:0:9009:HOH:O | 2.60 | 0.45 |
| 30:0:2828:G:C6 | 30:0:2913:A:C2 | 3.05 | 0.45 |
| 30:0:407:A:H3' | 38:0:4468:HOH:O | 2.16 | 0.45 |
| 27:1:16:HIS:CD2 | 30:0:470:U:O2' | 2.68 | 0.45 |
| 30:0:1626:A:H2' | 30:0:1627:G:C5' | 2.47 | 0.45 |
| 16:P:20:ARG:NH1 | 16:P:54:LYS:HD3 | 2.32 | 0.45 |
| 13:M:81:ARG:HG3 | 13:M:85:ARG:HB2 | 1.99 | 0.45 |
| 30:0:2624:A:O2' | 30:0:2625:C:H5' | 2.17 | 0.45 |
| 18:R:40:ALA:O | 18:R:44:VAL:HG23 | 2.16 | 0.45 |
| 30:0:884:C:H3' | 38:0:9406:HOH:O | 2.17 | 0.45 |
| 8:H:31:ILE:HG23 | 38:H:233:HOH:O | 2.16 | 0.45 |
| 14:N:37:ARG:NH1 | 31:9:6:C:OP1 | 2.50 | 0.44 |
| 30:0:2269:C:H2' | 30:0:2270:G:C5' | 2.47 | 0.44 |
| 30:0:2653:A:H2' | 30:0:2654:C:C6 | 2.52 | 0.44 |
| 1:A:179:MET:HA | 1:A:179:MET:CE | 2.47 | 0.44 |
| 3:C:46:TYR:CE1 | 3:C:92:PRO:HB3 | 2.51 | 0.44 |
| 23:W:122:ARG:HH12 | 23:W:154:ARG:N | 2.14 | 0.44 |
| 17:Q:26:PRO:O | 17:Q:30:VAL:HG23 | 2.16 | 0.44 |
| 3:C:39:GLN:O | 3:C:43:LYS:HD3 | 2.18 | 0.44 |
| 2:B:214:PRO:C | 2:B:220:VAL:HG22 | 2.37 | 0.44 |
| 30:0:1735:C:H2' | 30:0:1736:A:H8 | 1.82 | 0.44 |
| 4:D:12:GLU:O | 4:D:15:GLU:HG2 | 2.17 | 0.44 |
| 16:P:1:THR:O | 30:0:1396:C:H1' | 2.17 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1718:G:O2' | 30:0:1719:G:H5' | 2.17 | 0.44 |
| 5:E:75:GLY:HA3 | 5:E:136:PRO:O | 2.18 | 0.44 |
| 30:0:45:A:H5" | 30:0:47:G:O4' | 2.17 | 0.44 |
| 9:I:121:LYS:HB3 | 30:0:1184:C:H4' | 1.98 | 0.44 |
| 31:9:14:G:H8 | 31:9:14:G:C5' | 2.20 | 0.44 |
| 30:0:2510:C:N4 | 30:0:2564:G:H22 | 2.12 | 0.44 |
| 3:C:1:MET:HG2 | 3:C:2:GLN:N | 2.27 | 0.44 |
| 23:W:13:MET:HE2 | 23:W:17:ILE:HG22 | 1.98 | 0.44 |
| 5:E:15:GLN:HG3 | 5:E:20:ILE:HG12 | 1.99 | 0.44 |
| 25:Y:235:GLU:CD | 25:Y:235:GLU:N | 2.70 | 0.44 |
| 30:0:1676:G:C2' | 30:0:1677:U:H5' | 2.47 | 0.44 |
| 28:2:8:LYS:NZ | 30:0:1677:U:OP2 | 2.48 | 0.44 |
| 30:0:255:A:H2' | 30:0:256:C:O4' | 2.17 | 0.44 |
| 2:B:27:ASN:HD21 | 30:0:2807:U:P | 2.40 | 0.44 |
| 18:R:29:LYS:HE2 | 30:0:524:A:H5' | 1.99 | 0.44 |
| 4:D:52:THR:HG21 | 30:0:2346:C:O2' | 2.17 | 0.44 |
| 14:N:22:GLN:HA | 14:N:25:ARG:CZ | 2.47 | 0.44 |
| 29:3:60:LYS:HG3 | 29:3:61:PRO:HD2 | 1.98 | 0.44 |
| 30:0:1894:C:N4 | 30:0:1939:U:H2' | 2.31 | 0.44 |
| 13:M:159:VAL:HG13 | 13:M:160:PHE:N | 2.32 | 0.44 |
| 2:B:10:SER:O | 2:B:16:ARG:NH1 | 2.49 | 0.44 |
| 11:K:8:VAL:HG13 | 11:K:80:ILE:HG22 | 1.98 | 0.44 |
| 30:0:271:C:C2 | 30:0:273:G:O4' | 2.70 | 0.44 |
| 30:0:542:A:H1' | 38:0:4691:HOH:O | 2.16 | 0.44 |
| 30:0:2526:C:C2' | 30:0:2527:U:H5' | 2.47 | 0.44 |
| 31:9:3:A:C8 | 31:9:26:C:N3 | 2.86 | 0.44 |
| 30:0:2505:G:H2' | 30:0:2506:A:H5' | 2.00 | 0.44 |
| 23:W:21:LEU:HB3 | 23:W:26:ILE:HG12 | 1.99 | 0.44 |
| 30:0:2587:OMU:H2' | 30:0:2589:U:H5" | 1.99 | 0.44 |
| 13:M:59:GLY:HA3 | 13:M:141:ILE:CD1 | 2.47 | 0.44 |
| 4:D:137:PRO:O | 31:9:30:C:OP1 | 2.35 | 0.44 |
| 31:9:65:A:N6 | 31:9:112:U:C6 | 2.85 | 0.44 |
| 30:0:74:G:H2' | 30:0:75:U:H6 | 1.82 | 0.44 |
| 12:L:6:ARG:NH1 | 30:0:1299:G:N7 | 2.65 | 0.44 |
| 3:C:95:GLU:CD | 3:C:95:GLU:H | 2.20 | 0.44 |
| 25:Y:126:PRO:HG2 | 25:Y:128:PHE:CZ | 2.52 | 0.44 |
| 25:Y:154:ARG:NH2 | 30:0:1071:G:H4' | 2.31 | 0.44 |
| 16:P:137:LEU:O | 16:P:141:ILE:HG13 | 2.17 | 0.44 |
| 8:H:77:ILE:HG23 | 8:H:82:GLU:HG2 | 2.00 | 0.44 |
| 30:0:649:U:O2' | 30:0:650:C:H5' | 2.16 | 0.44 |
| 13:M:184:ARG:HG3 | 13:M:185:PRO:HA | 2.00 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2502:C:O2' | 30:0:2503:A:H5' | 2.17 | 0.44 |
| 30:0:1116:U:N3 | 30:0:1246:A:N6 | 2.59 | 0.44 |
| 11:K:55:VAL:CG1 | 11:K:56:SER:N | 2.80 | 0.44 |
| 2:B:162:MET:CE | 2:B:310:ARG:HD3 | 2.46 | 0.44 |
| 30:0:2064:U:H4' | 30:0:2653:A:OP1 | 2.17 | 0.44 |
| 30:0:1503:U:H2' | 30:0:1504:A:O4' | 2.17 | 0.44 |
| 4:D:54:ALA:HB2 | 4:D:69:ILE:CD1 | 2.48 | 0.44 |
| 30:0:796:A:C2 | 30:0:797:A:C4 | 3.05 | 0.44 |
| 30:0:1268:C:O2' | 30:0:1269:G:H5' | 2.16 | 0.44 |
| 30:0:957:A:H8 | 30:0:957:A:O5' | 2.01 | 0.44 |
| 30:0:1850:U:H2' | 30:0:1851:G:H8 | 1.82 | 0.44 |
| 27:1:8:GLN:HG3 | 30:0:1688:G:H4' | 1.99 | 0.44 |
| 31:9:45:A:C5 | 31:9:46:C:C5 | 3.05 | 0.44 |
| 3:C:233:THR:HG22 | 3:C:234:VAL:N | 2.32 | 0.44 |
| 30:0:1925:G:O2' | 30:0:1926:G:H5' | 2.18 | 0.44 |
| 5:E:95:VAL:HG11 | 5:E:131:LEU:HD21 | 1.98 | 0.44 |
| 16:P:19:ASN:OD1 | 30:0:1720:C:H5 | 2.00 | 0.44 |
| 30:0:195:C:H2' | 30:0:196:G:H5' | 1.99 | 0.44 |
| 10:J:70:PHE:HE1 | 30:0:2676:C:H4' | 1.79 | 0.44 |
| 30:0:731:U:O2' | 30:0:732:C:H5' | 2.18 | 0.44 |
| 30:0:1268:C:H2' | 30:0:1269:G:C8 | 2.53 | 0.44 |
| 1:A:70:ALA:HA | 1:A:71:PRO:HD3 | 1.77 | 0.44 |
| 30:0:397:A:O2' | 30:0:417:G:N3 | 2.36 | 0.44 |
| 1:A:164:ARG:HB2 | 26:Z:92:SER:OG | 2.17 | 0.44 |
| 30:0:1416:G:C2' | 30:0:1417:G:H5' | 2.47 | 0.44 |
| 30:0:970:U:H2' | 38:0:6346:HOH:O | 2.18 | 0.44 |
| 30:0:2734:G:O2' | 30:0:2735:U:H5' | 2.18 | 0.44 |
| 30:0:348:C:H5 | 38:0:6349:HOH:O | 1.99 | 0.44 |
| 30:0:299:U:H5' | 38:0:7352:HOH:O | 2.16 | 0.44 |
| 30:0:283:U:H5 | 30:0:284:C:C4 | 2.36 | 0.44 |
| 30:0:816:G:H5' | 30:0:1598:A:H4' | 2.00 | 0.44 |
| 30:0:1058:A:H2' | 30:0:1060:C:C5' | 2.47 | 0.44 |
| 13:M:92:THR:HB | 30:0:401:C:O2' | 2.17 | 0.44 |
| 30:0:1421:C:H2' | 30:0:1422:U:H6 | 1.82 | 0.44 |
| 27:1:1:THR:O | 30:0:1836:A:H1' | 2.18 | 0.44 |
| 30:0:535:G:C6 | 30:0:2064:U:C5 | 3.06 | 0.44 |
| 30:0:2324:G:H21 | 30:0:2377:U:H1' | 1.83 | 0.44 |
| 30:0:312:U:C2 | 30:0:320:G:N2 | 2.86 | 0.44 |
| 27:1:28:HIS:CE1 | 27:1:31:LYS:HE2 | 2.53 | 0.44 |
| 30:0:99:A:C8 | 30:0:100:C:C5 | 3.06 | 0.44 |
| 30:0:354:A:H2' | 30:0:355:C:C6 | 2.53 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1020:A:H2' | 30:0:1021:G:C8 | 2.52 | 0.44 |
| 30:0:2612:A:H4' | 38:0:3687:HOH:O | 2.16 | 0.44 |
| 18:R:61:GLN:NE2 | 38:0:4737:HOH:O | 2.50 | 0.44 |
| 12:L:79:ASP:HB2 | 38:L:8858:HOH:O | 2.17 | 0.44 |
| 2:B:198:GLU:HA | 38:B:9123:HOH:O | 2.17 | 0.44 |
| 25:Y:122:ARG:NH2 | 38:Y:8101:HOH:O | 2.51 | 0.44 |
| 31:9:56:A:H2' | 31:9:57:A:C5' | 2.28 | 0.44 |
| 30:0:545:G:H8 | 30:0:545:G:C5' | 2.14 | 0.44 |
| 30:0:1666:C:C2' | 30:0:1667:A:H5' | 2.31 | 0.44 |
| 2:B:256:GLN:HG2 | 38:B:9122:HOH:O | 2.17 | 0.44 |
| 30:0:2672:C:H2' | 30:0:2673:U:C6 | 2.52 | 0.44 |
| 11:K:118:ALA:CA | 11:K:125:ALA:HB2 | 2.48 | 0.44 |
| 27:1:21:ARG:HD2 | 27:1:39:PHE:HB2 | 1.98 | 0.44 |
| 20:T:19:ARG:HD3 | 20:T:67:LEU:O | 2.18 | 0.44 |
| 5:E:35:TYR:CD2 | 5:E:36:PRO:HD2 | 2.53 | 0.44 |
| 30:0:1224:G:H2' | 30:0:1225:C:C6 | 2.52 | 0.44 |
| 30:0:565:A:C6 | 30:0:566:A:C6 | 3.05 | 0.44 |
| 24:X:34:ARG:NH1 | 24:X:48:VAL:O | 2.49 | 0.44 |
| 7:G:19:GLU:O | 7:G:23:ILE:HG13 | 2.18 | 0.44 |
| 14:N:160:SER:HB3 | 31:9:51:A:H5' | 1.99 | 0.44 |
| 6:F:107:ASP:O | 6:F:111:ILE:HG13 | 2.18 | 0.44 |
| 30:0:363:C:O2' | 30:0:364:U:H5' | 2.18 | 0.44 |
| 5:E:81:GLU:HG2 | 5:E:134:SER:CB | 2.45 | 0.44 |
| 1:A:48:ASP:HA | 1:A:49:PRO:HD3 | 1.86 | 0.44 |
| 30:0:1947:G:N2 | 30:0:1966:U:C2 | 2.86 | 0.44 |
| 3:C:40:ALA:O | 3:C:43:LYS:HB2 | 2.18 | 0.44 |
| 30:0:777:U:OP2 | 30:0:777:U:H4' | 2.17 | 0.44 |
| 18:R:113:HIS:HE1 | 18:R:144:GLU:CD | 2.21 | 0.44 |
| 13:M:169:ARG:HD2 | 38:M:8886:HOH:O | 2.16 | 0.44 |
| 14:N:154:LEU:C | 14:N:156:GLU:H | 2.20 | 0.44 |
| 23:W:75:GLY:HA3 | 38:W:5763:HOH:O | 2.17 | 0.44 |
| 4:D:84:LEU:HA | 4:D:87:ALA:HB3 | 1.99 | 0.44 |
| 3:C:153:VAL:O | 3:C:157:LEU:HG | 2.16 | 0.44 |
| 30:0:1186:C:N4 | 30:0:1187:U:C4 | 2.86 | 0.44 |
| 30:0:1206:U:C5' | 30:0:1206:U:H6 | 2.24 | 0.44 |
| 30:0:2456:A:H5' | 38:0:5708:HOH:O | 2.18 | 0.44 |
| 30:0:1236:A:H2' | 30:0:1237:U:O4' | 2.17 | 0.44 |
| 30:0:537:G:O4' | 30:0:538:C:C5 | 2.70 | 0.44 |
| 30:0:1520:G:C2 | 30:0:1521:C:C2 | 3.06 | 0.44 |
| 30:0:2310:G:C2 | 30:0:2311:A:C5 | 3.05 | 0.44 |
| 30:0:970:U:O5' | 30:0:970:U:H6 | 2.01 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:51:TYR:CE2 | 27:1:53:LYS:HB3 | 2.53 | 0.44 |
| 30:0:1079:A:OP2 | 30:0:1080:C:N4 | 2.46 | 0.44 |
| 30:0:2717:C:C2' | 30:0:2718:C:C5' | 2.81 | 0.43 |
| 30:0:1593:C:O2' | 30:0:1594:C:H5' | 2.18 | 0.43 |
| 30:0:1695:G:C6 | 30:0:1696:U:C4 | 3.06 | 0.43 |
| 30:0:2387:U:H2' | 30:0:2388:C:C6 | 2.53 | 0.43 |
| 30:0:758:A:H2' | 30:0:759:C:O4' | 2.17 | 0.43 |
| 15:O:65:LEU:HD13 | 30:0:746:A:C6 | 2.53 | 0.43 |
| 3:C:195:VAL:HA | 3:C:213:ALA:O | 2.17 | 0.43 |
| 12:L:27:ARG:HH21 | 12:L:30:ARG:HG2 | 1.82 | 0.43 |
| 30:0:2842:G:H2' | 30:0:2843:A:H5' | 2.00 | 0.43 |
| 30:0:2015:A:H2' | 30:0:2016:U:O4' | 2.18 | 0.43 |
| 13:M:115:LEU:HD13 | 13:M:116:ASN:HB2 | 2.00 | 0.43 |
| 30:0:192:A:H5' | 38:0:7657:HOH:O | 2.17 | 0.43 |
| 30:0:1164:U:H3 | 30:0:1192:A:H2 | 1.65 | 0.43 |
| 30:0:2269:C:H2' | 30:0:2270:G:H5' | 2.00 | 0.43 |
| 17:Q:94:GLN:O | 17:Q:95:GLU:HB2 | 2.18 | 0.43 |
| 30:0:2642:G:H2' | 30:0:2643:G:O4' | 2.18 | 0.43 |
| 5:E:84:MET:HG2 | 5:E:168:ILE:HD13 | 2.00 | 0.43 |
| 30:0:958:G:H2' | 30:0:959:C:C6 | 2.53 | 0.43 |
| 10:J:88:PRO:CA | 35:J:8802:CL:CL | 3.03 | 0.43 |
| 30:0:1626:A:C2' | 30:0:1627:G:H5' | 2.48 | 0.43 |
| 30:0:327:A:H4' | 30:0:329:A:C8 | 2.52 | 0.43 |
| 30:0:2649:A:H5' | 30:0:2649:A:C8 | 2.53 | 0.43 |
| 30:0:705:C:H2' | 30:0:705:C:O2 | 2.17 | 0.43 |
| 22:V:4:HIS:O | 22:V:8:ILE:HG13 | 2.18 | 0.43 |
| 30:0:2595:U:O2' | 30:0:2596:A:H5' | 2.18 | 0.43 |
| 30:0:682:A:H2' | 30:0:683:G:O4' | 2.18 | 0.43 |
| 5:E:53:GLU:HB3 | 5:E:55:ASN:ND2 | 2.33 | 0.43 |
| 30:0:2906:A:H5' | 30:0:2907:C:O4' | 2.17 | 0.43 |
| 30:0:1069:C:H2' | 30:0:1070:A:O4' | 2.18 | 0.43 |
| 30:0:2107:U:O2' | 30:0:2108:A:H5' | 2.19 | 0.43 |
| 18:R:80:TYR:O | 30:0:2050:G:H5" | 2.18 | 0.43 |
| 30:0:1205:U:H5 | 38:0:4448:HOH:O | 2.00 | 0.43 |
| 9:I:87:PRO:HG3 | 38:0:7132:HOH:O | 2.18 | 0.43 |
| 31:9:23:U:C2' | 31:9:24:U:H4' | 2.48 | 0.43 |
| 30:0:711:G:C2 | 30:0:718:C:N3 | 2.87 | 0.43 |
| 30:0:1889:C:O2 | 30:0:2010:A:H2 | 2.02 | 0.43 |
| 27:1:9:GLY:HA3 | 30:0:1695:G:H1' | 2.00 | 0.43 |
| 30:0:1631:A:C6 | 30:0:1632:A:N1 | 2.86 | 0.43 |
| 30:0:1298:U:H2' | 30:0:1299:G:C8 | 2.53 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:130:C:H4' | 38:0:5803:HOH:O | 2.17 | 0.43 |
| 16:P:73:HIS:HE1 | 30:0:1789:G:O6 | 2.01 | 0.43 |
| 30:0:100:C:H2' | 30:0:101:C:H6 | 1.84 | 0.43 |
| 7:G:23:ILE:O | 7:G:27:ILE:HG13 | 2.18 | 0.43 |
| 30:0:745:G:H5" | 30:0:746:A:OP1 | 2.18 | 0.43 |
| 30:0:2801:A:H2' | 30:0:2801:A:N3 | 2.33 | 0.43 |
| 30:0:2349:G:O2' | 30:0:2350:G:H5' | 2.17 | 0.43 |
| 30:0:622:G:O2' | 30:0:623:U:H5' | 2.19 | 0.43 |
| 4:D:146:LYS:HE2 | 14:N:107:ASN:ND2 | 2.34 | 0.43 |
| 30:0:871:G:H4' | 38:0:4418:HOH:O | 2.18 | 0.43 |
| 8:H:12:ILE:HG23 | 8:H:129:ARG:CZ | 2.48 | 0.43 |
| 30:0:483:C:N4 | 30:0:484:A:C6 | 2.86 | 0.43 |
| 6:F:91:VAL:CG1 | 6:F:92:GLY:N | 2.81 | 0.43 |
| 30:0:367:G:OP2 | 30:0:367:G:H8 | 2.01 | 0.43 |
| 30:0:2315:C:H4' | 30:0:2425:A:C6 | 2.53 | 0.43 |
| 30:0:1503:U:H3' | 30:0:1503:U:H6 | 1.82 | 0.43 |
| 30:0:2040:C:H5" | 30:0:2759:C:O2' | 2.18 | 0.43 |
| 30:0:2649:A:H5' | 30:0:2649:A:H8 | 1.83 | 0.43 |
| 30:0:1368:U:H6 | 30:0:1368:U:O5' | 2.01 | 0.43 |
| 13:M:67:VAL:HB | 13:M:97:ILE:HG23 | 2.01 | 0.43 |
| 10:J:80:LYS:HE3 | 10:J:101:VAL:O | 2.19 | 0.43 |
| 16:P:98:ILE:HD12 | 16:P:102:ARG:CZ | 2.48 | 0.43 |
| 31:9:110:G:C5 | 31:9:111:U:C5 | 3.07 | 0.43 |
| 30:0:1074:G:H4' | 30:0:1260:G:C6 | 2.54 | 0.43 |
| 14:N:37:ARG:HH21 | 14:N:105:GLY:N | 2.16 | 0.43 |
| 15:O:32:ARG:HH21 | 15:O:35:LYS:HZ2 | 1.67 | 0.43 |
| 14:N:86:LEU:HD23 | 14:N:179:LEU:HD12 | 1.98 | 0.43 |
| 30:0:2010:A:C2' | 38:0:5975:HOH:O | 2.59 | 0.43 |
| 16:P:59:ARG:NH2 | 16:P:66:GLN:HE22 | 2.17 | 0.43 |
| 16:P:83:LYS:HG2 | 30:0:793:A:H5" | 1.99 | 0.43 |
