# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 08:47 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 1N32 |
| Title | : | Structure of the Thermus thermophilus 30S ribosomal subunit bound to codon and near-cognate transfer RNA anticodon stem-loop mismatched at the first codon position at the a site with paromomycin |
| Authors | : | Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V. |
| Deposited on | : | 2002-10-25 |
| Resolution | : | 3.00 Å(reported) |

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

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

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

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

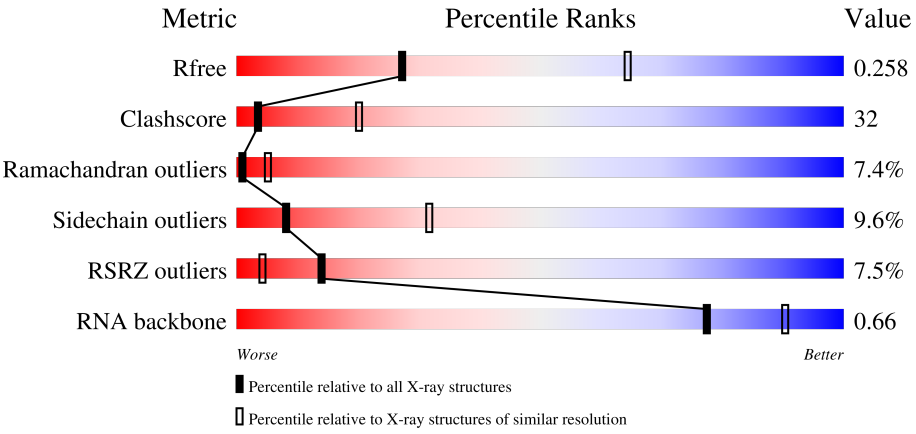
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36.2 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 3.00 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2092 (3.00-3.00) |
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |
| RNA backbone | 3102 | 1173 (3.30-2.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1522 | 11% 34% 51% 11% |
| 2 | Y | 17 | 29% 47% 12% 12% |
| 3 | Z | 6 | 17% 50% 17% 33% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | B | 256 | 4% 24% 53% 13% 9% |
| 5 | C | 239 | 4% 20% 51% 14% 14% |
| 6 | D | 208 | 3% 41% 51% 7% |
| 7 | E | 161 | % 35% 48% 9% 7% |
| 8 | F | 101 | 4% 36% 53% 11% |
| 9 | G | 155 | % 40% 55% 5% |
| 10 | H | 138 | % 47% 46% 7% |
| 11 | I | 128 | 10% 24% 63% 10% |
| 12 | J | 104 | 28% 14% 60% 19% 6% |
| 13 | K | 129 | 2% 40% 42% 11% 8% |
| 14 | L | 135 | % 39% 44% 8% 8% |
| 15 | M | 126 | 4% 27% 53% 13% 6% |
| 16 | N | 60 | 13% 25% 57% 13% 5% |
| 17 | O | 88 | 5% 52% 40% 8% |
| 18 | P | 88 | % 36% 49% 9% 6% |
| 19 | Q | 104 | 8% 44% 46% 9% |
| 20 | R | 88 | 2% 35% 42% 6% 17% |
| 21 | S | 92 | 14% 27% 49% 10% 13% |
| 22 | T | 106 | % 39% 44% 9% 7% |
| 23 | V | 26 | 8% 46% 46% 8% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 25 | MG | A | 1549 | - | - | - | X |
| 25 | MG | A | 1567 | - | - | - | X |
| 25 | MG | A | 1572 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 25 | MG | A | 1615 | - | - | - | X |
| 25 | MG | A | 1617 | - | - | - | X |
| 25 | MG | A | 1618 | - | - | - | X |
| 25 | MG | A | 1619 | - | - | - | X |
| 25 | MG | A | 1624 | - | - | - | X |
| 25 | MG | A | 1632 | - | - | - | X |
| 25 | MG | A | 1641 | - | - | - | X |
| 25 | MG | A | 1644 | - | - | - | X |
| 25 | MG | A | 1645 | - | - | - | X |
| 25 | MG | A | 1655 | - | - | - | X |
| 25 | MG | A | 1675 | - | - | - | X |
| 25 | MG | A | 1678 | - | - | - | X |
| 25 | MG | A | 1680 | - | - | - | X |

# 2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 52275 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | A | 1513 | 32508 | 14472 | 6016 | 10509 | 1511 | 0 | 0 | 0 |

- Molecule 2 is a RNA chain called ANTICODON STEM-LOOP OF LEU-2 TRANSFER RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 2 | Y | 15 | 318 | 143 | 56 | 105 | 14 | 0 | 0 | 0 |

- Molecule 3 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 3 | Z | 4 | 77 | 36 | 8 | 30 | 3 | 0 | 0 | 0 |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | B | 234 | 1900 | 1213 | 341 | 341 | 5 | 0 | 0 | 0 |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | C | 206 | 1612 | 1016 | 314 | 281 | 1 | 0 | 0 | 0 |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | D | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | E | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1146 | 724 | 217 | 201 | 4 | | | |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | F | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | G | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | H | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| H | 25 | ASP | GLU | conflict | UNP P24319 |
| H | 37 | ARG | LYS | conflict | UNP P24319 |
| H | 52 | ASP | GLU | conflict | UNP P24319 |
| H | 61 | VAL | ILE | conflict | UNP P24319 |
| H | 62 | TYR | HIS | conflict | UNP P24319 |
| H | 81 | HIS | LYS | conflict | UNP P24319 |
| H | 88 | LYS | ARG | conflict | UNP P24319 |
| H | 115 | SER | PRO | conflict | UNP P24319 |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | I | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1011 | 639 | 198 | 174 | | | |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | J | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 792 | 498 | 156 | 137 | 1 | | | |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | K | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | L | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 970 | 611 | 195 | 163 | 1 | | | |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | M | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 937 | 579 | 193 | 163 | 2 | | | |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | N | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | O | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 18 | P | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 700 | 443 | 139 | 117 | 1 | | | |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | Q | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 547 | 161 | 147 | 2 | | | |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Q | 50 | LYS | ARG | conflict | UNP P24321 |
| Q | 53 | LEU | VAL | conflict | UNP P24321 |
| Q | 62 | SER | ALA | conflict | UNP P24321 |
| Q | 79 | SER | GLU | conflict | UNP P24321 |
| Q | 82 | MET | LEU | conflict | UNP P24321 |
| Q | 90 | ILE | VAL | conflict | UNP P24321 |
| Q | 96 | GLN | ALA | conflict | UNP P24321 |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | R | 73 | Total | C | N | O | 0 | 0 | 0 |
| | | | 597 | 380 | 118 | 99 | | | |

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | S | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 647 | 414 | 119 | 112 | 2 | | | |

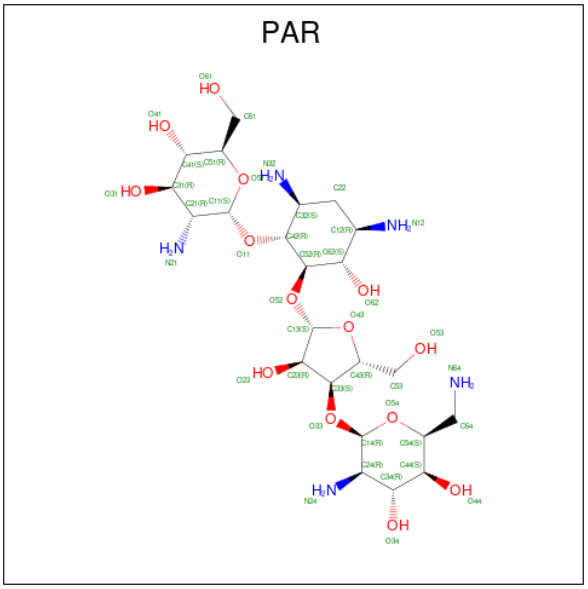
- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | T | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | V | 24 | Total | C | N | O | 0 | 0 | 0 |
| | | | 208 | 128 | 50 | 30 | | | |

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 24 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 25 | A | 153 | Total | Mg | 0 | 0 |
| | | | 153 | 153 | | |
| 25 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | J | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | M | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

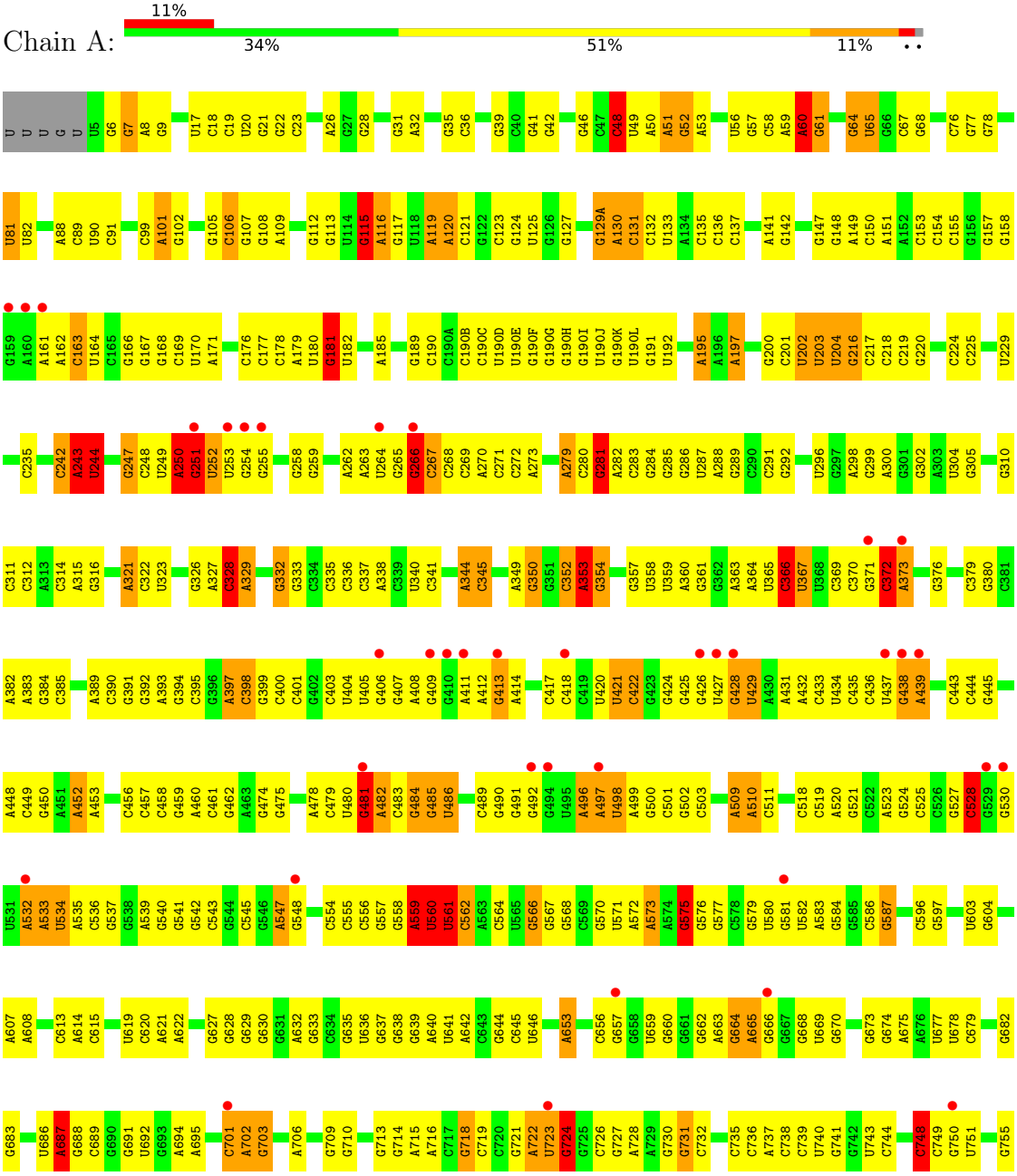
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 26 | D | 1 | Total Zn<br>1 1 | 0 | 0 |
| 26 | N | 1 | Total Zn<br>1 1 | 0 | 0 |

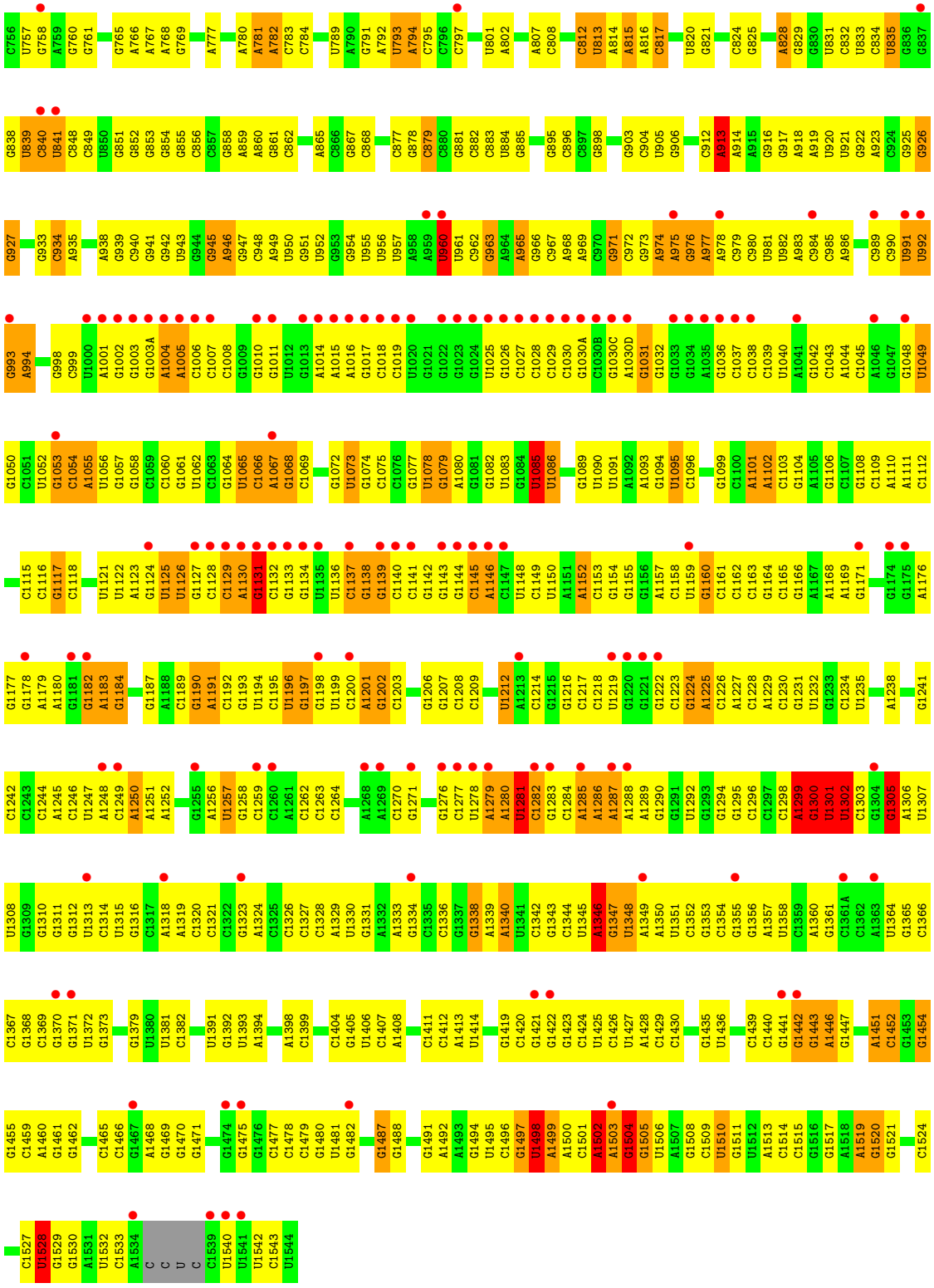
# 3 Residue-property plots (i)

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

- Molecule 1: 16S RIBOSOMAL RNA

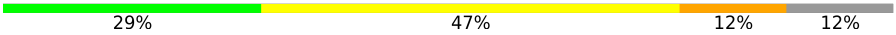
Chain A:

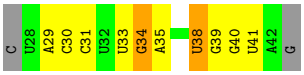




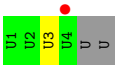
• Molecule 2: ANTICODON STEM-LOOP OF LEU-2 TRANSFER RNA

Chain Y:

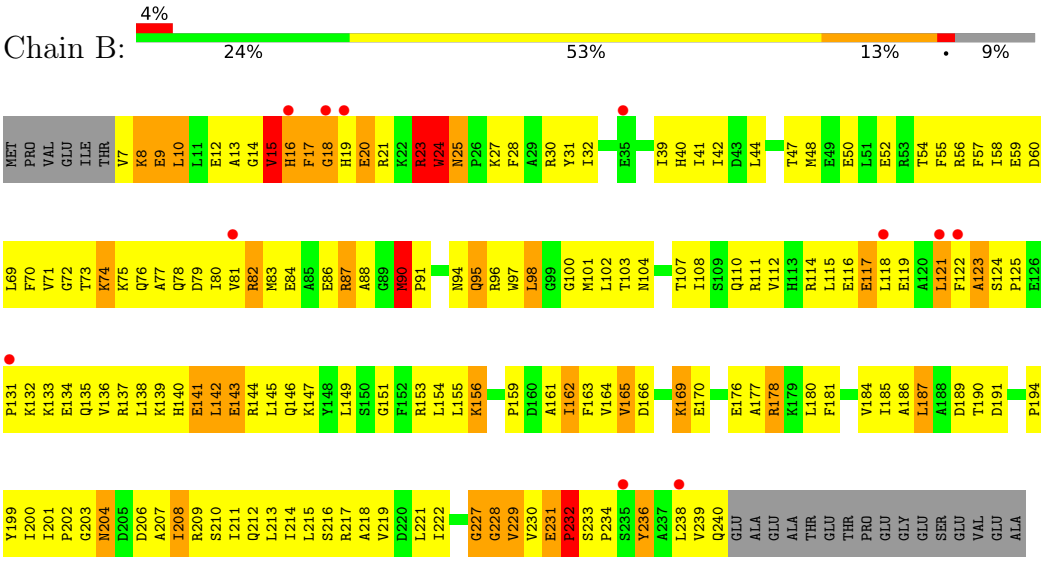





• Molecule 3: A-SITE MESSENGER RNA FRAGMENT

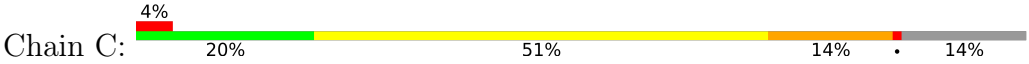

• Molecule 4: 30S RIBOSOMAL PROTEIN S2

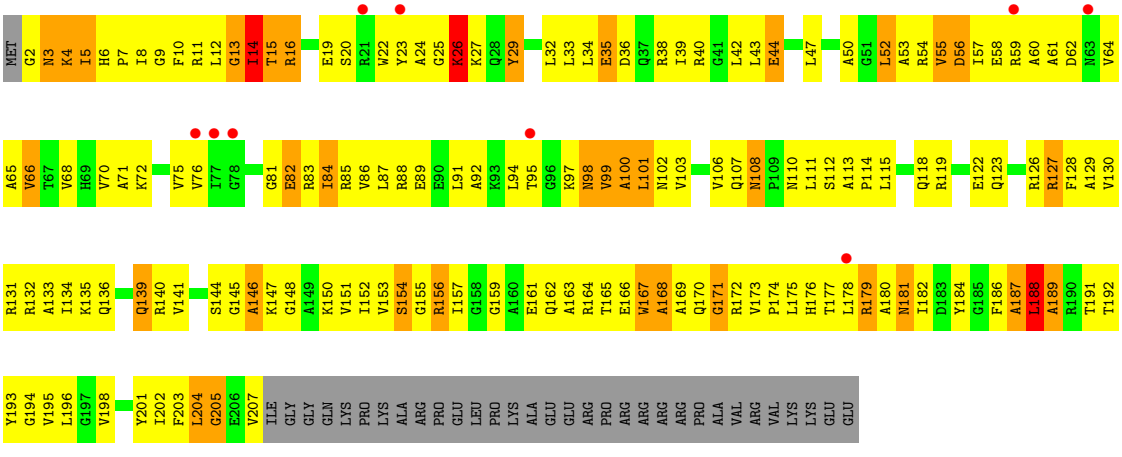




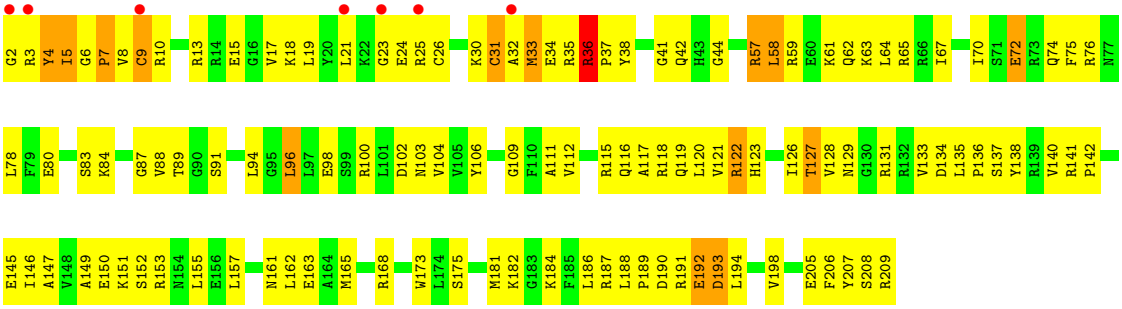


• Molecule 5: 30S RIBOSOMAL PROTEIN S3

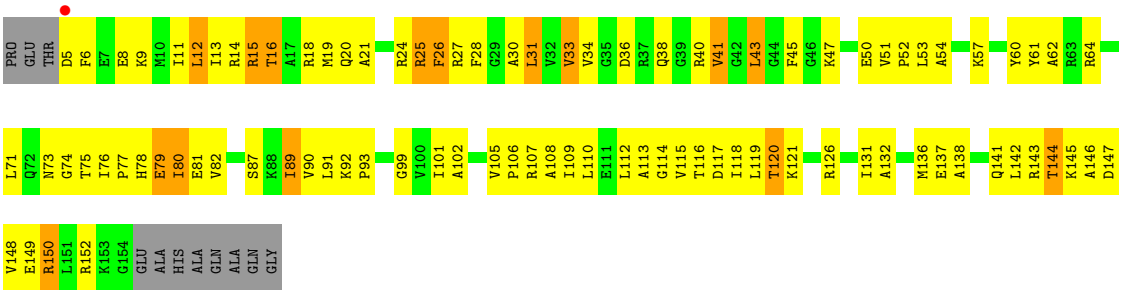


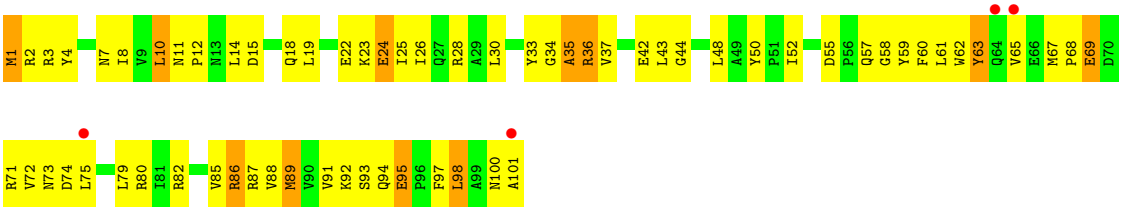

• Molecule 6: 30S RIBOSOMAL PROTEIN S4




• Molecule 7: 30S RIBOSOMAL PROTEIN S5

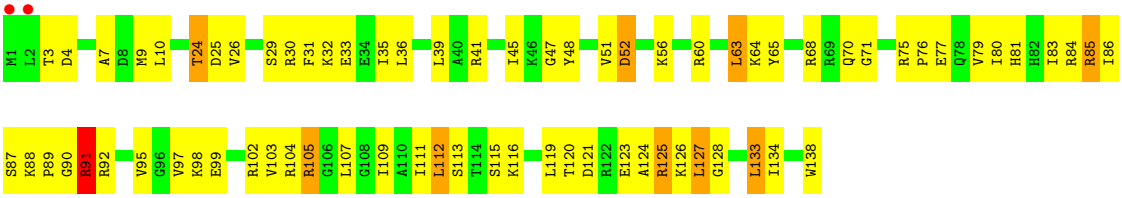

• Molecule 8: 30S RIBOSOMAL PROTEIN S6


• Molecule 9: 30S RIBOSOMAL PROTEIN S7



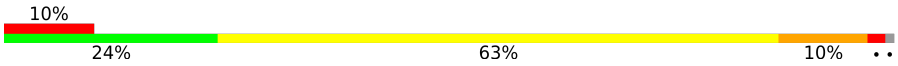
• Molecule 10: 30S RIBOSOMAL PROTEIN S8

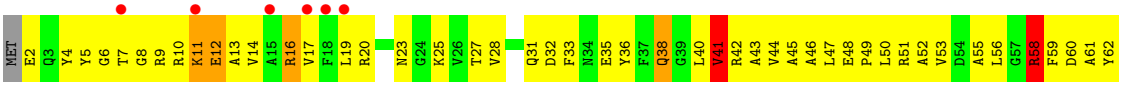


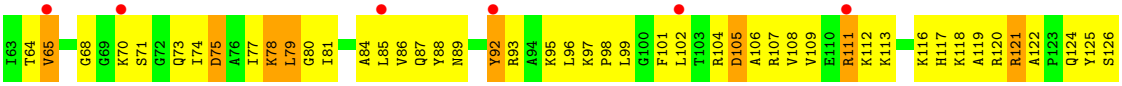


• Molecule 11: 30S RIBOSOMAL PROTEIN S9

Chain I:

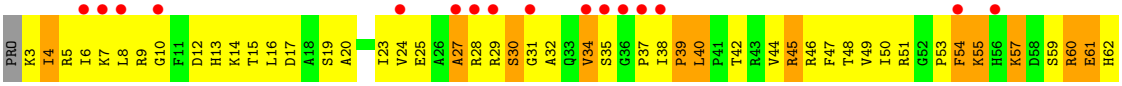


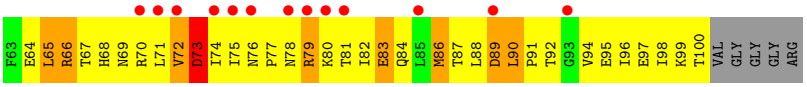





• Molecule 12: 30S RIBOSOMAL PROTEIN S10

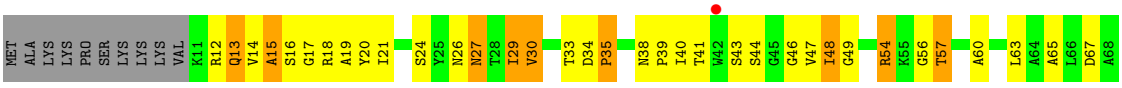
Chain J:

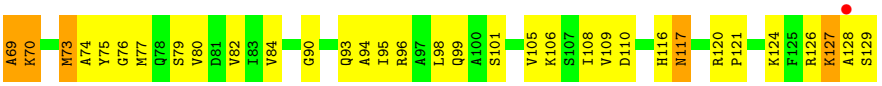





• Molecule 13: 30S RIBOSOMAL PROTEIN S11

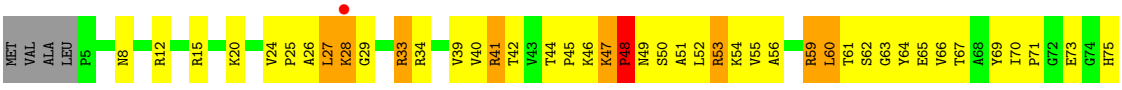
Chain K:

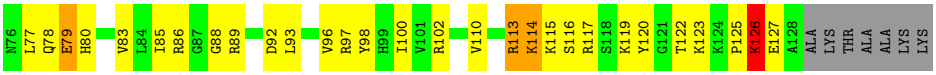





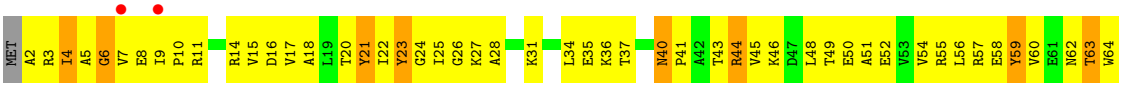
• Molecule 14: 30S RIBOSOMAL PROTEIN S12

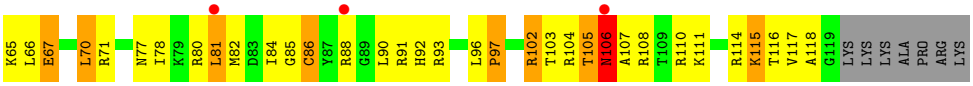
Chain L:

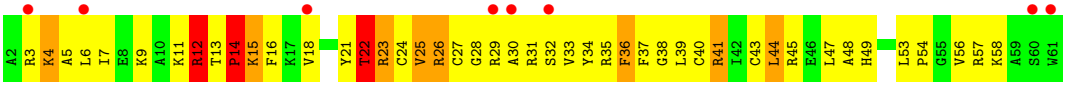



• Molecule 15: 30S RIBOSOMAL PROTEIN S13

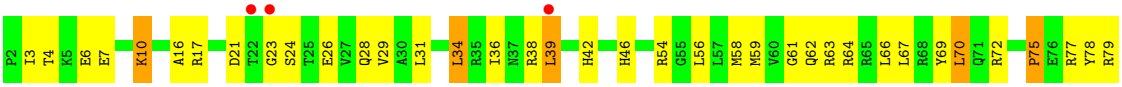



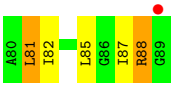




• Molecule 16: 30S RIBOSOMAL PROTEIN S14

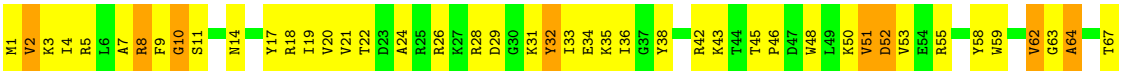



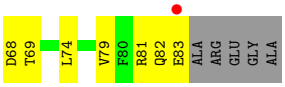

• Molecule 17: 30S RIBOSOMAL PROTEIN S15

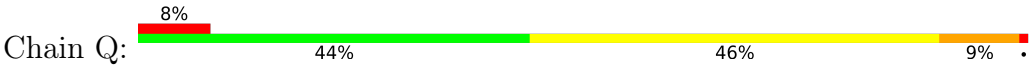



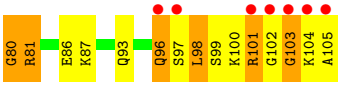

• Molecule 18: 30S RIBOSOMAL PROTEIN S16

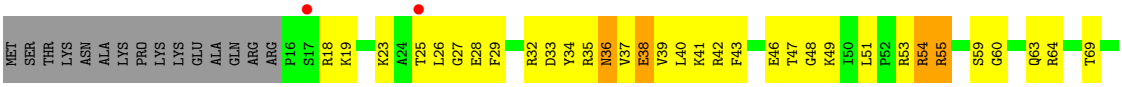

• Molecule 19: 30S RIBOSOMAL PROTEIN S17

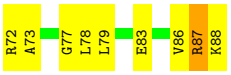



• Molecule 20: 30S RIBOSOMAL PROTEIN S18

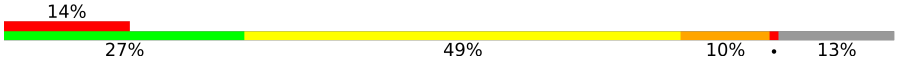
Chain R:

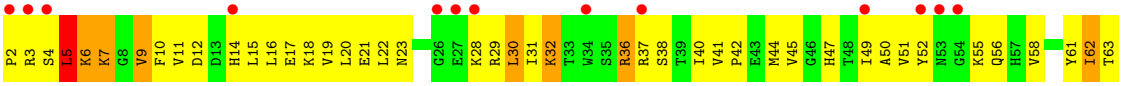



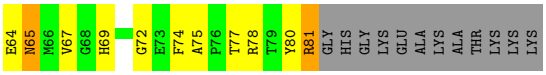




• Molecule 21: 30S RIBOSOMAL PROTEIN S19

Chain S:

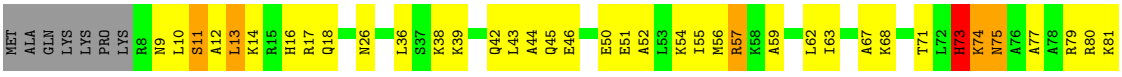



• Molecule 22: 30S RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 23: 30S RIBOSOMAL PROTEIN THX

Chain V:


# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 41 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 400.30Å 400.30Å 175.48Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 141.42 – 3.00<br>131.95 – 2.99 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 91.9 (141.42-3.00)<br>91.1 (131.95-2.99) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.13 | Depositor |
| $< I/\sigma(I) >$ [1] | 2.41 (at 3.01Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.227 , 0.270<br>0.215 , 0.258 | Depositor<br>DCC |
| $R_{free}$ test set | 13179 reflections (5.08%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 67.3 | Xtriage |
| Anisotropy | 0.222 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.31 , 86.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.89 | EDS |
| Total number of atoms | 52275 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 70.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, ZN, PAR, MG

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 | 0.46 | 0/36387 | 0.74 | 39/56789 (0.1%) |
| 2 | Y | 0.41 | 0/333 | 0.71 | 0/518 |
| 3 | Z | 0.49 | 0/84 | 0.82 | 0/128 |
| 4 | B | 0.32 | 0/1935 | 0.64 | 0/2609 |
| 5 | C | 0.35 | 0/1636 | 0.62 | 0/2205 |
| 6 | D | 0.38 | 0/1733 | 0.67 | 0/2318 |
| 7 | E | 0.44 | 0/1162 | 0.71 | 0/1564 |
| 8 | F | 0.31 | 0/856 | 0.60 | 0/1154 |
| 9 | G | 0.36 | 0/1276 | 0.59 | 0/1709 |
| 10 | H | 0.44 | 0/1136 | 0.77 | 0/1527 |
| 11 | I | 0.35 | 0/1029 | 0.64 | 0/1378 |
| 12 | J | 0.36 | 0/805 | 0.64 | 0/1082 |
| 13 | K | 0.39 | 0/900 | 0.73 | 0/1213 |
| 14 | L | 0.43 | 0/986 | 0.77 | 0/1320 |
| 15 | M | 0.33 | 0/947 | 0.65 | 0/1270 |
| 16 | N | 0.41 | 0/501 | 0.68 | 0/664 |
| 17 | O | 0.36 | 0/745 | 0.58 | 0/992 |
| 18 | P | 0.45 | 0/716 | 0.73 | 0/963 |
| 19 | Q | 0.44 | 0/870 | 0.75 | 0/1159 |
| 20 | R | 0.33 | 0/603 | 0.62 | 0/799 |
| 21 | S | 0.32 | 0/661 | 0.64 | 0/890 |
| 22 | T | 0.39 | 0/765 | 0.71 | 0/1007 |
| 23 | V | 0.44 | 0/212 | 0.76 | 0/277 |
| All | All | 0.44 | 0/56278 | 0.72 | 39/83535 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 4 | 35 |
| 18 | P | 0 | 1 |
| All | All | 4 | 36 |

There are no bond length outliers.

All (39) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 48 | C | C2'-C3'-O3' | 11.02 | 133.74 | 109.50 |
| 1 | A | 1498 | U | C2'-C3'-O3' | 10.16 | 131.86 | 109.50 |
| 1 | A | 243 | A | C2'-C3'-O3' | 9.62 | 130.66 | 109.50 |
| 1 | A | 281 | G | C2'-C3'-O3' | 9.39 | 130.16 | 109.50 |
| 1 | A | 115 | G | C2'-C3'-O3' | 9.27 | 129.88 | 109.50 |
| 1 | A | 1302 | U | C2'-C3'-O3' | 9.24 | 129.82 | 109.50 |
| 1 | A | 328 | C | C2'-C3'-O3' | 8.65 | 128.54 | 109.50 |
| 1 | A | 575 | G | C2'-C3'-O3' | 8.59 | 128.40 | 109.50 |
| 1 | A | 1528 | U | C2'-C3'-O3' | 8.57 | 128.35 | 109.50 |
| 1 | A | 687 | A | C2'-C3'-O3' | 8.17 | 127.48 | 109.50 |
| 1 | A | 1503 | A | C2'-C3'-O3' | 7.62 | 126.27 | 109.50 |
| 1 | A | 1502 | A | N9-C1'-C2' | 7.62 | 123.90 | 114.00 |
| 1 | A | 181 | G | C2'-C3'-O3' | 7.60 | 126.22 | 109.50 |
| 1 | A | 60 | A | C2'-C3'-O3' | 7.59 | 126.19 | 109.50 |
| 1 | A | 913 | A | C2'-C3'-O3' | 7.41 | 125.81 | 109.50 |
| 1 | A | 965 | A | C2'-C3'-O3' | 7.35 | 125.67 | 109.50 |
| 1 | A | 266 | G | C2'-C3'-O3' | 7.21 | 125.35 | 109.50 |
| 1 | A | 1504 | G | C2'-C3'-O3' | 7.16 | 125.26 | 109.50 |
| 1 | A | 372 | C | C2'-C3'-O3' | 7.10 | 125.12 | 109.50 |
| 1 | A | 509 | A | C2'-C3'-O3' | 7.07 | 125.05 | 109.50 |
| 1 | A | 1299 | A | N9-C1'-C2' | 6.68 | 122.68 | 114.00 |
| 1 | A | 366 | C | C2'-C3'-O3' | 6.45 | 124.02 | 113.70 |
| 1 | A | 1346 | A | C2'-C3'-O3' | 6.37 | 123.90 | 113.70 |
| 1 | A | 748 | C | N1-C1'-C2' | 5.87 | 121.64 | 114.00 |
| 1 | A | 1085 | U | C2'-C3'-O3' | 5.86 | 123.08 | 113.70 |
| 1 | A | 353 | A | C5'-C4'-O4' | -5.79 | 102.15 | 109.10 |
| 1 | A | 559 | A | C2'-C3'-O3' | 5.76 | 122.91 | 113.70 |
| 1 | A | 960 | U | N1-C1'-C2' | 5.70 | 121.41 | 114.00 |
| 1 | A | 244 | U | C5'-C4'-C3' | -5.68 | 106.90 | 116.00 |
| 1 | A | 1528 | U | C4'-C3'-O3' | 5.52 | 124.04 | 113.00 |
| 1 | A | 7 | G | C2'-C3'-O3' | 5.43 | 122.39 | 113.70 |
| 1 | A | 460 | A | N9-C1'-C2' | 5.31 | 120.90 | 114.00 |
| 1 | A | 694 | A | C5'-C4'-C3' | -5.25 | 107.60 | 116.00 |
| 1 | A | 1305 | G | N9-C1'-C2' | 5.21 | 120.78 | 114.00 |
| 1 | A | 1301 | U | C2'-C3'-O3' | 5.16 | 121.96 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 281 | G | C4'-C3'-O3' | 5.14 | 123.27 | 113.00 |
| 1 | A | 528 | C | C5'-C4'-C3' | 5.14 | 124.22 | 116.00 |
| 1 | A | 560 | U | C2'-C3'-O3' | 5.10 | 121.86 | 113.70 |
| 1 | A | 1281 | U | C2'-C3'-O3' | 5.08 | 121.83 | 113.70 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | A | 48 | C | C3' |
| 1 | A | 243 | A | C3' |
| 1 | A | 281 | G | C3' |
| 1 | A | 1528 | U | C3' |

All (36) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 106 | C | Sidechain |
| 1 | A | 1073 | U | Sidechain |
| 1 | A | 1077 | G | Sidechain |
| 1 | A | 1078 | U | Sidechain |
| 1 | A | 1079 | G | Sidechain |
| 1 | A | 1131 | G | Sidechain |
| 1 | A | 1299 | A | Sidechain |
| 1 | A | 1300 | G | Sidechain |
| 1 | A | 1301 | U | Sidechain |
| 1 | A | 1340 | A | Sidechain |
| 1 | A | 1414 | U | Sidechain |
| 1 | A | 1454 | G | Sidechain |
| 1 | A | 1510 | U | Sidechain |
| 1 | A | 1519 | A | Sidechain |
| 1 | A | 229 | U | Sidechain |
| 1 | A | 242 | C | Sidechain |
| 1 | A | 250 | A | Sidechain |
| 1 | A | 251 | G | Sidechain |
| 1 | A | 481 | G | Sidechain |
| 1 | A | 528 | C | Sidechain |
| 1 | A | 561 | U | Sidechain |
| 1 | A | 566 | G | Sidechain |
| 1 | A | 573 | A | Sidechain |
| 1 | A | 575 | G | Sidechain |
| 1 | A | 587 | G | Sidechain |
| 1 | A | 664 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 724 | G | Sidechain |
| 1 | A | 727 | G | Sidechain |
| 1 | A | 835 | U | Sidechain |
| 1 | A | 879 | C | Sidechain |
| 1 | A | 898 | G | Sidechain |
| 1 | A | 905 | U | Sidechain |
| 1 | A | 946 | A | Sidechain |
| 1 | A | 960 | U | Sidechain |
| 1 | A | 963 | G | Sidechain |
| 18 | P | 32 | 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 | 32508 | 0 | 16413 | 1088 | 0 |
| 2 | Y | 318 | 0 | 162 | 14 | 0 |
| 3 | Z | 77 | 0 | 42 | 1 | 0 |
| 4 | B | 1900 | 0 | 1951 | 255 | 0 |
| 5 | C | 1612 | 0 | 1677 | 229 | 0 |
| 6 | D | 1703 | 0 | 1763 | 134 | 0 |
| 7 | E | 1146 | 0 | 1207 | 105 | 0 |
| 8 | F | 843 | 0 | 857 | 95 | 0 |
| 9 | G | 1257 | 0 | 1296 | 107 | 0 |
| 10 | H | 1116 | 0 | 1177 | 80 | 0 |
| 11 | I | 1011 | 0 | 1043 | 124 | 0 |
| 12 | J | 792 | 0 | 835 | 131 | 0 |
| 13 | K | 885 | 0 | 904 | 75 | 0 |
| 14 | L | 970 | 0 | 1057 | 101 | 0 |
| 15 | M | 937 | 0 | 995 | 110 | 0 |
| 16 | N | 492 | 0 | 530 | 71 | 0 |
| 17 | O | 734 | 0 | 771 | 41 | 0 |
| 18 | P | 700 | 0 | 720 | 56 | 0 |
| 19 | Q | 857 | 0 | 930 | 69 | 0 |
| 20 | R | 597 | 0 | 668 | 63 | 0 |
| 21 | S | 647 | 0 | 673 | 86 | 0 |
| 22 | T | 763 | 0 | 861 | 79 | 0 |
| 23 | V | 208 | 0 | 221 | 14 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 24 | A | 42 | 0 | 45 | 2 | 0 |
| 25 | A | 153 | 0 | 0 | 0 | 0 |
| 25 | D | 1 | 0 | 0 | 0 | 0 |
| 25 | E | 1 | 0 | 0 | 0 | 0 |
| 25 | J | 1 | 0 | 0 | 0 | 0 |
| 25 | M | 1 | 0 | 0 | 0 | 0 |
| 25 | Y | 1 | 0 | 0 | 0 | 0 |
| 26 | D | 1 | 0 | 0 | 0 | 0 |
| 26 | N | 1 | 0 | 0 | 0 | 0 |
| All | All | 52275 | 0 | 36798 | 2844 | 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 32.