| 30:0:1568:G:C6 | 30:0:1569:U:C4 | 3.06 | 0.43 |
| 30:0:1626:A:H2' | 30:0:1627:G:H5' | 1.99 | 0.43 |
| 1:A:64:ASP:OD1 | 1:A:66:ARG:HD3 | 2.18 | 0.43 |
| 30:0:1416:G:H2' | 30:0:1417:G:H5' | 1.99 | 0.43 |
| 30:0:666:A:H2' | 30:0:667:C:O4' | 2.18 | 0.43 |
| 30:0:113:A:H2' | 30:0:115:U:O4 | 2.19 | 0.43 |
| 30:0:2902:A:H4' | 30:0:2903:C:OP1 | 2.19 | 0.43 |
| 31:9:117:G:H2' | 31:9:118:C:H6 | 1.83 | 0.43 |
| 30:0:2470:A:H5" | 38:0:3249:HOH:O | 2.18 | 0.43 |
| 15:O:29:VAL:HG11 | 15:O:98:LEU:HD21 | 1.99 | 0.43 |
| 30:0:725:C:H2' | 30:0:726:C:O5' | 2.17 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1163:G:H1 | 30:0:1184:C:N4 | 2.17 | 0.43 |
| 15:O:3:THR:HG22 | 30:0:656:G:C5' | 2.31 | 0.43 |
| 30:0:2829:G:N2 | 30:0:2912:C:C2 | 2.86 | 0.43 |
| 23:W:139:GLY:O | 23:W:141:HIS:CD2 | 2.71 | 0.43 |
| 22:V:59:ILE:O | 22:V:63:GLU:HG2 | 2.17 | 0.43 |
| 3:C:27:ARG:NH1 | 3:C:29:ASP:OD1 | 2.50 | 0.43 |
| 3:C:96:LYS:NZ | 30:0:1351:G:OP1 | 2.39 | 0.43 |
| 25:Y:204:ARG:NH2 | 30:0:1324:G:H21 | 2.16 | 0.43 |
| 30:0:1023:C:H2' | 30:0:1024:G:O4' | 2.18 | 0.43 |
| 15:O:25:VAL:HG11 | 30:0:710:G:H5' | 1.99 | 0.43 |
| 30:0:1314:U:H5" | 30:0:1316:G:O4' | 2.19 | 0.43 |
| 16:P:94:TRP:CH2 | 16:P:98:ILE:HG13 | 2.53 | 0.43 |
| 30:0:1585:C:H2' | 30:0:1586:G:H8 | 1.84 | 0.43 |
| 17:Q:47:VAL:HA | 17:Q:48:PRO:HD3 | 1.81 | 0.43 |
| 30:0:1181:A:O2' | 30:0:1182:C:H5' | 2.18 | 0.43 |
| 30:0:2716:G:O2' | 30:0:2717:C:H5' | 2.19 | 0.43 |
| 30:0:1474:C:C5' | 30:0:1474:C:H6 | 2.18 | 0.43 |
| 30:0:2421:G:H3' | 30:0:2422:U:H5" | 2.00 | 0.43 |
| 1:A:94:LEU:N | 1:A:94:LEU:HD23 | 2.33 | 0.43 |
| 1:A:94:LEU:HD12 | 1:A:98:GLU:HB2 | 2.00 | 0.43 |
| 3:C:118:THR:HG22 | 3:C:137:PRO:HB3 | 1.99 | 0.43 |
| 31:9:64:C:O2' | 31:9:65:A:H5' | 2.18 | 0.43 |
| 2:B:51:VAL:CG2 | 2:B:330:VAL:HG22 | 2.48 | 0.43 |
| 15:O:24:ALA:HB3 | 30:0:710:G:OP1 | 2.19 | 0.43 |
| 31:9:59:C:H2' | 31:9:60:C:H6 | 1.83 | 0.43 |
| 30:0:1626:A:H2' | 30:0:1627:G:O4' | 2.19 | 0.43 |
| 30:0:790:A:H2' | 30:0:791:A:O4' | 2.18 | 0.43 |
| 30:0:1950:G:O2' | 30:0:1951:G:H5' | 2.19 | 0.43 |
| 5:E:7:ILE:HG22 | 5:E:45:ASP:O | 2.19 | 0.43 |
| 30:0:912:A:C4 | 30:0:1294:A:C2 | 3.06 | 0.43 |
| 30:0:1175:G:O2' | 30:0:1193:A:H2' | 2.19 | 0.43 |
| 30:0:1132:A:H3' | 38:0:4832:HOH:O | 2.18 | 0.43 |
| 30:0:1453:G:N2 | 30:0:1675:C:C2 | 2.87 | 0.43 |
| 30:0:512:G:O3' | 30:0:513:A:C8 | 2.70 | 0.43 |
| 30:0:1705:C:H2' | 30:0:1706:G:O4' | 2.19 | 0.43 |
| 12:L:67:ARG:O | 12:L:71:GLU:HG3 | 2.19 | 0.43 |
| 14:N:108:SER:HA | 14:N:109:PRO:HD3 | 1.78 | 0.43 |
| 2:B:242:TRP:CZ2 | 30:0:2607:U:C4 | 3.06 | 0.43 |
| 13:M:49:ALA:C | 13:M:54:TYR:HB3 | 2.39 | 0.43 |
| 3:C:25:PRO:HG2 | 38:C:8520:HOH:O | 2.17 | 0.43 |
| 4:D:154:LYS:H | 4:D:154:LYS:CD | 2.20 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2589:U:H2' | 30:0:2590:U:C6 | 2.54 | 0.43 |
| 30:0:2362:A:H2' | 30:0:2363:G:C8 | 2.54 | 0.43 |
| 31:9:65:A:C2' | 31:9:66:G:OP2 | 2.66 | 0.43 |
| 30:0:2241:C:H2' | 30:0:2242:U:C6 | 2.54 | 0.43 |
| 30:0:1971:G:H5" | 38:0:7084:HOH:O | 2.18 | 0.43 |
| 30:0:64:G:H2' | 30:0:65:C:O4' | 2.19 | 0.43 |
| 6:F:61:MET:HB3 | 13:M:19:GLN:OE1 | 2.19 | 0.43 |
| 30:0:590:A:C2' | 30:0:591:A:H5' | 2.48 | 0.43 |
| 1:A:217:ARG:NH2 | 30:0:1853:C:O2' | 2.48 | 0.43 |
| 30:0:1463:U:H2' | 30:0:1464:C:H6 | 1.83 | 0.43 |
| 31:9:117:G:H2' | 31:9:118:C:C6 | 2.53 | 0.43 |
| 30:0:1138:G:H4' | 38:0:5722:HOH:O | 2.18 | 0.43 |
| 23:W:119:HIS:HE1 | 38:0:9560:HOH:O | 2.02 | 0.43 |
| 6:F:59:ILE:CD1 | 30:0:263:U:C2 | 3.02 | 0.43 |
| 14:N:44:ARG:HG3 | 14:N:45:ALA:N | 2.34 | 0.43 |
| 30:0:2761:A:H2' | 38:0:5654:HOH:O | 2.19 | 0.43 |
| 20:T:71:VAL:HG11 | 20:T:90:PRO:HB3 | 1.99 | 0.43 |
| 30:0:1158:G:O2' | 30:0:1159:G:H5' | 2.19 | 0.43 |
| 10:J:75:PRO:HD3 | 10:J:136:SER:OG | 2.18 | 0.43 |
| 30:0:1528:A:H61 | 30:0:1663:G:H1' | 1.84 | 0.43 |
| 23:W:26:ILE:HB | 38:W:5420:HOH:O | 2.18 | 0.43 |
| 30:0:779:U:H5' | 30:0:1836:A:C2 | 2.54 | 0.43 |
| 3:C:27:ARG:HG3 | 3:C:27:ARG:HH11 | 1.83 | 0.43 |
| 30:0:2249:G:C2 | 30:0:2253:G:C6 | 3.07 | 0.43 |
| 30:0:2314:G:O2' | 30:0:2315:C:H5' | 2.19 | 0.43 |
| 18:R:29:LYS:HE2 | 30:0:524:A:H5" | 2.01 | 0.43 |
| 30:0:1559:A:OP2 | 30:0:1559:A:H8 | 2.02 | 0.43 |
| 30:0:1483:C:O2' | 30:0:1484:G:H5' | 2.18 | 0.43 |
| 30:0:1829:A:C8 | 30:0:1885:A:C8 | 3.07 | 0.43 |
| 30:0:1015:C:H2' | 30:0:1016:U:C6 | 2.54 | 0.43 |
| 1:A:217:ARG:CG | 1:A:217:ARG:HH11 | 2.32 | 0.43 |
| 5:E:108:LEU:CD1 | 5:E:164:ASP:HB2 | 2.49 | 0.43 |
| 7:G:63:ARG:O | 7:G:67:LEU:HG | 2.18 | 0.43 |
| 31:9:121:C:H6 | 31:9:121:C:O5' | 2.02 | 0.43 |
| 30:0:764:C:H2' | 30:0:765:G:O4' | 2.19 | 0.43 |
| 4:D:96:SER:O | 30:0:2337:G:H5" | 2.19 | 0.43 |
| 30:0:1409:G:C2 | 30:0:1410:G:C8 | 3.07 | 0.43 |
| 1:A:173:GLY:O | 1:A:176:HIS:HB3 | 2.19 | 0.43 |
| 30:0:69:A:C8 | 30:0:69:A:C5' | 2.98 | 0.42 |
| 30:0:1213:C:C2' | 30:0:1214:G:H5' | 2.48 | 0.42 |
| 14:N:29:SER:HB3 | 30:0:2415:A:O2' | 2.19 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2374:G:H2' | 30:0:2375:A:H8 | 1.83 | 0.42 |
| 30:0:1482:A:H1' | 38:0:9422:HOH:O | 2.19 | 0.42 |
| 24:X:61:ARG:HD2 | 24:X:65:ASN:O | 2.19 | 0.42 |
| 2:B:82:VAL:HG12 | 2:B:82:VAL:O | 2.19 | 0.42 |
| 30:0:1413:A:H2' | 30:0:1414:A:O4' | 2.19 | 0.42 |
| 30:0:2293:G:C2 | 30:0:2316:G:C6 | 3.07 | 0.42 |
| 30:0:1555:G:H4' | 30:0:1630:A:H2 | 1.84 | 0.42 |
| 28:2:20:ARG:HG2 | 28:2:21:VAL:N | 2.33 | 0.42 |
| 30:0:1116:U:C2 | 30:0:1246:A:N6 | 2.87 | 0.42 |
| 23:W:6:GLN:HB2 | 23:W:26:ILE:HD11 | 1.98 | 0.42 |
| 30:0:56:G:N3 | 30:0:70:A:C2 | 2.87 | 0.42 |
| 20:T:9:LYS:HE3 | 20:T:13:ARG:NH1 | 2.33 | 0.42 |
| 18:R:128:ARG:HH22 | 30:0:2054:A:H2 | 1.65 | 0.42 |
| 30:0:137:U:H3' | 30:0:139:C:H41 | 1.83 | 0.42 |
| 30:0:808:A:C5 | 30:0:809:G:H1' | 2.54 | 0.42 |
| 30:0:319:A:H4' | 30:0:338:C:C4 | 2.53 | 0.42 |
| 30:0:2347:C:H2' | 30:0:2348:C:C6 | 2.54 | 0.42 |
| 30:0:1406:A:H4' | 30:0:1407:A:C5' | 2.50 | 0.42 |
| 5:E:91:PHE:HA | 5:E:92:PRO:HD3 | 1.80 | 0.42 |
| 30:0:941:G:C6 | 30:0:942:U:C4 | 3.08 | 0.42 |
| 30:0:1769:C:C4 | 30:0:1770:U:C4 | 3.08 | 0.42 |
| 30:0:2519:C:H2' | 30:0:2520:G:O4' | 2.19 | 0.42 |
| 30:0:917:U:H6 | 30:0:917:U:O5' | 2.02 | 0.42 |
| 14:N:73:ALA:HB1 | 14:N:74:PRO:CD | 2.49 | 0.42 |
| 30:0:216:A:O2' | 30:0:217:C:H5' | 2.19 | 0.42 |
| 17:Q:55:ARG:HD2 | 38:Q:2875:HOH:O | 2.18 | 0.42 |
| 30:0:2726:U:O2 | 30:0:2749:U:O5' | 2.36 | 0.42 |
| 30:0:1185:U:C5' | 38:0:7483:HOH:O | 2.66 | 0.42 |
| 30:0:2822:C:O2' | 30:0:2827:A:H4' | 2.19 | 0.42 |
| 1:A:211:LYS:HG2 | 38:0:7044:HOH:O | 2.19 | 0.42 |
| 21:U:52:THR:HG22 | 21:U:54:THR:N | 2.32 | 0.42 |
| 5:E:107:PHE:CZ | 5:E:152:THR:HB | 2.55 | 0.42 |
| 30:0:2755:G:H1' | 38:0:4696:HOH:O | 2.19 | 0.42 |
| 4:D:22:VAL:HA | 4:D:73:VAL:O | 2.19 | 0.42 |
| 2:B:70:PRO:HG3 | 30:0:2719:A:C2 | 2.54 | 0.42 |
| 30:0:78:G:C6 | 30:0:79:G:C6 | 3.07 | 0.42 |
| 30:0:699:C:C6 | 30:0:744:G:C4 | 3.07 | 0.42 |
| 5:E:77:THR:OG1 | 5:E:78:GLU:N | 2.53 | 0.42 |
| 30:0:1167:G:H3' | 38:0:7514:HOH:O | 2.19 | 0.42 |
| 30:0:1163:G:N2 | 30:0:1184:C:N3 | 2.67 | 0.42 |
| 30:0:1189:A:N7 | 30:0:1190:G:N7 | 2.67 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1603:A:H5' | 30:0:1605:G:C5' | 2.48 | 0.42 |
| 30:0:69:A:C2' | 30:0:70:A:OP2 | 2.67 | 0.42 |
| 30:0:536:A:H8 | 38:0:5057:HOH:O | 2.01 | 0.42 |
| 26:Z:40:ALA:HA | 30:0:1773:G:C8 | 2.54 | 0.42 |
| 30:0:2456:A:H2' | 30:0:2457:U:C6 | 2.55 | 0.42 |
| 30:0:1211:G:H2' | 30:0:1212:C:C6 | 2.48 | 0.42 |
| 30:0:2512:U:O5' | 30:0:2512:U:H6 | 2.02 | 0.42 |
| 30:0:305:A:C6 | 30:0:329:A:N3 | 2.87 | 0.42 |
| 4:D:23:VAL:HG21 | 4:D:45:THR:CG2 | 2.49 | 0.42 |
| 16:P:16:VAL:HG22 | 16:P:20:ARG:CZ | 2.50 | 0.42 |
| 30:0:1400:C:C2' | 30:0:1401:G:H5' | 2.49 | 0.42 |
| 30:0:2061:C:H2' | 30:0:2062:A:H5' | 2.00 | 0.42 |
| 30:0:1850:U:H2' | 30:0:1851:G:C8 | 2.53 | 0.42 |
| 30:0:2119:C:O2' | 30:0:2120:U:H5' | 2.19 | 0.42 |
| 30:0:1057:A:H1' | 30:0:2492:U:O2' | 2.19 | 0.42 |
| 9:I:82:THR:HG22 | 30:0:1168:C:H5" | 2.00 | 0.42 |
| 30:0:2661:U:H3 | 30:0:2812:A:H62 | 1.66 | 0.42 |
| 31:9:14:G:C8 | 31:9:14:G:C5' | 2.99 | 0.42 |
| 14:N:55:ASP:OD2 | 31:9:7:G:H4' | 2.20 | 0.42 |
| 30:0:138:U:OP2 | 30:0:139:C:H5 | 2.02 | 0.42 |
| 2:B:304:PRO:HD2 | 2:B:307:ARG:HE | 1.84 | 0.42 |
| 30:0:807:A:H2' | 30:0:808:A:O4' | 2.19 | 0.42 |
| 30:0:2879:A:H2' | 30:0:2880:A:O4' | 2.19 | 0.42 |
| 30:0:470:U:H2' | 30:0:471:G:O4' | 2.20 | 0.42 |
| 30:0:952:G:H4' | 38:0:4039:HOH:O | 2.19 | 0.42 |
| 31:9:39:U:H1' | 31:9:44:A:N6 | 2.35 | 0.42 |
| 4:D:76:ARG:NH1 | 31:9:42:C:O2 | 2.53 | 0.42 |
| 30:0:1015:C:H2' | 30:0:1016:U:H6 | 1.85 | 0.42 |
| 30:0:2310:G:N1 | 30:0:2311:A:C5 | 2.88 | 0.42 |
| 30:0:939:A:C2 | 30:0:1027:G:N3 | 2.88 | 0.42 |
| 30:0:1381:A:N3 | 30:0:1382:G:H1' | 2.35 | 0.42 |
| 2:B:275:GLY:O | 2:B:291:ASP:HA | 2.19 | 0.42 |
| 30:0:459:A:H4' | 38:0:9454:HOH:O | 2.20 | 0.42 |
| 9:I:118:ASN:HB3 | 30:0:1185:U:C5' | 2.49 | 0.42 |
| 9:I:130:LEU:HD21 | 30:0:1167:G:H4' | 2.02 | 0.42 |
| 30:0:1603:A:C5' | 30:0:1605:G:C5' | 2.96 | 0.42 |
| 28:2:48:ASP:O | 28:2:49:GLU:HB2 | 2.19 | 0.42 |
| 30:0:1211:G:O2' | 30:0:1212:C:H5' | 2.19 | 0.42 |
| 30:0:191:A:C4 | 30:0:237:G:N7 | 2.88 | 0.42 |
| 30:0:657:G:H2' | 30:0:658:C:C6 | 2.55 | 0.42 |
| 2:B:310:ARG:HD2 | 38:B:9114:HOH:O | 2.19 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1966:U:H2' | 30:0:1967:U:H2' | 2.00 | 0.42 |
| 3:C:206:ASN:HB2 | 30:0:329:A:OP2 | 2.19 | 0.42 |
| 30:0:1976:G:O2' | 30:0:1977:U:C5' | 2.68 | 0.42 |
| 30:0:2388:C:O2' | 30:0:2389:U:H5' | 2.19 | 0.42 |
| 4:D:101:THR:HG22 | 4:D:101:THR:O | 2.19 | 0.42 |
| 30:0:849:C:H1' | 38:0:6632:HOH:O | 2.19 | 0.42 |
| 28:2:10:ARG:NH2 | 30:0:121:U:OP2 | 2.39 | 0.42 |
| 30:0:2816:A:H5" | 30:0:2817:G:H5' | 2.01 | 0.42 |
| 18:R:72:VAL:CG1 | 18:R:75:TRP:HB3 | 2.50 | 0.42 |
| 30:0:722:G:H22 | 30:0:938:G:P | 2.42 | 0.42 |
| 30:0:1193:A:H1' | 30:0:1194:A:N7 | 2.35 | 0.42 |
| 30:0:2524:G:H5" | 38:0:4744:HOH:O | 2.19 | 0.42 |
| 30:0:212:A:O4' | 30:0:214:U:C6 | 2.72 | 0.42 |
| 30:0:307:G:H3' | 30:0:342:C:OP2 | 2.19 | 0.42 |
| 18:R:99:ALA:O | 18:R:104:PHE:HB2 | 2.19 | 0.42 |
| 30:0:137:U:H6 | 30:0:137:U:O5' | 2.02 | 0.42 |
| 30:0:120:A:H2' | 30:0:120:A:N3 | 2.34 | 0.42 |
| 2:B:140:LEU:HD13 | 2:B:175:LEU:HA | 2.01 | 0.42 |
| 38:W:7873:HOH:O | 30:0:1287:A:H8 | 2.03 | 0.42 |
| 30:0:1754:A:H2' | 30:0:1755:A:O4' | 2.19 | 0.42 |
| 30:0:1097:A:C6 | 30:0:1098:A:C6 | 3.08 | 0.42 |
| 3:C:73:GLN:HA | 3:C:73:GLN:NE2 | 2.35 | 0.42 |
| 30:0:485:A:H4' | 30:0:486:A:OP1 | 2.20 | 0.42 |
| 30:0:287:C:O5' | 30:0:287:C:H6 | 2.03 | 0.42 |
| 30:0:85:C:H5" | 30:0:86:A:OP2 | 2.20 | 0.42 |
| 30:0:2355:G:H2' | 38:0:5650:HOH:O | 2.18 | 0.42 |
| 8:H:6:ALA:CA | 8:H:61:ARG:HH12 | 2.29 | 0.42 |
| 2:B:254:GLN:NE2 | 38:B:9058:HOH:O | 2.52 | 0.42 |
| 20:T:41:ARG:NH1 | 20:T:42:VAL:O | 2.53 | 0.42 |
| 30:0:2333:G:H2' | 30:0:2334:C:H6 | 1.84 | 0.42 |
| 1:A:30:ARG:HG2 | 1:A:31:LYS:N | 2.35 | 0.42 |
| 30:0:2575:C:H2' | 30:0:2576:A:O4' | 2.19 | 0.42 |
| 30:0:2497:A:C2 | 30:0:2524:G:C2 | 3.07 | 0.42 |
| 20:T:9:LYS:HB2 | 38:0:7442:HOH:O | 2.20 | 0.42 |
| 2:B:53:LEU:HD21 | 2:B:270:ILE:HD12 | 2.01 | 0.42 |
| 30:0:2324:G:C2 | 30:0:2377:U:O2 | 2.73 | 0.42 |
| 30:0:293:A:C4 | 30:0:360:A:C2 | 3.08 | 0.42 |
| 2:B:137:LEU:HD21 | 2:B:140:LEU:HD21 | 2.02 | 0.42 |
| 4:D:21:VAL:HA | 4:D:131:THR:O | 2.20 | 0.42 |
| 4:D:19:GLU:O | 4:D:76:ARG:HG2 | 2.19 | 0.42 |
| 4:D:51:ARG:HD3 | 38:D:7636:HOH:O | 2.20 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:834:G:H4' | 30:0:835:U:OP2 | 2.19 | 0.42 |