All (2844) 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) |
|---|---|---|---|
| 6:D:36:ARG:H | 6:D:37:PRO:HD3 | 1.02 | 1.18 |
| 15:M:10:PRO:HB2 | 15:M:18:ALA:HB1 | 1.29 | 1.14 |
| 7:E:15:ARG:HD3 | 7:E:26:PHE:HD2 | 1.13 | 1.11 |
| 1:A:975:A:H4' | 1:A:976:G:H5" | 1.31 | 1.11 |
| 1:A:1532:U:H2' | 1:A:1533:C:H5" | 1.19 | 1.09 |
| 1:A:723:U:H2' | 1:A:724:G:H5' | 1.33 | 1.07 |
| 1:A:760:G:H1 | 19:Q:105:ALA:HB2 | 1.19 | 1.07 |
| 5:C:108:ASN:HD22 | 5:C:111:LEU:HG | 1.09 | 1.07 |
| 13:K:48:ILE:HG22 | 13:K:49:GLY:H | 1.10 | 1.06 |
| 9:G:90:GLU:HG3 | 9:G:155:ARG:HH22 | 1.19 | 1.06 |
| 13:K:40:ILE:HG22 | 13:K:41:THR:HG23 | 1.38 | 1.05 |
| 4:B:77:ALA:HB2 | 4:B:211:ILE:HD13 | 1.36 | 1.05 |
| 12:J:4:ILE:HD12 | 12:J:74:ILE:HB | 1.33 | 1.04 |
| 12:J:38:ILE:HB | 12:J:71:LEU:HB2 | 1.38 | 1.03 |
| 1:A:243:A:H4' | 1:A:244:U:H5' | 1.36 | 1.03 |
| 1:A:737:A:H1' | 8:F:73:ASN:HD21 | 1.22 | 1.03 |
| 21:S:28:LYS:HG2 | 21:S:29:ARG:H | 1.25 | 1.01 |
| 1:A:349:A:H2' | 1:A:350:G:H5" | 1.43 | 1.01 |
| 1:A:1443:G:H5" | 1:A:1446:A:H5' | 1.03 | 1.00 |
| 1:A:877:C:O2 | 10:H:3:THR:HG21 | 1.60 | 0.99 |
| 12:J:45:ARG:HB3 | 12:J:45:ARG:HH11 | 1.22 | 0.99 |
| 1:A:1250:A:H4' | 11:I:68:GLY:H | 1.28 | 0.98 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 0.97 | 0.97 |
| 17:O:3:ILE:HD13 | 17:O:34:LEU:HD13 | 1.45 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1443:G:C5' | 1:A:1446:A:H5' | 1.95 | 0.97 |
| 1:A:1305:G:O2' | 1:A:1306:A:H8 | 1.48 | 0.96 |
| 22:T:13:LEU:H | 22:T:13:LEU:HD12 | 1.30 | 0.96 |
| 7:E:15:ARG:HD3 | 7:E:26:PHE:CD2 | 2.00 | 0.96 |
| 1:A:371:G:O2' | 1:A:372:C:H5' | 1.66 | 0.96 |
| 7:E:80:ILE:CD1 | 7:E:91:LEU:HB2 | 1.95 | 0.96 |
| 8:F:33:TYR:HB2 | 8:F:75:LEU:HD23 | 1.47 | 0.96 |
| 1:A:579:G:H5' | 1:A:728:A:H1' | 1.48 | 0.96 |
| 7:E:79:GLU:HG3 | 7:E:93:PRO:HD2 | 1.46 | 0.95 |
| 1:A:1101:A:H4' | 1:A:1102:A:O5' | 1.63 | 0.95 |
| 6:D:151:LYS:H | 6:D:151:LYS:HD2 | 1.33 | 0.94 |
| 5:C:14:ILE:HD13 | 5:C:14:ILE:H | 1.32 | 0.94 |
| 1:A:266:G:H5" | 1:A:268:C:H41 | 1.31 | 0.94 |
| 22:T:57:ARG:NE | 22:T:102:GLY:HA3 | 1.81 | 0.93 |
| 1:A:1532:U:C2' | 1:A:1533:C:H5" | 1.98 | 0.93 |
| 6:D:36:ARG:N | 6:D:37:PRO:HD3 | 1.83 | 0.93 |
| 1:A:1127:G:H21 | 1:A:1146:A:H62 | 1.18 | 0.92 |
| 7:E:81:GLU:HG2 | 7:E:90:VAL:HG22 | 1.49 | 0.92 |
| 4:B:102:LEU:HD21 | 4:B:162:ILE:HD11 | 1.52 | 0.92 |
| 12:J:34:VAL:HG22 | 12:J:74:ILE:HG23 | 1.51 | 0.92 |
| 5:C:108:ASN:ND2 | 5:C:111:LEU:HG | 1.83 | 0.92 |
| 20:R:47:THR:HA | 20:R:83:GLU:HB2 | 1.51 | 0.92 |
| 10:H:121:ASP:HB2 | 10:H:125:ARG:HH21 | 1.32 | 0.91 |
| 12:J:51:ARG:HG2 | 12:J:60:ARG:O | 1.69 | 0.91 |
| 11:I:93:ARG:HD3 | 11:I:97:LYS:HZ1 | 1.34 | 0.91 |
| 5:C:191:THR:HB | 5:C:194:GLY:O | 1.70 | 0.91 |
| 11:I:8:GLY:HA2 | 11:I:79:LEU:HD13 | 1.52 | 0.91 |
| 1:A:1057:G:H5" | 5:C:154:SER:HB2 | 1.53 | 0.91 |
| 6:D:8:VAL:HG13 | 6:D:21:LEU:HD12 | 1.53 | 0.90 |
| 8:F:87:ARG:HH11 | 8:F:87:ARG:HG3 | 1.35 | 0.90 |
| 8:F:100:ASN:HD22 | 20:R:23:LYS:HG2 | 1.35 | 0.90 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.18 | 0.90 |
| 1:A:1443:G:H5" | 1:A:1446:A:C5' | 1.97 | 0.90 |
| 14:L:47:LYS:HB3 | 14:L:48:PRO:CD | 2.03 | 0.89 |
| 1:A:838:G:H2' | 1:A:839:U:H5" | 1.51 | 0.89 |
| 1:A:1502:A:H2 | 1:A:1505:G:N1 | 1.71 | 0.89 |
| 1:A:723:U:H2' | 1:A:724:G:C5' | 2.03 | 0.89 |
| 5:C:91:LEU:HD21 | 5:C:99:VAL:HG13 | 1.55 | 0.89 |
| 1:A:972:C:H4' | 12:J:57:LYS:HG2 | 1.53 | 0.89 |
| 19:Q:93:GLN:O | 19:Q:96:GLN:HB2 | 1.71 | 0.89 |
| 5:C:7:PRO:O | 5:C:11:ARG:HD2 | 1.71 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:132:LYS:HA | 4:B:135:GLN:HB3 | 1.55 | 0.88 |
| 14:L:47:LYS:HB3 | 14:L:48:PRO:HD3 | 1.52 | 0.88 |
| 1:A:1305:G:HO2' | 1:A:1306:A:H8 | 0.90 | 0.88 |
| 1:A:1195:C:H3' | 1:A:1196:U:H5" | 1.53 | 0.88 |
| 1:A:1319:A:H4' | 21:S:37:ARG:NH1 | 1.88 | 0.88 |
| 4:B:116:GLU:HG2 | 4:B:153:ARG:HH12 | 1.35 | 0.88 |
| 13:K:48:ILE:HG22 | 13:K:49:GLY:N | 1.85 | 0.88 |
| 5:C:50:ALA:HB1 | 5:C:70:VAL:HG11 | 1.54 | 0.88 |
| 1:A:760:G:N1 | 19:Q:105:ALA:HB2 | 1.88 | 0.87 |
| 1:A:975:A:H5' | 1:A:975:A:H8 | 1.38 | 0.87 |
| 5:C:64:VAL:HB | 5:C:99:VAL:HB | 1.54 | 0.87 |
| 1:A:1127:G:N2 | 1:A:1146:A:H62 | 1.73 | 0.87 |
| 12:J:12:ASP:HB3 | 12:J:15:THR:HG22 | 1.55 | 0.87 |
| 17:O:4:THR:OG1 | 17:O:7:GLU:HB2 | 1.75 | 0.87 |
| 15:M:8:GLU:HG3 | 15:M:22:ILE:HG12 | 1.58 | 0.86 |
| 1:A:1137:C:H4' | 1:A:1138:G:C2 | 2.10 | 0.86 |
| 6:D:70:ILE:HD11 | 6:D:100:ARG:HD2 | 1.56 | 0.86 |
| 4:B:84:GLU:HB3 | 4:B:219:VAL:HG21 | 1.56 | 0.86 |
| 1:A:1086:U:H3 | 1:A:1099:G:H22 | 1.20 | 0.86 |
| 6:D:8:VAL:HG21 | 6:D:115:ARG:NH1 | 1.90 | 0.86 |
| 22:T:57:ARG:HG2 | 22:T:102:GLY:O | 1.73 | 0.86 |
| 1:A:204:U:H4' | 1:A:216:G:O5' | 1.73 | 0.85 |
| 2:Y:33:U:H5' | 2:Y:34:G:OP2 | 1.76 | 0.85 |
| 15:M:34:LEU:HD13 | 15:M:41:PRO:HA | 1.57 | 0.85 |
| 6:D:190:ASP:HB3 | 6:D:193:ASP:OD1 | 1.76 | 0.85 |
| 1:A:975:A:H4' | 1:A:976:G:C5' | 2.05 | 0.85 |
| 4:B:77:ALA:HB2 | 4:B:211:ILE:CD1 | 2.06 | 0.85 |
| 22:T:54:LYS:HE3 | 22:T:100:ILE:HD11 | 1.57 | 0.85 |
| 5:C:26:LYS:H | 5:C:26:LYS:HD3 | 1.40 | 0.85 |
| 23:V:6:ARG:HD2 | 23:V:15:ARG:HH12 | 1.42 | 0.85 |
| 1:A:1152:A:H5" | 12:J:13:HIS:CD2 | 2.12 | 0.84 |
| 6:D:57:ARG:H | 6:D:57:ARG:HD3 | 1.42 | 0.84 |
| 6:D:127:THR:HG23 | 6:D:147:ALA:HB3 | 1.57 | 0.84 |
| 11:I:16:ARG:HG3 | 11:I:64:THR:HB | 1.57 | 0.84 |
| 22:T:12:ALA:H | 22:T:13:LEU:HD12 | 1.43 | 0.84 |
| 1:A:1238:A:H5' | 1:A:1336:C:H41 | 1.41 | 0.84 |
| 1:A:1367:C:H5' | 12:J:60:ARG:NH1 | 1.91 | 0.84 |
| 5:C:35:GLU:HG2 | 5:C:59:ARG:HH22 | 1.43 | 0.84 |
| 8:F:28:ARG:NH1 | 8:F:28:ARG:HB2 | 1.92 | 0.83 |
| 15:M:4:ILE:HG22 | 15:M:5:ALA:N | 1.93 | 0.83 |
| 1:A:129(A):G:O2' | 1:A:190(E):U:H2' | 1.78 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:231:GLU:HB2 | 4:B:232:PRO:HD2 | 1.57 | 0.83 |
| 1:A:1124:G:H5" | 12:J:35:SER:O | 1.78 | 0.83 |
| 22:T:50:GLU:HB2 | 22:T:99:LEU:HD12 | 1.58 | 0.83 |
| 5:C:34:LEU:HD12 | 16:N:25:VAL:HG21 | 1.59 | 0.83 |
| 6:D:36:ARG:H | 6:D:37:PRO:CD | 1.90 | 0.83 |
| 20:R:55:ARG:HB3 | 20:R:55:ARG:HH11 | 1.44 | 0.83 |
| 21:S:41:VAL:HG12 | 21:S:42:PRO:HD2 | 1.60 | 0.83 |
| 1:A:31:G:N1 | 1:A:48:C:H5" | 1.94 | 0.83 |
| 2:Y:29:A:H2' | 2:Y:30:C:C6 | 2.14 | 0.83 |
| 1:A:1125:U:H3 | 12:J:5:ARG:HH21 | 1.26 | 0.82 |
| 10:H:24:THR:HG22 | 10:H:63:LEU:HD21 | 1.61 | 0.82 |
| 4:B:59:GLU:HB3 | 4:B:221:LEU:HD11 | 1.62 | 0.82 |
| 1:A:250:A:H4' | 1:A:251:G:O5' | 1.78 | 0.82 |
| 17:O:16:ALA:HB1 | 17:O:21:ASP:HB3 | 1.59 | 0.82 |
| 1:A:1366:C:H2' | 1:A:1367:C:H6 | 1.41 | 0.82 |
| 1:A:1250:A:H4' | 11:I:68:GLY:N | 1.94 | 0.82 |
| 15:M:102:ARG:HB2 | 15:M:102:ARG:HH11 | 1.44 | 0.82 |
| 1:A:1106:G:H5" | 5:C:172:ARG:HG2 | 1.62 | 0.82 |
| 1:A:1352:C:H2' | 1:A:1353:G:C8 | 2.14 | 0.82 |
| 12:J:7:LYS:HE3 | 12:J:40:LEU:HD11 | 1.61 | 0.82 |
| 5:C:35:GLU:HG2 | 5:C:59:ARG:NH2 | 1.93 | 0.82 |
| 13:K:48:ILE:CG2 | 13:K:49:GLY:H | 1.92 | 0.82 |
| 12:J:10:GLY:HA3 | 12:J:16:LEU:HD21 | 1.62 | 0.81 |
| 1:A:1128:C:H4' | 11:I:16:ARG:NH2 | 1.95 | 0.81 |
| 7:E:144:THR:HG22 | 7:E:147:ASP:H | 1.42 | 0.81 |
| 10:H:113:SER:HB2 | 10:H:134:ILE:HD11 | 1.63 | 0.81 |
| 1:A:1190:G:OP1 | 5:C:4:LYS:HA | 1.80 | 0.81 |
| 9:G:54:THR:HG22 | 9:G:56:GLN:H | 1.46 | 0.81 |
| 4:B:124:SER:HB2 | 4:B:125:PRO:HD2 | 1.62 | 0.81 |
| 1:A:1425:U:H2' | 1:A:1426:C:C6 | 2.17 | 0.80 |
| 5:C:24:ALA:HB2 | 5:C:32:LEU:HD12 | 1.62 | 0.80 |
| 1:A:1223:C:P | 21:S:78:ARG:HH12 | 2.05 | 0.80 |
| 5:C:180:ALA:O | 5:C:181:ASN:HB3 | 1.78 | 0.80 |
| 1:A:1003(A):G:H2' | 1:A:1004:A:H4' | 1.64 | 0.80 |
| 4:B:84:GLU:OE1 | 4:B:216:SER:HA | 1.81 | 0.80 |
| 5:C:191:THR:HG22 | 5:C:193:TYR:H | 1.45 | 0.80 |
| 1:A:192:U:H4' | 22:T:102:GLY:O | 1.82 | 0.80 |
| 8:F:2:ARG:HD2 | 8:F:69:GLU:HB3 | 1.64 | 0.80 |
| 21:S:28:LYS:HG2 | 21:S:29:ARG:N | 1.96 | 0.80 |
| 4:B:134:GLU:HA | 4:B:137:ARG:HH12 | 1.48 | 0.79 |
| 10:H:121:ASP:HB2 | 10:H:125:ARG:NH2 | 1.96 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:656:C:H4' | 17:O:62:GLN:HE22 | 1.47 | 0.79 |
| 1:A:1208:C:H2' | 1:A:1209:C:C6 | 2.17 | 0.79 |
| 10:H:102:ARG:HG2 | 10:H:125:ARG:HH12 | 1.46 | 0.79 |
| 13:K:84:VAL:HG23 | 13:K:110:ASP:HA | 1.64 | 0.79 |
| 7:E:51:VAL:HB | 7:E:52:PRO:HD3 | 1.63 | 0.79 |
| 1:A:349:A:C2' | 1:A:350:G:H5" | 2.12 | 0.79 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.18 | 0.79 |
| 9:G:90:GLU:HG3 | 9:G:155:ARG:NH2 | 1.98 | 0.78 |
| 1:A:132:C:O3' | 22:T:74:LYS:HE3 | 1.83 | 0.78 |
| 14:L:55:VAL:HG12 | 14:L:56:ALA:H | 1.49 | 0.78 |
| 1:A:438:G:H4' | 1:A:439:A:OP1 | 1.83 | 0.78 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.18 | 0.78 |
| 13:K:84:VAL:HG21 | 20:R:88:LYS:HD3 | 1.63 | 0.78 |
| 7:E:105:VAL:HB | 7:E:106:PRO:HD3 | 1.66 | 0.78 |
| 6:D:104:VAL:HG11 | 6:D:146:ILE:HG12 | 1.64 | 0.78 |
| 1:A:1065:U:H4' | 1:A:1066:C:O5' | 1.84 | 0.78 |
| 1:A:1208:C:H2' | 1:A:1209:C:H6 | 1.49 | 0.78 |
| 11:I:43:ALA:HA | 11:I:74:ILE:HD13 | 1.66 | 0.78 |
| 7:E:80:ILE:HD12 | 7:E:91:LEU:HB2 | 1.65 | 0.77 |
| 15:M:8:GLU:O | 15:M:9:ILE:HG23 | 1.83 | 0.77 |
| 20:R:86:VAL:O | 20:R:87:ARG:HB2 | 1.81 | 0.77 |
| 1:A:344:A:H4' | 1:A:345:C:OP2 | 1.84 | 0.77 |
| 4:B:80:ILE:HD11 | 4:B:208:ILE:HG23 | 1.65 | 0.77 |
| 11:I:10:ARG:HD2 | 11:I:75:ASP:CB | 2.13 | 0.77 |
| 7:E:8:GLU:HG2 | 7:E:34:VAL:HG22 | 1.67 | 0.77 |
| 1:A:1285:A:H4' | 1:A:1286:A:O5' | 1.84 | 0.77 |
| 4:B:77:ALA:CB | 4:B:211:ILE:HD13 | 2.11 | 0.77 |
| 5:C:191:THR:HG21 | 5:C:193:TYR:CE1 | 2.20 | 0.77 |
| 1:A:243:A:C4' | 1:A:244:U:H5' | 2.15 | 0.76 |
| 9:G:50:ILE:HG21 | 9:G:61:VAL:HG21 | 1.65 | 0.76 |
| 4:B:134:GLU:HA | 4:B:137:ARG:NH1 | 1.98 | 0.76 |
| 11:I:93:ARG:HB2 | 11:I:97:LYS:HE3 | 1.66 | 0.76 |
| 12:J:31:GLY:HA2 | 12:J:78:ASN:HD22 | 1.49 | 0.76 |
| 1:A:812:C:HO2' | 1:A:813:U:P | 2.08 | 0.76 |
| 12:J:49:VAL:HG13 | 16:N:41:ARG:HD2 | 1.67 | 0.76 |
| 1:A:328:C:O2 | 1:A:328:C:H2' | 1.84 | 0.76 |
| 6:D:23:GLY:HA3 | 6:D:112:VAL:HG12 | 1.68 | 0.76 |
| 12:J:49:VAL:HG11 | 16:N:41:ARG:O | 1.85 | 0.76 |
| 14:L:47:LYS:CB | 14:L:48:PRO:HD3 | 2.15 | 0.76 |
| 12:J:53:PRO:HA | 16:N:41:ARG:HH21 | 1.49 | 0.76 |
| 4:B:87:ARG:O | 4:B:87:ARG:HD2 | 1.86 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:J:30:SER:HB3 | 12:J:84:GLN:NE2 | 2.01 | 0.76 |
| 1:A:556:C:OP2 | 14:L:20:LYS:HE3 | 1.85 | 0.76 |
| 14:L:114:LYS:HA | 14:L:114:LYS:HE3 | 1.67 | 0.76 |
| 1:A:975:A:H5' | 1:A:975:A:C8 | 2.19 | 0.75 |
| 16:N:14:PRO:O | 16:N:15:LYS:HB2 | 1.85 | 0.75 |
| 21:S:16:LEU:O | 21:S:19:VAL:HG12 | 1.85 | 0.75 |
| 1:A:722:A:H4' | 1:A:723:U:OP1 | 1.85 | 0.75 |
| 1:A:1367:C:H5' | 12:J:60:ARG:HH12 | 1.50 | 0.75 |
| 8:F:10:LEU:HD12 | 8:F:59:TYR:HB3 | 1.69 | 0.75 |
| 12:J:45:ARG:HB3 | 12:J:45:ARG:NH1 | 2.01 | 0.75 |
| 4:B:218:ALA:O | 4:B:222:ILE:HG13 | 1.85 | 0.75 |
| 15:M:49:THR:HG22 | 15:M:51:ALA:H | 1.51 | 0.75 |
| 1:A:838:G:C2' | 1:A:839:U:H5" | 2.14 | 0.75 |
| 19:Q:97:SER:H | 19:Q:103:GLY:HA2 | 1.50 | 0.75 |
| 9:G:50:ILE:O | 9:G:54:THR:HB | 1.86 | 0.75 |
| 14:L:89:ARG:HG2 | 14:L:97:ARG:HA | 1.68 | 0.75 |
| 17:O:17:ARG:HG3 | 17:O:17:ARG:HH11 | 1.51 | 0.75 |
| 1:A:530:G:O6 | 3:Z:3:U:H1' | 1.87 | 0.75 |
| 1:A:1250:A:C4' | 11:I:68:GLY:H | 1.98 | 0.74 |
| 15:M:50:GLU:O | 15:M:54:VAL:HG23 | 1.87 | 0.74 |
| 22:T:54:LYS:HE3 | 22:T:100:ILE:CD1 | 2.16 | 0.74 |
| 1:A:1222:G:OP1 | 21:S:77:THR:HG21 | 1.87 | 0.74 |
| 18:P:20:VAL:HG11 | 18:P:32:TYR:CB | 2.16 | 0.74 |
| 8:F:28:ARG:HB2 | 8:F:28:ARG:HH11 | 1.49 | 0.74 |
| 21:S:42:PRO:HA | 21:S:45:VAL:HG23 | 1.68 | 0.74 |
| 1:A:939:G:H5" | 9:G:102:ARG:NH2 | 2.02 | 0.74 |
| 10:H:116:LYS:HD3 | 10:H:127:LEU:HD12 | 1.68 | 0.74 |
| 20:R:25:THR:CG2 | 20:R:42:ARG:HH22 | 2.00 | 0.74 |
| 1:A:1250:A:H2' | 1:A:1251:A:C8 | 2.22 | 0.74 |
| 11:I:106:ALA:O | 11:I:108:VAL:HG23 | 1.88 | 0.74 |
| 1:A:1343:G:H2' | 1:A:1344:C:C6 | 2.23 | 0.74 |
| 5:C:119:ARG:O | 5:C:122:GLU:HB2 | 1.86 | 0.74 |
| 8:F:4:TYR:CZ | 8:F:72:VAL:HG21 | 2.23 | 0.74 |
| 4:B:116:GLU:HG2 | 4:B:153:ARG:NH1 | 2.02 | 0.74 |
| 5:C:174:PRO:HB2 | 5:C:177:THR:HG22 | 1.69 | 0.74 |
| 7:E:76:ILE:HG23 | 7:E:77:PRO:HD2 | 1.68 | 0.74 |
| 1:A:839:U:H5' | 1:A:840:C:C5 | 2.23 | 0.74 |
| 7:E:144:THR:O | 7:E:148:VAL:HG23 | 1.88 | 0.74 |
| 15:M:49:THR:HB | 15:M:52:GLU:HG3 | 1.67 | 0.74 |
| 1:A:31:G:H1 | 1:A:48:C:H5" | 1.51 | 0.73 |
| 7:E:110:LEU:HD13 | 7:E:118:ILE:HG21 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1115:C:H2' | 1:A:1116:C:H6 | 1.52 | 0.73 |
| 1:A:1168:A:H2' | 1:A:1169:A:C8 | 2.23 | 0.73 |
| 1:A:269:C:H2' | 1:A:270:A:C8 | 2.23 | 0.73 |
| 1:A:1281:U:H5' | 1:A:1282:C:H5 | 1.51 | 0.73 |
| 4:B:178:ARG:HH11 | 4:B:178:ARG:HG3 | 1.53 | 0.73 |
| 4:B:15:VAL:HG21 | 4:B:209:ARG:HG3 | 1.68 | 0.73 |
| 1:A:1038:C:H2' | 1:A:1039:C:H6 | 1.53 | 0.73 |
| 1:A:1251:A:H2' | 1:A:1252:A:C8 | 2.24 | 0.73 |
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.22 | 0.73 |
| 5:C:64:VAL:HB | 5:C:99:VAL:CB | 2.19 | 0.73 |
| 1:A:1381:U:O2' | 1:A:1382:C:H5' | 1.88 | 0.73 |
| 14:L:71:PRO:O | 14:L:102:ARG:HD2 | 1.89 | 0.73 |
| 1:A:1005:A:H2' | 1:A:1006:C:H5' | 1.71 | 0.73 |
| 1:A:1368:G:O2' | 1:A:1369:C:H5' | 1.87 | 0.73 |
| 1:A:371:G:C2' | 1:A:372:C:H5' | 2.18 | 0.72 |
| 1:A:706:A:O4' | 13:K:29:ILE:HD11 | 1.89 | 0.72 |
| 22:T:73:HIS:O | 22:T:74:LYS:HB2 | 1.88 | 0.72 |
| 1:A:112:G:H21 | 1:A:354:G:H5' | 1.53 | 0.72 |
| 1:A:662:G:H2' | 1:A:663:A:C8 | 2.24 | 0.72 |
| 1:A:923:A:OP1 | 7:E:21:ALA:HB2 | 1.89 | 0.72 |
| 1:A:1356:G:H2' | 1:A:1357:A:C8 | 2.23 | 0.72 |
| 9:G:37:ASN:ND2 | 11:I:41:VAL:HG23 | 2.04 | 0.72 |
| 9:G:72:ARG:HH12 | 9:G:138:LYS:NZ | 1.88 | 0.72 |
| 17:O:39:LEU:HD13 | 17:O:56:LEU:HB2 | 1.70 | 0.72 |
| 1:A:163:C:O2' | 1:A:164:U:H5' | 1.90 | 0.72 |
| 1:A:539:A:H2' | 1:A:540:G:C8 | 2.25 | 0.72 |
| 1:A:1095:U:H2' | 1:A:1096:C:C6 | 2.25 | 0.72 |
| 13:K:106:LYS:HE2 | 13:K:106:LYS:HA | 1.70 | 0.72 |
| 4:B:16:HIS:HA | 4:B:204:ASN:HB2 | 1.72 | 0.72 |
| 1:A:1128:C:H4' | 11:I:16:ARG:HH22 | 1.53 | 0.72 |
| 8:F:12:PRO:HG3 | 8:F:57:GLN:O | 1.90 | 0.72 |
| 11:I:47:LEU:C | 11:I:49:PRO:HD2 | 2.10 | 0.72 |
| 18:P:74:LEU:O | 18:P:79:VAL:HG23 | 1.89 | 0.72 |
| 1:A:202:U:H5" | 1:A:203:U:OP2 | 1.89 | 0.71 |
| 8:F:14:LEU:HA | 8:F:18:GLN:NE2 | 2.04 | 0.71 |
| 10:H:112:LEU:HD23 | 10:H:112:LEU:H | 1.55 | 0.71 |
| 15:M:40:ASN:HD22 | 15:M:41:PRO:CD | 2.03 | 0.71 |
| 12:J:57:LYS:HD2 | 12:J:57:LYS:O | 1.90 | 0.71 |
| 11:I:31:GLN:HE21 | 11:I:35:GLU:HG3 | 1.55 | 0.71 |
| 16:N:27:CYS:SG | 16:N:29:ARG:HB2 | 2.30 | 0.71 |
| 1:A:1003(A):G:H2' | 1:A:1004:A:C4' | 2.20 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:I:10:ARG:HD2 | 11:I:75:ASP:HB3 | 1.72 | 0.71 |
| 1:A:384:G:H2' | 1:A:385:C:H6 | 1.55 | 0.71 |
| 21:S:4:SER:O | 21:S:5:LEU:HB2 | 1.89 | 0.71 |
| 5:C:6:HIS:HD2 | 5:C:8:ILE:H | 1.37 | 0.71 |
| 12:J:7:LYS:HE3 | 12:J:40:LEU:CD1 | 2.21 | 0.71 |
| 1:A:437:U:H5" | 6:D:155:LEU:HD22 | 1.72 | 0.71 |
| 1:A:1201:A:H4' | 1:A:1202:G:O5' | 1.91 | 0.71 |
| 4:B:95:GLN:O | 4:B:96:ARG:HD2 | 1.89 | 0.71 |
| 5:C:58:GLU:HB3 | 12:J:92:THR:HG21 | 1.73 | 0.71 |
| 1:A:113:G:H1' | 1:A:354:G:H5' | 1.72 | 0.71 |
| 1:A:1256:A:H5' | 1:A:1258:G:C1' | 2.20 | 0.71 |
| 14:L:110:VAL:O | 14:L:122:THR:HG21 | 1.90 | 0.71 |
| 1:A:824:C:H2' | 1:A:825:G:H8 | 1.56 | 0.70 |
| 1:A:1106:G:OP1 | 5:C:172:ARG:HD3 | 1.91 | 0.70 |
| 1:A:1425:U:H3 | 1:A:1475:G:H1 | 1.36 | 0.70 |
| 21:S:55:LYS:HG2 | 21:S:56:GLN:HE21 | 1.56 | 0.70 |
| 1:A:781:A:H2' | 1:A:782:A:H5' | 1.72 | 0.70 |
| 14:L:53:ARG:HG2 | 14:L:69:TYR:HE1 | 1.56 | 0.70 |
| 16:N:45:ARG:HH11 | 16:N:45:ARG:HG3 | 1.56 | 0.70 |
| 1:A:393:A:O2' | 1:A:394:G:H5' | 1.90 | 0.70 |
| 1:A:524:G:H2' | 1:A:525:C:C6 | 2.26 | 0.70 |
| 1:A:853:G:O2' | 1:A:854:G:H5' | 1.91 | 0.70 |
| 1:A:1061:G:O2' | 1:A:1062:U:H5' | 1.92 | 0.70 |
| 1:A:1123:A:H4' | 12:J:37:PRO:HD2 | 1.73 | 0.70 |
| 1:A:1499:A:H1' | 1:A:1520:G:H5' | 1.73 | 0.70 |
| 11:I:81:ILE:O | 11:I:85:LEU:HB2 | 1.92 | 0.70 |
| 15:M:81:LEU:O | 15:M:86:CYS:HB3 | 1.92 | 0.70 |
| 21:S:45:VAL:HA | 21:S:62:ILE:CG2 | 2.20 | 0.70 |
| 1:A:64:G:H4' | 1:A:65:U:O5' | 1.92 | 0.70 |
| 1:A:1427:U:H2' | 1:A:1428:A:C8 | 2.26 | 0.70 |
| 4:B:231:GLU:HB2 | 4:B:232:PRO:CD | 2.22 | 0.70 |
| 1:A:35:G:H2' | 1:A:36:C:C6 | 2.25 | 0.70 |
| 1:A:1314:C:H3' | 21:S:6:LYS:NZ | 2.06 | 0.70 |
| 1:A:835:U:OP1 | 20:R:64:ARG:NH2 | 2.24 | 0.70 |
| 5:C:70:VAL:HG12 | 5:C:71:ALA:H | 1.57 | 0.70 |
| 1:A:1207:G:O2' | 1:A:1208:C:H5' | 1.92 | 0.70 |
| 1:A:1263:C:H2' | 1:A:1264:C:C6 | 2.27 | 0.70 |
| 1:A:1278:U:H4' | 1:A:1279:A:C5' | 2.22 | 0.70 |
| 8:F:8:ILE:HD11 | 8:F:79:LEU:HD13 | 1.73 | 0.70 |
| 9:G:50:ILE:CG2 | 9:G:61:VAL:HG21 | 2.22 | 0.70 |
| 17:O:4:THR:HG1 | 17:O:7:GLU:HB2 | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:639:G:O2' | 1:A:640:A:H5' | 1.92 | 0.70 |
| 1:A:1054:C:O2 | 1:A:1054:C:H3' | 1.91 | 0.70 |
| 8:F:94:GLN:NE2 | 20:R:32:ARG:HD3 | 2.06 | 0.70 |
| 14:L:83:VAL:HG13 | 14:L:100:ILE:HG23 | 1.72 | 0.70 |
| 22:T:43:LEU:HD13 | 22:T:51:GLU:HG3 | 1.73 | 0.70 |
| 1:A:478:A:O2' | 1:A:479:C:H5' | 1.91 | 0.69 |
| 1:A:1152:A:H2' | 1:A:1153:C:C6 | 2.27 | 0.69 |
| 4:B:209:ARG:HH12 | 4:B:236:TYR:HE2 | 1.40 | 0.69 |
| 5:C:14:ILE:O | 5:C:16:ARG:N | 2.24 | 0.69 |
| 1:A:780:A:O2' | 1:A:781:A:H5" | 1.91 | 0.69 |
| 1:A:1191:A:P | 5:C:3:ASN:ND2 | 2.65 | 0.69 |
| 15:M:84:ILE:HG22 | 21:S:65:ASN:HD22 | 1.56 | 0.69 |
| 16:N:57:ARG:HG2 | 16:N:58:LYS:H | 1.57 | 0.69 |
| 1:A:556:C:O2' | 1:A:557:G:H5' | 1.92 | 0.69 |
| 1:A:1319:A:H4' | 21:S:37:ARG:HH12 | 1.53 | 0.69 |
| 5:C:83:ARG:HA | 5:C:86:VAL:HG23 | 1.73 | 0.69 |
| 6:D:8:VAL:CG1 | 6:D:21:LEU:HD12 | 2.23 | 0.69 |
| 10:H:112:LEU:HD23 | 10:H:112:LEU:N | 2.08 | 0.69 |
| 5:C:52:LEU:HD23 | 5:C:52:LEU:H | 1.56 | 0.69 |
| 18:P:22:THR:HA | 18:P:33:ILE:HG13 | 1.73 | 0.69 |
| 1:A:1057:G:H5" | 5:C:154:SER:CB | 2.23 | 0.69 |
| 9:G:38:LEU:O | 9:G:42:ILE:HG13 | 1.91 | 0.69 |
| 13:K:34:ASP:OD2 | 13:K:38:ASN:HB2 | 1.92 | 0.69 |
| 1:A:677:U:H3 | 1:A:713:G:H22 | 1.38 | 0.69 |
| 1:A:1116:C:H2' | 1:A:1117:G:H5" | 1.75 | 0.69 |
| 5:C:94:LEU:HD22 | 5:C:95:THR:HG23 | 1.74 | 0.69 |
| 6:D:57:ARG:HB3 | 6:D:206:PHE:HB2 | 1.75 | 0.69 |
| 12:J:4:ILE:HD11 | 12:J:77:PRO:HB3 | 1.74 | 0.69 |
| 14:L:70:ILE:HD13 | 14:L:77:LEU:HD12 | 1.73 | 0.69 |
| 22:T:89:ARG:HG3 | 22:T:104:LEU:HD13 | 1.73 | 0.69 |
| 4:B:208:ILE:HA | 4:B:211:ILE:HD12 | 1.74 | 0.69 |
| 13:K:93:GLN:HE21 | 13:K:96:ARG:HH21 | 1.38 | 0.69 |
| 21:S:28:LYS:CG | 21:S:29:ARG:H | 2.03 | 0.69 |
| 8:F:10:LEU:CD1 | 8:F:59:TYR:HB3 | 2.22 | 0.69 |
| 1:A:1195:C:H3' | 1:A:1196:U:C5' | 2.22 | 0.69 |
| 1:A:1305:G:H5' | 23:V:4:GLY:HA3 | 1.75 | 0.69 |
| 17:O:26:GLU:OE1 | 17:O:77:ARG:HD2 | 1.92 | 0.69 |
| 1:A:390:C:H2' | 1:A:391:G:H8 | 1.55 | 0.68 |
| 1:A:656:C:H4' | 17:O:62:GLN:NE2 | 2.07 | 0.68 |
| 1:A:1086:U:H3 | 1:A:1099:G:N2 | 1.91 | 0.68 |
| 1:A:1279:A:H5" | 1:A:1280:A:OP1 | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:D:187:ARG:HA | 6:D:187:ARG:HE | 1.59 | 0.68 |
| 12:J:3:LYS:N | 12:J:75:ILE:HA | 2.08 | 0.68 |
| 1:A:443:C:H2' | 1:A:444:C:H6 | 1.58 | 0.68 |
| 13:K:30:VAL:HG21 | 13:K:65:ALA:HA | 1.75 | 0.68 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.27 | 0.68 |
| 5:C:179:ARG:HD3 | 5:C:207:VAL:HA | 1.74 | 0.68 |
| 1:A:627:G:O2' | 1:A:628:G:H5' | 1.93 | 0.68 |
| 4:B:15:VAL:HG11 | 4:B:209:ARG:HB3 | 1.73 | 0.68 |
| 22:T:54:LYS:HG3 | 22:T:100:ILE:HD12 | 1.75 | 0.68 |
| 1:A:1320:C:O2 | 21:S:72:GLY:HA3 | 1.93 | 0.68 |
| 4:B:219:VAL:HA | 4:B:222:ILE:HD12 | 1.74 | 0.68 |
| 5:C:91:LEU:HD23 | 5:C:92:ALA:N | 2.08 | 0.68 |
| 6:D:6:GLY:O | 6:D:8:VAL:HG23 | 1.94 | 0.68 |
| 1:A:191:G:C4 | 22:T:105:SER:HB3 | 2.28 | 0.68 |
| 1:A:539:A:H2' | 1:A:540:G:H8 | 1.59 | 0.68 |
| 14:L:56:ALA:O | 14:L:67:THR:HA | 1.93 | 0.68 |
| 1:A:1191:A:P | 5:C:3:ASN:HD21 | 2.17 | 0.68 |
| 1:A:1404:C:H2' | 1:A:1405:G:C8 | 2.29 | 0.68 |
| 14:L:25:PRO:C | 14:L:27:LEU:H | 1.95 | 0.68 |
| 1:A:877:C:H1' | 10:H:3:THR:CG2 | 2.24 | 0.68 |
| 15:M:23:TYR:O | 15:M:25:ILE:N | 2.26 | 0.68 |
| 20:R:55:ARG:HB3 | 20:R:55:ARG:NH1 | 2.07 | 0.68 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.58 | 0.68 |
| 9:G:126:ASP:OD1 | 9:G:131:LYS:HE3 | 1.94 | 0.68 |
| 14:L:27:LEU:O | 14:L:29:GLY:N | 2.27 | 0.68 |
| 14:L:27:LEU:C | 14:L:29:GLY:H | 1.97 | 0.68 |
| 1:A:357:G:O2' | 1:A:358:U:H5' | 1.95 | 0.67 |
| 11:I:70:LYS:O | 11:I:74:ILE:HG13 | 1.94 | 0.67 |
| 1:A:41:G:H2' | 1:A:42:G:H8 | 1.59 | 0.67 |
| 12:J:46:ARG:NH1 | 12:J:64:GLU:HB3 | 2.09 | 0.67 |
| 15:M:62:ASN:O | 15:M:63:THR:HB | 1.94 | 0.67 |
| 1:A:266:G:H5' | 1:A:266:G:C8 | 2.29 | 0.67 |
| 1:A:580:U:H2' | 1:A:581:G:O4' | 1.95 | 0.67 |
| 1:A:839:U:H5' | 1:A:840:C:H5 | 1.59 | 0.67 |
| 4:B:197:VAL:HB | 4:B:200:ILE:HG12 | 1.75 | 0.67 |
| 19:Q:63:ARG:O | 19:Q:65:ILE:HD12 | 1.94 | 0.67 |
| 1:A:1016:A:H2' | 1:A:1017:G:O4' | 1.94 | 0.67 |
| 7:E:92:LYS:HB3 | 7:E:119:LEU:HB2 | 1.76 | 0.67 |
| 6:D:8:VAL:C | 6:D:10:ARG:H | 1.98 | 0.67 |
| 1:A:384:G:H2' | 1:A:385:C:C6 | 2.30 | 0.67 |
| 1:A:1343:G:H2' | 1:A:1344:C:H6 | 1.59 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1310:G:N7 | 21:S:2:PRO:HD3 | 2.09 | 0.67 |
| 1:A:1497:G:C2' | 1:A:1498:U:H5' | 2.25 | 0.67 |
| 8:F:2:ARG:HH11 | 8:F:69:GLU:HB3 | 1.58 | 0.67 |
| 14:L:75:HIS:HD2 | 14:L:77:LEU:H | 1.42 | 0.67 |
| 1:A:192:U:H4' | 22:T:102:GLY:C | 2.14 | 0.67 |
| 4:B:10:LEU:HD22 | 4:B:48:MET:CE | 2.24 | 0.67 |
| 16:N:26:ARG:HH11 | 16:N:43:CYS:HB3 | 1.58 | 0.67 |
| 1:A:1306:A:N6 | 1:A:1331:G:H1' | 2.09 | 0.67 |
| 4:B:135:GLN:O | 4:B:139:LYS:HG2 | 1.94 | 0.67 |
| 15:M:40:ASN:HD22 | 15:M:41:PRO:HD2 | 1.60 | 0.67 |
| 1:A:1330:U:OP1 | 15:M:23:TYR:O | 2.12 | 0.67 |
| 12:J:4:ILE:HA | 12:J:100:THR:CB | 2.25 | 0.67 |
| 21:S:41:VAL:CG1 | 21:S:42:PRO:HD2 | 2.25 | 0.67 |
| 1:A:939:G:H2' | 1:A:940:C:C6 | 2.30 | 0.66 |
| 10:H:90:GLY:O | 10:H:91:ARG:HB2 | 1.94 | 0.66 |
| 14:L:41:ARG:HG2 | 14:L:42:THR:N | 2.09 | 0.66 |
| 1:A:975:A:C4' | 1:A:976:G:H5" | 2.18 | 0.66 |
| 1:A:41:G:H2' | 1:A:42:G:C8 | 2.30 | 0.66 |
| 1:A:443:C:H2' | 1:A:444:C:C6 | 2.31 | 0.66 |
| 1:A:737:A:H1' | 8:F:73:ASN:ND2 | 2.03 | 0.66 |
| 4:B:19:HIS:CE1 | 4:B:206:ASP:HB3 | 2.30 | 0.66 |
| 5:C:76:VAL:HG11 | 5:C:103:VAL:HG21 | 1.77 | 0.66 |
| 14:L:89:ARG:NH2 | 14:L:97:ARG:HH21 | 1.91 | 0.66 |
| 1:A:1125:U:H3 | 12:J:5:ARG:NH2 | 1.93 | 0.66 |
| 5:C:111:LEU:HD21 | 5:C:144:SER:O | 1.94 | 0.66 |
| 6:D:70:ILE:HD11 | 6:D:100:ARG:CD | 2.26 | 0.66 |
| 21:S:31:ILE:HG22 | 21:S:32:LYS:H | 1.59 | 0.66 |
| 1:A:912:C:O2' | 1:A:913:A:H5' | 1.94 | 0.66 |
| 1:A:1280:A:H5' | 12:J:40:LEU:HD22 | 1.77 | 0.66 |
| 1:A:1154:G:H2' | 1:A:1155:G:H8 | 1.60 | 0.66 |
| 5:C:10:PHE:CE2 | 5:C:178:LEU:HD13 | 2.31 | 0.66 |
| 5:C:64:VAL:HB | 5:C:99:VAL:CG2 | 2.26 | 0.66 |
| 1:A:149:A:H2' | 1:A:150:C:C6 | 2.31 | 0.66 |
| 1:A:421:U:H5' | 1:A:422:C:OP2 | 1.94 | 0.66 |
| 15:M:37:THR:HG23 | 15:M:55:ARG:HD2 | 1.76 | 0.66 |
| 1:A:940:C:H2' | 1:A:941:G:H8 | 1.59 | 0.66 |
| 1:A:1366:C:H2' | 1:A:1367:C:C6 | 2.27 | 0.66 |
| 4:B:87:ARG:HH22 | 4:B:233:SER:HB2 | 1.59 | 0.66 |
| 1:A:1056:U:H5' | 5:C:163:ALA:CB | 2.26 | 0.66 |
| 1:A:1115:C:H2' | 1:A:1116:C:C6 | 2.31 | 0.66 |
| 5:C:15:THR:O | 5:C:16:ARG:HB2 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:I:97:LYS:HG2 | 11:I:102:LEU:HD12 | 1.76 | 0.66 |
| 4:B:12:GLU:C | 4:B:14:GLY:H | 1.98 | 0.66 |
| 12:J:8:LEU:HD23 | 12:J:96:ILE:HG12 | 1.78 | 0.66 |
| 12:J:12:ASP:HB3 | 12:J:15:THR:CG2 | 2.24 | 0.66 |
| 1:A:1189:C:P | 12:J:51:ARG:HH22 | 2.19 | 0.65 |
| 5:C:52:LEU:H | 5:C:52:LEU:CD2 | 2.09 | 0.65 |
| 15:M:54:VAL:O | 15:M:58:GLU:HG2 | 1.96 | 0.65 |
| 1:A:337:C:H2' | 1:A:338:A:H8 | 1.61 | 0.65 |
| 6:D:7:PRO:HB2 | 6:D:10:ARG:HD2 | 1.78 | 0.65 |
| 7:E:71:LEU:HD11 | 7:E:114:GLY:HA3 | 1.76 | 0.65 |
| 11:I:8:GLY:HA2 | 11:I:79:LEU:CD1 | 2.25 | 0.65 |
| 12:J:61:GLU:OE1 | 16:N:45:ARG:NH1 | 2.29 | 0.65 |
| 20:R:26:LEU:HD11 | 20:R:29:PHE:CD2 | 2.31 | 0.65 |
| 1:A:112:G:H4' | 1:A:389:A:H5" | 1.77 | 0.65 |
| 1:A:1225:A:H5' | 1:A:1226:C:OP2 | 1.96 | 0.65 |
| 4:B:213:LEU:O | 4:B:217:ARG:HG2 | 1.97 | 0.65 |
| 6:D:61:LYS:HD2 | 6:D:207:TYR:OH | 1.97 | 0.65 |
| 6:D:151:LYS:H | 6:D:151:LYS:CD | 2.08 | 0.65 |
| 19:Q:66:SER:OG | 19:Q:69:LYS:HB3 | 1.95 | 0.65 |
| 20:R:87:ARG:HG2 | 20:R:87:ARG:HH11 | 1.62 | 0.65 |
| 8:F:33:TYR:HA | 8:F:71:ARG:NH2 | 2.10 | 0.65 |
| 1:A:1527:C:O2' | 1:A:1528:U:H5' | 1.95 | 0.65 |
| 11:I:40:LEU:O | 11:I:42:ARG:N | 2.29 | 0.65 |
| 22:T:51:GLU:HA | 22:T:54:LYS:HB2 | 1.78 | 0.65 |
| 1:A:1014:A:C2 | 1:A:1219:U:H1' | 2.31 | 0.65 |
| 13:K:110:ASP:HB2 | 20:R:88:LYS:HD2 | 1.78 | 0.65 |
| 18:P:18:ARG:O | 18:P:20:VAL:HG23 | 1.95 | 0.65 |
| 19:Q:80:GLY:O | 19:Q:81:ARG:HB3 | 1.97 | 0.65 |
| 1:A:1141:C:O2' | 1:A:1142:G:H5' | 1.97 | 0.65 |
| 1:A:1262:C:O2' | 1:A:1263:C:H5' | 1.97 | 0.65 |
| 13:K:48:ILE:HD13 | 13:K:63:LEU:HB3 | 1.78 | 0.65 |
| 1:A:413:G:H2' | 1:A:428:G:N2 | 2.11 | 0.65 |
| 4:B:7:VAL:HG11 | 4:B:221:LEU:HD23 | 1.79 | 0.65 |
| 6:D:111:ALA:HA | 6:D:161:ASN:ND2 | 2.11 | 0.65 |
| 7:E:75:THR:HG23 | 7:E:76:ILE:N | 2.11 | 0.65 |
| 12:J:30:SER:HB3 | 12:J:84:GLN:HE22 | 1.61 | 0.65 |
| 18:P:3:LYS:O | 18:P:21:VAL:HA | 1.97 | 0.65 |
| 18:P:19:ILE:HG22 | 18:P:36:ILE:HG13 | 1.78 | 0.65 |
| 18:P:20:VAL:CG1 | 18:P:32:TYR:HB2 | 2.26 | 0.65 |
| 22:T:96:GLY:O | 22:T:97:ALA:HB3 | 1.96 | 0.65 |
| 1:A:1133:G:H2' | 1:A:1134:G:H8 | 1.59 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1314:C:C6 | 21:S:6:LYS:HE2 | 2.32 | 0.65 |
| 1:A:1003:G:H22 | 1:A:1039:C:H1' | 1.61 | 0.65 |
| 1:A:1372:U:OP1 | 11:I:71:SER:HB3 | 1.97 | 0.65 |
| 4:B:239:VAL:O | 4:B:239:VAL:HG12 | 1.97 | 0.65 |
| 7:E:76:ILE:HG22 | 7:E:78:HIS:H | 1.62 | 0.65 |
| 1:A:1241:G:H2' | 1:A:1242:C:C6 | 2.32 | 0.64 |
| 9:G:37:ASN:HD21 | 11:I:41:VAL:HG23 | 1.60 | 0.64 |
| 11:I:10:ARG:HD2 | 11:I:75:ASP:HB2 | 1.77 | 0.64 |
| 15:M:4:ILE:HG22 | 15:M:5:ALA:H | 1.62 | 0.64 |
| 1:A:991:U:O4 | 1:A:1212:U:H1' | 1.97 | 0.64 |
| 4:B:86:GLU:C | 4:B:88:ALA:H | 2.00 | 0.64 |
| 9:G:65:ALA:O | 9:G:69:VAL:HG23 | 1.97 | 0.64 |
| 19:Q:27:PHE:HB2 | 19:Q:28:PRO:HD2 | 1.79 | 0.64 |
| 22:T:11:SER:HA | 22:T:13:LEU:CD1 | 2.27 | 0.64 |
| 1:A:353:A:H5' | 1:A:353:A:H8 | 1.63 | 0.64 |
| 1:A:1116:C:C2' | 1:A:1117:G:H5" | 2.27 | 0.64 |
| 1:A:812:C:O2' | 1:A:813:U:P | 2.55 | 0.64 |
| 1:A:1305:G:H22 | 1:A:1331:G:H2' | 1.61 | 0.64 |
| 5:C:129:ALA:HB3 | 5:C:132:ARG:HH12 | 1.62 | 0.64 |
| 12:J:44:VAL:HG22 | 12:J:66:ARG:HB3 | 1.78 | 0.64 |
| 13:K:110:ASP:OD2 | 20:R:88:LYS:NZ | 2.30 | 0.64 |
| 16:N:26:ARG:NH1 | 16:N:47:LEU:HG | 2.13 | 0.64 |
| 5:C:155:GLY:O | 5:C:156:ARG:HB2 | 1.96 | 0.64 |
| 1:A:1292:U:P | 9:G:41:ARG:HH22 | 2.21 | 0.64 |
| 5:C:34:LEU:HD23 | 5:C:34:LEU:C | 2.18 | 0.64 |
| 10:H:85:ARG:NE | 10:H:87:SER:O | 2.30 | 0.64 |
| 19:Q:68:ARG:HG2 | 19:Q:68:ARG:HH11 | 1.61 | 0.64 |
| 21:S:77:THR:HG22 | 21:S:78:ARG:HG3 | 1.79 | 0.64 |
| 1:A:985:C:H2' | 1:A:986:A:C8 | 2.33 | 0.64 |
| 12:J:50:ILE:HA | 12:J:60:ARG:HA | 1.79 | 0.64 |
| 21:S:22:LEU:HD22 | 21:S:28:LYS:HD2 | 1.79 | 0.64 |
| 5:C:129:ALA:HB3 | 5:C:132:ARG:NH1 | 2.13 | 0.64 |
| 21:S:14:HIS:O | 21:S:18:LYS:HE3 | 1.98 | 0.64 |
| 1:A:403:C:O2' | 1:A:404:U:H5' | 1.98 | 0.64 |
| 5:C:177:THR:HG23 | 5:C:180:ALA:HB2 | 1.80 | 0.64 |
| 9:G:146:GLU:O | 9:G:149:ARG:HG2 | 1.98 | 0.64 |
| 10:H:51:VAL:HG12 | 10:H:52:ASP:N | 2.13 | 0.64 |
| 1:A:107:G:C2' | 1:A:108:G:H5' | 2.28 | 0.64 |
| 1:A:950:U:H5 | 15:M:102:ARG:HE | 1.45 | 0.64 |
| 1:A:954:G:H2' | 1:A:955:U:C6 | 2.33 | 0.64 |
| 1:A:1039:C:H2' | 1:A:1040:U:C6 | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1281:U:H5' | 1:A:1282:C:C5 | 2.31 | 0.63 |
| 5:C:186:PHE:CG | 5:C:187:ALA:N | 2.65 | 0.63 |
| 12:J:78:ASN:O | 12:J:80:LYS:N | 2.31 | 0.63 |
| 1:A:750:G:N3 | 17:O:23:GLY:HA3 | 2.13 | 0.63 |
| 4:B:15:VAL:CG2 | 4:B:209:ARG:HG3 | 2.28 | 0.63 |
| 4:B:16:HIS:NE2 | 4:B:214:ILE:HD11 | 2.13 | 0.63 |
| 5:C:204:LEU:HD12 | 5:C:204:LEU:O | 1.97 | 0.63 |
| 8:F:15:ASP:H | 8:F:18:GLN:NE2 | 1.96 | 0.63 |
| 9:G:69:VAL:HG21 | 9:G:104:LEU:HD21 | 1.81 | 0.63 |
| 11:I:42:ARG:NH2 | 11:I:71:SER:OG | 2.31 | 0.63 |
| 19:Q:97:SER:O | 19:Q:99:SER:N | 2.25 | 0.63 |
| 1:A:807:A:H2' | 1:A:808:C:C6 | 2.33 | 0.63 |
| 15:M:31:LYS:O | 15:M:35:GLU:HB2 | 1.98 | 0.63 |
| 17:O:78:TYR:CZ | 17:O:82:ILE:HD11 | 2.32 | 0.63 |
| 1:A:411:A:C4 | 1:A:413:G:H1' | 2.33 | 0.63 |
| 4:B:211:ILE:O | 4:B:215:LEU:HB2 | 1.98 | 0.63 |
| 5:C:54:ARG:HG2 | 5:C:55:VAL:N | 2.14 | 0.63 |
| 5:C:150:LYS:HE2 | 5:C:152:ILE:HD11 | 1.79 | 0.63 |
| 4:B:9:GLU:HB3 | 4:B:12:GLU:OE2 | 1.99 | 0.63 |
| 6:D:146:ILE:N | 6:D:146:ILE:HD12 | 2.13 | 0.63 |
| 8:F:35:ALA:O | 8:F:36:ARG:HB2 | 1.99 | 0.63 |
| 20:R:38:GLU:HA | 20:R:41:LYS:HE2 | 1.81 | 0.63 |
| 1:A:328:C:O2 | 1:A:328:C:C2' | 2.47 | 0.63 |
| 1:A:1142:G:H2' | 1:A:1143:G:O4' | 1.99 | 0.63 |
| 8:F:100:ASN:ND2 | 20:R:23:LYS:HG2 | 2.11 | 0.63 |
| 11:I:4:TYR:CD2 | 11:I:88:TYR:HA | 2.33 | 0.63 |
| 22:T:83:ARG:O | 22:T:87:LYS:HG3 | 1.99 | 0.63 |
| 1:A:701:C:H5" | 1:A:703:G:O4' | 1.98 | 0.63 |
| 1:A:877:C:H1' | 10:H:3:THR:HG21 | 1.81 | 0.63 |
| 5:C:83:ARG:C | 5:C:85:ARG:H | 2.02 | 0.63 |
| 10:H:120:THR:OG1 | 10:H:123:GLU:HG3 | 1.99 | 0.63 |
| 1:A:1127:G:H21 | 1:A:1146:A:N6 | 1.92 | 0.63 |
| 1:A:1305:G:C5' | 23:V:4:GLY:HA3 | 2.27 | 0.63 |
| 4:B:181:PHE:CD2 | 10:H:70:GLN:HB3 | 2.33 | 0.63 |
| 9:G:15:ASP:HB3 | 9:G:20:ASP:H | 1.64 | 0.63 |
| 10:H:111:ILE:O | 10:H:134:ILE:HB | 1.99 | 0.63 |
| 13:K:57:THR:CG2 | 13:K:60:ALA:H | 2.11 | 0.63 |
| 15:M:102:ARG:HB2 | 15:M:102:ARG:NH1 | 2.14 | 0.63 |
| 1:A:180:U:H2' | 1:A:181:G:H5' | 1.80 | 0.63 |
| 2:Y:34:G:H2' | 2:Y:35:A:H8 | 1.63 | 0.63 |
| 5:C:83:ARG:HE | 5:C:87:LEU:HD11 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:D:57:ARG:HD3 | 6:D:57:ARG:N | 2.14 | 0.63 |
| 13:K:15:ALA:O | 13:K:77:MET:HG3 | 1.98 | 0.63 |
| 1:A:112:G:O2' | 1:A:113:G:H5' | 1.98 | 0.62 |
| 1:A:1031:G:H2' | 1:A:1032:G:H8 | 1.64 | 0.62 |
| 1:A:428:G:H4' | 1:A:429:U:O5' | 1.98 | 0.62 |
| 1:A:1182:G:O2' | 1:A:1183:A:OP2 | 2.12 | 0.62 |
| 8:F:100:ASN:HD22 | 20:R:23:LYS:CG | 2.12 | 0.62 |
| 14:L:27:LEU:HG | 14:L:28:LYS:H | 1.63 | 0.62 |
| 21:S:49:ILE:N | 21:S:49:ILE:HD12 | 2.14 | 0.62 |
| 4:B:59:GLU:HG3 | 4:B:60:ASP:N | 2.13 | 0.62 |
| 4:B:178:ARG:HG3 | 4:B:178:ARG:NH1 | 2.13 | 0.62 |
| 5:C:25:GLY:O | 5:C:27:LYS:N | 2.33 | 0.62 |
| 5:C:83:ARG:O | 5:C:85:ARG:N | 2.24 | 0.62 |
| 5:C:100:ALA:O | 5:C:101:LEU:HB2 | 1.98 | 0.62 |
| 8:F:33:TYR:CB | 8:F:75:LEU:HD23 | 2.25 | 0.62 |
| 17:O:87:ILE:O | 17:O:88:ARG:HB2 | 1.99 | 0.62 |
| 20:R:34:TYR:HA | 20:R:69:THR:HG23 | 1.82 | 0.62 |
| 11:I:85:LEU:O | 11:I:92:TYR:HD1 | 1.81 | 0.62 |
| 13:K:121:PRO:HG2 | 13:K:126:ARG:HG2 | 1.80 | 0.62 |
| 15:M:78:ILE:O | 15:M:81:LEU:HD23 | 1.99 | 0.62 |
| 22:T:79:ARG:HD2 | 22:T:83:ARG:HH12 | 1.63 | 0.62 |
| 1:A:689:C:P | 13:K:46:GLY:HA3 | 2.39 | 0.62 |
| 4:B:27:LYS:HD3 | 4:B:195:ASP:OD2 | 2.00 | 0.62 |
| 4:B:139:LYS:O | 4:B:143:GLU:HG2 | 2.00 | 0.62 |
| 14:L:24:VAL:O | 14:L:26:ALA:N | 2.26 | 0.62 |
| 23:V:12:LYS:HB3 | 23:V:22:ARG:HD2 | 1.81 | 0.62 |
| 1:A:556:C:C2' | 1:A:557:G:H5' | 2.29 | 0.62 |
| 1:A:1195:C:H2' | 1:A:1197:G:H5' | 1.81 | 0.62 |
| 1:A:1347:G:N2 | 1:A:1373:G:H2' | 2.13 | 0.62 |
| 4:B:13:ALA:HB1 | 4:B:17:PHE:HE2 | 1.65 | 0.62 |
| 4:B:102:LEU:HD21 | 4:B:162:ILE:CD1 | 2.28 | 0.62 |
| 19:Q:59:ILE:HG22 | 19:Q:71:PHE:CD1 | 2.35 | 0.62 |
| 20:R:25:THR:HG22 | 20:R:42:ARG:HH22 | 1.62 | 0.62 |
| 1:A:148:G:H2' | 1:A:149:A:C8 | 2.35 | 0.62 |
| 1:A:1048:G:H5" | 16:N:3:ARG:HG3 | 1.82 | 0.62 |
| 1:A:1052:U:H2' | 1:A:1055:A:OP1 | 2.00 | 0.62 |
| 4:B:166:ASP:OD2 | 4:B:169:LYS:HB2 | 1.99 | 0.62 |
| 5:C:191:THR:HG21 | 5:C:193:TYR:CZ | 2.35 | 0.62 |
| 6:D:62:GLN:HE22 | 6:D:65:ARG:NH1 | 1.97 | 0.62 |
| 9:G:145:ALA:O | 9:G:147:ALA:N | 2.30 | 0.62 |
| 21:S:50:ALA:HA | 21:S:58:VAL:O | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:T:57:ARG:HE | 22:T:102:GLY:HA3 | 1.59 | 0.62 |
| 1:A:1031:G:H2' | 1:A:1032:G:C8 | 2.35 | 0.62 |
| 4:B:80:ILE:HD12 | 4:B:208:ILE:HG12 | 1.82 | 0.62 |
| 10:H:80:ILE:O | 10:H:80:ILE:HG22 | 1.99 | 0.62 |
| 1:A:1315:U:OP2 | 21:S:6:LYS:NZ | 2.33 | 0.62 |
| 14:L:24:VAL:O | 14:L:24:VAL:HG12 | 2.00 | 0.62 |
| 14:L:34:ARG:O | 14:L:61:THR:HG23 | 2.00 | 0.62 |
| 1:A:112:G:N2 | 1:A:354:G:H5' | 2.14 | 0.61 |
| 2:Y:34:G:H2' | 2:Y:35:A:C8 | 2.35 | 0.61 |
| 7:E:5:ASP:CG | 7:E:6:PHE:H | 2.04 | 0.61 |
| 12:J:39:PRO:O | 12:J:40:LEU:HB2 | 2.00 | 0.61 |
| 15:M:78:ILE:HA | 15:M:81:LEU:HD21 | 1.82 | 0.61 |
| 21:S:51:VAL:O | 21:S:58:VAL:HG22 | 2.00 | 0.61 |
| 1:A:794:A:H2' | 1:A:795:C:C6 | 2.34 | 0.61 |
| 1:A:1369:C:H2' | 1:A:1370:G:C8 | 2.34 | 0.61 |
| 5:C:112:SER:HB3 | 5:C:115:LEU:HD12 | 1.81 | 0.61 |
| 5:C:126:ARG:O | 5:C:127:ARG:HB2 | 1.99 | 0.61 |
| 6:D:64:LEU:HD12 | 6:D:75:PHE:CZ | 2.35 | 0.61 |
| 12:J:16:LEU:HD22 | 12:J:94:VAL:HG22 | 1.82 | 0.61 |
| 1:A:353:A:H5' | 1:A:353:A:C8 | 2.35 | 0.61 |
| 4:B:59:GLU:HG3 | 4:B:60:ASP:H | 1.65 | 0.61 |
| 14:L:75:HIS:CD2 | 14:L:77:LEU:H | 2.18 | 0.61 |
| 18:P:74:LEU:HB3 | 18:P:79:VAL:HG21 | 1.82 | 0.61 |
| 4:B:76:GLN:NE2 | 4:B:207:ALA:N | 2.49 | 0.61 |
| 5:C:177:THR:HG23 | 5:C:177:THR:O | 2.00 | 0.61 |
| 18:P:51:VAL:O | 18:P:52:ASP:HB2 | 2.01 | 0.61 |
| 1:A:269:C:H2' | 1:A:270:A:H8 | 1.62 | 0.61 |
| 1:A:792:A:H4' | 1:A:793:U:H5" | 1.82 | 0.61 |
| 1:A:1292:U:H5' | 11:I:38:GLN:NE2 | 2.16 | 0.61 |
| 4:B:101:MET:CE | 4:B:108:ILE:HG21 | 2.30 | 0.61 |
| 18:P:20:VAL:HG11 | 18:P:32:TYR:HB2 | 1.81 | 0.61 |
| 20:R:46:GLU:H | 20:R:46:GLU:CD | 2.04 | 0.61 |
| 1:A:148:G:H2' | 1:A:149:A:H8 | 1.64 | 0.61 |
| 1:A:523:A:H61 | 14:L:92:ASP:HB2 | 1.65 | 0.61 |
| 1:A:1193:G:O2' | 1:A:1194:U:H5' | 1.99 | 0.61 |
| 4:B:76:GLN:HE21 | 4:B:207:ALA:H | 1.47 | 0.61 |
| 5:C:91:LEU:HD21 | 5:C:99:VAL:CG1 | 2.28 | 0.61 |
| 12:J:49:VAL:O | 12:J:60:ARG:HA | 2.00 | 0.61 |
| 18:P:4:ILE:HG23 | 18:P:36:ILE:HD11 | 1.82 | 0.61 |
| 1:A:1259:C:H42 | 1:A:1276:G:H1 | 1.48 | 0.61 |
| 1:A:1286:A:H2' | 1:A:1287:A:H4' | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:201:ILE:HG21 | 4:B:214:ILE:HG21 | 1.81 | 0.61 |
| 5:C:34:LEU:HD23 | 5:C:34:LEU:O | 2.01 | 0.61 |
| 10:H:103:VAL:HG21 | 10:H:109:ILE:O | 2.01 | 0.61 |
| 20:R:26:LEU:HD23 | 20:R:42:ARG:HD3 | 1.83 | 0.61 |
| 22:T:67:ALA:HB2 | 22:T:77:ALA:HB2 | 1.83 | 0.61 |
| 1:A:64:G:O2' | 1:A:65:U:OP2 | 2.19 | 0.61 |
| 15:M:49:THR:HG22 | 15:M:51:ALA:N | 2.15 | 0.61 |
| 21:S:36:ARG:NH2 | 21:S:75:ALA:O | 2.34 | 0.61 |
| 1:A:77:G:O2' | 1:A:78:G:H5' | 2.01 | 0.61 |
| 1:A:190(L):U:O2 | 22:T:105:SER:HB2 | 2.00 | 0.61 |
| 1:A:840:C:H5" | 1:A:841:U:OP1 | 2.01 | 0.61 |
| 1:A:989:C:O2' | 1:A:990:C:H5' | 2.00 | 0.61 |
| 1:A:1427:U:H2' | 1:A:1428:A:H8 | 1.65 | 0.61 |
| 6:D:13:ARG:HD2 | 6:D:38:TYR:O | 2.01 | 0.61 |
| 7:E:26:PHE:CD1 | 7:E:26:PHE:N | 2.69 | 0.61 |
| 11:I:32:ASP:HB3 | 11:I:35:GLU:HB2 | 1.83 | 0.61 |
| 12:J:45:ARG:HH11 | 12:J:45:ARG:CB | 2.06 | 0.61 |
| 15:M:36:LYS:HB2 | 15:M:59:TYR:HE2 | 1.66 | 0.61 |
| 1:A:496:A:H4' | 1:A:497:A:OP1 | 1.99 | 0.61 |
| 1:A:979:C:H2' | 1:A:980:C:H5' | 1.83 | 0.61 |
| 1:A:1116:C:H2' | 1:A:1117:G:C5' | 2.30 | 0.61 |
| 1:A:1117:G:H5' | 1:A:1117:G:H8 | 1.66 | 0.61 |
| 1:A:1347:G:O2' | 1:A:1348:U:P | 2.59 | 0.61 |
| 1:A:1477:C:H2' | 1:A:1478:C:C6 | 2.36 | 0.61 |
| 4:B:156:LYS:HA | 4:B:156:LYS:NZ | 2.15 | 0.61 |
| 7:E:11:ILE:HB | 7:E:31:LEU:HB3 | 1.83 | 0.61 |
| 7:E:12:LEU:CD1 | 7:E:31:LEU:HB2 | 2.31 | 0.61 |
| 14:L:126:LYS:H | 14:L:126:LYS:HE3 | 1.65 | 0.61 |
| 16:N:36:PHE:O | 16:N:36:PHE:CD1 | 2.54 | 0.61 |