| 2:B:215:VAL:HA | 2:B:220:VAL:HG22 | 2.01 | 0.42 |
| 1:A:164:ARG:NH2 | 30:0:1876:C:O3' | 2.53 | 0.42 |
| 30:0:295:C:H2' | 30:0:296:G:O4' | 2.20 | 0.42 |
| 11:K:78:LYS:HA | 11:K:79:PRO:HD3 | 1.94 | 0.42 |
| 30:0:2911:C:H2' | 30:0:2912:C:C6 | 2.54 | 0.42 |
| 30:0:2727:A:C6 | 30:0:2756:U:C2 | 3.08 | 0.42 |
| 27:1:25:LYS:HG3 | 28:2:49:GLU:H | 1.85 | 0.42 |
| 23:W:48:VAL:HG12 | 23:W:48:VAL:O | 2.20 | 0.42 |
| 17:Q:18:PRO:O | 17:Q:21:ARG:HB2 | 2.20 | 0.42 |
| 30:0:130:C:H5' | 38:0:5226:HOH:O | 2.20 | 0.42 |
| 30:0:2134:G:C6 | 30:0:2258:A:C8 | 3.08 | 0.42 |
| 30:0:1544:U:H2' | 30:0:1545:C:C6 | 2.53 | 0.42 |
| 21:U:50:GLU:HB2 | 30:0:2866:U:C5 | 2.54 | 0.42 |
| 30:0:844:A:C6 | 30:0:882:A:C6 | 3.08 | 0.42 |
| 2:B:75:GLU:C | 2:B:77:PRO:HD3 | 2.39 | 0.42 |
| 30:0:264:G:H1' | 30:0:265:U:H5 | 1.85 | 0.42 |
| 30:0:1175:G:H1' | 30:0:1193:A:N9 | 2.33 | 0.41 |
| 30:0:2269:C:C2' | 30:0:2270:G:H5' | 2.50 | 0.41 |
| 30:0:583:C:C2 | 30:0:584:U:C5 | 3.08 | 0.41 |
| 17:Q:40:HIS:HE1 | 30:0:949:U:O2' | 2.03 | 0.41 |
| 30:0:212:A:N1 | 30:0:226:A:H5" | 2.35 | 0.41 |
| 30:0:2534:C:H2' | 30:0:2535:A:C8 | 2.55 | 0.41 |
| 20:T:48:VAL:HG22 | 20:T:97:ARG:O | 2.19 | 0.41 |
| 11:K:14:LYS:CB | 11:K:45:PRO:HG2 | 2.50 | 0.41 |
| 30:0:2297:U:H2' | 30:0:2298:C:C6 | 2.53 | 0.41 |
| 2:B:84:LEU:O | 2:B:99:GLU:HA | 2.20 | 0.41 |
| 30:0:803:C:H2' | 30:0:804:C:C6 | 2.55 | 0.41 |
| 30:0:2333:G:H2' | 30:0:2334:C:C6 | 2.55 | 0.41 |
| 7:G:20:VAL:O | 7:G:24:VAL:HG23 | 2.20 | 0.41 |
| 12:L:57:VAL:O | 12:L:57:VAL:HG12 | 2.20 | 0.41 |
| 12:L:57:VAL:HG21 | 30:0:2443:C:H5' | 2.02 | 0.41 |
| 13:M:47:ASP:CG | 13:M:48:LYS:N | 2.74 | 0.41 |
| 30:0:226:A:H1' | 30:0:393:G:C5 | 2.55 | 0.41 |
| 6:F:99:THR:HG23 | 6:F:99:THR:O | 2.20 | 0.41 |
| 13:M:9:ARG:HD2 | 30:0:380:A:OP2 | 2.20 | 0.41 |
| 1:A:179:MET:HG2 | 1:A:186:TRP:HB2 | 2.02 | 0.41 |
| 30:0:636:G:H5' | 30:0:2059:U:OP2 | 2.20 | 0.41 |
| 10:J:107:ASN:HD22 | 10:J:107:ASN:C | 2.24 | 0.41 |
| 11:K:41:LYS:O | 11:K:42:ASN:HB2 | 2.20 | 0.41 |
| 26:Z:34:SER:CB | 30:0:797:A:H4' | 2.50 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:229:ARG:HD2 | 38:B:8989:HOH:O | 2.20 | 0.41 |
| 18:R:79:ARG:HB3 | 30:0:2050:G:OP1 | 2.20 | 0.41 |
| 30:0:2350:G:H2' | 30:0:2351:C:C6 | 2.56 | 0.41 |
| 20:T:71:VAL:CG1 | 20:T:90:PRO:HB3 | 2.50 | 0.41 |
| 8:H:91:ARG:HG2 | 8:H:91:ARG:H | 1.54 | 0.41 |
| 30:0:830:G:C5 | 30:0:831:U:C4 | 3.08 | 0.41 |
| 1:A:97:ALA:HB2 | 1:A:150:PRO:HB2 | 2.02 | 0.41 |
| 20:T:28:SER:O | 20:T:32:ARG:HG3 | 2.19 | 0.41 |
| 30:0:1355:A:H4' | 38:0:5766:HOH:O | 2.19 | 0.41 |
| 5:E:10:ASP:HA | 38:E:6017:HOH:O | 2.20 | 0.41 |
| 18:R:96:VAL:HG13 | 18:R:106:GLY:HA3 | 2.02 | 0.41 |
| 30:0:1162:G:C6 | 30:0:1163:G:C6 | 3.09 | 0.41 |
| 31:9:3:A:C6 | 31:9:22:G:H1' | 2.52 | 0.41 |
| 30:0:1598:A:C2 | 30:0:1599:U:C2 | 3.07 | 0.41 |
| 1:A:141:PRO:HG2 | 30:0:1855:G:O6 | 2.20 | 0.41 |
| 30:0:567:U:H5" | 38:0:5300:HOH:O | 2.19 | 0.41 |
| 30:0:1172:G:H1' | 38:0:4984:HOH:O | 2.20 | 0.41 |
| 30:0:1971:G:C5' | 38:0:7084:HOH:O | 2.67 | 0.41 |
| 23:W:35:VAL:HA | 23:W:36:PRO:HD3 | 1.83 | 0.41 |
| 18:R:132:ARG:NH2 | 38:R:8987:HOH:O | 2.53 | 0.41 |
| 30:0:349:U:O2' | 30:0:350:G:H5' | 2.20 | 0.41 |
| 2:B:199:TYR:CE2 | 2:B:268:ARG:HB2 | 2.54 | 0.41 |
| 30:0:2766:A:O2' | 30:0:2767:C:H5' | 2.20 | 0.41 |
| 30:0:1056:U:H2' | 30:0:1057:A:O4' | 2.20 | 0.41 |
| 2:B:124:ALA:O | 2:B:128:ILE:HG13 | 2.21 | 0.41 |
| 30:0:696:C:O2' | 30:0:697:G:H5' | 2.19 | 0.41 |
| 30:0:1154:A:H2' | 30:0:1155:G:O4' | 2.20 | 0.41 |
| 30:0:283:U:C5 | 30:0:284:C:N3 | 2.87 | 0.41 |
| 30:0:1421:C:H2' | 30:0:1422:U:C6 | 2.55 | 0.41 |
| 30:0:594:C:C4 | 30:0:595:U:C4 | 3.09 | 0.41 |
| 4:D:129:ASP:OD1 | 30:0:2338:G:H2' | 2.20 | 0.41 |
| 30:0:1904:A:C2 | 30:0:1905:U:H1' | 2.54 | 0.41 |
| 30:0:2600:A:H2' | 30:0:2601:A:O4' | 2.20 | 0.41 |
| 23:W:74:GLU:OE1 | 30:0:1285:U:H4' | 2.21 | 0.41 |
| 30:0:1471:A:H2' | 30:0:1472:C:C6 | 2.55 | 0.41 |
| 30:0:445:U:H2' | 30:0:446:G:C8 | 2.55 | 0.41 |
| 30:0:2310:G:C2 | 30:0:2311:A:C8 | 3.08 | 0.41 |
| 30:0:1149:U:H5" | 30:0:1151:G:O4' | 2.21 | 0.41 |
| 30:0:2699:A:H2' | 30:0:2700:G:O4' | 2.20 | 0.41 |
| 11:K:22:ASP:HB2 | 38:K:5264:HOH:O | 2.20 | 0.41 |
| 17:Q:34:ASP:O | 17:Q:37:GLU:HB2 | 2.20 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1946:C:O4' | 30:0:1969:A:C2 | 2.73 | 0.41 |
| 30:0:1139:U:H2' | 30:0:1140:C:C6 | 2.55 | 0.41 |
| 30:0:1795:G:H2' | 30:0:1796:A:O4' | 2.20 | 0.41 |
| 30:0:177:A:O2' | 30:0:892:G:H4' | 2.20 | 0.41 |
| 8:H:46:TYR:HA | 8:H:47:PRO:HD3 | 1.88 | 0.41 |
| 30:0:30:U:O2 | 30:0:460:A:C2 | 2.74 | 0.41 |
| 30:0:815:U:O2' | 30:0:1598:A:H4' | 2.20 | 0.41 |
| 29:3:38:ARG:HD2 | 30:0:396:U:OP2 | 2.20 | 0.41 |
| 30:0:1060:C:H6 | 30:0:1060:C:C5' | 2.29 | 0.41 |
| 30:0:968:G:H2' | 30:0:969:G:C8 | 2.54 | 0.41 |
| 30:0:625:U:H3' | 38:0:3262:HOH:O | 2.20 | 0.41 |
| 24:X:43:VAL:HG12 | 24:X:44:ASP:H | 1.85 | 0.41 |
| 30:0:154:C:O2' | 30:0:155:C:H5' | 2.20 | 0.41 |
| 30:0:2250:G:N2 | 30:0:2251:G:H1' | 2.36 | 0.41 |
| 3:C:184:ARG:HD2 | 30:0:1306:U:OP1 | 2.21 | 0.41 |
| 2:B:248:ARG:NH2 | 30:0:2549:C:H1' | 2.35 | 0.41 |
| 31:9:110:G:C6 | 31:9:111:U:C5 | 3.08 | 0.41 |
| 30:0:113:A:OP2 | 30:0:114:A:H2' | 2.20 | 0.41 |
| 5:E:19:ASP:HA | 5:E:31:ARG:O | 2.21 | 0.41 |
| 30:0:1933:G:O2' | 30:0:1934:A:H5' | 2.20 | 0.41 |
| 5:E:111:LYS:CE | 30:0:2690:U:H4' | 2.50 | 0.41 |
| 13:M:72:ALA:HB2 | 13:M:93:ARG:HG2 | 2.01 | 0.41 |
| 30:0:1163:G:C2 | 30:0:1184:C:N3 | 2.89 | 0.41 |
| 30:0:1184:C:O2' | 30:0:1185:U:OP2 | 2.35 | 0.41 |
| 30:0:1189:A:C8 | 30:0:1190:G:C8 | 3.09 | 0.41 |
| 31:9:28:U:O2 | 31:9:57:A:N6 | 2.53 | 0.41 |
| 16:P:115:SER:OG | 16:P:118:GLN:HG3 | 2.21 | 0.41 |
| 30:0:563:C:H2' | 30:0:564:G:O4' | 2.21 | 0.41 |
| 30:0:2003:U:O2' | 30:0:2004:U:H5 | 2.02 | 0.41 |
| 30:0:168:C:O5' | 30:0:168:C:H6 | 2.04 | 0.41 |
| 30:0:1947:G:H2' | 30:0:1948:G:C8 | 2.52 | 0.41 |
| 19:S:57:THR:HG22 | 19:S:59:ASP:N | 2.34 | 0.41 |
| 30:0:1006:A:N3 | 30:0:2298:C:O2' | 2.50 | 0.41 |
| 30:0:2328:U:C4 | 30:0:2329:C:C5 | 3.08 | 0.41 |
| 30:0:2891:A:C2 | 30:0:2892:G:C4 | 3.09 | 0.41 |
| 30:0:2722:G:C2 | 30:0:2761:A:C2 | 3.09 | 0.41 |
| 8:H:91:ARG:HA | 30:0:1002:G:O2' | 2.20 | 0.41 |
| 30:0:2860:G:H2' | 30:0:2861:G:O4' | 2.20 | 0.41 |
| 30:0:929:A:O5' | 30:0:929:A:H8 | 2.04 | 0.41 |
| 30:0:571:C:H6 | 30:0:571:C:O5' | 2.03 | 0.41 |
| 13:M:164:THR:CG2 | 13:M:165:GLY:N | 2.82 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:1733:A:H2' | 30:0:1734:C:O4' | 2.20 | 0.41 |
| 30:0:1615:A:H5' | 38:0:4187:HOH:O | 2.19 | 0.41 |
| 1:A:36:ASP:CB | 1:A:85:SER:H | 2.29 | 0.41 |
| 25:Y:234:VAL:HG12 | 25:Y:235:GLU:N | 2.36 | 0.41 |
| 30:0:681:G:H2' | 30:0:681:G:N3 | 2.36 | 0.41 |
| 21:U:56:ARG:NH1 | 30:0:2890:A:C2 | 2.89 | 0.41 |
| 12:L:30:ARG:NH1 | 38:L:8811:HOH:O | 2.48 | 0.41 |
| 30:0:940:G:C5 | 30:0:1027:G:C2 | 3.09 | 0.41 |
| 25:Y:145:LYS:HD2 | 38:0:9965:HOH:O | 2.20 | 0.41 |
| 30:0:301:C:O2' | 30:0:302:A:H5' | 2.21 | 0.41 |
| 19:S:6:LYS:HB2 | 19:S:27:ALA:O | 2.20 | 0.41 |
| 30:0:1051:C:H2' | 30:0:1052:G:O4' | 2.21 | 0.41 |
| 30:0:1797:A:H2' | 30:0:1799:G:O5' | 2.21 | 0.41 |
| 31:9:78:G:O2' | 31:9:79:U:OP2 | 2.38 | 0.41 |
| 9:I:87:PRO:HD2 | 30:0:1180:U:O2' | 2.20 | 0.41 |
| 31:9:23:U:H2' | 31:9:24:U:H4' | 2.03 | 0.41 |
| 30:0:506:G:N1 | 30:0:509:A:OP2 | 2.54 | 0.41 |
| 30:0:2712:G:O2' | 30:0:2713:G:H5' | 2.21 | 0.41 |
| 30:0:2756:U:C2 | 30:0:2896:A:H2 | 2.39 | 0.41 |
| 30:0:1597:A:C4 | 30:0:1598:A:C8 | 3.09 | 0.41 |
| 30:0:250:C:H2' | 30:0:251:C:C6 | 2.55 | 0.41 |
| 30:0:1730:G:N3 | 30:0:1730:G:H2' | 2.36 | 0.41 |
| 30:0:1819:G:C2' | 30:0:1820:G:C5' | 2.97 | 0.41 |
| 2:B:307:ARG:HD2 | 38:B:9119:HOH:O | 2.20 | 0.41 |
| 30:0:1517:C:O2 | 30:0:1670:A:C2 | 2.74 | 0.41 |
| 2:B:140:LEU:HA | 38:B:9045:HOH:O | 2.20 | 0.41 |
| 30:0:510:U:H5" | 30:0:512:G:OP2 | 2.21 | 0.41 |
| 25:Y:151:SER:HB3 | 25:Y:154:ARG:HB3 | 2.03 | 0.41 |
| 30:0:24:G:H22 | 30:0:518:G:H1' | 1.86 | 0.41 |
| 30:0:2866:U:H4' | 30:0:2867:G:H5' | 2.01 | 0.41 |
| 23:W:130:HIS:NE2 | 31:9:88:G:OP1 | 2.45 | 0.41 |
| 23:W:38:THR:HG22 | 23:W:39:ASP:N | 2.35 | 0.41 |
| 16:P:55:LYS:HA | 38:0:5633:HOH:O | 2.21 | 0.41 |
| 30:0:519:A:H4' | 30:0:1320:C:O3' | 2.21 | 0.41 |
| 30:0:1255:A:N3 | 38:0:7772:HOH:O | 2.37 | 0.41 |
| 30:0:271:C:H4' | 30:0:272:A:OP1 | 2.21 | 0.41 |
| 2:B:234:ARG:HD3 | 30:0:1734:C:OP1 | 2.21 | 0.41 |
| 23:W:88:THR:HG23 | 23:W:110:GLN:CB | 2.43 | 0.41 |
| 30:0:1840:A:H4' | 30:0:1841:C:O5' | 2.21 | 0.41 |
| 30:0:2756:U:N3 | 30:0:2896:A:H2 | 2.17 | 0.41 |
| 30:0:1597:A:C5 | 30:0:1598:A:C8 | 3.08 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:W:4:LEU:HD22 | 23:W:52:VAL:CG2 | 2.49 | 0.41 |
| 30:0:1873:G:C2' | 30:0:1874:U:H5' | 2.51 | 0.41 |
| 30:0:1942:A:C1' | 38:0:9044:HOH:O | 2.69 | 0.41 |
| 30:0:1890:U:H4' | 30:0:2010:A:C6 | 2.56 | 0.41 |
| 4:D:173:GLU:HG3 | 4:D:174:VAL:N | 2.36 | 0.41 |
| 30:0:2361:A:H2' | 30:0:2362:A:C8 | 2.55 | 0.41 |
| 31:9:65:A:O2' | 31:9:66:G:P | 2.79 | 0.41 |
| 30:0:694:A:H2' | 30:0:695:C:C5' | 2.50 | 0.41 |
| 14:N:7:LYS:HB3 | 30:0:2353:A:O2' | 2.20 | 0.41 |
| 30:0:652:G:H2' | 30:0:653:U:O4' | 2.20 | 0.41 |
| 25:Y:134:HIS:HE1 | 30:0:538:C:OP2 | 2.04 | 0.41 |
| 1:A:105:VAL:HG11 | 1:A:154:ALA:HB1 | 2.01 | 0.41 |
| 23:W:5:VAL:HG22 | 23:W:32:CYS:HB2 | 2.02 | 0.41 |
| 4:D:18:ILE:HG12 | 4:D:134:LEU:HD21 | 2.03 | 0.41 |
| 30:0:1706:G:C6 | 30:0:1707:G:N1 | 2.89 | 0.41 |
| 17:Q:30:VAL:O | 17:Q:30:VAL:HG12 | 2.21 | 0.41 |
| 30:0:822:C:H2' | 30:0:823:U:C6 | 2.54 | 0.41 |
| 30:0:2479:A:H5" | 38:0:4665:HOH:O | 2.21 | 0.41 |
| 2:B:254:GLN:HG3 | 38:0:9708:HOH:O | 2.21 | 0.41 |
| 23:W:125:HIS:HD2 | 23:W:127:GLY:H | 1.68 | 0.41 |
| 30:0:278:A:H2' | 30:0:279:C:O4' | 2.19 | 0.41 |
| 29:3:60:LYS:HG3 | 38:0:7573:HOH:O | 2.19 | 0.41 |
| 4:D:49:PRO:HA | 4:D:73:VAL:HG22 | 2.02 | 0.41 |
| 30:0:1718:G:C6 | 30:0:1719:G:C5 | 3.08 | 0.41 |
| 2:B:80:ARG:O | 2:B:82:VAL:HG23 | 2.21 | 0.41 |
| 30:0:2689:A:H2' | 30:0:2690:U:H5' | 2.02 | 0.41 |
| 30:0:106:A:H2' | 30:0:107:U:O4' | 2.21 | 0.41 |
| 18:R:17:MET:HE3 | 18:R:19:ARG:NH2 | 2.36 | 0.41 |
| 30:0:1222:A:H2' | 30:0:1223:G:O4' | 2.21 | 0.41 |
| 16:P:28:GLN:HE22 | 30:0:1387:G:C1' | 2.33 | 0.41 |
| 23:W:120:PRO:HG2 | 30:0:1095:U:O2 | 2.20 | 0.41 |
| 30:0:827:A:H2' | 30:0:828:G:O4' | 2.21 | 0.41 |
| 13:M:75:ARG:HH21 | 13:M:78:LYS:HE3 | 1.85 | 0.41 |
| 30:0:2864:U:C5 | 30:0:2865:G:C6 | 3.09 | 0.41 |
| 30:0:1305:C:H5' | 38:0:9844:HOH:O | 2.20 | 0.41 |
| 30:0:1364:G:H1' | 38:0:4812:HOH:O | 2.20 | 0.41 |
| 8:H:52:LEU:HD13 | 8:H:153:PHE:HB3 | 2.02 | 0.41 |
| 30:0:1175:G:H1' | 30:0:1193:A:H2' | 2.03 | 0.41 |
| 30:0:2780:C:H2' | 30:0:2781:U:C6 | 2.56 | 0.41 |
| 30:0:364:U:H2' | 30:0:365:G:O4' | 2.21 | 0.41 |
| 30:0:1819:G:H2' | 30:0:1820:G:H5' | 1.98 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:3:48:ASN:ND2 | 30:0:169:A:H1' | 2.36 | 0.41 |
| 30:0:424:C:C2 | 30:0:425:U:C5 | 3.09 | 0.41 |
| 3:C:73:GLN:HG2 | 30:0:475:G:OP1 | 2.20 | 0.41 |
| 30:0:2722:G:N3 | 30:0:2761:A:C2 | 2.89 | 0.41 |
| 30:0:580:A:O4' | 30:0:1111:U:H4' | 2.21 | 0.41 |
| 30:0:413:G:H2' | 30:0:414:C:C6 | 2.55 | 0.41 |
| 30:0:146:U:O2' | 30:0:147:G:H5' | 2.21 | 0.41 |
| 30:0:426:G:H2' | 30:0:427:C:O4' | 2.19 | 0.41 |
| 30:0:2002:C:H2' | 30:0:2003:U:H5' | 2.03 | 0.40 |
| 4:D:135:VAL:HG22 | 4:D:136:ARG:N | 2.36 | 0.40 |
| 10:J:41:ALA:HB3 | 38:J:8865:HOH:O | 2.19 | 0.40 |
| 30:0:1217:G:C2 | 30:0:1218:U:C2 | 3.09 | 0.40 |