| 4:B:76:GLN:HG3 | 4:B:206:ASP:OD1 | 2.01 | 0.60 |
| 7:E:43:LEU:HB2 | 7:E:136:MET:HE2 | 1.82 | 0.60 |
| 9:G:23:VAL:O | 9:G:27:ILE:HG13 | 2.00 | 0.60 |
| 16:N:9:LYS:HG3 | 16:N:21:TYR:O | 2.01 | 0.60 |
| 19:Q:70:ARG:HG3 | 19:Q:70:ARG:HH11 | 1.66 | 0.60 |
| 1:A:216:G:H2' | 1:A:217:C:C6 | 2.36 | 0.60 |
| 1:A:918:A:H2' | 1:A:919:A:C8 | 2.35 | 0.60 |
| 1:A:1223:C:P | 21:S:78:ARG:NH1 | 2.74 | 0.60 |
| 1:A:1250:A:H4' | 11:I:68:GLY:CA | 2.31 | 0.60 |
| 8:F:101:ALA:HA | 20:R:28:GLU:HB3 | 1.83 | 0.60 |
| 9:G:138:LYS:HE2 | 9:G:142:GLU:OE1 | 2.02 | 0.60 |
| 1:A:107:G:H2' | 1:A:108:G:H5' | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:242:C:H2' | 1:A:243:A:H5' | 1.84 | 0.60 |
| 6:D:102:ASP:OD1 | 6:D:103:ASN:N | 2.34 | 0.60 |
| 14:L:89:ARG:HG2 | 14:L:97:ARG:CA | 2.31 | 0.60 |
| 20:R:37:VAL:O | 20:R:41:LYS:HG2 | 2.01 | 0.60 |
| 1:A:1370:G:O2' | 1:A:1371:G:H5' | 2.01 | 0.60 |
| 5:C:64:VAL:O | 5:C:99:VAL:HG23 | 2.01 | 0.60 |
| 12:J:24:VAL:O | 12:J:28:ARG:HG3 | 2.02 | 0.60 |
| 21:S:3:ARG:HH22 | 21:S:69:HIS:CE1 | 2.19 | 0.60 |
| 1:A:247:G:OP2 | 19:Q:100:LYS:HG3 | 2.01 | 0.60 |
| 1:A:314:C:O2' | 1:A:315:A:H5' | 2.00 | 0.60 |
| 1:A:977:A:H2' | 1:A:978:A:H5" | 1.84 | 0.60 |
| 1:A:1278:U:H4' | 1:A:1279:A:O5' | 2.02 | 0.60 |
| 4:B:19:HIS:CD2 | 4:B:20:GLU:HG2 | 2.37 | 0.60 |
| 4:B:143:GLU:O | 4:B:147:LYS:HG3 | 2.02 | 0.60 |
| 9:G:135:VAL:O | 9:G:139:GLU:HG3 | 2.02 | 0.60 |
| 11:I:97:LYS:CG | 11:I:102:LEU:HD12 | 2.31 | 0.60 |
| 12:J:4:ILE:HA | 12:J:100:THR:HA | 1.84 | 0.60 |
| 18:P:34:GLU:OE2 | 18:P:55:ARG:HD3 | 2.02 | 0.60 |
| 18:P:51:VAL:HG12 | 18:P:52:ASP:N | 2.17 | 0.60 |
| 22:T:54:LYS:HA | 22:T:57:ARG:CD | 2.31 | 0.60 |
| 1:A:420:U:H2' | 1:A:422:C:C5 | 2.37 | 0.60 |
| 1:A:706:A:C1' | 13:K:29:ILE:HD11 | 2.31 | 0.60 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.37 | 0.60 |
| 4:B:135:GLN:HG2 | 4:B:139:LYS:NZ | 2.16 | 0.60 |
| 7:E:12:LEU:HD13 | 7:E:31:LEU:HB2 | 1.83 | 0.60 |
| 8:F:97:PHE:HB2 | 20:R:32:ARG:HH21 | 1.66 | 0.60 |
| 14:L:41:ARG:HG2 | 14:L:42:THR:O | 2.02 | 0.60 |
| 15:M:84:ILE:CG2 | 21:S:65:ASN:HD22 | 2.14 | 0.60 |
| 19:Q:66:SER:O | 19:Q:70:ARG:NH1 | 2.34 | 0.60 |
| 20:R:53:ARG:HH11 | 20:R:59:SER:HA | 1.66 | 0.60 |
| 20:R:86:VAL:O | 20:R:87:ARG:CB | 2.50 | 0.60 |
| 1:A:743:U:H2' | 1:A:744:C:C6 | 2.35 | 0.60 |
| 4:B:71:VAL:O | 4:B:165:VAL:HG23 | 2.02 | 0.60 |
| 5:C:94:LEU:HD22 | 5:C:95:THR:CG2 | 2.31 | 0.60 |
| 6:D:4:TYR:O | 6:D:5:ILE:HB | 2.00 | 0.60 |
| 11:I:48:GLU:N | 11:I:49:PRO:HD2 | 2.16 | 0.60 |
| 1:A:76:C:O2' | 1:A:77:G:H5' | 2.01 | 0.60 |
| 19:Q:97:SER:HB2 | 19:Q:102:GLY:O | 2.00 | 0.60 |
| 21:S:16:LEU:C | 21:S:18:LYS:H | 2.05 | 0.60 |
| 1:A:542:G:H2' | 1:A:543:C:H6 | 1.67 | 0.60 |
| 1:A:1004:A:H5" | 1:A:1025:U:O4 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1064:G:H4' | 1:A:1065:U:C5' | 2.32 | 0.60 |
| 5:C:84:ILE:O | 5:C:88:ARG:HD2 | 2.02 | 0.60 |
| 9:G:71:PRO:HD3 | 9:G:103:TRP:HZ3 | 1.67 | 0.60 |
| 12:J:49:VAL:HG13 | 16:N:41:ARG:HB2 | 1.84 | 0.60 |
| 15:M:78:ILE:HA | 15:M:81:LEU:CD2 | 2.31 | 0.60 |
| 21:S:41:VAL:HG12 | 21:S:42:PRO:CD | 2.32 | 0.60 |
| 4:B:28:PHE:CZ | 4:B:189:ASP:HA | 2.37 | 0.60 |
| 5:C:145:GLY:O | 5:C:146:ALA:HB3 | 2.02 | 0.60 |
| 12:J:8:LEU:HB2 | 12:J:70:ARG:HB2 | 1.83 | 0.60 |
| 15:M:22:ILE:CD1 | 15:M:25:ILE:HD12 | 2.32 | 0.60 |
| 17:O:75:PRO:O | 17:O:79:ARG:HG3 | 2.02 | 0.60 |
| 1:A:542:G:OP1 | 6:D:10:ARG:NH2 | 2.35 | 0.59 |
| 1:A:748:C:HO2' | 1:A:749:C:H6 | 1.43 | 0.59 |
| 1:A:1060:C:O2' | 1:A:1061:G:H5' | 2.01 | 0.59 |
| 1:A:1108:G:H5' | 1:A:1191:A:H4' | 1.82 | 0.59 |
| 4:B:187:LEU:HD23 | 4:B:201:ILE:O | 2.02 | 0.59 |
| 1:A:19:C:H2' | 1:A:20:U:H6 | 1.68 | 0.59 |
| 1:A:484:G:H4' | 1:A:485:G:O5' | 2.02 | 0.59 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.37 | 0.59 |
| 7:E:57:LYS:HG2 | 7:E:61:TYR:CE2 | 2.37 | 0.59 |
| 9:G:48:LYS:O | 9:G:51:GLN:HB2 | 2.02 | 0.59 |
| 12:J:89:ASP:C | 12:J:90:LEU:HD12 | 2.23 | 0.59 |
| 13:K:74:ALA:C | 13:K:76:GLY:H | 2.06 | 0.59 |
| 15:M:5:ALA:O | 15:M:7:VAL:N | 2.35 | 0.59 |
| 1:A:219:C:H2' | 1:A:220:G:O4' | 2.02 | 0.59 |
| 1:A:285:G:O2' | 1:A:286:G:H5' | 2.01 | 0.59 |
| 1:A:1250:A:H5" | 11:I:68:GLY:N | 2.17 | 0.59 |
| 6:D:150:GLU:HG3 | 6:D:153:ARG:CZ | 2.33 | 0.59 |
| 8:F:80:ARG:NH1 | 8:F:88:VAL:HB | 2.17 | 0.59 |
| 9:G:149:ARG:HB3 | 9:G:149:ARG:HH11 | 1.66 | 0.59 |
| 10:H:95:VAL:HB | 10:H:99:GLU:HB2 | 1.83 | 0.59 |
| 12:J:38:ILE:HB | 12:J:71:LEU:CB | 2.24 | 0.59 |
| 1:A:1104:G:OP1 | 4:B:111:ARG:HD2 | 2.03 | 0.59 |
| 4:B:181:PHE:HD2 | 10:H:70:GLN:HB3 | 1.66 | 0.59 |
| 13:K:98:LEU:HA | 13:K:101:SER:HB3 | 1.84 | 0.59 |
| 18:P:20:VAL:HG11 | 18:P:32:TYR:CG | 2.38 | 0.59 |
| 5:C:40:ARG:O | 5:C:44:GLU:HB2 | 2.02 | 0.59 |
| 6:D:8:VAL:HG11 | 6:D:21:LEU:HB2 | 1.84 | 0.59 |
| 10:H:86:ILE:O | 10:H:88:LYS:HG3 | 2.02 | 0.59 |
| 20:R:26:LEU:HD12 | 20:R:27:GLY:O | 2.02 | 0.59 |
| 1:A:254:G:OP1 | 19:Q:67:LYS:O | 2.20 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1241:G:H2' | 1:A:1242:C:H6 | 1.68 | 0.59 |
| 5:C:191:THR:HG22 | 5:C:193:TYR:N | 2.15 | 0.59 |
| 6:D:23:GLY:HA3 | 6:D:112:VAL:CG1 | 2.32 | 0.59 |
| 6:D:111:ALA:HA | 6:D:161:ASN:HD22 | 1.68 | 0.59 |
| 9:G:51:GLN:HE21 | 9:G:58:PRO:HD3 | 1.68 | 0.59 |
| 17:O:10:LYS:HA | 17:O:10:LYS:NZ | 2.18 | 0.59 |
| 1:A:1053:G:C3' | 1:A:1054:C:H5' | 2.33 | 0.59 |
| 8:F:2:ARG:HD2 | 8:F:69:GLU:CB | 2.33 | 0.59 |
| 18:P:67:THR:HG22 | 18:P:68:ASP:N | 2.18 | 0.59 |
| 4:B:73:THR:HG23 | 4:B:95:GLN:O | 2.02 | 0.59 |
| 4:B:156:LYS:HA | 4:B:156:LYS:HZ3 | 1.68 | 0.59 |
| 6:D:64:LEU:HD12 | 6:D:75:PHE:HZ | 1.68 | 0.59 |
| 7:E:9:LYS:HB2 | 7:E:112:LEU:HD11 | 1.84 | 0.59 |
| 20:R:26:LEU:HD11 | 20:R:29:PHE:CE2 | 2.37 | 0.59 |
| 1:A:407:G:O2' | 6:D:116:GLN:HG3 | 2.02 | 0.59 |
| 1:A:1118:C:H1' | 1:A:1179:A:C4 | 2.37 | 0.59 |
| 5:C:19:GLU:O | 5:C:40:ARG:NH2 | 2.35 | 0.59 |
| 7:E:74:GLY:HA3 | 7:E:116:THR:HG22 | 1.85 | 0.59 |
| 18:P:21:VAL:HG21 | 18:P:59:TRP:CD1 | 2.37 | 0.59 |
| 4:B:9:GLU:HB3 | 4:B:12:GLU:CD | 2.22 | 0.59 |
| 4:B:76:GLN:OE1 | 4:B:208:ILE:HG13 | 2.02 | 0.59 |
| 7:E:87:SER:HB3 | 7:E:131:ILE:HD13 | 1.84 | 0.59 |
| 7:E:89:ILE:HD13 | 7:E:90:VAL:H | 1.67 | 0.59 |
| 12:J:20:ALA:O | 12:J:24:VAL:HG23 | 2.03 | 0.59 |
| 1:A:376:G:OP2 | 18:P:67:THR:HG21 | 2.02 | 0.58 |
| 5:C:91:LEU:CD2 | 5:C:99:VAL:HG13 | 2.32 | 0.58 |
| 5:C:107:GLN:O | 5:C:108:ASN:HB3 | 2.01 | 0.58 |
| 19:Q:68:ARG:HH11 | 19:Q:68:ARG:CG | 2.16 | 0.58 |
| 1:A:620:C:N1 | 6:D:135:LEU:HD13 | 2.18 | 0.58 |
| 1:A:1454:G:H2' | 1:A:1455:G:H8 | 1.68 | 0.58 |
| 4:B:50:GLU:HB3 | 4:B:200:ILE:O | 2.02 | 0.58 |
| 5:C:33:LEU:HD11 | 16:N:53:LEU:HD23 | 1.83 | 0.58 |
| 5:C:55:VAL:O | 5:C:55:VAL:HG12 | 2.02 | 0.58 |
| 7:E:80:ILE:HD12 | 7:E:80:ILE:H | 1.67 | 0.58 |
| 1:A:424:G:O2' | 1:A:425:G:H5' | 2.03 | 0.58 |
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.38 | 0.58 |
| 1:A:1497:G:H2' | 1:A:1498:U:H5' | 1.85 | 0.58 |
| 4:B:77:ALA:CB | 4:B:211:ILE:HG21 | 2.32 | 0.58 |
| 4:B:87:ARG:HH12 | 4:B:233:SER:HA | 1.68 | 0.58 |
| 8:F:98:LEU:H | 8:F:98:LEU:HD12 | 1.67 | 0.58 |
| 1:A:168:G:O2' | 1:A:169:C:H5' | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:370:C:O2' | 1:A:371:G:H5' | 2.04 | 0.58 |
| 1:A:620:C:C1' | 6:D:135:LEU:HD13 | 2.34 | 0.58 |
| 6:D:145:GLU:OE2 | 6:D:182:LYS:HD2 | 2.04 | 0.58 |
| 11:I:111:ARG:HD3 | 11:I:112:LYS:N | 2.18 | 0.58 |
| 1:A:255:G:H1' | 19:Q:16:GLN:NE2 | 2.19 | 0.58 |
| 4:B:10:LEU:HD22 | 4:B:48:MET:HE1 | 1.84 | 0.58 |
| 4:B:112:VAL:C | 4:B:114:ARG:H | 2.06 | 0.58 |
| 4:B:140:HIS:HA | 4:B:143:GLU:CG | 2.33 | 0.58 |
| 5:C:154:SER:O | 5:C:165:THR:HA | 2.03 | 0.58 |
| 6:D:150:GLU:HA | 6:D:153:ARG:HG3 | 1.85 | 0.58 |
| 8:F:95:GLU:CD | 8:F:95:GLU:H | 2.06 | 0.58 |
| 1:A:1423:G:O2' | 1:A:1424:C:H5' | 2.03 | 0.58 |
| 1:A:1425:U:H2' | 1:A:1426:C:H6 | 1.69 | 0.58 |
| 4:B:19:HIS:NE2 | 4:B:206:ASP:HB3 | 2.19 | 0.58 |
| 9:G:115:ARG:HH11 | 9:G:115:ARG:HB2 | 1.69 | 0.58 |
| 9:G:146:GLU:C | 9:G:148:ASN:H | 2.07 | 0.58 |
| 1:A:883:C:O2' | 1:A:884:U:H5' | 2.04 | 0.58 |
| 1:A:1061:G:C2' | 1:A:1062:U:H5' | 2.34 | 0.58 |
| 4:B:60:ASP:O | 4:B:64:ARG:NH1 | 2.37 | 0.58 |
| 4:B:111:ARG:HB3 | 4:B:149:LEU:HD11 | 1.85 | 0.58 |
| 5:C:34:LEU:HD21 | 5:C:38:ARG:CZ | 2.34 | 0.58 |
| 5:C:54:ARG:HG2 | 5:C:55:VAL:H | 1.67 | 0.58 |
| 5:C:84:ILE:O | 5:C:84:ILE:HG12 | 2.04 | 0.58 |
| 5:C:113:ALA:HB3 | 5:C:114:PRO:HD3 | 1.86 | 0.58 |
| 10:H:64:LYS:HG2 | 10:H:79:VAL:HG21 | 1.86 | 0.58 |
| 14:L:27:LEU:C | 14:L:29:GLY:N | 2.57 | 0.58 |
| 15:M:37:THR:HG22 | 15:M:37:THR:O | 2.03 | 0.58 |
| 17:O:29:VAL:HG11 | 17:O:67:LEU:HD21 | 1.85 | 0.58 |
| 22:T:36:LEU:HD12 | 22:T:62:LEU:HD12 | 1.84 | 0.58 |
| 22:T:67:ALA:HA | 22:T:73:HIS:H | 1.68 | 0.58 |
| 22:T:94:ALA:O | 22:T:95:ALA:HB3 | 2.02 | 0.58 |
| 1:A:337:C:H2' | 1:A:338:A:C8 | 2.38 | 0.58 |
| 1:A:940:C:H2' | 1:A:941:G:C8 | 2.37 | 0.58 |
| 4:B:91:PRO:HG3 | 4:B:154:LEU:HB2 | 1.86 | 0.58 |
| 5:C:179:ARG:HH11 | 5:C:179:ARG:HG3 | 1.68 | 0.58 |
| 11:I:117:HIS:C | 11:I:118:LYS:HG3 | 2.24 | 0.58 |
| 12:J:3:LYS:N | 12:J:75:ILE:HG12 | 2.18 | 0.58 |
| 13:K:21:ILE:HD13 | 13:K:94:ALA:HB3 | 1.86 | 0.58 |
| 13:K:126:ARG:O | 13:K:127:LYS:HB2 | 2.03 | 0.58 |
| 1:A:1149:C:H2' | 1:A:1150:U:C6 | 2.38 | 0.58 |
| 4:B:82:ARG:O | 4:B:86:GLU:HG3 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:D:24:GLU:HG2 | 6:D:25:ARG:N | 2.19 | 0.58 |
| 12:J:84:GLN:O | 12:J:88:LEU:HD12 | 2.04 | 0.58 |
| 19:Q:96:GLN:HB3 | 19:Q:103:GLY:HA2 | 1.85 | 0.58 |
| 1:A:444:C:H2' | 1:A:445:G:H8 | 1.69 | 0.58 |
| 1:A:740:U:O2' | 1:A:741:G:H5' | 2.03 | 0.58 |
| 1:A:1320:C:N3 | 21:S:36:ARG:HG3 | 2.19 | 0.58 |
| 1:A:1454:G:O2' | 1:A:1455:G:H5' | 2.04 | 0.58 |
| 7:E:144:THR:H | 7:E:147:ASP:HB2 | 1.68 | 0.58 |
| 8:F:50:TYR:CE1 | 20:R:77:GLY:HA2 | 2.39 | 0.58 |
| 10:H:86:ILE:HD12 | 10:H:133:LEU:HD22 | 1.86 | 0.58 |
| 22:T:10:LEU:O | 22:T:12:ALA:N | 2.36 | 0.58 |
| 1:A:824:C:H2' | 1:A:825:G:C8 | 2.36 | 0.57 |
| 1:A:1216:G:H5" | 16:N:5:ALA:HB2 | 1.86 | 0.57 |
| 1:A:1352:C:H2' | 1:A:1353:G:H8 | 1.68 | 0.57 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.38 | 0.57 |
| 5:C:139:GLN:CA | 5:C:139:GLN:HE21 | 2.17 | 0.57 |
| 5:C:191:THR:CG2 | 5:C:192:THR:N | 2.67 | 0.57 |
| 9:G:52:GLU:C | 9:G:53:LYS:HD2 | 2.24 | 0.57 |
| 9:G:113:GLU:HG2 | 9:G:119:ARG:HG2 | 1.85 | 0.57 |
| 16:N:37:PHE:CE2 | 16:N:53:LEU:HD13 | 2.39 | 0.57 |
| 1:A:243:A:H4' | 1:A:244:U:C5' | 2.24 | 0.57 |
| 1:A:895:G:H2' | 1:A:896:C:C6 | 2.39 | 0.57 |
| 1:A:1238:A:H5' | 1:A:1336:C:N4 | 2.15 | 0.57 |
| 4:B:100:GLY:C | 4:B:108:ILE:HD12 | 2.25 | 0.57 |
| 5:C:159:GLY:HA2 | 5:C:193:TYR:CZ | 2.39 | 0.57 |
| 8:F:4:TYR:CE2 | 8:F:72:VAL:HG21 | 2.39 | 0.57 |
| 8:F:86:ARG:HG2 | 8:F:86:ARG:HH11 | 1.69 | 0.57 |
| 11:I:111:ARG:HD3 | 11:I:112:LYS:C | 2.23 | 0.57 |
| 19:Q:101:ARG:CZ | 19:Q:101:ARG:HA | 2.34 | 0.57 |
| 1:A:390:C:O3' | 18:P:28:ARG:NH2 | 2.37 | 0.57 |
| 1:A:765:G:H1 | 1:A:812:C:H2' | 1.68 | 0.57 |
| 1:A:949:A:N7 | 15:M:106:ASN:ND2 | 2.52 | 0.57 |
| 1:A:1152:A:H5" | 12:J:13:HIS:CG | 2.39 | 0.57 |
| 1:A:1342:C:O2' | 1:A:1343:G:H5' | 2.03 | 0.57 |
| 10:H:119:LEU:HD12 | 10:H:124:ALA:HA | 1.85 | 0.57 |
| 20:R:33:ASP:OD2 | 20:R:36:ASN:HB2 | 2.04 | 0.57 |
| 1:A:976:G:H5' | 1:A:1358:U:O2' | 2.05 | 0.57 |
| 1:A:1054:C:N3 | 2:Y:34:G:O4' | 2.37 | 0.57 |
| 4:B:101:MET:HE3 | 4:B:108:ILE:HD13 | 1.86 | 0.57 |
| 5:C:188:LEU:O | 5:C:189:ALA:HB2 | 2.05 | 0.57 |
| 18:P:67:THR:HG22 | 18:P:69:THR:H | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:407:G:H2' | 1:A:408:A:H8 | 1.70 | 0.57 |
| 1:A:1256:A:H5' | 1:A:1258:G:H1' | 1.86 | 0.57 |
| 1:A:1424:C:O2' | 1:A:1425:U:H5' | 2.04 | 0.57 |
| 16:N:29:ARG:HG2 | 16:N:29:ARG:HH11 | 1.69 | 0.57 |
| 1:A:1030(C):G:H2' | 1:A:1030(D):A:C8 | 2.39 | 0.57 |
| 1:A:1258:G:O2' | 1:A:1259:C:H5' | 2.04 | 0.57 |
| 7:E:79:GLU:HG3 | 7:E:93:PRO:CD | 2.28 | 0.57 |
| 7:E:80:ILE:HD11 | 7:E:91:LEU:HB2 | 1.81 | 0.57 |
| 14:L:42:THR:HA | 14:L:53:ARG:O | 2.04 | 0.57 |
| 16:N:25:VAL:HG12 | 16:N:38:GLY:O | 2.03 | 0.57 |
| 19:Q:27:PHE:CE1 | 19:Q:36:ILE:HD11 | 2.38 | 0.57 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.40 | 0.57 |
| 1:A:560:U:H5' | 1:A:566:G:N2 | 2.20 | 0.57 |
| 1:A:954:G:H2' | 1:A:955:U:H6 | 1.69 | 0.57 |
| 1:A:1157:A:H4' | 1:A:1158:C:O5' | 2.04 | 0.57 |
| 1:A:1338:G:H2' | 1:A:1339:A:C8 | 2.40 | 0.57 |
| 4:B:30:ARG:HG3 | 4:B:31:TYR:CD2 | 2.40 | 0.57 |
| 10:H:68:ARG:HG2 | 10:H:68:ARG:HH11 | 1.69 | 0.57 |
| 14:L:60:LEU:HD21 | 14:L:85:ILE:HD12 | 1.85 | 0.57 |
| 18:P:58:TYR:O | 18:P:62:VAL:HG23 | 2.04 | 0.57 |
| 19:Q:45:HIS:CD2 | 19:Q:47:PRO:HG3 | 2.39 | 0.57 |
| 21:S:19:VAL:HG13 | 21:S:20:LEU:N | 2.20 | 0.57 |
| 1:A:1053:G:C4' | 1:A:1054:C:H5' | 2.34 | 0.57 |
| 1:A:1053:G:HO2' | 1:A:1199:U:H5 | 1.53 | 0.57 |
| 1:A:1128:C:H42 | 1:A:1143:G:H1 | 1.53 | 0.57 |
| 1:A:1227:A:O3' | 15:M:115:LYS:HE3 | 2.05 | 0.57 |
| 5:C:136:GLN:O | 5:C:139:GLN:HB2 | 2.05 | 0.57 |
| 6:D:191:ARG:O | 6:D:191:ARG:HD2 | 2.05 | 0.57 |
| 8:F:19:LEU:C | 8:F:19:LEU:HD23 | 2.24 | 0.57 |
| 12:J:6:ILE:HG22 | 12:J:98:ILE:HG23 | 1.87 | 0.57 |
| 21:S:20:LEU:HA | 21:S:23:ASN:ND2 | 2.19 | 0.57 |
| 1:A:939:G:H5" | 9:G:102:ARG:HH22 | 1.70 | 0.57 |
| 1:A:950:U:OP2 | 15:M:102:ARG:HG2 | 2.05 | 0.57 |
| 1:A:1060:C:C5 | 5:C:2:GLY:HA3 | 2.40 | 0.57 |
| 1:A:1117:G:H21 | 1:A:1180:A:H1' | 1.69 | 0.57 |
| 19:Q:59:ILE:HG23 | 19:Q:71:PHE:HB3 | 1.87 | 0.57 |
| 1:A:1056:U:H5' | 5:C:163:ALA:HB2 | 1.85 | 0.57 |
| 9:G:15:ASP:OD1 | 9:G:17:VAL:N | 2.38 | 0.57 |
| 9:G:114:ARG:HG2 | 9:G:114:ARG:HH11 | 1.70 | 0.57 |
| 21:S:7:LYS:HG2 | 21:S:7:LYS:O | 2.04 | 0.57 |
| 1:A:364:A:H62 | 14:L:28:LYS:NZ | 2.02 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:865:A:H5' | 1:A:1078:U:O4 | 2.05 | 0.56 |
| 5:C:70:VAL:HG12 | 5:C:71:ALA:N | 2.18 | 0.56 |
| 7:E:30:ALA:O | 7:E:45:PHE:HA | 2.05 | 0.56 |
| 9:G:38:LEU:O | 9:G:38:LEU:HD12 | 2.05 | 0.56 |
| 9:G:85:TYR:HD1 | 9:G:154:TYR:HE1 | 1.53 | 0.56 |
| 1:A:1477:C:H2' | 1:A:1478:C:H6 | 1.70 | 0.56 |
| 8:F:48:LEU:HD13 | 8:F:52:ILE:HG13 | 1.87 | 0.56 |
| 11:I:10:ARG:O | 11:I:12:GLU:N | 2.38 | 0.56 |
| 20:R:88:LYS:OXT | 20:R:88:LYS:HG2 | 2.05 | 0.56 |
| 1:A:748:C:O2' | 1:A:749:C:C6 | 2.56 | 0.56 |
| 1:A:882:C:O2' | 1:A:883:C:H5' | 2.04 | 0.56 |
| 1:A:1015:A:H2' | 1:A:1016:A:C8 | 2.40 | 0.56 |
| 1:A:1468:A:H2' | 1:A:1469:G:O4' | 2.06 | 0.56 |
| 2:Y:30:C:O2' | 2:Y:31:C:H5' | 2.04 | 0.56 |
| 4:B:230:VAL:HG12 | 4:B:231:GLU:N | 2.20 | 0.56 |
| 12:J:51:ARG:HG3 | 12:J:59:SER:HB2 | 1.87 | 0.56 |
| 14:L:8:ASN:O | 14:L:12:ARG:HG3 | 2.05 | 0.56 |
| 14:L:47:LYS:CG | 14:L:48:PRO:HD3 | 2.35 | 0.56 |
| 14:L:89:ARG:HH22 | 14:L:97:ARG:HH21 | 1.52 | 0.56 |
| 1:A:127:G:HO2' | 19:Q:2:PRO:N | 2.03 | 0.56 |
| 1:A:176:C:H2' | 1:A:177:C:H6 | 1.71 | 0.56 |
| 1:A:748:C:O2' | 1:A:749:C:H6 | 1.87 | 0.56 |
| 1:A:1121:U:H2' | 1:A:1122:U:H6 | 1.71 | 0.56 |
| 8:F:97:PHE:HB2 | 20:R:32:ARG:NH2 | 2.20 | 0.56 |
| 21:S:20:LEU:HD12 | 21:S:21:GLU:N | 2.20 | 0.56 |
| 1:A:112:G:H21 | 1:A:354:G:C5' | 2.17 | 0.56 |
| 1:A:1163:C:H2' | 1:A:1164:G:H8 | 1.70 | 0.56 |
| 1:A:1176:A:H2' | 1:A:1177:G:C8 | 2.41 | 0.56 |
| 4:B:64:ARG:HG2 | 4:B:64:ARG:O | 2.05 | 0.56 |
| 6:D:58:LEU:O | 6:D:62:GLN:HG2 | 2.05 | 0.56 |
| 6:D:111:ALA:HB2 | 6:D:120:LEU:HD12 | 1.86 | 0.56 |
| 6:D:131:ARG:H | 6:D:131:ARG:HD2 | 1.71 | 0.56 |
| 11:I:127:LYS:HZ3 | 11:I:127:LYS:H | 1.51 | 0.56 |
| 12:J:38:ILE:O | 12:J:70:ARG:HA | 2.06 | 0.56 |
| 1:A:1054:C:H2' | 1:A:1055:A:H5" | 1.88 | 0.56 |
| 1:A:1125:U:H3 | 12:J:5:ARG:HE | 1.54 | 0.56 |
| 1:A:1305:G:H5" | 23:V:4:GLY:C | 2.26 | 0.56 |
| 4:B:140:HIS:HA | 4:B:143:GLU:HG2 | 1.88 | 0.56 |
| 6:D:63:LYS:HD2 | 6:D:198:VAL:HG22 | 1.87 | 0.56 |
| 1:A:748:C:OP2 | 1:A:748:C:H6 | 1.89 | 0.56 |
| 1:A:1007:C:H2' | 1:A:1008:C:H6 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1222:G:P | 21:S:77:THR:HG21 | 2.46 | 0.56 |
| 5:C:131:ARG:O | 5:C:135:LYS:HG3 | 2.06 | 0.56 |
| 7:E:24:ARG:HG2 | 7:E:24:ARG:HH11 | 1.70 | 0.56 |
| 7:E:82:VAL:HG11 | 7:E:137:GLU:HB3 | 1.87 | 0.56 |
| 15:M:10:PRO:CB | 15:M:18:ALA:HB1 | 2.20 | 0.56 |
| 21:S:42:PRO:HA | 21:S:45:VAL:CG2 | 2.36 | 0.56 |
| 22:T:59:ALA:O | 22:T:63:ILE:HG13 | 2.05 | 0.56 |
| 1:A:1005:A:C2' | 1:A:1006:C:H5' | 2.34 | 0.56 |
| 1:A:1187:G:OP1 | 11:I:113:LYS:HE2 | 2.05 | 0.56 |
| 1:A:1227:A:OP2 | 15:M:111:LYS:HE3 | 2.05 | 0.56 |
| 1:A:1311:G:N7 | 21:S:2:PRO:HA | 2.21 | 0.56 |
| 1:A:1312:G:O2' | 1:A:1313:U:H5' | 2.05 | 0.56 |
| 5:C:85:ARG:HA | 5:C:88:ARG:HB2 | 1.88 | 0.56 |
| 6:D:121:VAL:O | 6:D:134:ASP:HA | 2.06 | 0.56 |
| 11:I:44:VAL:HG12 | 11:I:51:ARG:NH2 | 2.21 | 0.56 |
| 1:A:1234:C:O2' | 1:A:1235:U:H5' | 2.06 | 0.56 |
| 1:A:1256:A:O3' | 1:A:1257:U:H4' | 2.06 | 0.56 |
| 1:A:1305:G:C8 | 1:A:1305:G:OP2 | 2.59 | 0.56 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.41 | 0.56 |
| 4:B:162:ILE:CG2 | 4:B:164:VAL:HG23 | 2.36 | 0.56 |
| 11:I:17:VAL:HG11 | 11:I:81:ILE:HA | 1.88 | 0.56 |
| 19:Q:24:GLU:CD | 19:Q:37:LYS:HD3 | 2.26 | 0.56 |
| 1:A:112:G:H5' | 1:A:389:A:H4' | 1.88 | 0.56 |
| 8:F:22:GLU:O | 8:F:26:ILE:HG13 | 2.05 | 0.56 |
| 1:A:88:A:H2' | 1:A:89:C:O4' | 2.06 | 0.55 |
| 1:A:195:A:H4' | 22:T:68:LYS:HE2 | 1.88 | 0.55 |
| 1:A:328:C:H4' | 1:A:329:A:H5' | 1.88 | 0.55 |
| 1:A:861:G:O2' | 1:A:862:C:H5' | 2.06 | 0.55 |
| 1:A:1128:C:H1' | 1:A:1146:A:H61 | 1.70 | 0.55 |
| 5:C:26:LYS:HD3 | 5:C:26:LYS:N | 2.17 | 0.55 |
| 6:D:32:ALA:C | 6:D:34:GLU:N | 2.58 | 0.55 |
| 13:K:116:HIS:O | 13:K:117:ASN:HB2 | 2.04 | 0.55 |
| 1:A:135:C:O2 | 18:P:1:MET:HB2 | 2.07 | 0.55 |
| 1:A:1441:G:H4' | 1:A:1442:G:C5 | 2.40 | 0.55 |
| 4:B:25:ASN:HD22 | 4:B:25:ASN:C | 2.10 | 0.55 |
| 4:B:97:TRP:HH2 | 4:B:176:GLU:CD | 2.09 | 0.55 |
| 5:C:76:VAL:HG11 | 5:C:103:VAL:CG2 | 2.36 | 0.55 |