| 30:0:334:G:C5 | 30:0:335:U:C5 | 3.09 | 0.40 |
| 30:0:1250:C:O2' | 30:0:1251:C:H5' | 2.21 | 0.40 |
| 25:Y:144:ARG:CZ | 38:Y:8181:HOH:O | 2.69 | 0.40 |
| 30:0:772:G:H2' | 30:0:773:A:O4' | 2.21 | 0.40 |
| 19:S:38:ALA:O | 19:S:42:GLU:HG3 | 2.21 | 0.40 |
| 2:B:24:PRO:HD3 | 38:B:8991:HOH:O | 2.22 | 0.40 |
| 30:0:275:G:C2 | 30:0:376:C:N3 | 2.88 | 0.40 |
| 13:M:167:GLY:O | 13:M:171:ARG:HG3 | 2.21 | 0.40 |
| 30:0:371:U:H2' | 30:0:372:A:H8 | 1.86 | 0.40 |
| 3:C:236:THR:CG2 | 3:C:239:ALA:H | 2.34 | 0.40 |
| 30:0:921:G:H4' | 30:0:924:G:N1 | 2.36 | 0.40 |
| 30:0:921:G:H4' | 30:0:924:G:C6 | 2.56 | 0.40 |
| 30:0:1587:U:C4 | 30:0:1588:G:C5 | 3.09 | 0.40 |
| 30:0:423:A:C4 | 30:0:424:C:C6 | 3.09 | 0.40 |
| 30:0:1295:G:H2' | 30:0:1296:A:C8 | 2.56 | 0.40 |
| 30:0:293:A:C2 | 30:0:294:C:C6 | 3.09 | 0.40 |
| 30:0:1669:G:H2' | 30:0:1670:A:C8 | 2.56 | 0.40 |
| 8:H:27:PRO:HD3 | 8:H:123:ILE:HG22 | 2.02 | 0.40 |
| 7:G:63:ARG:NH1 | 30:0:1151:G:OP1 | 2.54 | 0.40 |
| 3:C:138:VAL:O | 3:C:234:VAL:HA | 2.21 | 0.40 |
| 30:0:725:C:C2' | 30:0:726:C:O5' | 2.69 | 0.40 |
| 30:0:1928:C:C2' | 30:0:1929:G:H5' | 2.51 | 0.40 |
| 23:W:11:VAL:HG11 | 30:0:1086:A:C6 | 2.55 | 0.40 |
| 25:Y:152:LYS:HB3 | 25:Y:160:LYS:HG3 | 2.03 | 0.40 |
| 30:0:2385:G:H2' | 30:0:2386:U:C6 | 2.56 | 0.40 |
| 30:0:2846:C:H3' | 38:0:7101:HOH:O | 2.20 | 0.40 |
| 21:U:31:PHE:CG | 21:U:37:GLU:HG2 | 2.56 | 0.40 |
| 30:0:1182:C:H1' | 30:0:1192:A:C8 | 2.41 | 0.40 |
| 30:0:1205:U:O2 | 30:0:1205:U:H2' | 2.21 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:0:2831:C:H2' | 30:0:2832:C:O4' | 2.22 | 0.40 |
| 2:B:209:LYS:HB2 | 2:B:257:THR:O | 2.21 | 0.40 |
| 23:W:139:GLY:O | 23:W:141:HIS:HD2 | 2.04 | 0.40 |
| 30:0:1198:U:H1' | 30:0:1201:C:H5 | 1.86 | 0.40 |
| 11:K:81:ARG:HD3 | 11:K:87:ARG:NH2 | 2.36 | 0.40 |
| 1:A:38:ILE:HA | 1:A:38:ILE:HD13 | 1.90 | 0.40 |
| 3:C:226:GLY:HA3 | 30:0:1308:A:O4' | 2.21 | 0.40 |
| 30:0:123:U:H2' | 30:0:124:C:C6 | 2.55 | 0.40 |
| 30:0:1947:G:OP1 | 30:0:1971:G:N7 | 2.54 | 0.40 |
| 30:0:319:A:H2' | 30:0:320:G:C8 | 2.56 | 0.40 |
| 23:W:5:VAL:HG11 | 23:W:153:MET:HE1 | 2.04 | 0.40 |
| 10:J:90:LYS:HB2 | 35:J:8802:CL:CL | 2.58 | 0.40 |
| 24:X:30:MET:HE1 | 24:X:55:ASN:HA | 2.03 | 0.40 |
| 30:0:303:C:N4 | 30:0:304:G:C6 | 2.89 | 0.40 |
| 13:M:42:ARG:HA | 13:M:43:PRO:HD3 | 1.93 | 0.40 |
| 16:P:87:ARG:HG2 | 38:0:5961:HOH:O | 2.22 | 0.40 |
| 30:0:2765:C:H2' | 30:0:2766:A:C8 | 2.56 | 0.40 |
| 25:Y:148:GLY:HA3 | 30:0:622:G:P | 2.61 | 0.40 |
| 17:Q:59:GLN:NE2 | 30:0:1018:A:H4' | 2.36 | 0.40 |
| 30:0:549:A:C6 | 30:0:550:C:C4 | 3.10 | 0.40 |
| 30:0:1375:A:C2' | 30:0:1376:G:H5' | 2.51 | 0.40 |
| 30:0:1167:G:O2' | 30:0:1168:C:H5' | 2.22 | 0.40 |
| 30:0:272:A:N1 | 30:0:369:G:H5" | 2.35 | 0.40 |
| 30:0:545:G:C8 | 30:0:545:G:C5' | 2.95 | 0.40 |
| 31:9:24:U:H3' | 31:9:24:U:H6 | 1.87 | 0.40 |
| 30:0:2505:G:HO2' | 30:0:2506:A:H5' | 1.80 | 0.40 |
| 20:T:21:LYS:HA | 20:T:24:ARG:HG3 | 2.04 | 0.40 |
| 28:2:41:HIS:CD2 | 28:2:44:ARG:H | 2.31 | 0.40 |
| 4:D:25:MET:HE1 | 4:D:37:ALA:O | 2.22 | 0.40 |
| 25:Y:187:VAL:HG13 | 25:Y:205:ILE:HA | 2.02 | 0.40 |
| 6:F:56:PRO:HB2 | 6:F:58:GLU:OE1 | 2.21 | 0.40 |
| 30:0:2887:G:H2' | 30:0:2888:U:O4' | 2.22 | 0.40 |
| 30:0:963:C:O2 | 30:0:1005:A:N1 | 2.54 | 0.40 |
| 24:X:79:GLU:CD | 24:X:80:GLU:H | 2.25 | 0.40 |
| 1:A:109:GLU:HG2 | 1:A:116:GLY:N | 2.36 | 0.40 |
| 30:0:803:C:H2' | 30:0:804:C:H6 | 1.87 | 0.40 |
| 30:0:2802:C:H2' | 30:0:2803:C:H6 | 1.85 | 0.40 |
| 12:L:30:ARG:HD3 | 30:0:164:G:H4' | 2.04 | 0.40 |
| 30:0:2118:A:C5 | 30:0:2470:A:C5 | 3.09 | 0.40 |
| 30:0:1386:G:O2' | 30:0:1387:G:H5' | 2.22 | 0.40 |
| 30:0:2437:A:H2' | 30:0:2438:G:C8 | 2.57 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:W:108:ARG:HG3 | 23:W:114:PRO:HG3 | 2.03 | 0.40 |
| 30:0:27:U:H5 | 38:0:5902:HOH:O | 2.04 | 0.40 |
| 30:0:1931:A:H2' | 30:0:1932:G:H5' | 2.04 | 0.40 |
| 30:0:1189:A:H1' | 30:0:1209:C:H1' | 2.02 | 0.40 |
| 30:0:1191:A:H2 | 30:0:1206:U:H3 | 1.69 | 0.40 |
| 30:0:1207:A:H5' | 30:0:1208:C:OP2 | 2.21 | 0.40 |
| 30:0:2712:G:P | 38:0:5233:HOH:O | 2.79 | 0.40 |
| 30:0:1342:C:H2' | 30:0:1343:C:C5' | 2.47 | 0.40 |
| 30:0:365:G:C6 | 30:0:366:U:C4 | 3.09 | 0.40 |
| 20:T:49:GLU:OE2 | 20:T:97:ARG:HD2 | 2.22 | 0.40 |
| 30:0:1589:G:H4' | 38:0:6875:HOH:O | 2.20 | 0.40 |
| 30:0:2133:U:H4' | 30:0:2134:G:H5' | 2.02 | 0.40 |
| 18:R:132:ARG:CZ | 38:R:8987:HOH:O | 2.70 | 0.40 |
| 30:0:820:G:H5' | 30:0:821:U:H5' | 2.02 | 0.40 |
| 30:0:2346:C:O5' | 30:0:2346:C:C6 | 2.74 | 0.40 |
| 12:L:113:GLN:C | 30:0:700:A:H62 | 2.24 | 0.40 |
| 14:N:143:ARG:HG2 | 14:N:172:PHE:CD2 | 2.56 | 0.40 |
| 30:0:1102:C:H4' | 38:0:9561:HOH:O | 2.20 | 0.40 |
| 15:O:44:ASN:OD1 | 15:O:65:LEU:HB2 | 2.22 | 0.40 |
| 30:0:2304:G:C6 | 30:0:2305:A:C5 | 3.10 | 0.40 |
| 7:G:64:ASN:N | 7:G:64:ASN:HD22 | 2.18 | 0.40 |
| 30:0:2237:G:O2' | 30:0:2238:A:C8 | 2.72 | 0.40 |
| 16:P:104:LYS:HE2 | 16:P:138:GLU:OE2 | 2.20 | 0.40 |
| 30:0:2543:G:H2' | 30:0:2544:G:O4' | 2.21 | 0.40 |
| 25:Y:133:HIS:HD2 | 38:Y:8150:HOH:O | 2.04 | 0.40 |
| 18:R:46:TYR:O | 18:R:50:VAL:HG23 | 2.22 | 0.40 |
| 26:Z:50:VAL:O | 26:Z:54:GLU:HG3 | 2.21 | 0.40 |
| 30:0:461:C:N3 | 30:0:479:G:H5' | 2.36 | 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%) | 211 (90%) | 22 (9%) | 2 (1%) | 21 52 |
| 2 | B | 335/338 (99%) | 309 (92%) | 21 (6%) | 5 (2%) | 13 36 |
| 3 | C | 244/246 (99%) | 228 (93%) | 16 (7%) | 0 | 100 100 |
| 4 | D | 134/177 (76%) | 110 (82%) | 22 (16%) | 2 (2%) | 13 36 |
| 5 | E | 170/178 (96%) | 160 (94%) | 9 (5%) | 1 (1%) | 30 62 |
| 6 | F | 117/120 (98%) | 107 (92%) | 8 (7%) | 2 (2%) | 11 32 |
| 7 | G | 25/348 (7%) | 23 (92%) | 2 (8%) | 0 | 100 100 |
| 8 | H | 156/177 (88%) | 141 (90%) | 14 (9%) | 1 (1%) | 30 62 |
| 9 | I | 68/162 (42%) | 53 (78%) | 13 (19%) | 2 (3%) | 6 17 |
| 10 | J | 140/145 (97%) | 131 (94%) | 8 (6%) | 1 (1%) | 26 59 |
| 11 | K | 130/132 (98%) | 122 (94%) | 8 (6%) | 0 | 100 100 |
| 12 | L | 141/165 (86%) | 125 (89%) | 13 (9%) | 3 (2%) | 9 25 |
| 13 | M | 192/196 (98%) | 181 (94%) | 10 (5%) | 1 (0%) | 34 67 |
| 14 | N | 184/187 (98%) | 164 (89%) | 16 (9%) | 4 (2%) | 8 24 |
| 15 | O | 113/116 (97%) | 110 (97%) | 3 (3%) | 0 | 100 100 |
| 16 | P | 141/149 (95%) | 137 (97%) | 4 (3%) | 0 | 100 100 |
| 17 | Q | 93/96 (97%) | 89 (96%) | 3 (3%) | 1 (1%) | 17 46 |
| 18 | R | 148/155 (96%) | 141 (95%) | 7 (5%) | 0 | 100 100 |
| 19 | S | 79/85 (93%) | 74 (94%) | 5 (6%) | 0 | 100 100 |
| 20 | T | 117/120 (98%) | 108 (92%) | 8 (7%) | 1 (1%) | 21 52 |
| 21 | U | 51/67 (76%) | 48 (94%) | 3 (6%) | 0 | 100 100 |
| 22 | V | 63/71 (89%) | 59 (94%) | 3 (5%) | 1 (2%) | 12 34 |
| 23 | W | 152/154 (99%) | 146 (96%) | 6 (4%) | 0 | 100 100 |
| 24 | X | 80/92 (87%) | 73 (91%) | 5 (6%) | 2 (2%) | 7 21 |
| 25 | Y | 140/241 (58%) | 139 (99%) | 1 (1%) | 0 | 100 100 |
| 26 | Z | 71/116 (61%) | 62 (87%) | 9 (13%) | 0 | 100 100 |
| 27 | 1 | 54/57 (95%) | 52 (96%) | 2 (4%) | 0 | 100 100 |
| 28 | 2 | 42/50 (84%) | 41 (98%) | 1 (2%) | 0 | 100 100 |
| 29 | 3 | 90/92 (98%) | 88 (98%) | 2 (2%) | 0 | 100 100 |
| All | All | 3705/4472 (83%) | 3432 (93%) | 244 (7%) | 29 (1%) | 24 55 |

All (29) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 37 | VAL |
| 8 | H | 19 | ARG |
| 10 | J | 5 | GLU |
| 14 | N | 154 | LEU |
| 14 | N | 183 | ASP |
| 14 | N | 184 | ILE |
| 2 | B | 184 | ASP |
| 9 | I | 107 | LYS |
| 12 | L | 149 | ARG |
| 14 | N | 162 | ASP |
| 1 | A | 34 | ASP |
| 2 | B | 34 | GLY |
| 6 | F | 101 | ALA |
| 12 | L | 80 | ASP |
| 2 | B | 2 | GLN |
| 2 | B | 245 | SER |
| 4 | D | 56 | ARG |
| 12 | L | 21 | ARG |
| 20 | T | 53 | GLY |
| 24 | X | 87 | ALA |
| 4 | D | 137 | PRO |
| 6 | F | 100 | ASP |
| 24 | X | 70 | ILE |
| 22 | V | 39 | ALA |
| 2 | B | 185 | GLY |
| 17 | Q | 78 | GLY |
| 5 | E | 44 | GLY |
| 9 | I | 83 | GLY |
| 13 | M | 88 | 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%) | 166 (93%) | 13 (7%) | 17 41 |
| 2 | B | 282/283 (100%) | 264 (94%) | 18 (6%) | 22 49 |
| 3 | C | 193/193 (100%) | 179 (93%) | 14 (7%) | 17 41 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 4 | D | 117/148 (79%) | 113 (97%) | 4 (3%) | 44 76 |
| 5 | E | 152/156 (97%) | 150 (99%) | 2 (1%) | 76 93 |
| 6 | F | 93/94 (99%) | 92 (99%) | 1 (1%) | 80 94 |
| 7 | G | 27/282 (10%) | 25 (93%) | 2 (7%) | 17 40 |
| 8 | H | 134/145 (92%) | 129 (96%) | 5 (4%) | 41 74 |
| 9 | I | 58/130 (45%) | 58 (100%) | 0 | 100 100 |
| 10 | J | 118/121 (98%) | 112 (95%) | 6 (5%) | 29 61 |
| 11 | K | 106/106 (100%) | 105 (99%) | 1 (1%) | 84 95 |
| 12 | L | 113/127 (89%) | 107 (95%) | 6 (5%) | 28 58 |
| 13 | M | 158/160 (99%) | 152 (96%) | 6 (4%) | 40 73 |
| 14 | N | 149/150 (99%) | 142 (95%) | 7 (5%) | 32 64 |
| 15 | O | 93/94 (99%) | 93 (100%) | 0 | 100 100 |
| 16 | P | 113/117 (97%) | 110 (97%) | 3 (3%) | 52 83 |
| 17 | Q | 79/80 (99%) | 75 (95%) | 4 (5%) | 29 61 |
| 18 | R | 117/122 (96%) | 111 (95%) | 6 (5%) | 29 61 |
| 19 | S | 71/74 (96%) | 70 (99%) | 1 (1%) | 74 92 |
| 20 | T | 105/106 (99%) | 98 (93%) | 7 (7%) | 20 46 |
| 21 | U | 44/53 (83%) | 44 (100%) | 0 | 100 100 |
| 22 | V | 51/57 (90%) | 50 (98%) | 1 (2%) | 63 89 |
| 23 | W | 130/130 (100%) | 126 (97%) | 4 (3%) | 47 79 |
| 24 | X | 66/74 (89%) | 62 (94%) | 4 (6%) | 23 52 |
| 25 | Y | 120/196 (61%) | 116 (97%) | 4 (3%) | 45 77 |
| 26 | Z | 60/94 (64%) | 59 (98%) | 1 (2%) | 68 90 |
| 27 | 1 | 46/47 (98%) | 45 (98%) | 1 (2%) | 60 87 |
| 28 | 2 | 42/46 (91%) | 41 (98%) | 1 (2%) | 57 86 |
| 29 | 3 | 79/79 (100%) | 76 (96%) | 3 (4%) | 40 73 |
| All | All | 3095/3646 (85%) | 2970 (96%) | 125 (4%) | 38 71 |

All (125) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3 | ARG |
| 1 | A | 26 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 36 | ASP |
| 1 | A | 38 | ILE |
| 1 | A | 68 | ILE |
| 1 | A | 69 | LEU |
| 1 | A | 94 | LEU |
| 1 | A | 131 | HIS |
| 1 | A | 165 | THR |
| 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 | 16 | ARG |
| 2 | B | 27 | ASN |
| 2 | B | 51 | VAL |
| 2 | B | 53 | LEU |
| 2 | B | 71 | VAL |
| 2 | B | 88 | GLU |
| 2 | B | 97 | LEU |
| 2 | B | 98 | THR |
| 2 | B | 132 | HIS |
| 2 | B | 149 | ASP |
| 2 | B | 162 | MET |
| 2 | B | 175 | LEU |
| 2 | B | 234 | ARG |
| 2 | B | 254 | GLN |
| 2 | B | 257 | THR |
| 2 | B | 265 | LEU |
| 3 | C | 78 | ARG |
| 3 | C | 91 | PRO |
| 3 | C | 94 | THR |
| 3 | C | 101 | ASP |
| 3 | C | 115 | LEU |
| 3 | C | 132 | ASP |
| 3 | C | 136 | VAL |
| 3 | C | 162 | VAL |
| 3 | C | 187 | ARG |
| 3 | C | 214 | THR |
| 3 | C | 222 | ASP |
| 3 | C | 223 | LEU |
| 3 | C | 234 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 243 | VAL |
| 4 | D | 24 | HIS |
| 4 | D | 29 | HIS |
| 4 | D | 50 | VAL |
| 4 | D | 161 | ASP |
| 5 | E | 102 | VAL |
| 5 | E | 156 | ASP |
| 6 | F | 12 | LEU |
| 7 | G | 72 | ASP |
| 7 | G | 73 | ASP |
| 8 | H | 21 | GLU |
| 8 | H | 62 | HIS |
| 8 | H | 87 | LYS |
| 8 | H | 91 | ARG |
| 8 | H | 157 | TYR |
| 10 | J | 46 | ILE |
| 10 | J | 52 | GLN |
| 10 | J | 74 | ARG |
| 10 | J | 79 | PHE |
| 10 | J | 93 | ARG |
| 10 | J | 107 | ASN |
| 11 | K | 10 | GLN |
| 12 | L | 35 | ARG |
| 12 | L | 37 | LYS |
| 12 | L | 102 | ASP |
| 12 | L | 104 | ASP |
| 12 | L | 114 | VAL |
| 12 | L | 140 | VAL |
| 13 | M | 46 | LEU |
| 13 | M | 68 | ARG |
| 13 | M | 93 | ARG |
| 13 | M | 99 | ARG |
| 13 | M | 116 | ASN |
| 13 | M | 164 | THR |
| 14 | N | 23 | ARG |
| 14 | N | 26 | LEU |
| 14 | N | 49 | THR |
| 14 | N | 101 | VAL |
| 14 | N | 127 | LEU |
| 14 | N | 139 | TRP |
| 14 | N | 173 | ASP |
| 16 | P | 16 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | P | 91 | LYS |
| 16 | P | 98 | ILE |
| 17 | Q | 11 | ARG |
| 17 | Q | 16 | ASN |
| 17 | Q | 18 | PRO |
| 17 | Q | 57 | ASP |
| 18 | R | 39 | THR |
| 18 | R | 82 | GLU |
| 18 | R | 119 | VAL |
| 18 | R | 132 | ARG |
| 18 | R | 143 | VAL |
| 18 | R | 150 | PRO |
| 19 | S | 44 | GLN |
| 20 | T | 39 | ASN |
| 20 | T | 48 | VAL |
| 20 | T | 71 | VAL |
| 20 | T | 73 | HIS |
| 20 | T | 89 | ARG |
| 20 | T | 115 | GLU |
| 20 | T | 117 | ASP |
| 22 | V | 12 | THR |
| 23 | W | 26 | ILE |
| 23 | W | 52 | VAL |
| 23 | W | 108 | ARG |
| 23 | W | 146 | ILE |
| 24 | X | 27 | ASP |
| 24 | X | 52 | PRO |
| 24 | X | 72 | VAL |
| 24 | X | 82 | GLU |
| 25 | Y | 95 | THR |
| 25 | Y | 189 | ASN |
| 25 | Y | 191 | ASP |
| 25 | Y | 203 | VAL |
| 26 | Z | 68 | GLU |
| 27 | 1 | 14 | THR |
| 28 | 2 | 18 | ASN |
| 29 | 3 | 14 | CYS |
| 29 | 3 | 56 | PRO |
| 29 | 3 | 87 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 47 | HIS |
| 1 | A | 199 | HIS |
| 2 | B | 2 | GLN |
| 2 | B | 27 | ASN |
| 2 | B | 106 | HIS |
| 2 | B | 145 | HIS |
| 2 | B | 221 | GLN |
| 2 | B | 238 | ASN |
| 2 | B | 256 | GLN |
| 2 | B | 260 | HIS |
| 2 | B | 320 | GLN |
| 2 | B | 332 | ASN |
| 3 | C | 73 | GLN |
| 3 | C | 129 | HIS |
| 3 | C | 151 | GLN |
| 3 | C | 163 | HIS |
| 4 | D | 85 | GLN |
| 4 | D | 103 | ASN |
| 5 | E | 143 | GLN |
| 7 | G | 64 | ASN |
| 8 | H | 34 | HIS |
| 8 | H | 59 | GLN |
| 8 | H | 62 | HIS |
| 10 | J | 52 | GLN |
| 10 | J | 107 | ASN |
| 10 | J | 126 | ASN |
| 10 | J | 142 | ASN |
| 11 | K | 10 | GLN |
| 11 | K | 44 | HIS |
| 11 | K | 67 | GLN |
| 12 | L | 18 | HIS |
| 12 | L | 41 | HIS |
| 13 | M | 24 | GLN |
| 13 | M | 58 | GLN |
| 13 | M | 137 | ASN |
| 13 | M | 143 | ASN |
| 13 | M | 170 | ASN |
| 14 | N | 40 | ASN |
| 14 | N | 53 | ASN |
| 14 | N | 107 | ASN |
| 14 | N | 132 | ASN |
| 16 | P | 50 | GLN |
| 16 | P | 66 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | P | 73 | HIS |
| 16 | P | 88 | GLN |
| 16 | P | 118 | GLN |
| 17 | Q | 40 | HIS |
| 18 | R | 22 | GLN |
| 18 | R | 61 | GLN |
| 18 | R | 94 | ASN |
| 18 | R | 98 | ASN |
| 18 | R | 113 | HIS |
| 18 | R | 117 | HIS |
| 18 | R | 122 | GLN |
| 18 | R | 123 | GLN |
| 19 | S | 44 | GLN |
| 19 | S | 53 | ASN |
| 20 | T | 39 | ASN |
| 21 | U | 39 | ASN |
| 22 | V | 60 | GLN |
| 23 | W | 27 | HIS |
| 23 | W | 110 | GLN |
| 23 | W | 119 | HIS |
| 23 | W | 125 | HIS |
| 23 | W | 141 | HIS |
| 24 | X | 23 | HIS |
| 25 | Y | 134 | HIS |
| 25 | Y | 189 | ASN |
| 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 | 15 | ASN |
| 29 | 3 | 20 | HIS |
| 29 | 3 | 48 | ASN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 30 | 0 | 2745/2923 (93%) | 232 (8%) | 18 (0%) |
| 31 | 9 | 121/122 (99%) | 16 (13%) | 1 (0%) |
| All | All | 2866/3045 (94%) | 248 (8%) | 19 (0%) |

All (248) 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 | 130 | C |
| 30 | 0 | 141 | C |
| 30 | 0 | 151 | A |
| 30 | 0 | 166 | A |
| 30 | 0 | 169 | A |
| 30 | 0 | 186 | A |
| 30 | 0 | 191 | A |
| 30 | 0 | 192 | A |
| 30 | 0 | 198 | A |
| 30 | 0 | 200 | C |
| 30 | 0 | 204 | A |
| 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 | 368 | C |
| 30 | 0 | 381 | G |
| 30 | 0 | 397 | A |
| 30 | 0 | 417 | G |
| 30 | 0 | 461 | C |
| 30 | 0 | 487 | G |
| 30 | 0 | 498 | A |
| 30 | 0 | 510 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 | 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 | 701 | U |
| 30 | 0 | 746 | A |
| 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 | 857 | A |
| 30 | 0 | 858 | U |
| 30 | 0 | 868 | G |
| 30 | 0 | 869 | G |
| 30 | 0 | 871 | G |
| 30 | 0 | 872 | U |
| 30 | 0 | 875 | A |
| 30 | 0 | 877 | G |
| 30 | 0 | 878 | G |
| 30 | 0 | 884 | C |
| 30 | 0 | 885 | 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 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 | 1124 | A |
| 30 | 0 | 1130 | U |
| 30 | 0 | 1151 | G |
| 30 | 0 | 1165 | G |
| 30 | 0 | 1174 | A |
| 30 | 0 | 1175 | G |
| 30 | 0 | 1185 | U |
| 30 | 0 | 1192 | A |
| 30 | 0 | 1193 | A |
| 30 | 0 | 1206 | U |
| 30 | 0 | 1208 | C |
| 30 | 0 | 1216 | G |
| 30 | 0 | 1237 | U |
| 30 | 0 | 1238 | C |
| 30 | 0 | 1239 | G |
| 30 | 0 | 1242 | A |
| 30 | 0 | 1279 | U |
| 30 | 0 | 1289 | C |
| 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 | 1409 | G |
| 30 | 0 | 1474 | C |
| 30 | 0 | 1505 | U |
| 30 | 0 | 1506 | U |
| 30 | 0 | 1524 | U |
| 30 | 0 | 1525 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 1526 | A |
| 30 | 0 | 1535 | G |
| 30 | 0 | 1562 | C |
| 30 | 0 | 1592 | G |
| 30 | 0 | 1605 | 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 |
| 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 | 1731 | C |
| 30 | 0 | 1732 | A |
| 30 | 0 | 1742 | A |
| 30 | 0 | 1752 | G |
| 30 | 0 | 1778 | A |
| 30 | 0 | 1798 | C |
| 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 | 1979 | G |
| 30 | 0 | 1980 | U |
| 30 | 0 | 1996 | U |
| 30 | 0 | 2006 | C |
| 30 | 0 | 2008 | U |
| 30 | 0 | 2011 | A |
| 30 | 0 | 2012 | U |
| 30 | 0 | 2013 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 |
| 30 | 0 | 2110 | G |
| 30 | 0 | 2238 | A |
| 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 | 2354 | A |
| 30 | 0 | 2361 | A |
| 30 | 0 | 2369 | A |
| 30 | 0 | 2379 | G |
| 30 | 0 | 2422 | U |
| 30 | 0 | 2462 | G |
| 30 | 0 | 2465 | A |
| 30 | 0 | 2467 | A |
| 30 | 0 | 2476 | C |
| 30 | 0 | 2483 | A |
| 30 | 0 | 2507 | G |
| 30 | 0 | 2509 | A |
| 30 | 0 | 2511 | A |
| 30 | 0 | 2533 | C |
| 30 | 0 | 2537 | G |
| 30 | 0 | 2541 | U |
| 30 | 0 | 2553 | A |
| 30 | 0 | 2564 | G |
| 30 | 0 | 2589 | U |
| 30 | 0 | 2601 | A |
| 30 | 0 | 2602 | G |
| 30 | 0 | 2608 | C |
| 30 | 0 | 2613 | G |
| 30 | 0 | 2637 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 2638 | G |
| 30 | 0 | 2649 | A |
| 30 | 0 | 2664 | A |
| 30 | 0 | 2681 | A |
| 30 | 0 | 2682 | C |
| 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 | 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 | 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 | 40 | C |
| 31 | 9 | 41 | C |
| 31 | 9 | 43 | G |
| 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 (19) RNA pucker outliers are listed below:

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 0 | 129 | A |
| 30 | 0 | 603 | A |
| 30 | 0 | 699 | C |
| 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 | 1506 | U |
| 30 | 0 | 1685 | A |
| 30 | 0 | 1979 | G |
| 30 | 0 | 2467 | A |
| 30 | 0 | 2649 | A |
| 30 | 0 | 2718 | C |
| 30 | 0 | 2726 | U |
| 30 | 0 | 2761 | A |
| 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 | OMU | 0 | 2587 | 30 | 12,22,23 | 0.99 | 1 (8%) | 19,31,34 | 3.13 | 2 (10%) |
| 30 | OMG | 0 | 2588 | 30 | 17,26,27 | 1.06 | 1 (5%) | 21,38,41 | 2.52 | 3 (14%) |
| 30 | UR3 | 0 | 2619 | 30 | 12,22,23 | 0.74 | 0 | 16,32,35 | 0.75 | 0 |
| 30 | PSU | 0 | 2621 | 30 | 13,21,22 | 1.72 | 2 (15%) | 18,30,33 | 6.16 | 3 (16%) |
| 30 | 1MA | 0 | 628 | 30,34 | 14,25,26 | 0.97 | 1 (7%) | 15,37,40 | 1.12 | 1 (6%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 30 | OMU | 0 | 2587 | 30 | - | 0/5/27/28 | 0/2/2/2 |
| 30 | OMG | 0 | 2588 | 30 | - | 0/5/27/28 | 0/3/3/3 |
| 30 | UR3 | 0 | 2619 | 30 | - | 0/3/25/26 | 0/2/2/2 |
| 30 | PSU | 0 | 2621 | 30 | - | 0/7/25/26 | 0/2/2/2 |
| 30 | 1MA | 0 | 628 | 30,34 | - | 0/3/25/26 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 0 | 2621 | PSU | C5-C1' | -5.23 | 1.47 | 1.52 |
| 30 | 0 | 2587 | OMU | C4-N3 | 2.44 | 1.37 | 1.33 |
| 30 | 0 | 628 | 1MA | C6-N6 | 2.68 | 1.34 | 1.29 |
| 30 | 0 | 2621 | PSU | C4-N3 | 2.70 | 1.38 | 1.33 |
| 30 | 0 | 2588 | OMG | C6-N1 | 3.25 | 1.39 | 1.33 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 0 | 2621 | PSU | N1-C2-N3 | -21.71 | 114.48 | 128.33 |
| 30 | 0 | 2588 | OMG | C5-C6-N1 | -8.66 | 111.74 | 123.59 |
| 30 | 0 | 628 | 1MA | C2-N3-C4 | -3.59 | 110.84 | 116.40 |
| 30 | 0 | 2587 | OMU | C5-C4-N3 | -3.31 | 114.63 | 123.12 |
| 30 | 0 | 2588 | OMG | N3-C2-N1 | -2.30 | 123.94 | 127.44 |
| 30 | 0 | 2621 | PSU | C6-N1-C2 | 2.75 | 119.90 | 115.47 |
| 30 | 0 | 2588 | OMG | C6-N1-C2 | 6.63 | 125.14 | 115.94 |
| 30 | 0 | 2587 | OMU | C4-N3-C2 | 13.02 | 127.04 | 114.14 |
| 30 | 0 | 2621 | PSU | C4-N3-C2 | 13.78 | 127.16 | 115.25 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 30 | 0 | 2587 | OMU | 2 | 0 |

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%) | 0.82 | 28 (11%) 6 4 | 22, 47, 83, 108 | 0 |
| 2 | B | 337/338 (99%) | 0.54 | 16 (4%) 35 28 | 25, 51, 79, 90 | 0 |
| 3 | C | 246/246 (100%) | -0.03 | 5 (2%) 68 63 | 19, 42, 65, 81 | 0 |
| 4 | D | 140/177 (79%) | 2.05 | 58 (41%) 0 0 | 58, 101, 124, 135 | 0 |
| 5 | E | 172/178 (96%) | 0.68 | 16 (9%) 11 7 | 42, 66, 89, 94 | 0 |
| 6 | F | 119/120 (99%) | 0.97 | 19 (15%) 3 2 | 44, 69, 96, 114 | 0 |
| 7 | G | 29/348 (8%) | 1.64 | 10 (34%) 0 0 | 71, 91, 100, 102 | 0 |
| 8 | H | 160/177 (90%) | 1.31 | 40 (25%) 1 0 | 55, 73, 100, 106 | 0 |
| 9 | I | 70/162 (43%) | 3.52 | 50 (71%) 0 0 | 127, 145, 163, 164 | 0 |
| 10 | J | 142/145 (97%) | 0.40 | 5 (3%) 48 41 | 34, 51, 71, 94 | 0 |
| 11 | K | 132/132 (100%) | 0.69 | 8 (6%) 25 18 | 29, 47, 68, 77 | 0 |
| 12 | L | 145/165 (87%) | 0.47 | 11 (7%) 17 11 | 26, 62, 111, 125 | 0 |
| 13 | M | 194/196 (98%) | 0.25 | 3 (1%) 76 72 | 24, 38, 55, 62 | 0 |
| 14 | N | 186/187 (99%) | 0.59 | 16 (8%) 13 8 | 40, 65, 111, 120 | 0 |
| 15 | O | 115/116 (99%) | -0.21 | 0 100 100 | 34, 49, 67, 76 | 0 |
| 16 | P | 143/149 (95%) | 0.83 | 15 (10%) 8 5 | 34, 51, 67, 75 | 0 |
| 17 | Q | 95/96 (98%) | 0.13 | 0 100 100 | 34, 45, 61, 74 | 0 |
| 18 | R | 150/155 (96%) | 0.34 | 3 (2%) 68 63 | 28, 44, 64, 74 | 0 |
| 19 | S | 81/85 (95%) | 0.45 | 4 (4%) 33 26 | 35, 53, 73, 86 | 0 |
| 20 | T | 119/120 (99%) | 0.21 | 5 (4%) 40 33 | 34, 52, 80, 109 | 0 |
| 21 | U | 53/67 (79%) | 1.00 | 8 (15%) 3 2 | 39, 54, 73, 82 | 0 |
| 22 | V | 65/71 (91%) | 1.10 | 8 (12%) 5 3 | 42, 66, 113, 122 | 0 |
| 23 | W | 154/154 (100%) | 0.06 | 2 (1%) 79 75 | 36, 49, 67, 83 | 0 |
| 24 | X | 82/92 (89%) | 0.97 | 10 (12%) 5 3 | 37, 57, 82, 98 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 25 | Y | 142/241 (58%) | -0.09 | 2 (1%) 78 73 | 23, 44, 65, 87 | 0 |
| 26 | Z | 73/116 (62%) | 1.28 | 17 (23%) 1 1 | 47, 66, 82, 97 | 0 |
| 27 | 1 | 56/57 (98%) | 0.44 | 0 100 100 | 21, 28, 35, 45 | 0 |
| 28 | 2 | 46/50 (92%) | 0.75 | 5 (10%) 7 4 | 28, 58, 88, 95 | 0 |
| 29 | 3 | 92/92 (100%) | 0.23 | 0 100 100 | 35, 54, 67, 83 | 0 |
| 30 | 0 | 2749/2923 (94%) | 0.01 | 38 (1%) 78 73 | 19, 43, 89, 167 | 0 |
| 31 | 9 | 122/122 (100%) | -0.44 | 2 (1%) 74 70 | 37, 67, 86, 146 | 0 |
| All | All | 6646/7517 (88%) | 0.35 | 404 (6%) 25 18 | 19, 49, 99, 167 | 0 |

All (404) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 22 | V | 1 | THR | 16.2 |
| 9 | I | 100 | VAL | 12.0 |
| 4 | D | 63 | ILE | 11.4 |
| 9 | I | 74 | ILE | 10.4 |
| 4 | D | 66 | GLY | 9.0 |
| 9 | I | 128 | THR | 9.0 |
| 4 | D | 93 | LEU | 9.0 |
| 9 | I | 104 | ALA | 9.0 |
| 1 | A | 237 | GLY | 7.4 |
| 9 | I | 113 | SER | 7.1 |
| 22 | V | 40 | PRO | 6.8 |
| 9 | I | 70 | THR | 6.7 |
| 4 | D | 81 | GLU | 6.6 |
| 22 | V | 39 | ALA | 6.6 |
| 22 | V | 43 | PRO | 6.6 |
| 9 | I | 97 | VAL | 6.4 |
| 9 | I | 91 | PHE | 6.4 |