| 13:K:93:GLN:HE21 | 13:K:96:ARG:NH2 | 2.05 | 0.55 |
| 16:N:57:ARG:HG2 | 16:N:58:LYS:N | 2.20 | 0.55 |
| 1:A:178:C:O2' | 1:A:179:A:H5' | 2.06 | 0.55 |
| 1:A:450:G:N7 | 1:A:481:G:C6 | 2.74 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:629:G:O2' | 1:A:630:G:H5' | 2.06 | 0.55 |
| 1:A:1090:U:O2' | 1:A:1091:U:H5' | 2.06 | 0.55 |
| 10:H:51:VAL:HG12 | 10:H:52:ASP:H | 1.71 | 0.55 |
| 12:J:75:ILE:O | 12:J:76:ASN:HB2 | 2.05 | 0.55 |
| 18:P:51:VAL:O | 18:P:52:ASP:CB | 2.55 | 0.55 |
| 1:A:1064:G:H4' | 1:A:1065:U:H5' | 1.87 | 0.55 |
| 1:A:1139:G:H4' | 1:A:1140:C:H5' | 1.87 | 0.55 |
| 1:A:1412:C:H2' | 1:A:1413:A:C8 | 2.41 | 0.55 |
| 1:A:1461:G:O2' | 1:A:1462:G:H5' | 2.06 | 0.55 |
| 16:N:25:VAL:O | 16:N:25:VAL:HG22 | 2.06 | 0.55 |
| 18:P:81:ARG:NH1 | 18:P:81:ARG:HB2 | 2.20 | 0.55 |
| 20:R:47:THR:HG23 | 20:R:83:GLU:H | 1.70 | 0.55 |
| 1:A:1392:G:O2' | 1:A:1393:U:H5' | 2.07 | 0.55 |
| 4:B:18:GLY:HA2 | 4:B:41:ILE:HA | 1.88 | 0.55 |
| 4:B:55:PHE:HA | 4:B:58:ILE:HD12 | 1.88 | 0.55 |
| 4:B:83:MET:HE2 | 4:B:234:PRO:HG2 | 1.87 | 0.55 |
| 5:C:52:LEU:HD23 | 5:C:52:LEU:N | 2.21 | 0.55 |
| 5:C:134:ILE:HG22 | 5:C:168:ALA:HB3 | 1.88 | 0.55 |
| 7:E:28:PHE:O | 7:E:47:LYS:HA | 2.06 | 0.55 |
| 10:H:86:ILE:HG22 | 10:H:87:SER:N | 2.21 | 0.55 |
| 11:I:9:ARG:HG2 | 11:I:13:ALA:O | 2.06 | 0.55 |
| 11:I:93:ARG:HD3 | 11:I:97:LYS:NZ | 2.16 | 0.55 |
| 21:S:44:MET:HA | 21:S:47:HIS:HD2 | 1.71 | 0.55 |
| 1:A:406:G:H2' | 1:A:407:G:H8 | 1.72 | 0.55 |
| 4:B:69:LEU:HD12 | 4:B:155:LEU:HD11 | 1.87 | 0.55 |
| 5:C:23:TYR:OH | 12:J:9:ARG:HD3 | 2.06 | 0.55 |
| 19:Q:65:ILE:HD12 | 19:Q:65:ILE:N | 2.21 | 0.55 |
| 1:A:832:C:O2' | 1:A:833:U:H5' | 2.06 | 0.55 |
| 1:A:993:G:H4' | 1:A:994:A:OP2 | 2.06 | 0.55 |
| 1:A:1091:U:O2 | 1:A:1093:A:C8 | 2.60 | 0.55 |
| 1:A:1216:G:O2' | 1:A:1217:C:H5' | 2.07 | 0.55 |
| 4:B:47:THR:HA | 4:B:202:PRO:HG2 | 1.88 | 0.55 |
| 5:C:139:GLN:HA | 5:C:139:GLN:NE2 | 2.22 | 0.55 |
| 11:I:108:VAL:HG12 | 11:I:109:VAL:N | 2.22 | 0.55 |
| 21:S:64:GLU:O | 21:S:67:VAL:HG23 | 2.06 | 0.55 |
| 1:A:414:A:OP2 | 1:A:428:G:N2 | 2.33 | 0.55 |
| 1:A:1145:C:O2' | 1:A:1146:A:H8 | 1.90 | 0.55 |
| 1:A:1315:U:H2' | 1:A:1316:G:O4' | 2.07 | 0.55 |
| 4:B:136:VAL:HA | 4:B:139:LYS:CG | 2.36 | 0.55 |
| 6:D:30:LYS:C | 6:D:32:ALA:H | 2.09 | 0.55 |
| 8:F:14:LEU:HA | 8:F:18:GLN:HE21 | 1.69 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:Q:45:HIS:NE2 | 19:Q:47:PRO:HG3 | 2.22 | 0.55 |
| 1:A:192:U:C1' | 22:T:103:GLY:HA2 | 2.37 | 0.55 |
| 1:A:701:C:O2' | 1:A:702:A:OP2 | 2.21 | 0.55 |
| 8:F:87:ARG:HG3 | 8:F:87:ARG:NH1 | 2.10 | 0.55 |
| 18:P:10:GLY:HA3 | 18:P:14:ASN:O | 2.06 | 0.55 |
| 1:A:248:C:O2' | 1:A:249:U:H5' | 2.06 | 0.55 |
| 1:A:640:A:O2' | 1:A:641:U:H5' | 2.07 | 0.55 |
| 1:A:858:G:O2' | 1:A:859:A:H5' | 2.07 | 0.55 |
| 1:A:961:U:C2' | 1:A:962:C:H5' | 2.37 | 0.55 |
| 4:B:12:GLU:C | 4:B:14:GLY:N | 2.60 | 0.55 |
| 4:B:80:ILE:CD1 | 4:B:208:ILE:HG23 | 2.35 | 0.55 |
| 4:B:142:LEU:O | 4:B:144:ARG:N | 2.40 | 0.55 |
| 5:C:70:VAL:O | 5:C:106:VAL:HG23 | 2.06 | 0.55 |
| 12:J:46:ARG:HH11 | 12:J:64:GLU:HB3 | 1.71 | 0.55 |
| 1:A:1109:C:OP2 | 5:C:176:HIS:CD2 | 2.60 | 0.54 |
| 4:B:59:GLU:HB3 | 4:B:221:LEU:CD1 | 2.35 | 0.54 |
| 4:B:127:ILE:HB | 4:B:128:GLU:OE2 | 2.06 | 0.54 |
| 6:D:122:ARG:HH21 | 6:D:134:ASP:CG | 2.09 | 0.54 |
| 6:D:151:LYS:HD2 | 6:D:151:LYS:N | 2.14 | 0.54 |
| 9:G:90:GLU:H | 9:G:155:ARG:HH12 | 1.54 | 0.54 |
| 11:I:93:ARG:HA | 11:I:96:LEU:HB3 | 1.89 | 0.54 |
| 15:M:36:LYS:HD2 | 15:M:59:TYR:CE2 | 2.42 | 0.54 |
| 1:A:731:G:OP1 | 1:A:766:A:H1' | 2.07 | 0.54 |
| 1:A:838:G:H2' | 1:A:839:U:C5' | 2.30 | 0.54 |
| 1:A:1072:G:H2' | 1:A:1073:U:C6 | 2.42 | 0.54 |
| 1:A:1148:U:H2' | 1:A:1149:C:O4' | 2.08 | 0.54 |
| 4:B:98:LEU:HD23 | 4:B:98:LEU:N | 2.22 | 0.54 |
| 8:F:91:VAL:HG13 | 20:R:72:ARG:NH2 | 2.22 | 0.54 |
| 10:H:119:LEU:HB3 | 10:H:123:GLU:HB2 | 1.89 | 0.54 |
| 15:M:22:ILE:HD12 | 15:M:25:ILE:HD12 | 1.88 | 0.54 |
| 1:A:268:C:O2' | 1:A:269:C:H5' | 2.07 | 0.54 |
| 1:A:860:A:H2' | 1:A:861:G:O4' | 2.07 | 0.54 |
| 4:B:17:PHE:O | 4:B:18:GLY:C | 2.45 | 0.54 |
| 4:B:87:ARG:HH12 | 4:B:233:SER:CA | 2.21 | 0.54 |
| 5:C:19:GLU:HB3 | 5:C:40:ARG:NH2 | 2.22 | 0.54 |
| 5:C:171:GLY:O | 5:C:173:VAL:HG23 | 2.07 | 0.54 |
| 9:G:145:ALA:O | 9:G:146:GLU:HB2 | 2.06 | 0.54 |
| 11:I:19:LEU:HB3 | 11:I:59:PHE:CD2 | 2.42 | 0.54 |
| 11:I:116:LYS:HE2 | 11:I:122:ALA:HB2 | 1.90 | 0.54 |
| 21:S:30:LEU:HD13 | 21:S:31:ILE:N | 2.22 | 0.54 |
| 1:A:1420:C:H2' | 1:A:1421:G:H8 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:87:ARG:HH12 | 4:B:233:SER:CB | 2.21 | 0.54 |
| 9:G:140:ASP:HA | 9:G:143:ARG:HD2 | 1.87 | 0.54 |
| 15:M:37:THR:CG2 | 15:M:55:ARG:HD2 | 2.38 | 0.54 |
| 1:A:149:A:H2' | 1:A:150:C:H6 | 1.70 | 0.54 |
| 1:A:540:G:H2' | 1:A:541:G:O4' | 2.08 | 0.54 |
| 1:A:1128:C:H2' | 1:A:1129:C:H5" | 1.89 | 0.54 |
| 4:B:25:ASN:HD22 | 4:B:27:LYS:H | 1.53 | 0.54 |
| 4:B:52:GLU:O | 4:B:56:ARG:HG3 | 2.08 | 0.54 |
| 5:C:177:THR:CG2 | 5:C:180:ALA:HB2 | 2.38 | 0.54 |
| 14:L:59:ARG:NE | 14:L:65:GLU:HG3 | 2.22 | 0.54 |
| 18:P:81:ARG:HB2 | 18:P:81:ARG:HH11 | 1.73 | 0.54 |
| 19:Q:60:ILE:HD13 | 19:Q:61:GLU:N | 2.22 | 0.54 |
| 1:A:485:G:O2' | 1:A:486:U:P | 2.65 | 0.54 |
| 1:A:583:A:H2' | 1:A:584:G:O4' | 2.08 | 0.54 |
| 1:A:789:U:H5' | 1:A:1540:U:O2 | 2.07 | 0.54 |
| 1:A:1125:U:H5" | 1:A:1126:U:H5 | 1.73 | 0.54 |
| 4:B:10:LEU:HD22 | 4:B:48:MET:HE2 | 1.88 | 0.54 |
| 4:B:80:ILE:O | 4:B:80:ILE:HG22 | 2.06 | 0.54 |
| 5:C:15:THR:HG21 | 5:C:179:ARG:O | 2.07 | 0.54 |
| 5:C:110:ASN:O | 5:C:141:VAL:HG22 | 2.08 | 0.54 |
| 6:D:57:ARG:NH1 | 6:D:205:GLU:OE2 | 2.40 | 0.54 |
| 12:J:46:ARG:HH11 | 12:J:46:ARG:HG2 | 1.71 | 0.54 |
| 15:M:107:ALA:O | 15:M:111:LYS:HG3 | 2.08 | 0.54 |
| 1:A:344:A:H5" | 1:A:345:C:H5 | 1.71 | 0.54 |
| 1:A:1305:G:N2 | 1:A:1331:G:C2' | 2.71 | 0.54 |
| 4:B:23:ARG:HH11 | 4:B:24:TRP:HA | 1.72 | 0.54 |
| 6:D:78:LEU:HD22 | 6:D:96:LEU:HB3 | 1.89 | 0.54 |
| 8:F:94:GLN:HE21 | 20:R:32:ARG:HH11 | 1.54 | 0.54 |
| 13:K:13:GLN:HA | 13:K:75:TYR:O | 2.07 | 0.54 |
| 15:M:6:GLY:O | 15:M:7:VAL:HG22 | 2.08 | 0.54 |
| 16:N:3:ARG:NH2 | 16:N:6:LEU:HD11 | 2.23 | 0.54 |
| 1:A:1054:C:N4 | 2:Y:34:G:C8 | 2.76 | 0.54 |
| 6:D:192:GLU:HA | 6:D:192:GLU:OE1 | 2.08 | 0.54 |
| 15:M:5:ALA:O | 15:M:6:GLY:C | 2.46 | 0.54 |
| 17:O:6:GLU:H | 17:O:6:GLU:CD | 2.09 | 0.54 |
| 18:P:38:TYR:CE2 | 18:P:50:LYS:HE2 | 2.43 | 0.54 |
| 20:R:53:ARG:NH1 | 20:R:59:SER:HA | 2.22 | 0.54 |
| 22:T:101:GLY:C | 22:T:103:GLY:H | 2.11 | 0.54 |
| 1:A:659:U:O2' | 1:A:660:G:H5' | 2.08 | 0.54 |
| 1:A:757:U:H2' | 1:A:758:G:O4' | 2.08 | 0.54 |
| 19:Q:67:LYS:HG2 | 19:Q:68:ARG:N | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:105:G:H2' | 1:A:106:C:C6 | 2.42 | 0.54 |
| 1:A:1038:C:H2' | 1:A:1039:C:C6 | 2.39 | 0.54 |
| 1:A:1057:G:H2' | 1:A:1058:G:O4' | 2.08 | 0.54 |
| 1:A:1307:U:H2' | 1:A:1308:U:C6 | 2.43 | 0.54 |
| 5:C:108:ASN:HD21 | 5:C:110:ASN:HB2 | 1.73 | 0.54 |
| 11:I:23:ASN:HD21 | 11:I:25:LYS:HD2 | 1.73 | 0.54 |
| 15:M:59:TYR:O | 15:M:63:THR:HG22 | 2.08 | 0.54 |
| 22:T:56:MET:HE2 | 22:T:88:VAL:HB | 1.89 | 0.54 |
| 1:A:190(D):U:O2' | 1:A:190(E):U:H5' | 2.09 | 0.53 |
| 1:A:985:C:H2' | 1:A:986:A:H8 | 1.71 | 0.53 |
| 4:B:115:LEU:O | 4:B:119:GLU:HG2 | 2.08 | 0.53 |
| 4:B:137:ARG:HB3 | 4:B:137:ARG:HH11 | 1.73 | 0.53 |
| 4:B:187:LEU:HA | 4:B:201:ILE:HB | 1.89 | 0.53 |
| 7:E:116:THR:HG23 | 7:E:117:ASP:OD2 | 2.07 | 0.53 |
| 8:F:2:ARG:HH11 | 8:F:69:GLU:CB | 2.20 | 0.53 |
| 8:F:63:TYR:HD2 | 8:F:63:TYR:N | 2.06 | 0.53 |
| 18:P:28:ARG:HG3 | 18:P:29:ASP:OD2 | 2.08 | 0.53 |
| 19:Q:4:LYS:HE3 | 19:Q:6:LEU:HD21 | 1.89 | 0.53 |
| 1:A:352:C:H4' | 1:A:354:G:OP1 | 2.08 | 0.53 |
| 5:C:36:ASP:O | 5:C:39:ILE:HB | 2.07 | 0.53 |
| 6:D:135:LEU:HB2 | 6:D:138:TYR:HB2 | 1.91 | 0.53 |
| 1:A:405:U:H3' | 1:A:406:G:H5' | 1.90 | 0.53 |
| 1:A:1305:G:N2 | 1:A:1331:G:O2' | 2.41 | 0.53 |
| 4:B:121:LEU:O | 4:B:127:ILE:HG12 | 2.07 | 0.53 |
| 6:D:2:GLY:O | 6:D:3:ARG:HD3 | 2.07 | 0.53 |
| 13:K:54:ARG:HG3 | 13:K:54:ARG:NH1 | 2.24 | 0.53 |
| 14:L:49:ASN:ND2 | 14:L:92:ASP:OD2 | 2.42 | 0.53 |
| 14:L:85:ILE:HG22 | 14:L:86:ARG:N | 2.24 | 0.53 |
| 15:M:80:ARG:C | 15:M:82:MET:H | 2.10 | 0.53 |
| 16:N:12:ARG:O | 16:N:14:PRO:HD3 | 2.09 | 0.53 |
| 22:T:11:SER:HA | 22:T:13:LEU:HD12 | 1.90 | 0.53 |
| 1:A:1057:G:O2' | 1:A:1058:G:H5' | 2.07 | 0.53 |
| 1:A:1481:U:O2' | 1:A:1482:G:H5' | 2.07 | 0.53 |
| 4:B:136:VAL:HA | 4:B:139:LYS:HG2 | 1.89 | 0.53 |
| 6:D:98:GLU:HG2 | 6:D:189:PRO:HG3 | 1.91 | 0.53 |
| 8:F:22:GLU:OE1 | 8:F:25:ILE:HD12 | 2.08 | 0.53 |
| 14:L:26:ALA:O | 14:L:27:LEU:O | 2.26 | 0.53 |
| 16:N:14:PRO:O | 16:N:15:LYS:CB | 2.55 | 0.53 |
| 21:S:30:LEU:O | 21:S:31:ILE:HD13 | 2.08 | 0.53 |
| 1:A:1108:G:H4' | 1:A:1191:A:O4' | 2.07 | 0.53 |
| 1:A:1281:U:H3' | 1:A:1281:U:H6 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1326:C:C5 | 23:V:6:ARG:NH2 | 2.76 | 0.53 |
| 6:D:165:MET:SD | 6:D:168:ARG:HD3 | 2.48 | 0.53 |
| 18:P:20:VAL:HG13 | 18:P:34:GLU:O | 2.08 | 0.53 |
| 1:A:21:G:H2' | 1:A:22:G:C8 | 2.44 | 0.53 |
| 1:A:456:C:H2' | 1:A:457:C:C6 | 2.44 | 0.53 |
| 1:A:1004:A:H5" | 1:A:1025:U:C4 | 2.44 | 0.53 |
| 1:A:1207:G:H2' | 1:A:1208:C:H6 | 1.73 | 0.53 |
| 1:A:1222:G:O2' | 1:A:1223:C:H5' | 2.07 | 0.53 |
| 4:B:10:LEU:N | 4:B:10:LEU:HD23 | 2.23 | 0.53 |
| 8:F:44:GLY:HA3 | 8:F:59:TYR:CE1 | 2.44 | 0.53 |
| 13:K:57:THR:HG22 | 13:K:60:ALA:CB | 2.39 | 0.53 |
| 20:R:59:SER:O | 20:R:60:GLY:C | 2.47 | 0.53 |
| 1:A:131:C:H2' | 1:A:132:C:H6 | 1.74 | 0.53 |
| 1:A:162:A:H2' | 1:A:163:C:O4' | 2.09 | 0.53 |
| 1:A:1054:C:C2' | 1:A:1055:A:H5" | 2.38 | 0.53 |
| 1:A:1399:C:C2 | 1:A:1502:A:N6 | 2.77 | 0.53 |
| 1:A:1405:G:O4' | 1:A:1519:A:H4' | 2.09 | 0.53 |
| 4:B:17:PHE:HA | 4:B:42:ILE:HB | 1.90 | 0.53 |
| 5:C:23:TYR:CE1 | 5:C:24:ALA:O | 2.62 | 0.53 |
| 5:C:186:PHE:O | 5:C:187:ALA:HB2 | 2.08 | 0.53 |
| 6:D:62:GLN:HE22 | 6:D:65:ARG:HH12 | 1.54 | 0.53 |
| 6:D:141:ARG:HG2 | 6:D:141:ARG:HH11 | 1.73 | 0.53 |
| 18:P:43:LYS:HA | 18:P:48:TRP:HB3 | 1.90 | 0.53 |
| 19:Q:79:SER:O | 19:Q:80:GLY:O | 2.26 | 0.53 |
| 1:A:332:G:O2' | 1:A:333:G:H5' | 2.08 | 0.53 |
| 1:A:404:U:O2' | 1:A:405:U:H5' | 2.09 | 0.53 |
| 1:A:955:U:O2' | 1:A:956:U:H5' | 2.09 | 0.53 |
| 1:A:1060:C:H5" | 12:J:51:ARG:HB3 | 1.90 | 0.53 |
| 8:F:2:ARG:HD2 | 8:F:69:GLU:CG | 2.39 | 0.53 |
| 15:M:85:GLY:O | 15:M:86:CYS:O | 2.27 | 0.53 |
| 1:A:401:C:H1' | 1:A:622:A:H1' | 1.90 | 0.53 |
| 1:A:1347:G:C2' | 1:A:1348:U:OP2 | 2.56 | 0.53 |
| 1:A:1497:G:O2' | 1:A:1498:U:H5' | 2.09 | 0.53 |
| 4:B:142:LEU:HD22 | 4:B:146:GLN:CD | 2.29 | 0.53 |
| 6:D:100:ARG:HH12 | 6:D:137:SER:HB3 | 1.72 | 0.53 |
| 11:I:49:PRO:O | 11:I:52:ALA:HB3 | 2.09 | 0.53 |
| 12:J:6:ILE:HD11 | 12:J:72:VAL:HG11 | 1.90 | 0.53 |
| 1:A:287:U:O2' | 1:A:288:A:H5' | 2.10 | 0.53 |
| 1:A:562:C:H1' | 14:L:15:ARG:HB3 | 1.90 | 0.53 |
| 1:A:974:A:OP2 | 16:N:41:ARG:NH1 | 2.42 | 0.53 |
| 1:A:1085:U:H3' | 1:A:1086:U:C5 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:G:144:MET:C | 9:G:145:ALA:O | 2.45 | 0.53 |
| 13:K:16:SER:HA | 13:K:79:SER:O | 2.09 | 0.53 |
| 17:O:17:ARG:HG3 | 17:O:17:ARG:NH1 | 2.21 | 0.53 |
| 1:A:456:C:H2' | 1:A:457:C:H6 | 1.73 | 0.52 |
| 5:C:150:LYS:HG3 | 5:C:169:ALA:HB2 | 1.90 | 0.52 |
| 6:D:140:VAL:HG11 | 6:D:146:ILE:HD11 | 1.90 | 0.52 |
| 14:L:39:VAL:HG12 | 14:L:40:VAL:N | 2.23 | 0.52 |
| 14:L:119:LYS:O | 14:L:120:TYR:HB2 | 2.10 | 0.52 |
| 17:O:10:LYS:HA | 17:O:10:LYS:HZ3 | 1.74 | 0.52 |
| 1:A:364:A:H61 | 14:L:28:LYS:HE2 | 1.74 | 0.52 |
| 1:A:1004:A:H5" | 1:A:1025:U:C5 | 2.45 | 0.52 |
| 1:A:1124:G:C5' | 12:J:35:SER:O | 2.55 | 0.52 |
| 1:A:1286:A:C8 | 1:A:1287:A:H4' | 2.44 | 0.52 |
| 2:Y:29:A:H2' | 2:Y:30:C:C5 | 2.44 | 0.52 |
| 4:B:101:MET:N | 4:B:108:ILE:HD12 | 2.24 | 0.52 |
| 5:C:43:LEU:HD22 | 5:C:68:VAL:HG21 | 1.91 | 0.52 |
| 6:D:30:LYS:O | 6:D:32:ALA:N | 2.43 | 0.52 |
| 7:E:93:PRO:HG2 | 10:H:105:ARG:CZ | 2.39 | 0.52 |
| 9:G:20:ASP:HB3 | 9:G:23:VAL:HG23 | 1.92 | 0.52 |
| 9:G:108:ALA:O | 9:G:119:ARG:HD2 | 2.10 | 0.52 |
| 11:I:53:VAL:HG21 | 11:I:85:LEU:HD21 | 1.90 | 0.52 |
| 14:L:54:LYS:N | 14:L:54:LYS:HD2 | 2.24 | 0.52 |
| 15:M:17:VAL:O | 15:M:20:THR:HB | 2.09 | 0.52 |
| 20:R:26:LEU:HD12 | 20:R:26:LEU:C | 2.29 | 0.52 |
| 22:T:43:LEU:HD11 | 22:T:55:ILE:HD12 | 1.91 | 0.52 |
| 1:A:528:C:H5' | 1:A:535:A:C6 | 2.43 | 0.52 |
| 1:A:922:G:H2' | 1:A:923:A:C8 | 2.43 | 0.52 |
| 1:A:957:U:H3 | 1:A:960:U:H5" | 1.75 | 0.52 |
| 1:A:1054:C:O2' | 1:A:1055:A:H5" | 2.09 | 0.52 |
| 1:A:1250:A:C5' | 11:I:68:GLY:H | 2.22 | 0.52 |
| 4:B:76:GLN:HE21 | 4:B:207:ALA:N | 2.07 | 0.52 |
| 7:E:18:ARG:HH21 | 7:E:25:ARG:HB3 | 1.74 | 0.52 |
| 9:G:124:LEU:O | 9:G:127:ALA:HB3 | 2.09 | 0.52 |
| 1:A:532:A:H2' | 1:A:533:A:C5' | 2.40 | 0.52 |
| 1:A:545:C:H5" | 6:D:72:GLU:HG3 | 1.90 | 0.52 |
| 1:A:1351:U:H4' | 9:G:33:ASP:OD2 | 2.10 | 0.52 |
| 4:B:132:LYS:HD3 | 4:B:135:GLN:OE1 | 2.09 | 0.52 |
| 7:E:107:ARG:HG2 | 7:E:108:ALA:N | 2.24 | 0.52 |
| 8:F:43:LEU:HD22 | 8:F:43:LEU:N | 2.25 | 0.52 |
| 8:F:63:TYR:N | 8:F:63:TYR:CD2 | 2.75 | 0.52 |
| 22:T:54:LYS:HA | 22:T:57:ARG:HD2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1054:C:O2 | 1:A:1054:C:C3' | 2.57 | 0.52 |
| 4:B:73:THR:O | 4:B:75:LYS:N | 2.43 | 0.52 |
| 7:E:144:THR:HG23 | 7:E:146:ALA:H | 1.75 | 0.52 |
| 11:I:19:LEU:HB3 | 11:I:59:PHE:CE2 | 2.45 | 0.52 |
| 1:A:124:G:C6 | 1:A:125:U:C4 | 2.97 | 0.52 |
| 1:A:190(F):G:H4' | 1:A:190(G):G:OP2 | 2.10 | 0.52 |
| 1:A:457:C:H2' | 1:A:458:C:C6 | 2.45 | 0.52 |
| 1:A:1080:A:O3' | 7:E:16:THR:OG1 | 2.27 | 0.52 |
| 4:B:100:GLY:HA3 | 4:B:104:ASN:HB3 | 1.92 | 0.52 |
| 4:B:138:LEU:HA | 4:B:141:GLU:HB2 | 1.92 | 0.52 |
| 4:B:200:ILE:HG22 | 4:B:202:PRO:HD3 | 1.92 | 0.52 |
| 7:E:60:TYR:HE1 | 7:E:64:ARG:NH2 | 2.07 | 0.52 |
| 7:E:76:ILE:HD11 | 7:E:115:VAL:CG2 | 2.40 | 0.52 |
| 12:J:16:LEU:CD2 | 12:J:94:VAL:HG22 | 2.39 | 0.52 |
| 21:S:28:LYS:HD3 | 21:S:31:ILE:CD1 | 2.40 | 0.52 |
| 1:A:392:G:H2' | 1:A:393:A:H8 | 1.75 | 0.52 |
| 1:A:586:C:O2' | 1:A:587:G:H5' | 2.10 | 0.52 |
| 1:A:1300:G:O2' | 1:A:1301:U:H6 | 1.93 | 0.52 |
| 1:A:1422:G:O2' | 1:A:1423:G:H5' | 2.09 | 0.52 |
| 4:B:54:THR:HG23 | 4:B:199:TYR:HB3 | 1.92 | 0.52 |
| 4:B:76:GLN:HE22 | 4:B:208:ILE:N | 2.08 | 0.52 |
| 12:J:19:SER:HB2 | 12:J:91:PRO:HG3 | 1.91 | 0.52 |
| 15:M:22:ILE:O | 15:M:23:TYR:O | 2.28 | 0.52 |
| 1:A:457:C:H2' | 1:A:458:C:H6 | 1.74 | 0.52 |
| 1:A:1206:G:H2' | 1:A:1207:G:C8 | 2.45 | 0.52 |
| 4:B:57:PHE:CE2 | 4:B:185:ILE:HD11 | 2.45 | 0.52 |
| 13:K:54:ARG:HG3 | 13:K:54:ARG:HH11 | 1.75 | 0.52 |
| 16:N:33:VAL:HA | 16:N:40:CYS:HA | 1.92 | 0.52 |
| 17:O:87:ILE:O | 17:O:88:ARG:CB | 2.58 | 0.52 |
| 1:A:1160:G:O2' | 1:A:1161:C:H5' | 2.10 | 0.52 |
| 1:A:1394:A:C5 | 1:A:1501:C:H4' | 2.44 | 0.52 |
| 1:A:1470:G:O2' | 1:A:1471:G:H5' | 2.09 | 0.52 |
| 5:C:91:LEU:HD11 | 5:C:99:VAL:HG13 | 1.92 | 0.52 |
| 7:E:36:ASP:OD1 | 7:E:38:GLN:N | 2.40 | 0.52 |
| 8:F:24:GLU:HG3 | 8:F:25:ILE:N | 2.25 | 0.52 |
| 11:I:118:LYS:O | 11:I:119:ALA:HB3 | 2.10 | 0.52 |
| 18:P:2:VAL:O | 18:P:64:ALA:HA | 2.10 | 0.52 |
| 1:A:270:A:H2' | 1:A:271:C:C6 | 2.45 | 0.52 |
| 1:A:828:A:H2' | 1:A:829:G:O4' | 2.09 | 0.52 |
| 1:A:1300:G:HO2' | 1:A:1301:U:H6 | 1.57 | 0.52 |
| 1:A:1373:G:O6 | 11:I:11:LYS:HE2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:G:146:GLU:HA | 9:G:149:ARG:HG2 | 1.91 | 0.52 |
| 16:N:35:ARG:C | 16:N:37:PHE:H | 2.13 | 0.52 |
| 18:P:11:SER:OG | 18:P:14:ASN:HB3 | 2.09 | 0.52 |
| 1:A:392:G:H2' | 1:A:393:A:C8 | 2.44 | 0.51 |
| 1:A:434:U:H2' | 1:A:435:C:C6 | 2.45 | 0.51 |
| 1:A:636:U:H2' | 1:A:637:G:H8 | 1.74 | 0.51 |
| 1:A:1030:C:O2' | 1:A:1030(A):G:H5' | 2.10 | 0.51 |
| 1:A:1030(C):G:H2' | 1:A:1030(D):A:H8 | 1.76 | 0.51 |
| 7:E:18:ARG:HE | 7:E:25:ARG:HB2 | 1.74 | 0.51 |
| 9:G:122:HIS:HD2 | 9:G:125:MET:CE | 2.23 | 0.51 |
| 14:L:59:ARG:HH21 | 14:L:65:GLU:HB3 | 1.75 | 0.51 |
| 14:L:85:ILE:CG2 | 14:L:98:TYR:HB3 | 2.40 | 0.51 |
| 21:S:9:VAL:HG12 | 21:S:10:PHE:N | 2.25 | 0.51 |
| 23:V:6:ARG:CD | 23:V:15:ARG:HH12 | 2.19 | 0.51 |
| 1:A:498:U:O2' | 1:A:499:A:H5' | 2.10 | 0.51 |
| 1:A:730:G:N2 | 1:A:765:G:H5" | 2.25 | 0.51 |
| 4:B:227:GLY:O | 4:B:229:VAL:N | 2.39 | 0.51 |
| 5:C:47:LEU:N | 5:C:47:LEU:HD12 | 2.25 | 0.51 |
| 5:C:181:ASN:C | 5:C:182:ILE:HD12 | 2.30 | 0.51 |
| 10:H:83:ILE:HG23 | 10:H:83:ILE:O | 2.10 | 0.51 |
| 12:J:4:ILE:HG13 | 12:J:74:ILE:O | 2.11 | 0.51 |
| 16:N:25:VAL:O | 16:N:25:VAL:HG13 | 2.10 | 0.51 |
| 17:O:36:ILE:HG12 | 17:O:59:MET:HE3 | 1.92 | 0.51 |
| 21:S:45:VAL:HA | 21:S:62:ILE:HG22 | 1.92 | 0.51 |
| 1:A:52:G:O2' | 1:A:53:A:H5' | 2.11 | 0.51 |
| 1:A:664:G:H2' | 1:A:666:G:OP1 | 2.10 | 0.51 |
| 1:A:782:A:H2' | 1:A:783:C:O4' | 2.11 | 0.51 |
| 1:A:948:C:O2' | 1:A:949:A:H5' | 2.11 | 0.51 |
| 4:B:47:THR:HG23 | 4:B:202:PRO:O | 2.10 | 0.51 |
| 4:B:178:ARG:HH21 | 4:B:196:LEU:HA | 1.75 | 0.51 |
| 7:E:120:THR:HG23 | 7:E:121:LYS:N | 2.25 | 0.51 |
| 12:J:8:LEU:CD2 | 12:J:96:ILE:HG12 | 2.39 | 0.51 |
| 14:L:50:SER:O | 14:L:51:ALA:HB2 | 2.09 | 0.51 |
| 14:L:126:LYS:H | 14:L:126:LYS:CE | 2.23 | 0.51 |
| 19:Q:98:LEU:HD12 | 19:Q:98:LEU:O | 2.09 | 0.51 |
| 1:A:192:U:H1' | 22:T:103:GLY:HA2 | 1.93 | 0.51 |
| 1:A:537:G:OP1 | 14:L:113:ARG:NH2 | 2.43 | 0.51 |
| 1:A:945:G:C2 | 1:A:946:A:C8 | 2.97 | 0.51 |
| 4:B:124:SER:CB | 4:B:125:PRO:HD2 | 2.37 | 0.51 |
| 5:C:20:SER:O | 16:N:54:PRO:HB3 | 2.11 | 0.51 |
| 9:G:51:GLN:NE2 | 9:G:56:GLN:O | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:H:85:ARG:CD | 10:H:87:SER:O | 2.59 | 0.51 |
| 13:K:121:PRO:HG2 | 13:K:126:ARG:CG | 2.40 | 0.51 |
| 16:N:22:THR:O | 16:N:23:ARG:HB2 | 2.08 | 0.51 |
| 1:A:190(L):U:C2 | 22:T:105:SER:HB2 | 2.46 | 0.51 |
| 1:A:393:A:C2' | 1:A:394:G:H5' | 2.41 | 0.51 |
| 4:B:78:GLN:O | 4:B:94:ASN:OD1 | 2.29 | 0.51 |
| 5:C:14:ILE:HD13 | 5:C:14:ILE:N | 2.13 | 0.51 |
| 6:D:127:THR:CG2 | 6:D:147:ALA:HB3 | 2.36 | 0.51 |
| 13:K:46:GLY:O | 13:K:48:ILE:O | 2.29 | 0.51 |
| 15:M:14:ARG:HH12 | 15:M:16:ASP:CG | 2.13 | 0.51 |
| 20:R:25:THR:HG22 | 20:R:42:ARG:NH2 | 2.25 | 0.51 |
| 21:S:40:ILE:HD13 | 21:S:62:ILE:HD11 | 1.91 | 0.51 |
| 1:A:404:U:H2' | 1:A:405:U:C6 | 2.46 | 0.51 |
| 1:A:1132:C:H2' | 1:A:1133:G:C8 | 2.46 | 0.51 |
| 5:C:70:VAL:HG21 | 5:C:76:VAL:HG21 | 1.93 | 0.51 |
| 5:C:195:VAL:O | 5:C:196:LEU:HD23 | 2.09 | 0.51 |
| 6:D:8:VAL:HG13 | 6:D:21:LEU:CD1 | 2.33 | 0.51 |
| 15:M:62:ASN:O | 15:M:63:THR:CB | 2.58 | 0.51 |
| 17:O:54:ARG:O | 17:O:58:MET:HG3 | 2.11 | 0.51 |
| 22:T:50:GLU:HG3 | 22:T:100:ILE:HG13 | 1.92 | 0.51 |
| 1:A:51:A:H4' | 1:A:52:G:C5' | 2.41 | 0.51 |
| 1:A:1206:G:H2' | 1:A:1207:G:H8 | 1.76 | 0.51 |
| 4:B:57:PHE:CD2 | 4:B:185:ILE:HD11 | 2.46 | 0.51 |
| 6:D:103:ASN:O | 6:D:106:TYR:HB3 | 2.11 | 0.51 |
| 9:G:28:ASN:OD1 | 9:G:36:LYS:NZ | 2.44 | 0.51 |
| 12:J:34:VAL:HG12 | 12:J:35:SER:N | 2.25 | 0.51 |
| 1:A:161:A:H2' | 1:A:162:A:C8 | 2.46 | 0.51 |
| 1:A:973:G:H3' | 1:A:974:A:H5" | 1.93 | 0.51 |
| 8:F:7:ASN:HB2 | 8:F:89:MET:HB3 | 1.92 | 0.51 |
| 11:I:48:GLU:HG3 | 11:I:101:PHE:CZ | 2.46 | 0.51 |
| 12:J:87:THR:O | 12:J:87:THR:HG22 | 2.11 | 0.51 |
| 16:N:23:ARG:NH1 | 16:N:30:ALA:HB2 | 2.26 | 0.51 |
| 18:P:4:ILE:CG2 | 18:P:36:ILE:HD11 | 2.40 | 0.51 |
| 19:Q:97:SER:N | 19:Q:103:GLY:HA2 | 2.23 | 0.51 |
| 21:S:52:TYR:HA | 21:S:56:GLN:O | 2.11 | 0.51 |
| 1:A:502:G:H2' | 1:A:503:C:C6 | 2.46 | 0.51 |
| 1:A:991:U:C4 | 1:A:1212:U:H1' | 2.46 | 0.51 |
| 4:B:189:ASP:O | 4:B:191:ASP:N | 2.43 | 0.51 |
| 5:C:114:PRO:O | 5:C:118:GLN:HB2 | 2.10 | 0.51 |
| 9:G:16:LEU:H | 9:G:16:LEU:HD22 | 1.75 | 0.51 |
| 10:H:4:ASP:OD2 | 10:H:7:ALA:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:I:32:ASP:O | 11:I:35:GLU:HB3 | 2.11 | 0.51 |
| 12:J:4:ILE:HA | 12:J:100:THR:CA | 2.41 | 0.51 |
| 12:J:4:ILE:O | 12:J:73:ASP:HA | 2.11 | 0.51 |
| 13:K:126:ARG:O | 13:K:127:LYS:CB | 2.59 | 0.51 |
| 21:S:11:VAL:HG13 | 21:S:38:SER:HB2 | 1.92 | 0.51 |
| 1:A:922:G:H5' | 7:E:20:GLN:NE2 | 2.25 | 0.51 |
| 1:A:1110:A:H8 | 1:A:1110:A:O5' | 1.94 | 0.51 |
| 1:A:1165:C:O2' | 1:A:1166:G:H5' | 2.10 | 0.51 |
| 1:A:1299:A:C8 | 1:A:1301:U:H1' | 2.45 | 0.51 |
| 2:Y:38:PSU:H2' | 2:Y:39:G:O4' | 2.11 | 0.51 |
| 4:B:14:GLY:C | 4:B:15:VAL:HG22 | 2.31 | 0.51 |
| 4:B:42:ILE:HD11 | 4:B:189:ASP:HB2 | 1.92 | 0.51 |
| 16:N:9:LYS:HD3 | 16:N:9:LYS:C | 2.31 | 0.51 |
| 21:S:30:LEU:HD13 | 21:S:31:ILE:O | 2.11 | 0.51 |
| 1:A:532:A:H2' | 1:A:533:A:H5" | 1.93 | 0.50 |
| 1:A:575:G:OP1 | 1:A:575:G:H4' | 2.11 | 0.50 |
| 1:A:730:G:H21 | 1:A:765:G:H5" | 1.76 | 0.50 |
| 1:A:877:C:H1' | 10:H:3:THR:HG23 | 1.90 | 0.50 |
| 1:A:1152:A:H2' | 1:A:1153:C:H6 | 1.74 | 0.50 |
| 4:B:42:ILE:HD12 | 4:B:203:GLY:HA2 | 1.94 | 0.50 |
| 9:G:156:TRP:CD1 | 9:G:156:TRP:C | 2.84 | 0.50 |
| 11:I:77:ILE:O | 11:I:79:LEU:N | 2.43 | 0.50 |
| 18:P:19:ILE:HD12 | 18:P:19:ILE:N | 2.26 | 0.50 |
| 19:Q:81:ARG:HG3 | 19:Q:81:ARG:O | 2.11 | 0.50 |
| 21:S:81:ARG:O | 21:S:81:ARG:HD3 | 2.11 | 0.50 |
| 22:T:94:ALA:O | 22:T:95:ALA:CB | 2.59 | 0.50 |
| 1:A:106:C:O2 | 1:A:379:C:H4' | 2.11 | 0.50 |
| 1:A:112:G:H4' | 1:A:389:A:C5' | 2.41 | 0.50 |
| 1:A:258:G:O2' | 1:A:259:G:H5' | 2.12 | 0.50 |
| 1:A:1270:C:O2' | 1:A:1271:G:H5' | 2.12 | 0.50 |
| 8:F:87:ARG:HH11 | 8:F:87:ARG:CG | 2.15 | 0.50 |
| 13:K:84:VAL:CG2 | 13:K:110:ASP:HA | 2.37 | 0.50 |
| 13:K:93:GLN:NE2 | 13:K:96:ARG:HH21 | 2.09 | 0.50 |
| 19:Q:12:SER:HB3 | 19:Q:20:THR:HB | 1.93 | 0.50 |
| 19:Q:80:GLY:O | 19:Q:81:ARG:CB | 2.60 | 0.50 |
| 22:T:100:ILE:C | 22:T:102:GLY:N | 2.63 | 0.50 |
| 23:V:24:ARG:O | 23:V:25:LYS:CB | 2.59 | 0.50 |
| 1:A:1195:C:C3' | 1:A:1196:U:H5" | 2.35 | 0.50 |
| 4:B:98:LEU:O | 4:B:101:MET:HG2 | 2.12 | 0.50 |
| 4:B:204:ASN:ND2 | 4:B:206:ASP:H | 2.09 | 0.50 |
| 10:H:30:ARG:O | 10:H:33:GLU:HB3 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:J:82:ILE:O | 12:J:86:MET:HB2 | 2.11 | 0.50 |
| 13:K:110:ASP:HB2 | 20:R:88:LYS:CD | 2.40 | 0.50 |
| 14:L:115:LYS:O | 14:L:117:ARG:N | 2.40 | 0.50 |
| 19:Q:2:PRO:O | 19:Q:3:LYS:C | 2.50 | 0.50 |
| 1:A:217:C:H2' | 1:A:218:C:H6 | 1.77 | 0.50 |
| 1:A:397:A:H5' | 1:A:398:C:OP1 | 2.10 | 0.50 |
| 1:A:438:G:C4' | 1:A:439:A:OP1 | 2.57 | 0.50 |
| 1:A:547:A:H4' | 1:A:548:G:O5' | 2.11 | 0.50 |
| 1:A:554:C:H2' | 1:A:555:C:C6 | 2.47 | 0.50 |
| 1:A:691:G:O2' | 1:A:797:C:H4' | 2.11 | 0.50 |
| 4:B:16:HIS:O | 4:B:17:PHE:O | 2.30 | 0.50 |
| 4:B:134:GLU:HG2 | 4:B:134:GLU:O | 2.12 | 0.50 |
| 15:M:26:GLY:O | 15:M:28:ALA:N | 2.44 | 0.50 |
| 21:S:16:LEU:O | 21:S:18:LYS:N | 2.44 | 0.50 |
| 1:A:189:G:H2' | 1:A:190:C:C6 | 2.47 | 0.50 |
| 1:A:335:C:H2' | 1:A:336:C:C6 | 2.47 | 0.50 |
| 1:A:485:G:C2' | 1:A:486:U:OP2 | 2.59 | 0.50 |
| 1:A:939:G:H5" | 9:G:102:ARG:CZ | 2.40 | 0.50 |
| 1:A:1250:A:H5" | 11:I:68:GLY:H | 1.75 | 0.50 |
| 5:C:15:THR:HB | 5:C:181:ASN:HB2 | 1.94 | 0.50 |
| 5:C:134:ILE:HG23 | 5:C:151:VAL:HB | 1.93 | 0.50 |
| 22:T:44:ALA:C | 22:T:46:GLU:H | 2.15 | 0.50 |
| 1:A:458:C:H2' | 1:A:459:G:H8 | 1.76 | 0.50 |
| 1:A:1201:A:O2' | 1:A:1202:G:OP2 | 2.28 | 0.50 |
| 1:A:1298:C:H4' | 1:A:1299:A:O4' | 2.11 | 0.50 |
| 5:C:5:ILE:N | 5:C:5:ILE:HD12 | 2.26 | 0.50 |
| 5:C:42:LEU:HD12 | 5:C:94:LEU:HD12 | 1.92 | 0.50 |
| 11:I:48:GLU:HG3 | 11:I:101:PHE:HZ | 1.75 | 0.50 |
| 19:Q:33:GLY:O | 19:Q:34:LYS:C | 2.49 | 0.50 |
| 19:Q:68:ARG:CG | 19:Q:68:ARG:NH1 | 2.73 | 0.50 |
| 22:T:67:ALA:O | 22:T:73:HIS:ND1 | 2.44 | 0.50 |
| 1:A:657:G:H4' | 17:O:28:GLN:HG2 | 1.93 | 0.50 |
| 1:A:1491:G:C5 | 24:A:1545:PAR:H21 | 2.46 | 0.50 |
| 4:B:16:HIS:HA | 4:B:204:ASN:CB | 2.39 | 0.50 |
| 6:D:142:PRO:CB | 6:D:187:ARG:HH21 | 2.24 | 0.50 |
| 6:D:187:ARG:HG3 | 6:D:188:LEU:N | 2.27 | 0.50 |
| 9:G:16:LEU:HD22 | 9:G:16:LEU:N | 2.26 | 0.50 |
| 9:G:42:ILE:HG22 | 9:G:120:ILE:HD12 | 1.94 | 0.50 |
| 21:S:77:THR:HG22 | 21:S:78:ARG:N | 2.27 | 0.50 |
| 1:A:357:G:OP1 | 1:A:367:U:H2' | 2.11 | 0.50 |
| 1:A:731:G:H5' | 1:A:766:A:H4' | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1223:C:OP1 | 1:A:1224:G:H3' | 2.12 | 0.50 |
| 1:A:1256:A:H61 | 1:A:1278:U:H1' | 1.76 | 0.50 |
| 10:H:60:ARG:HH11 | 10:H:60:ARG:HG3 | 1.76 | 0.50 |
| 13:K:17:GLY:HA3 | 13:K:77:MET:HE1 | 1.94 | 0.50 |
| 14:L:60:LEU:N | 14:L:64:TYR:O | 2.37 | 0.50 |
| 22:T:26:ASN:OD1 | 22:T:71:THR:HA | 2.12 | 0.50 |
| 23:V:12:LYS:HG2 | 23:V:22:ARG:HB3 | 1.92 | 0.50 |
| 1:A:109:A:H2' | 1:A:326:G:N2 | 2.26 | 0.50 |
| 1:A:431:A:O2' | 1:A:432:A:H5' | 2.12 | 0.50 |
| 1:A:1090:U:H2' | 1:A:1091:U:H6 | 1.77 | 0.50 |
| 1:A:1347:G:H2' | 1:A:1373:G:H1 | 1.77 | 0.50 |
| 1:A:1499:A:C1' | 1:A:1520:G:H5' | 2.41 | 0.50 |
| 4:B:23:ARG:NH1 | 4:B:24:TRP:HA | 2.27 | 0.50 |
| 6:D:83:SER:HA | 6:D:89:THR:OG1 | 2.12 | 0.50 |
| 9:G:113:GLU:CD | 9:G:113:GLU:H | 2.16 | 0.50 |
| 11:I:17:VAL:HG21 | 11:I:81:ILE:N | 2.27 | 0.50 |
| 12:J:6:ILE:HA | 12:J:97:GLU:O | 2.12 | 0.50 |
| 15:M:88:ARG:HH11 | 21:S:3:ARG:HH21 | 1.58 | 0.50 |
| 18:P:45:THR:HB | 18:P:46:PRO:HD2 | 1.94 | 0.50 |
| 18:P:67:THR:CG2 | 18:P:68:ASP:N | 2.74 | 0.50 |
| 20:R:40:LEU:HB3 | 20:R:79:LEU:HD11 | 1.94 | 0.50 |
| 1:A:436:C:H2' | 1:A:437:U:C6 | 2.47 | 0.49 |
| 1:A:1405:G:O2' | 1:A:1406:U:H5' | 2.12 | 0.49 |
| 4:B:189:ASP:HB3 | 4:B:203:GLY:O | 2.12 | 0.49 |
| 5:C:14:ILE:H | 5:C:14:ILE:CD1 | 2.12 | 0.49 |
| 5:C:24:ALA:CB | 5:C:32:LEU:HD12 | 2.38 | 0.49 |
| 5:C:86:VAL:O | 5:C:89:GLU:HB3 | 2.12 | 0.49 |
| 7:E:150:ARG:HG3 | 7:E:150:ARG:HH11 | 1.75 | 0.49 |
| 9:G:51:GLN:C | 9:G:53:LYS:H | 2.15 | 0.49 |
| 12:J:47:PHE:HD2 | 16:N:34:TYR:CD2 | 2.30 | 0.49 |
| 14:L:61:THR:C | 14:L:63:GLY:H | 2.15 | 0.49 |
| 15:M:44:ARG:HB3 | 15:M:46:LYS:HG2 | 1.94 | 0.49 |
| 16:N:24:CYS:HB3 | 16:N:28:GLY:H | 1.77 | 0.49 |
| 16:N:44:LEU:HD12 | 16:N:44:LEU:O | 2.11 | 0.49 |
| 5:C:22:TRP:CG | 5:C:59:ARG:HD2 | 2.47 | 0.49 |
| 5:C:139:GLN:O | 5:C:140:ARG:C | 2.50 | 0.49 |
| 7:E:143:ARG:NH1 | 10:H:77:GLU:OE2 | 2.39 | 0.49 |
| 9:G:57:GLU:O | 9:G:60:LYS:HB2 | 2.11 | 0.49 |
| 11:I:7:THR:HG22 | 11:I:8:GLY:N | 2.26 | 0.49 |
| 16:N:45:ARG:HG3 | 16:N:45:ARG:NH1 | 2.26 | 0.49 |
| 17:O:70:LEU:HD13 | 17:O:78:TYR:HA | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:T:54:LYS:HA | 22:T:57:ARG:HD3 | 1.94 | 0.49 |
| 23:V:24:ARG:O | 23:V:25:LYS:HB2 | 2.12 | 0.49 |
| 1:A:413:G:N2 | 1:A:428:G:O2' | 2.42 | 0.49 |
| 1:A:533:A:O2' | 1:A:534:U:OP1 | 2.30 | 0.49 |
| 1:A:570:G:H2' | 1:A:571:U:C6 | 2.47 | 0.49 |
| 1:A:952:U:O4 | 15:M:104:ARG:HD3 | 2.12 | 0.49 |
| 1:A:1056:U:O2' | 1:A:1057:G:H5' | 2.12 | 0.49 |
| 1:A:1196:U:OP1 | 1:A:1197:G:H5' | 2.12 | 0.49 |
| 1:A:1368:G:OP1 | 12:J:62:HIS:HE1 | 1.94 | 0.49 |
| 4:B:87:ARG:NH2 | 4:B:233:SER:HB2 | 2.27 | 0.49 |
| 4:B:110:GLN:O | 4:B:114:ARG:HB2 | 2.12 | 0.49 |
| 4:B:119:GLU:HG3 | 4:B:153:ARG:HH22 | 1.77 | 0.49 |
| 9:G:71:PRO:HD3 | 9:G:103:TRP:CZ3 | 2.45 | 0.49 |
| 15:M:14:ARG:NH1 | 15:M:16:ASP:OD1 | 2.45 | 0.49 |
| 1:A:197:A:N1 | 1:A:220:G:O2' | 2.41 | 0.49 |
| 1:A:922:G:H4' | 7:E:20:GLN:HA | 1.95 | 0.49 |
| 1:A:939:G:H2' | 1:A:940:C:H6 | 1.78 | 0.49 |
| 4:B:97:TRP:HZ2 | 4:B:102:LEU:HD13 | 1.76 | 0.49 |
| 6:D:8:VAL:C | 6:D:10:ARG:N | 2.65 | 0.49 |
| 7:E:13:ILE:HG13 | 7:E:13:ILE:O | 2.11 | 0.49 |
| 9:G:146:GLU:C | 9:G:148:ASN:N | 2.66 | 0.49 |
| 10:H:45:ILE:HG13 | 10:H:47:GLY:H | 1.77 | 0.49 |
| 13:K:19:ALA:HB2 | 13:K:80:VAL:HG21 | 1.94 | 0.49 |
| 15:M:40:ASN:HB3 | 15:M:43:THR:HG23 | 1.94 | 0.49 |
| 1:A:99:C:H2' | 1:A:101:A:O4' | 2.13 | 0.49 |
| 1:A:200:G:H2' | 1:A:201:C:O4' | 2.11 | 0.49 |
| 1:A:653:A:C8 | 10:H:56:LYS:HG2 | 2.47 | 0.49 |
| 1:A:714:G:H2' | 1:A:715:A:C8 | 2.48 | 0.49 |
| 1:A:961:U:H2' | 1:A:962:C:H5' | 1.93 | 0.49 |
| 1:A:1053:G:N7 | 1:A:1200:C:H5' | 2.27 | 0.49 |
| 4:B:54:THR:O | 4:B:58:ILE:HG13 | 2.11 | 0.49 |
| 4:B:118:LEU:HD11 | 4:B:141:GLU:HB3 | 1.94 | 0.49 |
| 5:C:6:HIS:CD2 | 5:C:8:ILE:H | 2.24 | 0.49 |
| 5:C:23:TYR:HE2 | 12:J:9:ARG:HG3 | 1.78 | 0.49 |
| 8:F:35:ALA:O | 8:F:36:ARG:CB | 2.59 | 0.49 |
| 11:I:126:SER:O | 11:I:128:ARG:N | 2.45 | 0.49 |
| 14:L:55:VAL:HG12 | 14:L:56:ALA:N | 2.24 | 0.49 |
| 1:A:668:G:O2' | 17:O:46:HIS:CD2 | 2.66 | 0.49 |
| 1:A:1121:U:H2' | 1:A:1122:U:C6 | 2.46 | 0.49 |
| 1:A:1251:A:H2' | 1:A:1252:A:H8 | 1.73 | 0.49 |
| 7:E:76:ILE:HD13 | 7:E:118:ILE:HD12 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:J:3:LYS:HG2 | 12:J:75:ILE:HG23 | 1.95 | 0.49 |
| 15:M:45:VAL:HA | 15:M:48:LEU:HG | 1.94 | 0.49 |
| 1:A:1278:U:C5' | 1:A:1279:A:H5' | 2.43 | 0.49 |
| 1:A:1314:C:H3' | 21:S:6:LYS:HZ3 | 1.75 | 0.49 |
| 4:B:97:TRP:CZ2 | 4:B:101:MET:HB2 | 2.48 | 0.49 |
| 4:B:114:ARG:O | 4:B:117:GLU:HB3 | 2.12 | 0.49 |
| 5:C:182:ILE:HD12 | 5:C:182:ILE:N | 2.27 | 0.49 |
| 7:E:101:ILE:HD12 | 7:E:119:LEU:HD23 | 1.95 | 0.49 |
| 11:I:51:ARG:NH1 | 11:I:51:ARG:HB2 | 2.27 | 0.49 |
| 12:J:34:VAL:HG22 | 12:J:74:ILE:CG2 | 2.35 | 0.49 |
| 12:J:49:VAL:O | 12:J:60:ARG:CA | 2.61 | 0.49 |
| 14:L:53:ARG:HG2 | 14:L:69:TYR:CE1 | 2.41 | 0.49 |
| 21:S:30:LEU:HD13 | 21:S:30:LEU:C | 2.32 | 0.49 |
| 1:A:971:G:OP1 | 1:A:972:C:H5" | 2.13 | 0.49 |
| 1:A:1085:U:H3' | 1:A:1086:U:H5 | 1.78 | 0.49 |
| 1:A:1228:C:H4' | 15:M:116:THR:HA | 1.95 | 0.49 |
| 6:D:119:GLN:CG | 6:D:123:HIS:CD2 | 2.95 | 0.49 |
| 9:G:87:VAL:HG11 | 9:G:154:TYR:O | 2.13 | 0.49 |
| 11:I:20:ARG:O | 11:I:60:ASP:N | 2.45 | 0.49 |
| 15:M:84:ILE:HG22 | 21:S:65:ASN:ND2 | 2.24 | 0.49 |
| 22:T:101:GLY:O | 22:T:103:GLY:N | 2.45 | 0.49 |
| 1:A:1073:U:H2' | 1:A:1074:G:C8 | 2.48 | 0.49 |
| 1:A:1111:A:H61 | 5:C:177:THR:HA | 1.78 | 0.49 |
| 1:A:1245:A:H2' | 1:A:1246:C:C6 | 2.48 | 0.49 |
| 1:A:1347:G:C8 | 11:I:107:ARG:NH1 | 2.81 | 0.49 |
| 4:B:74:LYS:HZ2 | 4:B:206:ASP:HA | 1.77 | 0.49 |
| 5:C:139:GLN:HE21 | 5:C:139:GLN:HA | 1.77 | 0.49 |
| 9:G:115:ARG:HB3 | 9:G:118:VAL:HG23 | 1.94 | 0.49 |
| 12:J:3:LYS:C | 12:J:4:ILE:HG13 | 2.32 | 0.49 |
| 1:A:427:U:OP1 | 6:D:13:ARG:NH2 | 2.45 | 0.49 |
| 1:A:637:G:O2' | 1:A:638:G:H5' | 2.13 | 0.49 |
| 1:A:1480:G:O2' | 1:A:1481:U:H5' | 2.12 | 0.49 |
| 2:Y:40:G:H2' | 2:Y:41:U:C6 | 2.48 | 0.49 |
| 6:D:118:ARG:HG3 | 6:D:136:PRO:HB3 | 1.95 | 0.49 |
| 7:E:145:LYS:O | 7:E:149:GLU:HB2 | 2.12 | 0.49 |
| 13:K:27:ASN:HA | 13:K:56:GLY:HA2 | 1.95 | 0.49 |
| 13:K:57:THR:HG23 | 13:K:60:ALA:H | 1.76 | 0.49 |
| 1:A:613:C:O2' | 1:A:614:A:H5' | 2.13 | 0.48 |
| 1:A:1108:G:H5' | 1:A:1191:A:C4' | 2.43 | 0.48 |
| 4:B:13:ALA:C | 4:B:15:VAL:N | 2.66 | 0.48 |
| 4:B:102:LEU:N | 4:B:102:LEU:HD12 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:124:SER:HB2 | 4:B:125:PRO:CD | 2.39 | 0.48 |
| 7:E:15:ARG:O | 7:E:16:THR:O | 2.31 | 0.48 |
| 10:H:51:VAL:HG21 | 10:H:60:ARG:HG2 | 1.95 | 0.48 |
| 12:J:42:THR:HG23 | 12:J:67:THR:C | 2.34 | 0.48 |
| 15:M:65:LYS:O | 15:M:70:LEU:HG | 2.14 | 0.48 |
| 17:O:66:LEU:O | 17:O:69:TYR:HB3 | 2.13 | 0.48 |
| 22:T:12:ALA:N | 22:T:13:LEU:HD12 | 2.20 | 0.48 |
| 1:A:131:C:H2' | 1:A:132:C:C6 | 2.48 | 0.48 |
| 1:A:349:A:C3' | 1:A:350:G:H5" | 2.43 | 0.48 |
| 1:A:596:C:O2' | 1:A:597:G:H5' | 2.12 | 0.48 |
| 1:A:735:C:O2' | 1:A:736:C:H5' | 2.12 | 0.48 |
| 1:A:797:C:OP1 | 13:K:124:LYS:HD3 | 2.12 | 0.48 |
| 1:A:980:C:H2' | 1:A:981:U:O4' | 2.12 | 0.48 |
| 1:A:1499:A:O2' | 1:A:1500:A:H5' | 2.12 | 0.48 |
| 4:B:97:TRP:CE2 | 4:B:101:MET:HG3 | 2.48 | 0.48 |
| 8:F:48:LEU:HD13 | 8:F:52:ILE:CG1 | 2.43 | 0.48 |
| 12:J:35:SER:HB2 | 12:J:72:VAL:O | 2.12 | 0.48 |
| 13:K:48:ILE:CG2 | 13:K:49:GLY:N | 2.58 | 0.48 |
| 21:S:63:THR:HG22 | 21:S:64:GLU:N | 2.28 | 0.48 |
| 22:T:96:GLY:O | 22:T:97:ALA:CB | 2.61 | 0.48 |
| 1:A:60:A:H4' | 1:A:61:G:O5' | 2.13 | 0.48 |
| 1:A:350:G:H5' | 1:A:350:G:H8 | 1.78 | 0.48 |
| 1:A:519:C:H2' | 1:A:520:A:C8 | 2.49 | 0.48 |
| 1:A:628:G:H2' | 1:A:629:G:H8 | 1.78 | 0.48 |
| 1:A:1278:U:H4' | 1:A:1279:A:O4' | 2.12 | 0.48 |
| 4:B:69:LEU:HD23 | 4:B:70:PHE:N | 2.27 | 0.48 |
| 4:B:141:GLU:O | 4:B:145:LEU:HG | 2.14 | 0.48 |
| 7:E:15:ARG:O | 7:E:27:ARG:O | 2.31 | 0.48 |
| 9:G:42:ILE:CG2 | 9:G:120:ILE:HD12 | 2.42 | 0.48 |
| 10:H:10:LEU:HD22 | 10:H:83:ILE:HD11 | 1.96 | 0.48 |
| 13:K:44:SER:H | 13:K:47:VAL:HB | 1.77 | 0.48 |
| 1:A:925:G:C6 | 1:A:927:G:N7 | 2.81 | 0.48 |
| 1:A:974:A:H8 | 1:A:974:A:OP1 | 1.95 | 0.48 |
| 1:A:1005:A:H2' | 1:A:1006:C:C5' | 2.42 | 0.48 |
| 5:C:10:PHE:O | 5:C:178:LEU:HD11 | 2.13 | 0.48 |
| 5:C:29:TYR:CZ | 16:N:54:PRO:HG2 | 2.49 | 0.48 |
| 5:C:58:GLU:H | 5:C:65:ALA:HB3 | 1.78 | 0.48 |
| 7:E:33:VAL:HG11 | 7:E:109:ILE:HA | 1.95 | 0.48 |
| 7:E:76:ILE:HD11 | 7:E:115:VAL:HG21 | 1.94 | 0.48 |
| 11:I:118:LYS:O | 11:I:120:ARG:N | 2.46 | 0.48 |
| 12:J:6:ILE:CG2 | 12:J:98:ILE:HG23 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:J:71:LEU:O | 12:J:72:VAL:HB | 2.12 | 0.48 |
| 12:J:84:GLN:C | 12:J:88:LEU:HD12 | 2.34 | 0.48 |
| 17:O:61:GLY:O | 17:O:64:ARG:HG2 | 2.13 | 0.48 |
| 18:P:19:ILE:HG22 | 18:P:36:ILE:CG1 | 2.43 | 0.48 |
| 1:A:115:G:H1' | 1:A:116:A:N7 | 2.29 | 0.48 |
| 1:A:407:G:H2' | 1:A:408:A:C8 | 2.47 | 0.48 |
| 1:A:1001:A:H2' | 1:A:1002:G:C8 | 2.48 | 0.48 |
| 7:E:41:VAL:HG13 | 7:E:113:ALA:HA | 1.94 | 0.48 |
| 10:H:3:THR:HG23 | 10:H:4:ASP:N | 2.29 | 0.48 |
| 11:I:19:LEU:HD23 | 11:I:61:ALA:HB2 | 1.95 | 0.48 |
| 1:A:22:G:H4' | 1:A:885:G:C8 | 2.49 | 0.48 |
| 1:A:119:A:H4' | 1:A:120:A:O5' | 2.14 | 0.48 |
| 1:A:364:A:N6 | 14:L:28:LYS:NZ | 2.61 | 0.48 |
| 1:A:1123:A:O2' | 1:A:1124:G:H5' | 2.13 | 0.48 |
| 1:A:1277:C:O2' | 1:A:1279:A:H1' | 2.14 | 0.48 |
| 1:A:1360:A:O2' | 1:A:1361:G:H5' | 2.14 | 0.48 |
| 4:B:13:ALA:C | 4:B:15:VAL:H | 2.15 | 0.48 |
| 5:C:29:TYR:OH | 16:N:54:PRO:HG2 | 2.13 | 0.48 |
| 5:C:119:ARG:O | 5:C:122:GLU:N | 2.46 | 0.48 |
| 6:D:119:GLN:HG3 | 6:D:123:HIS:CD2 | 2.48 | 0.48 |
| 10:H:45:ILE:C | 10:H:47:GLY:H | 2.17 | 0.48 |
| 1:A:35:G:H2' | 1:A:36:C:H6 | 1.76 | 0.48 |
| 1:A:157:G:O2' | 1:A:158:G:H5' | 2.13 | 0.48 |
| 1:A:452:A:HO2' | 1:A:453:A:H8 | 1.59 | 0.48 |
| 1:A:521:G:OP1 | 14:L:73:GLU:O | 2.31 | 0.48 |
| 1:A:1247:U:O2' | 1:A:1248:A:H5' | 2.14 | 0.48 |
| 1:A:1333:A:H2' | 1:A:1334:G:O4' | 2.14 | 0.48 |
| 4:B:17:PHE:HD2 | 4:B:44:LEU:HD11 | 1.79 | 0.48 |
| 4:B:238:LEU:C | 4:B:240:GLN:H | 2.16 | 0.48 |
| 6:D:59:ARG:NH2 | 6:D:62:GLN:HG3 | 2.29 | 0.48 |
| 6:D:80:GLU:O | 6:D:84:LYS:HG3 | 2.13 | 0.48 |
| 12:J:94:VAL:HG12 | 12:J:95:GLU:N | 2.27 | 0.48 |
| 13:K:109:VAL:HG22 | 20:R:86:VAL:HA | 1.95 | 0.48 |
| 15:M:40:ASN:HD22 | 15:M:41:PRO:N | 2.10 | 0.48 |
| 17:O:26:GLU:HA | 17:O:81:LEU:HD11 | 1.96 | 0.48 |
| 1:A:112:G:C2' | 1:A:113:G:H5' | 2.43 | 0.48 |
| 1:A:674:G:H2' | 1:A:675:A:H8 | 1.78 | 0.48 |
| 1:A:992:U:H4' | 1:A:993:G:O5' | 2.14 | 0.48 |
| 4:B:136:VAL:HG12 | 4:B:140:HIS:NE2 | 2.28 | 0.48 |
| 5:C:87:LEU:C | 5:C:89:GLU:N | 2.66 | 0.48 |
| 5:C:151:VAL:HG12 | 5:C:152:ILE:N | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:C:157:ILE:HG21 | 5:C:164:ARG:NH2 | 2.28 | 0.48 |
| 9:G:143:ARG:O | 9:G:145:ALA:O | 2.31 | 0.48 |
| 11:I:4:TYR:CZ | 11:I:88:TYR:HD1 | 2.32 | 0.48 |
| 14:L:126:LYS:HZ1 | 14:L:127:GLU:N | 2.11 | 0.48 |
| 15:M:11:ARG:HA | 15:M:45:VAL:HB | 1.96 | 0.48 |
| 15:M:80:ARG:C | 15:M:82:MET:N | 2.66 | 0.48 |
| 16:N:35:ARG:O | 16:N:37:PHE:N | 2.47 | 0.48 |
| 21:S:4:SER:O | 21:S:5:LEU:CB | 2.62 | 0.48 |
| 1:A:628:G:H2' | 1:A:629:G:C8 | 2.49 | 0.48 |
| 1:A:653:A:OP1 | 10:H:56:LYS:NZ | 2.40 | 0.48 |
| 1:A:983:A:H2 | 1:A:984:C:C6 | 2.31 | 0.48 |
| 1:A:1064:G:C4' | 1:A:1065:U:H5' | 2.43 | 0.48 |
| 1:A:1202:G:H2' | 1:A:1203:C:O4' | 2.14 | 0.48 |
| 4:B:25:ASN:ND2 | 4:B:27:LYS:H | 2.12 | 0.48 |
| 4:B:76:GLN:OE1 | 4:B:76:GLN:C | 2.51 | 0.48 |
| 6:D:94:LEU:HD12 | 6:D:191:ARG:HD3 | 1.96 | 0.48 |
| 7:E:57:LYS:HG2 | 7:E:61:TYR:HE2 | 1.77 | 0.48 |
| 10:H:103:VAL:HG21 | 10:H:109:ILE:C | 2.34 | 0.48 |