| 14 | N | 166 | ALA | 6.3 |
| 22 | V | 38 | GLY | 6.2 |
| 4 | D | 88 | LEU | 6.2 |
| 20 | T | 119 | ALA | 6.1 |
| 4 | D | 27 | ILE | 6.0 |
| 31 | 9 | 1 | U | 6.0 |
| 2 | B | 1 | PRO | 5.9 |
| 9 | I | 80 | PHE | 5.8 |
| 9 | I | 78 | ALA | 5.8 |
| 9 | I | 110 | ASP | 5.7 |
| 9 | I | 115 | ASP | 5.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | D | 64 | ARG | 5.3 |
| 4 | D | 57 | THR | 5.3 |
| 26 | Z | 43 | GLY | 5.2 |
| 9 | I | 108 | HIS | 5.2 |
| 4 | D | 26 | GLY | 5.2 |
| 9 | I | 117 | THR | 5.2 |
| 21 | U | 46 | ALA | 5.1 |
| 4 | D | 171 | ASP | 5.0 |
| 9 | I | 111 | LEU | 5.0 |
| 7 | G | 27 | ILE | 5.0 |
| 1 | A | 43 | VAL | 5.0 |
| 26 | Z | 67 | GLY | 5.0 |
| 4 | D | 69 | ILE | 4.9 |
| 9 | I | 103 | ILE | 4.9 |
| 4 | D | 134 | LEU | 4.9 |
| 8 | H | 48 | VAL | 4.8 |
| 4 | D | 95 | THR | 4.8 |
| 30 | 0 | 1172 | G | 4.8 |
| 9 | I | 95 | LEU | 4.7 |
| 26 | Z | 48 | ARG | 4.7 |
| 4 | D | 62 | ASP | 4.7 |
| 24 | X | 85 | VAL | 4.6 |
| 9 | I | 87 | PRO | 4.6 |
| 16 | P | 143 | ALA | 4.6 |
| 9 | I | 133 | THR | 4.6 |
| 28 | 2 | 39 | ARG | 4.5 |
| 19 | S | 81 | ILE | 4.5 |
| 22 | V | 41 | GLU | 4.5 |
| 8 | H | 76 | LEU | 4.4 |
| 9 | I | 132 | VAL | 4.4 |
| 4 | D | 170 | TYR | 4.4 |
| 8 | H | 150 | LYS | 4.4 |
| 4 | D | 85 | GLN | 4.3 |
| 5 | E | 87 | PHE | 4.3 |
| 14 | N | 162 | ASP | 4.2 |
| 9 | I | 99 | GLN | 4.2 |
| 8 | H | 123 | ILE | 4.2 |
| 24 | X | 10 | VAL | 4.2 |
| 5 | E | 100 | ASP | 4.2 |
| 8 | H | 53 | ILE | 4.2 |
| 30 | 0 | 2637 | A | 4.2 |
| 6 | F | 20 | LEU | 4.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | D | 19 | GLU | 4.1 |
| 14 | N | 185 | GLU | 4.1 |
| 6 | F | 115 | VAL | 4.1 |
| 1 | A | 89 | ALA | 4.1 |
| 8 | H | 97 | VAL | 4.1 |
| 9 | I | 68 | PRO | 4.1 |
| 8 | H | 30 | LYS | 4.1 |
| 8 | H | 89 | THR | 4.1 |
| 21 | U | 24 | LYS | 4.0 |
| 4 | D | 90 | LEU | 4.0 |
| 12 | L | 97 | VAL | 4.0 |
| 4 | D | 87 | ALA | 4.0 |
| 4 | D | 102 | GLY | 4.0 |
| 16 | P | 114 | LEU | 4.0 |
| 4 | D | 44 | ILE | 4.0 |
| 9 | I | 93 | ALA | 4.0 |
| 7 | G | 26 | MET | 3.9 |
| 30 | 0 | 1195 | G | 3.9 |
| 24 | X | 88 | GLU | 3.9 |
| 4 | D | 166 | ILE | 3.9 |
| 26 | Z | 46 | SER | 3.9 |
| 9 | I | 66 | GLY | 3.9 |
| 24 | X | 14 | LEU | 3.9 |
| 30 | 0 | 1196 | C | 3.9 |
| 4 | D | 128 | LEU | 3.8 |
| 26 | Z | 49 | ARG | 3.8 |
| 30 | 0 | 1170 | U | 3.8 |
| 22 | V | 37 | GLY | 3.8 |
| 9 | I | 118 | ASN | 3.8 |
| 9 | I | 96 | SER | 3.7 |
| 2 | B | 278 | PRO | 3.7 |
| 4 | D | 104 | PHE | 3.7 |
| 1 | A | 158 | VAL | 3.7 |
| 9 | I | 116 | LEU | 3.7 |
| 8 | H | 81 | GLY | 3.7 |
| 8 | H | 169 | GLU | 3.7 |
| 9 | I | 88 | GLN | 3.7 |
| 4 | D | 61 | PHE | 3.6 |
| 8 | H | 133 | GLY | 3.6 |
| 9 | I | 120 | ALA | 3.6 |
| 4 | D | 18 | ILE | 3.6 |
| 30 | 0 | 1951 | G | 3.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 99 | ILE | 3.6 |
| 4 | D | 75 | LEU | 3.6 |
| 12 | L | 100 | ALA | 3.6 |
| 23 | W | 96 | LEU | 3.6 |
| 2 | B | 119 | HIS | 3.6 |
| 30 | 0 | 1177 | A | 3.5 |
| 10 | J | 6 | PHE | 3.5 |
| 11 | K | 110 | LYS | 3.5 |
| 30 | 0 | 1950 | G | 3.5 |
| 4 | D | 10 | PHE | 3.5 |
| 30 | 0 | 2508 | C | 3.5 |
| 8 | H | 157 | TYR | 3.5 |
| 8 | H | 141 | CYS | 3.5 |
| 9 | I | 106 | GLN | 3.5 |
| 30 | 0 | 999 | C | 3.5 |
| 4 | D | 158 | ASN | 3.5 |
| 14 | N | 182 | GLY | 3.5 |
| 19 | S | 2 | TRP | 3.5 |
| 4 | D | 101 | THR | 3.4 |
| 21 | U | 52 | THR | 3.4 |
| 8 | H | 79 | GLU | 3.4 |
| 30 | 0 | 1171 | A | 3.4 |
| 16 | P | 137 | LEU | 3.4 |
| 5 | E | 159 | VAL | 3.4 |
| 4 | D | 165 | PHE | 3.4 |
| 16 | P | 116 | SER | 3.4 |
| 9 | I | 134 | ILE | 3.4 |
| 2 | B | 91 | PRO | 3.3 |
| 30 | 0 | 1169 | U | 3.3 |
| 28 | 2 | 27 | LEU | 3.3 |
| 4 | D | 172 | VAL | 3.3 |
| 6 | F | 17 | LEU | 3.3 |
| 9 | I | 79 | GLY | 3.3 |
| 26 | Z | 42 | TYR | 3.3 |
| 8 | H | 16 | ALA | 3.3 |
| 12 | L | 76 | LEU | 3.3 |
| 30 | 0 | 970 | U | 3.3 |
| 4 | D | 94 | ALA | 3.3 |
| 8 | H | 161 | THR | 3.3 |
| 7 | G | 70 | ALA | 3.3 |
| 8 | H | 146 | ALA | 3.3 |
| 4 | D | 80 | ALA | 3.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 30 | 0 | 1182 | C | 3.2 |
| 30 | 0 | 2510 | C | 3.2 |
| 9 | I | 102 | GLN | 3.2 |
| 6 | F | 19 | ALA | 3.2 |
| 1 | A | 36 | ASP | 3.2 |
| 6 | F | 44 | SER | 3.2 |
| 8 | H | 174 | LEU | 3.2 |
| 4 | D | 60 | GLU | 3.2 |
| 9 | I | 101 | LYS | 3.2 |
| 21 | U | 51 | TRP | 3.2 |
| 4 | D | 43 | GLU | 3.2 |
| 8 | H | 62 | HIS | 3.1 |
| 2 | B | 62 | ARG | 3.1 |
| 4 | D | 28 | GLY | 3.1 |
| 30 | 0 | 2507 | G | 3.1 |
| 7 | G | 73 | ASP | 3.1 |
| 8 | H | 77 | ILE | 3.1 |
| 3 | C | 62 | GLY | 3.1 |
| 1 | A | 82 | VAL | 3.1 |
| 7 | G | 68 | GLU | 3.1 |
| 9 | I | 82 | THR | 3.0 |
| 1 | A | 80 | LEU | 3.0 |
| 30 | 0 | 1198 | U | 3.0 |
| 2 | B | 138 | GLY | 3.0 |
| 4 | D | 89 | PRO | 3.0 |
| 1 | A | 124 | VAL | 3.0 |
| 14 | N | 95 | ALA | 3.0 |
| 2 | B | 118 | ASP | 3.0 |
| 26 | Z | 44 | ARG | 3.0 |
| 8 | H | 54 | VAL | 3.0 |
| 9 | I | 83 | GLY | 3.0 |
| 4 | D | 129 | ASP | 3.0 |
| 12 | L | 95 | ASP | 3.0 |
| 16 | P | 112 | GLY | 3.0 |
| 12 | L | 93 | VAL | 3.0 |
| 11 | K | 128 | ALA | 2.9 |
| 6 | F | 49 | PHE | 2.9 |
| 14 | N | 164 | ASP | 2.9 |
| 11 | K | 85 | GLY | 2.9 |
| 7 | G | 23 | ILE | 2.9 |
| 1 | A | 211 | LYS | 2.9 |
| 14 | N | 147 | ILE | 2.9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | D | 50 | VAL | 2.9 |
| 5 | E | 129 | GLU | 2.9 |
| 26 | Z | 50 | VAL | 2.9 |
| 9 | I | 112 | LEU | 2.9 |
| 4 | D | 135 | VAL | 2.9 |
| 8 | H | 85 | ASP | 2.9 |
| 21 | U | 31 | PHE | 2.9 |
| 5 | E | 168 | ILE | 2.9 |
| 30 | 0 | 2506 | A | 2.9 |
| 8 | H | 156 | ALA | 2.9 |
| 14 | N | 163 | PHE | 2.8 |
| 1 | A | 37 | VAL | 2.8 |
| 1 | A | 135 | VAL | 2.8 |
| 9 | I | 67 | VAL | 2.8 |
| 4 | D | 74 | THR | 2.8 |
| 8 | H | 170 | ARG | 2.8 |
| 8 | H | 39 | LYS | 2.8 |
| 5 | E | 112 | ALA | 2.8 |
| 28 | 2 | 49 | GLU | 2.8 |
| 8 | H | 61 | ARG | 2.8 |
| 9 | I | 75 | LYS | 2.8 |
| 6 | F | 100 | ASP | 2.8 |
| 30 | 0 | 497 | A | 2.8 |
| 30 | 0 | 1181 | A | 2.8 |
| 9 | I | 109 | PRO | 2.8 |
| 9 | I | 76 | ASP | 2.8 |
| 4 | D | 173 | GLU | 2.7 |
| 30 | 0 | 1197 | G | 2.7 |
| 5 | E | 127 | ASP | 2.7 |
| 26 | Z | 68 | GLU | 2.7 |
| 8 | H | 37 | GLY | 2.7 |
| 11 | K | 130 | MET | 2.7 |
| 6 | F | 105 | ASP | 2.7 |
| 5 | E | 91 | PHE | 2.7 |
| 8 | H | 40 | GLN | 2.7 |
| 9 | I | 114 | TYR | 2.7 |
| 30 | 0 | 1180 | U | 2.7 |
| 5 | E | 45 | ASP | 2.7 |
| 30 | 0 | 2538 | A | 2.7 |
| 12 | L | 77 | ALA | 2.7 |
| 30 | 0 | 1179 | C | 2.7 |
| 1 | A | 91 | GLY | 2.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | C | 61 | PHE | 2.7 |
| 6 | F | 16 | ALA | 2.7 |
| 12 | L | 145 | LEU | 2.6 |
| 5 | E | 44 | GLY | 2.6 |
| 6 | F | 91 | VAL | 2.6 |
| 12 | L | 44 | GLU | 2.6 |
| 24 | X | 8 | ARG | 2.6 |
| 10 | J | 94 | GLY | 2.6 |
| 25 | Y | 235 | GLU | 2.6 |
| 1 | A | 138 | VAL | 2.6 |
| 24 | X | 72 | VAL | 2.6 |
| 16 | P | 113 | THR | 2.6 |
| 9 | I | 73 | LEU | 2.6 |
| 30 | 0 | 1965 | C | 2.6 |
| 8 | H | 125 | GLY | 2.6 |
| 9 | I | 92 | VAL | 2.6 |
| 4 | D | 154 | LYS | 2.6 |
| 24 | X | 80 | GLU | 2.6 |
| 4 | D | 37 | ALA | 2.6 |
| 6 | F | 112 | ALA | 2.6 |
| 7 | G | 21 | ASP | 2.6 |
| 30 | 0 | 1200 | A | 2.6 |
| 4 | D | 23 | VAL | 2.6 |
| 3 | C | 64 | GLY | 2.5 |
| 5 | E | 154 | ILE | 2.5 |
| 19 | S | 1 | SER | 2.5 |
| 26 | Z | 106 | SER | 2.5 |
| 2 | B | 151 | VAL | 2.5 |
| 4 | D | 83 | PHE | 2.5 |
| 9 | I | 98 | ASP | 2.5 |
| 20 | T | 116 | ASP | 2.5 |
| 1 | A | 151 | GLN | 2.5 |
| 1 | A | 75 | GLY | 2.5 |
| 1 | A | 58 | VAL | 2.5 |
| 16 | P | 105 | LEU | 2.5 |
| 3 | C | 215 | ALA | 2.5 |
| 8 | H | 86 | TYR | 2.5 |
| 4 | D | 103 | ASN | 2.5 |
| 16 | P | 120 | ARG | 2.5 |
| 8 | H | 167 | LYS | 2.5 |
| 14 | N | 75 | THR | 2.5 |
| 22 | V | 24 | LYS | 2.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 8 | H | 114 | ASP | 2.5 |
| 14 | N | 136 | LEU | 2.4 |
| 30 | 0 | 1203 | G | 2.4 |
| 13 | M | 194 | GLY | 2.4 |
| 25 | Y | 108 | ASP | 2.4 |
| 3 | C | 65 | ARG | 2.4 |
| 28 | 2 | 21 | VAL | 2.4 |
| 1 | A | 145 | MET | 2.4 |
| 30 | 0 | 1000 | C | 2.4 |
| 14 | N | 159 | TYR | 2.4 |
| 6 | F | 119 | ARG | 2.4 |
| 1 | A | 69 | LEU | 2.4 |
| 7 | G | 66 | LEU | 2.4 |
| 1 | A | 88 | ILE | 2.4 |
| 16 | P | 98 | ILE | 2.4 |
| 2 | B | 175 | LEU | 2.4 |
| 19 | S | 20 | PHE | 2.4 |
| 30 | 0 | 1173 | A | 2.4 |
| 26 | Z | 61 | HIS | 2.4 |
| 6 | F | 23 | ALA | 2.4 |
| 9 | I | 105 | GLU | 2.4 |
| 11 | K | 127 | ALA | 2.4 |
| 5 | E | 155 | ASN | 2.4 |
| 18 | R | 106 | GLY | 2.3 |
| 1 | A | 42 | VAL | 2.3 |
| 10 | J | 41 | ALA | 2.3 |
| 1 | A | 83 | GLY | 2.3 |
| 6 | F | 117 | GLU | 2.3 |
| 8 | H | 91 | ARG | 2.3 |
| 4 | D | 141 | VAL | 2.3 |
| 30 | 0 | 280 | C | 2.3 |
| 11 | K | 68 | VAL | 2.3 |
| 4 | D | 41 | LEU | 2.3 |
| 30 | 0 | 2100 | A | 2.3 |
| 14 | N | 143 | ARG | 2.3 |
| 4 | D | 39 | ASP | 2.3 |
| 2 | B | 115 | VAL | 2.3 |
| 26 | Z | 58 | ASN | 2.3 |
| 6 | F | 99 | THR | 2.3 |
| 13 | M | 80 | GLY | 2.3 |
| 26 | Z | 64 | PRO | 2.3 |
| 8 | H | 132 | ALA | 2.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | E | 46 | THR | 2.3 |
| 16 | P | 141 | ILE | 2.3 |
| 21 | U | 8 | TYR | 2.3 |
| 4 | D | 92 | GLU | 2.3 |
| 5 | E | 65 | PHE | 2.3 |
| 4 | D | 105 | SER | 2.3 |
| 7 | G | 25 | GLU | 2.3 |
| 26 | Z | 85 | ASP | 2.3 |
| 9 | I | 71 | ALA | 2.3 |
| 10 | J | 97 | ALA | 2.3 |
| 1 | A | 55 | VAL | 2.3 |
| 12 | L | 25 | GLY | 2.3 |
| 16 | P | 82 | GLY | 2.3 |
| 5 | E | 5 | LEU | 2.2 |
| 18 | R | 1 | GLY | 2.2 |
| 4 | D | 106 | PHE | 2.2 |
| 30 | 0 | 1199 | A | 2.2 |
| 11 | K | 95 | ALA | 2.2 |
| 2 | B | 161 | VAL | 2.2 |
| 6 | F | 59 | ILE | 2.2 |
| 30 | 0 | 2237 | G | 2.2 |
| 10 | J | 122 | ASP | 2.2 |
| 24 | X | 79 | GLU | 2.2 |
| 8 | H | 152 | ALA | 2.2 |
| 5 | E | 22 | VAL | 2.2 |
| 26 | Z | 45 | VAL | 2.2 |
| 6 | F | 24 | ARG | 2.2 |
| 16 | P | 108 | LEU | 2.2 |
| 16 | P | 68 | LYS | 2.2 |
| 23 | W | 45 | VAL | 2.2 |
| 14 | N | 178 | THR | 2.2 |
| 9 | I | 125 | GLY | 2.2 |
| 30 | 0 | 282 | C | 2.2 |
| 24 | X | 74 | ALA | 2.2 |
| 26 | Z | 62 | ALA | 2.2 |
| 2 | B | 98 | THR | 2.2 |
| 6 | F | 25 | ASP | 2.2 |
| 16 | P | 102 | ARG | 2.2 |
| 7 | G | 22 | ALA | 2.2 |
| 14 | N | 70 | GLY | 2.1 |
| 20 | T | 60 | GLY | 2.1 |
| 4 | D | 136 | ARG | 2.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 79 | GLU | 2.1 |
| 4 | D | 45 | THR | 2.1 |
| 8 | H | 149 | VAL | 2.1 |
| 26 | Z | 34 | SER | 2.1 |
| 30 | 0 | 2509 | A | 2.1 |
| 4 | D | 24 | HIS | 2.1 |
| 1 | A | 64 | ASP | 2.1 |
| 20 | T | 72 | ILE | 2.1 |
| 30 | 0 | 1184 | C | 2.1 |
| 21 | U | 43 | GLY | 2.1 |
| 12 | L | 29 | GLY | 2.1 |
| 14 | N | 175 | LEU | 2.1 |
| 18 | R | 132 | ARG | 2.1 |
| 16 | P | 55 | LYS | 2.1 |
| 31 | 9 | 24 | U | 2.1 |
| 4 | D | 174 | VAL | 2.1 |
| 6 | F | 8 | VAL | 2.1 |
| 14 | N | 186 | LEU | 2.1 |
| 1 | A | 74 | VAL | 2.1 |
| 12 | L | 74 | THR | 2.1 |
| 21 | U | 22 | VAL | 2.1 |
| 2 | B | 18 | ARG | 2.1 |
| 9 | I | 90 | ASP | 2.1 |
| 24 | X | 75 | ALA | 2.1 |
| 9 | I | 86 | GLU | 2.0 |
| 30 | 0 | 969 | G | 2.0 |
| 1 | A | 40 | GLY | 2.0 |
| 2 | B | 86 | ALA | 2.0 |
| 1 | A | 133 | ARG | 2.0 |
| 20 | T | 115 | GLU | 2.0 |
| 2 | B | 106 | HIS | 2.0 |
| 11 | K | 58 | THR | 2.0 |
| 8 | H | 31 | ILE | 2.0 |
| 8 | H | 29 | SER | 2.0 |
| 8 | H | 71 | SER | 2.0 |
| 28 | 2 | 19 | SER | 2.0 |
| 2 | B | 53 | LEU | 2.0 |
| 8 | H | 6 | ALA | 2.0 |
| 13 | M | 30 | GLU | 2.0 |
| 30 | 0 | 2289 | G | 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ 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 | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 30 | 1MA | 0 | 628 | 23/24 | 0.89 | 0.23 | - | 25,27,30,31 | 0 |
| 30 | OMU | 0 | 2587 | 21/22 | 0.83 | 0.20 | - | 31,33,34,36 | 0 |
| 30 | OMG | 0 | 2588 | 24/25 | 0.90 | 0.17 | - | 30,31,35,36 | 0 |
| 30 | UR3 | 0 | 2619 | 21/22 | 0.88 | 0.20 | - | 33,35,38,43 | 0 |
| 30 | PSU | 0 | 2621 | 20/21 | 0.91 | 0.17 | - | 30,32,37,37 | 0 |

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ 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 | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 34 | NA | 0 | 8528 | 1/1 | 0.86 | 0.99 | 49.12 | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8511 | 1/1 | 0.74 | 0.65 | 36.02 | 54,54,54,54 | 0 |
| 34 | NA | 0 | 8512 | 1/1 | 0.33 | 0.42 | 27.63 | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8564 | 1/1 | 0.63 | 0.80 | 27.10 | 67,67,67,67 | 0 |
| 34 | NA | 0 | 8517 | 1/1 | 0.76 | 0.73 | 26.16 | 38,38,38,38 | 0 |
| 34 | NA | 0 | 8553 | 1/1 | 0.56 | 0.58 | 24.19 | 70,70,70,70 | 0 |
| 34 | NA | 0 | 8559 | 1/1 | 0.79 | 0.52 | 21.34 | 74,74,74,74 | 0 |
| 34 | NA | 0 | 8522 | 1/1 | 0.27 | 0.47 | 18.05 | 57,57,57,57 | 0 |
| 32 | MG | 0 | 8079 | 1/1 | -0.09 | 0.35 | 15.71 | 67,67,67,67 | 0 |
| 34 | NA | 0 | 8575 | 1/1 | 0.15 | 0.69 | 15.69 | 72,72,72,72 | 0 |
| 34 | NA | 0 | 8569 | 1/1 | 0.84 | 0.47 | 15.69 | 64,64,64,64 | 0 |
| 32 | MG | A | 8051 | 1/1 | 0.95 | 0.54 | 14.29 | 64,64,64,64 | 0 |
| 34 | NA | 0 | 8563 | 1/1 | 0.78 | 0.49 | 12.75 | 70,70,70,70 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 34 | NA | 0 | 8565 | 1/1 | 0.49 | 0.37 | 12.50 | 65,65,65,65 | 0 |
| 34 | NA | 0 | 8562 | 1/1 | 0.26 | 0.45 | 11.59 | 67,67,67,67 | 0 |
| 34 | NA | 0 | 8560 | 1/1 | 0.44 | 0.37 | 11.44 | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8556 | 1/1 | 0.69 | 0.83 | 9.99 | 35,35,35,35 | 0 |
| 34 | NA | 0 | 8523 | 1/1 | 0.52 | 0.42 | 9.55 | 62,62,62,62 | 0 |
| 34 | NA | Q | 8540 | 1/1 | 0.86 | 0.50 | 9.28 | 46,46,46,46 | 0 |
| 34 | NA | 0 | 8530 | 1/1 | 0.89 | 0.41 | 8.73 | 59,59,59,59 | 0 |
| 33 | K | 0 | 8401 | 1/1 | 0.60 | 0.57 | 8.21 | 149,149,149,149 | 0 |
| 36 | SR | B | 8987 | 1/1 | 0.14 | 0.44 | 7.32 | 200,200,200,200 | 0 |
| 34 | NA | 0 | 8547 | 1/1 | 0.62 | 0.32 | 7.06 | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8062 | 1/1 | 0.65 | 0.37 | 6.45 | 68,68,68,68 | 0 |
| 36 | SR | 0 | 8985 | 1/1 | 0.49 | 0.23 | 6.19 | 137,137,137,137 | 0 |
| 36 | SR | 0 | 8972 | 1/1 | 0.88 | 0.82 | 6.12 | 159,159,159,159 | 0 |
| 34 | NA | 0 | 8504 | 1/1 | 0.88 | 0.31 | 5.55 | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8008 | 1/1 | 0.96 | 0.24 | 5.39 | 18,18,18,18 | 0 |
| 34 | NA | 0 | 8519 | 1/1 | 0.85 | 0.29 | 5.10 | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8015 | 1/1 | 0.69 | 0.23 | 4.83 | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8534 | 1/1 | 0.78 | 0.30 | 4.75 | 35,35,35,35 | 0 |
| 34 | NA | 0 | 8533 | 1/1 | 0.19 | 0.33 | 4.68 | 65,65,65,65 | 0 |
| 34 | NA | 0 | 8507 | 1/1 | 0.40 | 0.34 | 4.62 | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8075 | 1/1 | 0.69 | 0.22 | 4.30 | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8546 | 1/1 | 0.51 | 0.32 | 4.09 | 57,57,57,57 | 0 |
| 34 | NA | 0 | 8555 | 1/1 | 0.96 | 0.30 | 3.81 | 58,58,58,58 | 0 |
| 36 | SR | A | 8929 | 1/1 | 0.46 | 0.34 | 3.08 | 135,135,135,135 | 0 |
| 34 | NA | 0 | 8521 | 1/1 | 0.86 | 0.25 | 2.11 | 42,42,42,42 | 0 |
| 32 | MG | 0 | 8084 | 1/1 | 0.95 | 0.18 | 1.95 | 30,30,30,30 | 0 |
| 36 | SR | 0 | 8969 | 1/1 | 0.81 | 0.28 | 1.85 | 143,143,143,143 | 0 |
| 33 | K | 0 | 8402 | 1/1 | 0.55 | 0.23 | 1.49 | 63,63,63,63 | 0 |
| 34 | NA | 0 | 8558 | 1/1 | 0.39 | 0.23 | 1.12 | 36,36,36,36 | 0 |
| 34 | NA | R | 8532 | 1/1 | 0.84 | 0.19 | 0.75 | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8052 | 1/1 | 0.96 | 0.21 | 0.65 | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8047 | 1/1 | 0.96 | 0.19 | 0.25 | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8044 | 1/1 | 0.30 | 0.21 | 0.21 | 40,40,40,40 | 0 |
| 32 | MG | B | 8042 | 1/1 | 0.86 | 0.19 | -0.02 | 48,48,48,48 | 0 |
| 36 | SR | 0 | 8903 | 1/1 | 0.59 | 0.18 | -0.02 | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8028 | 1/1 | 0.68 | 0.18 | -0.20 | 23,23,23,23 | 0 |
| 32 | MG | Y | 8086 | 1/1 | 0.69 | 0.17 | -0.36 | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8537 | 1/1 | 0.92 | 0.14 | -0.41 | 39,39,39,39 | 0 |
| 35 | CL | J | 8821 | 1/1 | 0.93 | 0.18 | -0.44 | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8043 | 1/1 | 0.81 | 0.16 | -0.52 | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8058 | 1/1 | 0.69 | 0.11 | -0.54 | 18,18,18,18 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 34 | NA | 0 | 8542 | 1/1 | 0.76 | 0.20 | -0.67 | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8012 | 1/1 | 0.95 | 0.16 | -0.72 | 16,16,16,16 | 0 |
| 34 | NA | J | 8538 | 1/1 | 0.59 | 0.18 | -0.73 | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8070 | 1/1 | 0.85 | 0.16 | -0.77 | 65,65,65,65 | 0 |
| 34 | NA | 0 | 8529 | 1/1 | 0.64 | 0.12 | -0.87 | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8025 | 1/1 | 0.86 | 0.17 | -0.88 | 16,16,16,16 | 0 |
| 32 | MG | 0 | 8034 | 1/1 | 0.37 | 0.19 | -0.92 | 28,28,28,28 | 0 |
| 35 | CL | 0 | 8812 | 1/1 | 0.67 | 0.16 | -1.03 | 35,35,35,35 | 0 |
| 35 | CL | O | 8808 | 1/1 | 0.78 | 0.10 | -1.13 | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8013 | 1/1 | 0.87 | 0.14 | -1.24 | 29,29,29,29 | 0 |
| 32 | MG | 0 | 8009 | 1/1 | 0.85 | 0.16 | -1.24 | 29,29,29,29 | 0 |
| 36 | SR | 0 | 8935 | 1/1 | 0.83 | 0.13 | -1.26 | 75,75,75,75 | 0 |
| 32 | MG | 0 | 8014 | 1/1 | 0.39 | 0.15 | -1.39 | 15,15,15,15 | 0 |
| 34 | NA | M | 8539 | 1/1 | 0.69 | 0.15 | -1.44 | 30,30,30,30 | 0 |
| 37 | CD | U | 8701 | 1/1 | 0.87 | 0.07 | -1.53 | 60,60,60,60 | 0 |
| 32 | MG | 0 | 8031 | 1/1 | 0.96 | 0.12 | -1.56 | 45,45,45,45 | 0 |
| 37 | CD | Z | 8703 | 1/1 | 0.71 | 0.08 | -1.58 | 64,64,64,64 | 0 |
| 32 | MG | T | 8057 | 1/1 | 0.34 | 0.13 | -1.64 | 54,54,54,54 | 0 |
| 36 | SR | 0 | 8975 | 1/1 | 0.72 | 0.08 | -1.72 | 146,146,146,146 | 0 |
| 32 | MG | K | 8054 | 1/1 | 0.51 | 0.12 | -1.73 | 29,29,29,29 | 0 |
| 35 | CL | 0 | 8803 | 1/1 | 0.81 | 0.15 | -1.78 | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8045 | 1/1 | 0.95 | 0.10 | -1.95 | 29,29,29,29 | 0 |
| 37 | CD | 1 | 8702 | 1/1 | 0.96 | 0.09 | -2.39 | 53,53,53,53 | 0 |
| 34 | NA | 0 | 8515 | 1/1 | 0.36 | 0.12 | -2.49 | 33,33,33,33 | 0 |
| 32 | MG | A | 8050 | 1/1 | 0.91 | 0.16 | -2.57 | 48,48,48,48 | 0 |
| 37 | CD | 3 | 8704 | 1/1 | 0.94 | 0.10 | -2.58 | 62,62,62,62 | 0 |
| 36 | SR | R | 8912 | 1/1 | 0.91 | 0.09 | -2.60 | 80,80,80,80 | 0 |
| 34 | NA | 0 | 8568 | 1/1 | 0.96 | 0.15 | -2.65 | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8006 | 1/1 | 0.95 | 0.11 | -2.68 | 34,34,34,34 | 0 |
| 34 | NA | 0 | 8527 | 1/1 | 0.91 | 0.17 | -2.81 | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8041 | 1/1 | 0.65 | 0.13 | -2.83 | 21,21,21,21 | 0 |
| 32 | MG | 0 | 8011 | 1/1 | 0.56 | 0.14 | -2.84 | 31,31,31,31 | 0 |
| 36 | SR | 0 | 8949 | 1/1 | 0.90 | 0.11 | -3.02 | 105,105,105,105 | 0 |
| 36 | SR | 0 | 8936 | 1/1 | 0.77 | 0.11 | -3.12 | 86,86,86,86 | 0 |
| 32 | MG | 0 | 8088 | 1/1 | 0.94 | 0.11 | -3.13 | 26,26,26,26 | 0 |
| 36 | SR | 0 | 8964 | 1/1 | 0.76 | 0.09 | -3.19 | 131,131,131,131 | 0 |
| 32 | MG | 0 | 8003 | 1/1 | 0.94 | 0.12 | -3.23 | 28,28,28,28 | 0 |
| 36 | SR | A | 8930 | 1/1 | 0.91 | 0.09 | -3.45 | 87,87,87,87 | 0 |
| 36 | SR | 0 | 8910 | 1/1 | 0.94 | 0.09 | -3.52 | 87,87,87,87 | 0 |
| 35 | CL | 3 | 8804 | 1/1 | 0.95 | 0.04 | -3.82 | 58,58,58,58 | 0 |
| 36 | SR | 0 | 8904 | 1/1 | 0.97 | 0.10 | -3.86 | 49,49,49,49 | 0 |
| 32 | MG | 0 | 8065 | 1/1 | 0.70 | 0.10 | -3.93 | 37,37,37,37 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 34 | NA | 0 | 8535 | 1/1 | 0.58 | 0.14 | -3.98 | 35,35,35,35 | 0 |
| 35 | CL | 0 | 8805 | 1/1 | 0.90 | 0.06 | -4.02 | 50,50,50,50 | 0 |
| 35 | CL | 0 | 8815 | 1/1 | 0.80 | 0.10 | -4.25 | 66,66,66,66 | 0 |
| 36 | SR | 0 | 8918 | 1/1 | 0.57 | 0.12 | -4.32 | 73,73,73,73 | 0 |
| 36 | SR | 1 | 8913 | 1/1 | 0.74 | 0.11 | -4.65 | 82,82,82,82 | 0 |
| 35 | CL | M | 8818 | 1/1 | 0.95 | 0.07 | -4.84 | 30,30,30,30 | 0 |
| 32 | MG | 0 | 8010 | 1/1 | 0.93 | 0.10 | -5.00 | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8004 | 1/1 | 0.98 | 0.10 | -5.07 | 26,26,26,26 | 0 |
| 32 | MG | 0 | 8001 | 1/1 | 0.88 | 0.08 | -5.08 | 27,27,27,27 | 0 |
| 36 | SR | 3 | 8932 | 1/1 | 0.50 | 0.09 | -5.13 | 68,68,68,68 | 0 |
| 35 | CL | B | 8819 | 1/1 | 0.96 | 0.10 | -5.17 | 49,49,49,49 | 0 |
| 36 | SR | 0 | 8945 | 1/1 | 0.88 | 0.09 | -5.35 | 113,113,113,113 | 0 |
| 36 | SR | 0 | 8984 | 1/1 | 0.98 | 0.08 | -5.37 | 106,106,106,106 | 0 |
| 36 | SR | 0 | 8943 | 1/1 | 0.63 | 0.08 | -5.71 | 113,113,113,113 | 0 |
| 32 | MG | 0 | 8002 | 1/1 | 0.96 | 0.07 | -5.79 | 26,26,26,26 | 0 |
| 34 | NA | 0 | 8557 | 1/1 | 0.81 | 0.08 | -5.86 | 57,57,57,57 | 0 |
| 36 | SR | 0 | 8992 | 1/1 | 0.86 | 0.06 | -6.66 | 123,123,123,123 | 0 |
| 36 | SR | 0 | 8902 | 1/1 | 0.88 | 0.09 | -6.84 | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8087 | 1/1 | 0.73 | 0.11 | -7.20 | 29,29,29,29 | 0 |
| 34 | NA | 9 | 8572 | 1/1 | 0.85 | 0.06 | -8.00 | 88,88,88,88 | 0 |
| 34 | NA | 0 | 8573 | 1/1 | 0.65 | 0.28 | - | 78,78,78,78 | 0 |
| 32 | MG | 0 | 8091 | 1/1 | 0.83 | 0.10 | - | 43,43,43,43 | 0 |
| 36 | SR | 1 | 8952 | 1/1 | 0.84 | 0.12 | - | 70,70,70,70 | 0 |
| 36 | SR | 0 | 8906 | 1/1 | 0.87 | 0.09 | - | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8566 | 1/1 | 0.10 | 1.21 | - | 40,40,40,40 | 0 |
| 36 | SR | 0 | 8923 | 1/1 | 0.86 | 0.05 | - | 104,104,104,104 | 0 |
| 36 | SR | 0 | 8971 | 1/1 | 0.63 | 0.18 | - | 172,172,172,172 | 0 |
| 32 | MG | 0 | 8082 | 1/1 | -0.06 | 0.63 | - | 76,76,76,76 | 0 |
| 36 | SR | 0 | 9006 | 1/1 | -0.04 | 1.42 | - | 200,200,200,200 | 0 |
| 36 | SR | 9 | 8978 | 1/1 | 0.77 | 0.13 | - | 150,150,150,150 | 0 |
| 34 | NA | 0 | 8514 | 1/1 | 0.72 | 0.54 | - | 52,52,52,52 | 0 |
| 35 | CL | J | 8802 | 1/1 | 0.79 | 0.24 | - | 70,70,70,70 | 0 |
| 32 | MG | 0 | 8037 | 1/1 | 0.86 | 0.34 | - | 77,77,77,77 | 0 |
| 32 | MG | 0 | 8039 | 1/1 | 0.57 | 0.23 | - | 55,55,55,55 | 0 |
| 32 | MG | 0 | 8067 | 1/1 | 0.64 | 0.22 | - | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8024 | 1/1 | 0.87 | 0.23 | - | 50,50,50,50 | 0 |
| 36 | SR | 9 | 9003 | 1/1 | 0.58 | 0.11 | - | 157,157,157,157 | 0 |
| 32 | MG | 0 | 8020 | 1/1 | 0.73 | 0.12 | - | 37,37,37,37 | 0 |
| 34 | NA | 0 | 8554 | 1/1 | 0.94 | 0.40 | - | 50,50,50,50 | 0 |
| 34 | NA | S | 8510 | 1/1 | 0.83 | 0.09 | - | 26,26,26,26 | 0 |
| 36 | SR | 0 | 8927 | 1/1 | 0.58 | 0.17 | - | 167,167,167,167 | 0 |
| 36 | SR | 0 | 8951 | 1/1 | 0.85 | 0.08 | - | 139,139,139,139 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 34 | NA | 0 | 8561 | 1/1 | 0.85 | 0.51 | - | 71,71,71,71 | 0 |
| 36 | SR | 0 | 8948 | 1/1 | 0.94 | 0.10 | - | 101,101,101,101 | 0 |
| 36 | SR | 0 | 9000 | 1/1 | 0.32 | 0.36 | - | 171,171,171,171 | 0 |
| 32 | MG | 0 | 8077 | 1/1 | 0.75 | 0.18 | - | 24,24,24,24 | 0 |
| 32 | MG | 0 | 8049 | 1/1 | 0.68 | 0.35 | - | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8032 | 1/1 | 0.95 | 0.10 | - | 29,29,29,29 | 0 |
| 34 | NA | 0 | 8509 | 1/1 | 0.09 | 0.35 | - | 64,64,64,64 | 0 |
| 36 | SR | 0 | 8924 | 1/1 | 0.51 | 0.15 | - | 140,140,140,140 | 0 |
| 34 | NA | 0 | 8571 | 1/1 | 0.28 | 0.40 | - | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8056 | 1/1 | 0.92 | 0.17 | - | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8046 | 1/1 | 0.73 | 0.13 | - | 28,28,28,28 | 0 |
| 36 | SR | 0 | 8998 | 1/1 | 0.62 | 0.16 | - | 134,134,134,134 | 0 |
| 36 | SR | 0 | 8989 | 1/1 | 0.28 | 0.20 | - | 182,182,182,182 | 0 |
| 34 | NA | 0 | 8552 | 1/1 | 0.63 | 0.50 | - | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8076 | 1/1 | 0.92 | 0.24 | - | 29,29,29,29 | 0 |
| 34 | NA | C | 8503 | 1/1 | 0.90 | 0.14 | - | 32,32,32,32 | 0 |
| 36 | SR | 0 | 8901 | 1/1 | 0.62 | 0.10 | - | 78,78,78,78 | 0 |
| 35 | CL | Q | 8811 | 1/1 | 0.96 | 0.17 | - | 57,57,57,57 | 0 |
| 32 | MG | 0 | 8019 | 1/1 | 0.95 | 0.18 | - | 24,24,24,24 | 0 |
| 36 | SR | 0 | 8942 | 1/1 | 0.65 | 0.12 | - | 109,109,109,109 | 0 |
| 36 | SR | 0 | 8954 | 1/1 | 0.71 | 0.12 | - | 94,94,94,94 | 0 |
| 36 | SR | 0 | 8940 | 1/1 | 0.92 | 0.10 | - | 79,79,79,79 | 0 |
| 36 | SR | 0 | 8925 | 1/1 | 0.83 | 0.06 | - | 90,90,90,90 | 0 |
| 36 | SR | 0 | 8995 | 1/1 | 0.96 | 0.14 | - | 140,140,140,140 | 0 |
| 36 | SR | 0 | 8966 | 1/1 | 0.68 | 0.12 | - | 97,97,97,97 | 0 |
| 36 | SR | F | 9005 | 1/1 | 0.18 | 0.12 | - | 130,130,130,130 | 0 |
| 36 | SR | 0 | 8986 | 1/1 | 0.42 | 0.17 | - | 200,200,200,200 | 0 |
| 36 | SR | 0 | 8937 | 1/1 | 0.89 | 0.09 | - | 101,101,101,101 | 0 |
| 36 | SR | 0 | 8916 | 1/1 | 0.76 | 0.10 | - | 107,107,107,107 | 0 |
| 36 | SR | 0 | 8922 | 1/1 | 0.97 | 0.22 | - | 177,177,177,177 | 0 |
| 32 | MG | 0 | 8089 | 1/1 | 0.30 | 0.60 | - | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8016 | 1/1 | 0.70 | 0.10 | - | 36,36,36,36 | 0 |
| 36 | SR | 0 | 9004 | 1/1 | 0.66 | 1.00 | - | 200,200,200,200 | 0 |
| 36 | SR | 0 | 9001 | 1/1 | 0.42 | 0.52 | - | 169,169,169,169 | 0 |
| 34 | NA | 0 | 8548 | 1/1 | 0.70 | 0.24 | - | 66,66,66,66 | 0 |
| 35 | CL | 0 | 8814 | 1/1 | 0.85 | 0.41 | - | 62,62,62,62 | 0 |
| 35 | CL | J | 8801 | 1/1 | 0.91 | 0.07 | - | 65,65,65,65 | 0 |
| 36 | SR | 0 | 8959 | 1/1 | 0.66 | 0.08 | - | 142,142,142,142 | 0 |
| 32 | MG | 0 | 8064 | 1/1 | 0.92 | 0.13 | - | 37,37,37,37 | 0 |
| 35 | CL | 0 | 8822 | 1/1 | 0.92 | 0.40 | - | 80,80,80,80 | 0 |
| 36 | SR | 0 | 8976 | 1/1 | 0.55 | 0.53 | - | 173,173,173,173 | 0 |
| 36 | SR | 0 | 8993 | 1/1 | 0.74 | 0.28 | - | 173,173,173,173 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 32 | MG | 0 | 8060 | 1/1 | 0.80 | 0.13 | - | 42,42,42,42 | 0 |
| 36 | SR | 0 | 8917 | 1/1 | 0.55 | 0.17 | - | 114,114,114,114 | 0 |
| 32 | MG | 0 | 8073 | 1/1 | 0.89 | 0.26 | - | 57,57,57,57 | 0 |
| 36 | SR | 0 | 8979 | 1/1 | 0.54 | 0.26 | - | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8033 | 1/1 | 0.13 | 0.20 | - | 46,46,46,46 | 0 |
| 36 | SR | 0 | 8962 | 1/1 | 0.84 | 0.45 | - | 157,157,157,157 | 0 |
| 36 | SR | 0 | 8911 | 1/1 | 0.82 | 0.11 | - | 70,70,70,70 | 0 |
| 36 | SR | 0 | 8958 | 1/1 | 0.60 | 0.11 | - | 99,99,99,99 | 0 |
| 32 | MG | 0 | 8021 | 1/1 | 0.69 | 0.15 | - | 32,32,32,32 | 0 |
| 36 | SR | 0 | 8983 | 1/1 | 0.15 | 0.23 | - | 183,183,183,183 | 0 |
| 32 | MG | 0 | 8048 | 1/1 | 0.97 | 0.23 | - | 20,20,20,20 | 0 |
| 32 | MG | 0 | 8092 | 1/1 | 0.48 | 0.38 | - | 40,40,40,40 | 0 |
| 35 | CL | 0 | 8813 | 1/1 | 0.93 | 0.10 | - | 45,45,45,45 | 0 |
| 34 | NA | 0 | 8520 | 1/1 | 0.93 | 0.28 | - | 55,55,55,55 | 0 |
| 36 | SR | 0 | 8939 | 1/1 | 0.62 | 0.08 | - | 129,129,129,129 | 0 |
| 32 | MG | 0 | 8027 | 1/1 | 0.94 | 0.09 | - | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8069 | 1/1 | 0.87 | 0.45 | - | 61,61,61,61 | 0 |
| 32 | MG | 0 | 8026 | 1/1 | 0.70 | 0.12 | - | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8005 | 1/1 | 0.96 | 0.10 | - | 25,25,25,25 | 0 |
| 36 | SR | 0 | 8967 | 1/1 | 0.75 | 0.23 | - | 145,145,145,145 | 0 |
| 35 | CL | L | 8810 | 1/1 | 0.94 | 0.06 | - | 57,57,57,57 | 0 |
| 32 | MG | 0 | 8081 | 1/1 | 0.86 | 0.17 | - | 48,48,48,48 | 0 |
| 34 | NA | 0 | 8551 | 1/1 | 0.66 | 0.26 | - | 39,39,39,39 | 0 |
| 35 | CL | 0 | 8816 | 1/1 | 0.76 | 0.18 | - | 62,62,62,62 | 0 |
| 34 | NA | 0 | 8524 | 1/1 | 0.78 | 0.29 | - | 56,56,56,56 | 0 |
| 36 | SR | 0 | 8919 | 1/1 | 0.07 | 0.15 | - | 144,144,144,144 | 0 |
| 35 | CL | N | 8807 | 1/1 | 0.81 | 0.11 | - | 59,59,59,59 | 0 |
| 36 | SR | 0 | 8914 | 1/1 | 0.80 | 0.22 | - | 105,105,105,105 | 0 |
| 36 | SR | 0 | 8944 | 1/1 | 0.55 | 0.10 | - | 148,148,148,148 | 0 |
| 34 | NA | 0 | 8502 | 1/1 | 0.44 | 1.21 | - | 78,78,78,78 | 0 |
| 32 | MG | 0 | 8072 | 1/1 | 0.96 | 0.24 | - | 68,68,68,68 | 0 |
| 34 | NA | 0 | 8526 | 1/1 | 0.57 | 0.36 | - | 31,31,31,31 | 0 |
| 36 | SR | 3 | 8999 | 1/1 | 0.75 | 0.10 | - | 95,95,95,95 | 0 |
| 36 | SR | 0 | 8965 | 1/1 | 0.69 | 0.13 | - | 125,125,125,125 | 0 |
| 32 | MG | 0 | 8090 | 1/1 | 0.87 | 0.25 | - | 45,45,45,45 | 0 |
| 34 | NA | 0 | 8516 | 1/1 | 0.66 | 0.26 | - | 31,31,31,31 | 0 |
| 36 | SR | 0 | 8905 | 1/1 | 0.87 | 0.14 | - | 55,55,55,55 | 0 |
| 32 | MG | 0 | 8022 | 1/1 | 0.49 | 0.20 | - | 24,24,24,24 | 0 |
| 37 | CD | O | 8705 | 1/1 | 0.96 | 0.07 | - | 81,81,81,81 | 0 |
| 36 | SR | 0 | 8955 | 1/1 | 0.78 | 0.16 | - | 174,174,174,174 | 0 |
| 34 | NA | 0 | 8570 | 1/1 | 0.72 | 0.18 | - | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8068 | 1/1 | 0.65 | 0.28 | - | 58,58,58,58 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 36 | SR | 0 | 8997 | 1/1 | 0.69 | 0.75 | - | 189,189,189,189 | 0 |
| 32 | MG | 0 | 8038 | 1/1 | 0.73 | 0.31 | - | 74,74,74,74 | 0 |
| 36 | SR | 0 | 8907 | 1/1 | 0.88 | 0.10 | - | 58,58,58,58 | 0 |
| 36 | SR | 0 | 8946 | 1/1 | 0.43 | 0.15 | - | 110,110,110,110 | 0 |
| 32 | MG | 0 | 8071 | 1/1 | 0.85 | 0.26 | - | 56,56,56,56 | 0 |
| 36 | SR | 0 | 8973 | 1/1 | 0.92 | 0.07 | - | 124,124,124,124 | 0 |
| 32 | MG | 0 | 8040 | 1/1 | 0.57 | 0.53 | - | 69,69,69,69 | 0 |
| 34 | NA | 0 | 8536 | 1/1 | 0.91 | 0.06 | - | 43,43,43,43 | 0 |
| 34 | NA | 0 | 8550 | 1/1 | 0.94 | 0.13 | - | 42,42,42,42 | 0 |
| 36 | SR | 0 | 8947 | 1/1 | 0.85 | 0.24 | - | 160,160,160,160 | 0 |
| 36 | SR | A | 8977 | 1/1 | 0.66 | 0.09 | - | 147,147,147,147 | 0 |
| 34 | NA | 9 | 8543 | 1/1 | 0.53 | 0.18 | - | 53,53,53,53 | 0 |
| 36 | SR | 0 | 8957 | 1/1 | 0.70 | 0.75 | - | 200,200,200,200 | 0 |
| 36 | SR | 0 | 8960 | 1/1 | 0.85 | 0.11 | - | 138,138,138,138 | 0 |
| 34 | NA | 0 | 8518 | 1/1 | 0.58 | 0.43 | - | 76,76,76,76 | 0 |
| 32 | MG | 9 | 8074 | 1/1 | 0.61 | 0.12 | - | 73,73,73,73 | 0 |
| 34 | NA | 0 | 8549 | 1/1 | 0.86 | 0.53 | - | 42,42,42,42 | 0 |
| 35 | CL | A | 8809 | 1/1 | 0.53 | 0.18 | - | 65,65,65,65 | 0 |
| 36 | SR | 0 | 8994 | 1/1 | 0.52 | 0.62 | - | 188,188,188,188 | 0 |
| 32 | MG | 0 | 8061 | 1/1 | 0.82 | 0.28 | - | 29,29,29,29 | 0 |
| 34 | NA | 0 | 8531 | 1/1 | 0.96 | 0.09 | - | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8078 | 1/1 | 0.72 | 0.22 | - | 41,41,41,41 | 0 |
| 36 | SR | 9 | 8968 | 1/1 | 0.91 | 0.38 | - | 178,178,178,178 | 0 |
| 36 | SR | 0 | 8988 | 1/1 | 0.65 | 0.19 | - | 144,144,144,144 | 0 |
| 36 | SR | 0 | 8934 | 1/1 | 0.96 | 0.15 | - | 100,100,100,100 | 0 |
| 34 | NA | 0 | 8567 | 1/1 | 0.39 | 0.25 | - | 57,57,57,57 | 0 |
| 32 | MG | 0 | 8083 | 1/1 | 0.76 | 0.10 | - | 30,30,30,30 | 0 |
| 36 | SR | 0 | 8928 | 1/1 | 0.83 | 0.12 | - | 167,167,167,167 | 0 |
| 35 | CL | 0 | 8817 | 1/1 | 0.68 | 0.09 | - | 60,60,60,60 | 0 |
| 36 | SR | 0 | 8953 | 1/1 | 0.77 | 0.11 | - | 130,130,130,130 | 0 |
| 34 | NA | 0 | 8513 | 1/1 | 0.49 | 0.49 | - | 44,44,44,44 | 0 |
| 36 | SR | 0 | 8991 | 1/1 | 0.20 | 0.30 | - | 176,176,176,176 | 0 |
| 36 | SR | 0 | 8990 | 1/1 | 0.86 | 0.19 | - | 109,109,109,109 | 0 |
| 36 | SR | 9 | 8980 | 1/1 | 0.74 | 0.16 | - | 154,154,154,154 | 0 |
| 32 | MG | 0 | 8055 | 1/1 | 0.85 | 0.15 | - | 28,28,28,28 | 0 |
| 36 | SR | 0 | 8956 | 1/1 | 0.96 | 0.12 | - | 167,167,167,167 | 0 |
| 34 | NA | 0 | 8545 | 1/1 | 0.94 | 0.29 | - | 30,30,30,30 | 0 |
| 36 | SR | 0 | 9007 | 1/1 | 0.68 | 0.51 | - | 181,181,181,181 | 0 |
| 32 | MG | 0 | 8093 | 1/1 | 0.54 | 0.12 | - | 35,35,35,35 | 0 |
| 36 | SR | 0 | 8982 | 1/1 | 0.12 | 0.49 | - | 186,186,186,186 | 0 |
| 36 | SR | 0 | 8938 | 1/1 | 0.66 | 0.15 | - | 175,175,175,175 | 0 |
| 32 | MG | 0 | 8029 | 1/1 | 0.97 | 0.14 | - | 40,40,40,40 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 32 | MG | 0 | 8066 | 1/1 | 0.64 | 0.19 | - | 53,53,53,53 | 0 |
| 34 | NA | 0 | 8505 | 1/1 | 0.79 | 0.76 | - | 36,36,36,36 | 0 |
| 36 | SR | 0 | 8970 | 1/1 | 0.88 | 0.06 | - | 121,121,121,121 | 0 |
| 36 | SR | 0 | 8921 | 1/1 | 0.79 | 0.11 | - | 74,74,74,74 | 0 |
| 36 | SR | 0 | 8981 | 1/1 | 0.88 | 0.10 | - | 140,140,140,140 | 0 |
| 32 | MG | 0 | 8085 | 1/1 | 0.64 | 0.71 | - | 82,82,82,82 | 0 |
| 36 | SR | 0 | 9002 | 1/1 | 0.67 | 0.15 | - | 170,170,170,170 | 0 |
| 32 | MG | 0 | 8035 | 1/1 | 0.87 | 0.12 | - | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8501 | 1/1 | 0.74 | 0.19 | - | 30,30,30,30 | 0 |
| 34 | NA | 0 | 8525 | 1/1 | 0.57 | 0.56 | - | 91,91,91,91 | 0 |
| 32 | MG | 0 | 8053 | 1/1 | 0.87 | 0.10 | - | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8023 | 1/1 | 0.89 | 0.14 | - | 27,27,27,27 | 0 |
| 36 | SR | 0 | 8920 | 1/1 | 0.89 | 0.17 | - | 106,106,106,106 | 0 |
| 32 | MG | 0 | 8036 | 1/1 | 0.42 | 0.13 | - | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8017 | 1/1 | 0.71 | 0.14 | - | 29,29,29,29 | 0 |
| 32 | MG | 0 | 8059 | 1/1 | 0.72 | 0.07 | - | 33,33,33,33 | 0 |
| 36 | SR | 0 | 8915 | 1/1 | 0.76 | 0.09 | - | 114,114,114,114 | 0 |
| 36 | SR | 0 | 8909 | 1/1 | 0.83 | 0.09 | - | 88,88,88,88 | 0 |
| 36 | SR | S | 8961 | 1/1 | 0.63 | 0.09 | - | 124,124,124,124 | 0 |
| 36 | SR | B | 8950 | 1/1 | 0.59 | 0.14 | - | 108,108,108,108 | 0 |
| 36 | SR | 0 | 8908 | 1/1 | 0.94 | 0.14 | - | 87,87,87,87 | 0 |
| 35 | CL | R | 8806 | 1/1 | 0.93 | 0.37 | - | 43,43,43,43 | 0 |
| 36 | SR | 0 | 8996 | 1/1 | 0.44 | 0.36 | - | 200,200,200,200 | 0 |
| 34 | NA | 0 | 8541 | 1/1 | 0.90 | 0.29 | - | 59,59,59,59 | 0 |
| 34 | NA | 0 | 8506 | 1/1 | 0.73 | 0.30 | - | 74,74,74,74 | 0 |
| 35 | CL | 0 | 8820 | 1/1 | 0.74 | 0.12 | - | 39,39,39,39 | 0 |
| 34 | NA | 0 | 8508 | 1/1 | 0.91 | 0.18 | - | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8030 | 1/1 | 0.56 | 0.46 | - | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8080 | 1/1 | 0.80 | 0.15 | - | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8063 | 1/1 | 0.51 | 0.67 | - | 98,98,98,98 | 0 |
| 36 | SR | 0 | 8933 | 1/1 | 0.65 | 0.14 | - | 134,134,134,134 | 0 |
| 36 | SR | 0 | 8974 | 1/1 | 0.65 | 0.17 | - | 155,155,155,155 | 0 |
| 36 | SR | 0 | 8926 | 1/1 | 0.79 | 0.14 | - | 145,145,145,145 | 0 |
| 34 | NA | 0 | 8574 | 1/1 | 0.52 | 0.19 | - | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8007 | 1/1 | 0.74 | 0.23 | - | 28,28,28,28 | 0 |
| 32 | MG | 0 | 8018 | 1/1 | 0.89 | 0.12 | - | 37,37,37,37 | 0 |
| 34 | NA | 0 | 8544 | 1/1 | 0.90 | 0.19 | - | 59,59,59,59 | 0 |
| 36 | SR | 0 | 8963 | 1/1 | 0.93 | 0.05 | - | 177,177,177,177 | 0 |
| 36 | SR | 0 | 8931 | 1/1 | 0.84 | 0.12 | - | 108,108,108,108 | 0 |
| 36 | SR | 0 | 8941 | 1/1 | 0.91 | 0.11 | - | 104,104,104,104 | 0 |
| 36 | SR | 0 | 9008 | 1/1 | 0.87 | 0.07 | - | 89,89,89,89 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.