| 12:J:16:LEU:O | 12:J:19:SER:N | 2.47 | 0.48 |
| 12:J:42:THR:HG23 | 12:J:68:HIS:HA | 1.94 | 0.48 |
| 14:L:25:PRO:C | 14:L:27:LEU:N | 2.66 | 0.48 |
| 1:A:176:C:H2' | 1:A:177:C:C6 | 2.48 | 0.48 |
| 1:A:738:C:OP1 | 8:F:92:LYS:HE2 | 2.13 | 0.48 |
| 1:A:1044:A:H2' | 1:A:1045:C:C5' | 2.43 | 0.48 |
| 1:A:1074:G:O3' | 4:B:103:THR:HG22 | 2.14 | 0.48 |
| 1:A:1178:G:P | 11:I:97:LYS:HZ2 | 2.36 | 0.48 |
| 1:A:1314:C:H3' | 21:S:6:LYS:HZ1 | 1.77 | 0.48 |
| 1:A:1371:G:OP1 | 11:I:11:LYS:O | 2.31 | 0.48 |
| 2:Y:30:C:H2' | 2:Y:31:C:H6 | 1.79 | 0.48 |
| 5:C:72:LYS:HE2 | 5:C:75:VAL:CG2 | 2.44 | 0.48 |
| 5:C:155:GLY:O | 5:C:156:ARG:CB | 2.62 | 0.48 |
| 5:C:157:ILE:CG2 | 5:C:164:ARG:HH21 | 2.26 | 0.48 |
| 5:C:179:ARG:HG3 | 5:C:179:ARG:NH1 | 2.29 | 0.48 |
| 6:D:76:ARG:HG2 | 6:D:76:ARG:HH11 | 1.79 | 0.48 |
| 7:E:51:VAL:CB | 7:E:52:PRO:HD3 | 2.41 | 0.48 |
| 10:H:63:LEU:HD22 | 10:H:63:LEU:H | 1.78 | 0.48 |
| 18:P:20:VAL:HG12 | 18:P:21:VAL:N | 2.29 | 0.48 |
| 20:R:38:GLU:HA | 20:R:38:GLU:OE2 | 2.14 | 0.48 |
| 1:A:941:G:O2' | 1:A:942:G:H5' | 2.14 | 0.47 |
| 1:A:1054:C:H42 | 2:Y:34:G:C1' | 2.27 | 0.47 |
| 1:A:1216:G:H5" | 16:N:5:ALA:CB | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1281:U:H3' | 1:A:1281:U:C6 | 2.48 | 0.47 |
| 1:A:1298:C:C4 | 9:G:114:ARG:HD3 | 2.49 | 0.47 |
| 1:A:1392:G:O2' | 1:A:1502:A:H5" | 2.13 | 0.47 |
| 4:B:144:ARG:HG3 | 4:B:145:LEU:N | 2.29 | 0.47 |
| 5:C:95:THR:C | 5:C:97:LYS:H | 2.18 | 0.47 |
| 5:C:130:VAL:HG21 | 5:C:157:ILE:HG23 | 1.96 | 0.47 |
| 7:E:74:GLY:CA | 7:E:116:THR:HG22 | 2.44 | 0.47 |
| 9:G:72:ARG:HH12 | 9:G:138:LYS:HZ1 | 1.60 | 0.47 |
| 10:H:112:LEU:N | 10:H:112:LEU:CD2 | 2.76 | 0.47 |
| 11:I:10:ARG:HH22 | 11:I:107:ARG:NH2 | 2.11 | 0.47 |
| 14:L:114:LYS:HE2 | 14:L:125:PRO:HG3 | 1.96 | 0.47 |
| 18:P:18:ARG:HD3 | 18:P:35:LYS:CD | 2.44 | 0.47 |
| 19:Q:3:LYS:HD3 | 19:Q:61:GLU:O | 2.13 | 0.47 |
| 1:A:322:C:O2' | 1:A:323:U:H5' | 2.14 | 0.47 |
| 1:A:353:A:H8 | 1:A:353:A:C5' | 2.27 | 0.47 |
| 1:A:567:G:H2' | 1:A:568:G:O4' | 2.14 | 0.47 |
| 1:A:1520:G:O2' | 1:A:1521:G:H5' | 2.14 | 0.47 |
| 5:C:95:THR:O | 5:C:97:LYS:N | 2.43 | 0.47 |
| 5:C:155:GLY:O | 5:C:196:LEU:HD22 | 2.14 | 0.47 |
| 9:G:72:ARG:HH12 | 9:G:138:LYS:HZ3 | 1.61 | 0.47 |
| 10:H:126:LYS:C | 10:H:128:GLY:H | 2.17 | 0.47 |
| 13:K:84:VAL:HG11 | 13:K:95:ILE:HD11 | 1.96 | 0.47 |
| 19:Q:67:LYS:O | 19:Q:69:LYS:N | 2.46 | 0.47 |
| 1:A:147:G:O2' | 1:A:148:G:H5' | 2.15 | 0.47 |
| 1:A:235:C:H5' | 19:Q:70:ARG:HD3 | 1.96 | 0.47 |
| 4:B:73:THR:O | 4:B:74:LYS:C | 2.52 | 0.47 |
| 4:B:102:LEU:N | 4:B:102:LEU:CD1 | 2.76 | 0.47 |
| 5:C:75:VAL:O | 5:C:83:ARG:HD3 | 2.14 | 0.47 |
| 5:C:130:VAL:O | 5:C:134:ILE:HG13 | 2.13 | 0.47 |
| 6:D:8:VAL:CG2 | 6:D:115:ARG:NH1 | 2.72 | 0.47 |
| 7:E:120:THR:CG2 | 7:E:121:LYS:N | 2.77 | 0.47 |
| 8:F:14:LEU:HB3 | 8:F:18:GLN:HB2 | 1.96 | 0.47 |
| 9:G:31:MET:SD | 9:G:34:GLY:HA2 | 2.55 | 0.47 |
| 9:G:43:PHE:O | 9:G:46:ALA:HB3 | 2.14 | 0.47 |
| 11:I:10:ARG:HG2 | 11:I:11:LYS:N | 2.29 | 0.47 |
| 18:P:67:THR:HG22 | 18:P:69:THR:N | 2.29 | 0.47 |
| 1:A:56:U:H2' | 1:A:57:G:C8 | 2.49 | 0.47 |
| 1:A:383:A:H2' | 1:A:384:G:H5' | 1.96 | 0.47 |
| 1:A:399:G:H2' | 1:A:400:C:C6 | 2.50 | 0.47 |
| 1:A:533:A:O2' | 1:A:534:U:P | 2.72 | 0.47 |
| 1:A:975:A:O2' | 16:N:32:SER:HA | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1056:U:C5' | 5:C:163:ALA:HB2 | 2.45 | 0.47 |
| 6:D:126:ILE:HG22 | 6:D:127:THR:N | 2.29 | 0.47 |
| 8:F:62:TRP:C | 8:F:63:TYR:HD2 | 2.17 | 0.47 |
| 13:K:108:ILE:O | 13:K:109:VAL:HG23 | 2.14 | 0.47 |
| 18:P:26:ARG:HD3 | 18:P:31:LYS:N | 2.28 | 0.47 |
| 1:A:411:A:N6 | 1:A:413:G:N2 | 2.63 | 0.47 |
| 1:A:1004:A:N7 | 1:A:1037:C:N3 | 2.61 | 0.47 |
| 1:A:1075:C:H5' | 4:B:103:THR:HG21 | 1.95 | 0.47 |
| 1:A:1176:A:H2' | 1:A:1177:G:H8 | 1.79 | 0.47 |
| 1:A:1277:C:HO2' | 1:A:1279:A:C1' | 2.27 | 0.47 |
| 4:B:15:VAL:HB | 4:B:210:SER:HB2 | 1.97 | 0.47 |
| 4:B:77:ALA:HB1 | 4:B:211:ILE:HG21 | 1.95 | 0.47 |
| 5:C:131:ARG:HG3 | 5:C:135:LYS:HE3 | 1.96 | 0.47 |
| 6:D:98:GLU:HG2 | 6:D:194:LEU:HD11 | 1.95 | 0.47 |
| 7:E:82:VAL:HG21 | 7:E:138:ALA:HA | 1.96 | 0.47 |
| 11:I:93:ARG:NH1 | 11:I:97:LYS:NZ | 2.62 | 0.47 |
| 18:P:3:LYS:HD2 | 18:P:24:ALA:HB2 | 1.95 | 0.47 |
| 20:R:34:TYR:O | 20:R:73:ALA:HB2 | 2.14 | 0.47 |
| 21:S:31:ILE:O | 21:S:32:LYS:HB3 | 2.14 | 0.47 |
| 1:A:781:A:H2' | 1:A:782:A:C5' | 2.44 | 0.47 |
| 1:A:1302:U:OP2 | 15:M:17:VAL:HG13 | 2.15 | 0.47 |
| 5:C:195:VAL:C | 5:C:196:LEU:HD23 | 2.35 | 0.47 |
| 7:E:102:ALA:HB1 | 7:E:120:THR:HG21 | 1.97 | 0.47 |
| 10:H:35:ILE:O | 10:H:39:LEU:HD22 | 2.14 | 0.47 |
| 11:I:10:ARG:O | 11:I:11:LYS:C | 2.52 | 0.47 |
| 18:P:43:LYS:HB3 | 18:P:48:TRP:CD1 | 2.50 | 0.47 |
| 19:Q:98:LEU:HA | 19:Q:102:GLY:HA2 | 1.96 | 0.47 |
| 1:A:427:U:OP2 | 6:D:36:ARG:NH2 | 2.47 | 0.47 |
| 1:A:920:U:H2' | 1:A:921:U:C6 | 2.49 | 0.47 |
| 1:A:979:C:N4 | 16:N:18:VAL:HG12 | 2.30 | 0.47 |
| 1:A:1300:G:O2' | 1:A:1301:U:P | 2.73 | 0.47 |
| 1:A:1501:C:OP2 | 1:A:1504:G:H2' | 2.15 | 0.47 |
| 4:B:231:GLU:CB | 4:B:232:PRO:CD | 2.89 | 0.47 |
| 5:C:15:THR:O | 5:C:16:ARG:CB | 2.62 | 0.47 |
| 5:C:113:ALA:HA | 5:C:202:ILE:HD11 | 1.97 | 0.47 |
| 5:C:132:ARG:O | 5:C:135:LYS:N | 2.48 | 0.47 |
| 6:D:36:ARG:N | 6:D:37:PRO:CD | 2.60 | 0.47 |
| 8:F:67:MET:HE1 | 8:F:72:VAL:HA | 1.96 | 0.47 |
| 11:I:10:ARG:HG2 | 11:I:10:ARG:HH11 | 1.78 | 0.47 |
| 12:J:60:ARG:HD2 | 12:J:60:ARG:N | 2.29 | 0.47 |
| 12:J:81:THR:C | 12:J:83:GLU:H | 2.18 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:K:34:ASP:HB2 | 13:K:35:PRO:HD2 | 1.95 | 0.47 |
| 15:M:31:LYS:O | 15:M:35:GLU:N | 2.46 | 0.47 |
| 1:A:921:U:H2' | 1:A:922:G:O4' | 2.15 | 0.47 |
| 1:A:1073:U:H2' | 1:A:1074:G:H8 | 1.80 | 0.47 |
| 1:A:1194:U:O2' | 1:A:1195:C:H5' | 2.15 | 0.47 |
| 1:A:1206:G:C6 | 1:A:1207:G:C6 | 3.03 | 0.47 |
| 1:A:1343:G:OP1 | 11:I:125:TYR:HE2 | 1.98 | 0.47 |
| 1:A:1439:C:H2' | 1:A:1440:C:C6 | 2.50 | 0.47 |
| 4:B:24:TRP:N | 4:B:24:TRP:CD1 | 2.83 | 0.47 |
| 5:C:72:LYS:HE2 | 5:C:75:VAL:HG21 | 1.97 | 0.47 |
| 6:D:35:ARG:O | 6:D:36:ARG:HB2 | 2.14 | 0.47 |
| 9:G:146:GLU:HA | 9:G:149:ARG:HD3 | 1.97 | 0.47 |
| 10:H:51:VAL:HG21 | 10:H:60:ARG:CG | 2.44 | 0.47 |
| 12:J:9:ARG:HB3 | 12:J:9:ARG:NH1 | 2.29 | 0.47 |
| 1:A:204:U:O5' | 1:A:204:U:H6 | 1.97 | 0.47 |
| 1:A:1226:C:C4 | 15:M:104:ARG:HG3 | 2.50 | 0.47 |
| 1:A:1232:U:P | 11:I:124:GLN:HE21 | 2.38 | 0.47 |
| 4:B:59:GLU:O | 4:B:63:MET:HG2 | 2.14 | 0.47 |
| 4:B:75:LYS:HA | 4:B:78:GLN:HB2 | 1.97 | 0.47 |
| 4:B:204:ASN:HD22 | 4:B:206:ASP:H | 1.61 | 0.47 |
| 5:C:35:GLU:O | 5:C:36:ASP:C | 2.53 | 0.47 |
| 5:C:180:ALA:HB1 | 5:C:203:PHE:CE1 | 2.49 | 0.47 |
| 6:D:173:TRP:HB2 | 6:D:187:ARG:O | 2.15 | 0.47 |
| 18:P:5:ARG:HH21 | 18:P:28:ARG:HA | 1.80 | 0.47 |
| 1:A:607:A:O2' | 1:A:608:A:H5' | 2.15 | 0.47 |
| 1:A:1042:G:O2' | 1:A:1043:C:H5' | 2.15 | 0.47 |
| 1:A:1066:C:O2' | 1:A:1067:A:H5' | 2.14 | 0.47 |
| 1:A:1244:C:O2' | 1:A:1245:A:H5' | 2.15 | 0.47 |
| 1:A:1347:G:O2' | 1:A:1348:U:OP2 | 2.33 | 0.47 |
| 4:B:194:PRO:O | 4:B:196:LEU:N | 2.48 | 0.47 |
| 6:D:19:LEU:HD22 | 6:D:67:ILE:CG1 | 2.45 | 0.47 |
| 6:D:70:ILE:HG23 | 6:D:74:GLN:HB2 | 1.97 | 0.47 |
| 7:E:43:LEU:HD11 | 7:E:132:ALA:HB1 | 1.96 | 0.47 |
| 11:I:48:GLU:N | 11:I:49:PRO:CD | 2.78 | 0.47 |
| 17:O:63:ARG:O | 17:O:66:LEU:N | 2.47 | 0.47 |
| 18:P:21:VAL:HG21 | 18:P:59:TRP:CG | 2.50 | 0.47 |
| 1:A:327:A:O3' | 1:A:328:C:H4' | 2.15 | 0.46 |
| 1:A:408:A:O2' | 1:A:409:G:H5' | 2.15 | 0.46 |
| 1:A:485:G:O2' | 1:A:486:U:OP2 | 2.33 | 0.46 |
| 1:A:603:U:H2' | 1:A:604:G:H8 | 1.80 | 0.46 |
| 1:A:922:G:H5' | 7:E:19:MET:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1017:G:H2' | 1:A:1018:C:C6 | 2.50 | 0.46 |
| 1:A:1111:A:N6 | 5:C:177:THR:HA | 2.30 | 0.46 |
| 1:A:1372:U:O2' | 1:A:1373:G:H5' | 2.15 | 0.46 |
| 6:D:61:LYS:NZ | 6:D:62:GLN:NE2 | 2.63 | 0.46 |
| 8:F:2:ARG:CD | 8:F:69:GLU:HG2 | 2.45 | 0.46 |
| 11:I:93:ARG:CD | 11:I:97:LYS:HZ1 | 2.17 | 0.46 |
| 13:K:26:ASN:O | 13:K:27:ASN:HB2 | 2.15 | 0.46 |
| 13:K:33:THR:HB | 13:K:38:ASN:C | 2.35 | 0.46 |
| 13:K:57:THR:HG22 | 13:K:60:ALA:HB2 | 1.97 | 0.46 |
| 15:M:23:TYR:CB | 15:M:67:GLU:HA | 2.46 | 0.46 |
| 22:T:100:ILE:O | 22:T:101:GLY:C | 2.53 | 0.46 |
| 1:A:376:G:O3' | 18:P:5:ARG:HD2 | 2.16 | 0.46 |
| 1:A:946:A:H2' | 1:A:947:G:H8 | 1.73 | 0.46 |
| 1:A:1481:U:H2' | 1:A:1482:G:O4' | 2.15 | 0.46 |
| 4:B:227:GLY:C | 4:B:229:VAL:H | 2.18 | 0.46 |
| 5:C:167:TRP:O | 5:C:168:ALA:HB3 | 2.15 | 0.46 |
| 13:K:74:ALA:C | 13:K:76:GLY:N | 2.69 | 0.46 |
| 14:L:51:ALA:O | 14:L:52:LEU:HD23 | 2.15 | 0.46 |
| 15:M:59:TYR:CD1 | 15:M:59:TYR:C | 2.88 | 0.46 |
| 18:P:9:PHE:CD2 | 18:P:18:ARG:HG3 | 2.51 | 0.46 |
| 18:P:82:GLN:O | 18:P:83:GLU:C | 2.53 | 0.46 |
| 21:S:30:LEU:C | 21:S:31:ILE:HD13 | 2.36 | 0.46 |
| 21:S:41:VAL:CG1 | 21:S:42:PRO:CD | 2.92 | 0.46 |
| 1:A:1060:C:O2 | 1:A:1198:G:C2 | 2.68 | 0.46 |
| 1:A:1060:C:H5 | 5:C:2:GLY:HA3 | 1.78 | 0.46 |
| 1:A:1125:U:H3 | 12:J:5:ARG:NE | 2.14 | 0.46 |
| 5:C:145:GLY:O | 5:C:146:ALA:CB | 2.64 | 0.46 |
| 5:C:174:PRO:HB2 | 5:C:177:THR:CG2 | 2.41 | 0.46 |
| 7:E:18:ARG:NE | 7:E:25:ARG:HB2 | 2.30 | 0.46 |
| 9:G:23:VAL:HG13 | 9:G:43:PHE:CE2 | 2.51 | 0.46 |
| 9:G:141:VAL:O | 9:G:144:MET:N | 2.48 | 0.46 |
| 12:J:48:THR:HG23 | 12:J:62:HIS:CD2 | 2.50 | 0.46 |
| 14:L:75:HIS:HD2 | 14:L:77:LEU:N | 2.11 | 0.46 |
| 1:A:113:G:C1' | 1:A:354:G:H5' | 2.44 | 0.46 |
| 1:A:1190:G:P | 5:C:5:ILE:HG13 | 2.56 | 0.46 |
| 1:A:1206:G:H1' | 5:C:193:TYR:O | 2.16 | 0.46 |
| 1:A:1406:U:OP2 | 24:A:1545:PAR:N24 | 2.43 | 0.46 |
| 5:C:5:ILE:HD12 | 5:C:5:ILE:H | 1.80 | 0.46 |
| 9:G:50:ILE:O | 9:G:50:ILE:HG22 | 2.16 | 0.46 |
| 9:G:51:GLN:C | 9:G:53:LYS:N | 2.68 | 0.46 |
| 9:G:78:ARG:HD2 | 9:G:156:TRP:CE3 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:H:104:ARG:O | 10:H:105:ARG:C | 2.54 | 0.46 |
| 12:J:38:ILE:HD12 | 12:J:71:LEU:CD1 | 2.46 | 0.46 |
| 14:L:93:LEU:O | 14:L:96:VAL:HG23 | 2.15 | 0.46 |
| 20:R:18:ARG:NE | 20:R:18:ARG:HA | 2.30 | 0.46 |
| 1:A:28:G:O2' | 1:A:296:U:OP1 | 2.33 | 0.46 |
| 1:A:359:U:O2' | 1:A:360:A:H5' | 2.16 | 0.46 |
| 1:A:628:G:O2' | 1:A:629:G:H5' | 2.15 | 0.46 |
| 1:A:769:G:H4' | 1:A:1513:A:H4' | 1.97 | 0.46 |
| 1:A:1229:A:H2' | 1:A:1230:C:C6 | 2.51 | 0.46 |
| 5:C:134:ILE:CG2 | 5:C:168:ALA:HB3 | 2.46 | 0.46 |
| 5:C:170:GLN:O | 5:C:171:GLY:O | 2.33 | 0.46 |
| 7:E:89:ILE:HD13 | 7:E:90:VAL:N | 2.30 | 0.46 |
| 8:F:1:MET:CE | 8:F:1:MET:H3 | 2.27 | 0.46 |
| 14:L:59:ARG:NH2 | 14:L:65:GLU:HB3 | 2.31 | 0.46 |
| 15:M:20:THR:C | 15:M:22:ILE:H | 2.18 | 0.46 |
| 22:T:13:LEU:HD12 | 22:T:13:LEU:N | 2.13 | 0.46 |
| 1:A:179:A:H2' | 1:A:180:U:C6 | 2.51 | 0.46 |
| 1:A:333:G:H4' | 22:T:16:HIS:NE2 | 2.30 | 0.46 |
| 1:A:636:U:H2' | 1:A:637:G:C8 | 2.50 | 0.46 |
| 1:A:760:G:H2' | 1:A:761:G:H5' | 1.98 | 0.46 |
| 1:A:967:C:O3' | 11:I:128:ARG:NH2 | 2.49 | 0.46 |
| 1:A:1320:C:C2 | 21:S:72:GLY:HA3 | 2.51 | 0.46 |
| 1:A:1441:G:H4' | 1:A:1442:G:C4 | 2.51 | 0.46 |
| 1:A:1478:C:O2' | 1:A:1479:C:H5' | 2.15 | 0.46 |
| 4:B:84:GLU:HB3 | 4:B:219:VAL:CG2 | 2.37 | 0.46 |
| 4:B:116:GLU:HA | 4:B:119:GLU:CG | 2.45 | 0.46 |
| 4:B:212:GLN:NE2 | 4:B:216:SER:HB2 | 2.31 | 0.46 |
| 6:D:163:GLU:HA | 6:D:163:GLU:OE2 | 2.15 | 0.46 |
| 10:H:63:LEU:HD22 | 10:H:63:LEU:N | 2.30 | 0.46 |
| 12:J:42:THR:HG21 | 12:J:66:ARG:HB2 | 1.98 | 0.46 |
| 15:M:36:LYS:CB | 15:M:59:TYR:HE2 | 2.29 | 0.46 |
| 19:Q:48:GLU:O | 19:Q:49:GLU:C | 2.53 | 0.46 |
| 19:Q:69:LYS:C | 19:Q:70:ARG:HG3 | 2.35 | 0.46 |
| 22:T:26:ASN:OD1 | 22:T:71:THR:HG23 | 2.16 | 0.46 |
| 22:T:26:ASN:HA | 22:T:71:THR:HG23 | 1.97 | 0.46 |
| 1:A:203:U:H4' | 1:A:204:U:OP1 | 2.16 | 0.46 |
| 1:A:674:G:H2' | 1:A:675:A:C8 | 2.51 | 0.46 |
| 1:A:1296:C:H4' | 1:A:1302:U:C5 | 2.51 | 0.46 |
| 8:F:2:ARG:HD2 | 8:F:69:GLU:HG2 | 1.96 | 0.46 |
| 10:H:9:MET:SD | 10:H:32:LYS:HB3 | 2.55 | 0.46 |
| 11:I:104:ARG:O | 11:I:105:ASP:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:J:9:ARG:NH1 | 12:J:9:ARG:CB | 2.78 | 0.46 |
| 14:L:119:LYS:O | 14:L:120:TYR:CB | 2.63 | 0.46 |
| 22:T:74:LYS:HB3 | 22:T:75:ASN:H | 1.48 | 0.46 |
| 1:A:6:G:H4' | 1:A:298:A:H4' | 1.98 | 0.46 |
| 1:A:528:C:N4 | 14:L:49:ASN:HD21 | 2.14 | 0.46 |
| 1:A:1053:G:O2' | 1:A:1199:U:H5 | 1.99 | 0.46 |
| 4:B:32:ILE:HD13 | 4:B:40:HIS:CD2 | 2.51 | 0.46 |
| 5:C:147:LYS:HE3 | 5:C:203:PHE:CE2 | 2.51 | 0.46 |
| 6:D:62:GLN:NE2 | 6:D:62:GLN:HA | 2.31 | 0.46 |
| 6:D:109:GLY:C | 6:D:111:ALA:N | 2.69 | 0.46 |
| 8:F:30:LEU:HB3 | 8:F:35:ALA:HB3 | 1.98 | 0.46 |
| 11:I:89:ASN:O | 11:I:92:TYR:HB2 | 2.16 | 0.46 |
| 15:M:108:ARG:HD3 | 15:M:114:ARG:NH1 | 2.31 | 0.46 |
| 18:P:7:ALA:O | 18:P:17:TYR:HA | 2.15 | 0.46 |
| 19:Q:70:ARG:HH11 | 19:Q:70:ARG:CG | 2.29 | 0.46 |
| 19:Q:97:SER:C | 19:Q:99:SER:H | 2.14 | 0.46 |
| 22:T:95:ALA:O | 22:T:96:GLY:C | 2.54 | 0.46 |
| 1:A:413:G:H2' | 1:A:428:G:H22 | 1.79 | 0.46 |
| 1:A:848:C:H2' | 1:A:849:C:C6 | 2.50 | 0.46 |
| 1:A:1353:G:O2' | 1:A:1354:C:H5' | 2.15 | 0.46 |
| 1:A:1381:U:C2' | 1:A:1382:C:H5' | 2.46 | 0.46 |
| 5:C:88:ARG:HG3 | 5:C:101:LEU:CD1 | 2.45 | 0.46 |
| 5:C:156:ARG:NH2 | 5:C:161:GLU:HA | 2.31 | 0.46 |
| 9:G:145:ALA:O | 9:G:146:GLU:CB | 2.63 | 0.46 |
| 17:O:70:LEU:C | 17:O:72:ARG:H | 2.19 | 0.46 |
| 20:R:87:ARG:HB3 | 20:R:88:LYS:H | 1.49 | 0.46 |
| 1:A:1183:A:O2' | 1:A:1184:G:P | 2.74 | 0.46 |
| 1:A:1230:C:O2' | 1:A:1231:G:H5' | 2.16 | 0.46 |
| 1:A:1441:G:H1' | 1:A:1460:A:H61 | 1.81 | 0.46 |
| 1:A:1495:U:H2' | 1:A:1496:C:H6 | 1.80 | 0.46 |
| 6:D:100:ARG:HH12 | 6:D:137:SER:CB | 2.29 | 0.46 |
| 9:G:79:ARG:HH12 | 9:G:82:GLY:HA2 | 1.80 | 0.46 |
| 11:I:8:GLY:CA | 11:I:79:LEU:HB3 | 2.46 | 0.46 |
| 11:I:111:ARG:HD3 | 11:I:112:LYS:O | 2.16 | 0.46 |
| 14:L:75:HIS:HA | 14:L:102:ARG:HH22 | 1.80 | 0.46 |
| 16:N:11:LYS:O | 16:N:13:THR:N | 2.48 | 0.46 |
| 21:S:40:ILE:CD1 | 21:S:62:ILE:HD11 | 2.46 | 0.46 |
| 1:A:102:G:N3 | 1:A:151:A:H2 | 2.14 | 0.45 |
| 1:A:190(H):G:O2' | 1:A:190(I):G:H5' | 2.16 | 0.45 |
| 1:A:244:U:O4 | 1:A:906:G:H1' | 2.16 | 0.45 |
| 1:A:813:U:OP1 | 1:A:904:C:H5' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1053:G:C4 | 1:A:1199:U:C5 | 3.04 | 0.45 |
| 1:A:1225:A:H2' | 1:A:1225:A:N3 | 2.31 | 0.45 |
| 1:A:1256:A:H5' | 1:A:1258:G:O4' | 2.16 | 0.45 |
| 1:A:1451:A:O2' | 1:A:1452:C:OP1 | 2.31 | 0.45 |
| 5:C:50:ALA:HB1 | 5:C:70:VAL:CG1 | 2.37 | 0.45 |
| 5:C:83:ARG:HA | 5:C:86:VAL:CG2 | 2.44 | 0.45 |
| 5:C:129:ALA:CB | 5:C:132:ARG:HH12 | 2.28 | 0.45 |
| 6:D:24:GLU:CG | 6:D:25:ARG:N | 2.79 | 0.45 |
| 6:D:26:CYS:HA | 6:D:31:CYS:HB2 | 1.98 | 0.45 |
| 9:G:32:ARG:O | 9:G:33:ASP:HB2 | 2.16 | 0.45 |
| 10:H:3:THR:HG23 | 10:H:4:ASP:H | 1.81 | 0.45 |
| 10:H:41:ARG:NH1 | 10:H:123:GLU:OE2 | 2.49 | 0.45 |
| 10:H:45:ILE:C | 10:H:47:GLY:N | 2.70 | 0.45 |
| 11:I:48:GLU:HA | 11:I:51:ARG:NH1 | 2.31 | 0.45 |
| 14:L:47:LYS:HG2 | 14:L:48:PRO:HD3 | 1.98 | 0.45 |
| 14:L:114:LYS:HE3 | 14:L:114:LYS:CA | 2.44 | 0.45 |
| 22:T:16:HIS:O | 22:T:17:ARG:C | 2.53 | 0.45 |
| 1:A:780:A:C2 | 1:A:801:U:C5 | 3.04 | 0.45 |
| 1:A:1439:C:OP2 | 22:T:38:LYS:NZ | 2.49 | 0.45 |
| 1:A:1542:U:H2' | 1:A:1543:C:O4' | 2.16 | 0.45 |
| 4:B:76:GLN:NE2 | 4:B:207:ALA:H | 2.10 | 0.45 |
| 4:B:77:ALA:O | 4:B:81:VAL:HG23 | 2.17 | 0.45 |
| 5:C:88:ARG:HG3 | 5:C:101:LEU:HD13 | 1.99 | 0.45 |
| 6:D:208:SER:O | 6:D:209:ARG:C | 2.55 | 0.45 |
| 11:I:5:TYR:CG | 11:I:6:GLY:N | 2.84 | 0.45 |
| 11:I:50:LEU:C | 11:I:52:ALA:H | 2.19 | 0.45 |
| 13:K:12:ARG:O | 13:K:13:GLN:C | 2.54 | 0.45 |
| 13:K:106:LYS:HA | 13:K:106:LYS:CE | 2.44 | 0.45 |
| 15:M:59:TYR:C | 15:M:59:TYR:HD1 | 2.19 | 0.45 |
| 19:Q:86:GLU:O | 19:Q:87:LYS:C | 2.51 | 0.45 |
| 20:R:53:ARG:NH1 | 20:R:60:GLY:N | 2.64 | 0.45 |
| 1:A:46:G:O2' | 1:A:365:U:H1' | 2.16 | 0.45 |
| 1:A:190(J):U:H2' | 1:A:190(K):G:C8 | 2.52 | 0.45 |
| 1:A:556:C:H2' | 1:A:557:G:H5' | 1.99 | 0.45 |
| 1:A:683:G:H21 | 13:K:38:ASN:ND2 | 2.14 | 0.45 |
| 1:A:1178:G:P | 11:I:97:LYS:NZ | 2.90 | 0.45 |
| 1:A:1349:A:H2' | 1:A:1350:A:H8 | 1.81 | 0.45 |
| 4:B:44:LEU:HA | 4:B:47:THR:OG1 | 2.16 | 0.45 |
| 5:C:62:ASP:HA | 5:C:97:LYS:HB3 | 1.99 | 0.45 |
| 6:D:33:MET:HE3 | 6:D:37:PRO:HB3 | 1.98 | 0.45 |
| 6:D:62:GLN:NE2 | 6:D:65:ARG:NH1 | 2.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:F:98:LEU:HD12 | 8:F:98:LEU:N | 2.32 | 0.45 |
| 11:I:58:ARG:HH11 | 11:I:58:ARG:HG3 | 1.80 | 0.45 |
| 16:N:4:LYS:O | 16:N:7:ILE:HG12 | 2.17 | 0.45 |
| 22:T:45:GLN:HB2 | 22:T:91:LEU:HD13 | 1.98 | 0.45 |
| 1:A:340:U:H2' | 1:A:341:C:C6 | 2.51 | 0.45 |
| 1:A:501:C:OP1 | 14:L:117:ARG:NH2 | 2.50 | 0.45 |
| 1:A:564:C:C2 | 19:Q:31:LEU:HD11 | 2.52 | 0.45 |
| 1:A:1044:A:C2' | 1:A:1045:C:H5' | 2.47 | 0.45 |
| 4:B:17:PHE:HD1 | 4:B:18:GLY:N | 2.14 | 0.45 |
| 4:B:153:ARG:HG2 | 4:B:153:ARG:HH11 | 1.82 | 0.45 |
| 5:C:82:GLU:O | 5:C:85:ARG:HB3 | 2.17 | 0.45 |
| 5:C:115:LEU:O | 5:C:119:ARG:N | 2.47 | 0.45 |
| 8:F:98:LEU:HD23 | 20:R:28:GLU:OE1 | 2.17 | 0.45 |
| 10:H:48:TYR:HB2 | 10:H:60:ARG:O | 2.17 | 0.45 |
| 11:I:20:ARG:HH12 | 11:I:62:TYR:HB3 | 1.81 | 0.45 |
| 11:I:48:GLU:CD | 11:I:51:ARG:HH12 | 2.19 | 0.45 |
| 14:L:83:VAL:CG1 | 14:L:100:ILE:HG23 | 2.44 | 0.45 |
| 1:A:448:A:H2' | 1:A:449:C:C6 | 2.52 | 0.45 |
| 1:A:1044:A:H2' | 1:A:1045:C:H5' | 1.99 | 0.45 |
| 1:A:1056:U:H5' | 5:C:163:ALA:HB3 | 1.96 | 0.45 |
| 1:A:1138:G:H3' | 1:A:1138:G:N3 | 2.32 | 0.45 |
| 1:A:1206:G:C6 | 1:A:1207:G:C5 | 3.05 | 0.45 |
| 7:E:18:ARG:NH2 | 7:E:25:ARG:HB3 | 2.30 | 0.45 |
| 11:I:77:ILE:HG22 | 11:I:78:LYS:N | 2.32 | 0.45 |
| 14:L:33:ARG:HG2 | 14:L:62:SER:HB3 | 1.99 | 0.45 |
| 15:M:59:TYR:CD1 | 15:M:63:THR:HG21 | 2.52 | 0.45 |
| 15:M:115:LYS:HD3 | 15:M:115:LYS:N | 2.31 | 0.45 |
| 20:R:54:ARG:H | 20:R:54:ARG:HG3 | 1.56 | 0.45 |
| 1:A:133:U:P | 22:T:74:LYS:HE3 | 2.56 | 0.45 |
| 1:A:258:G:H2' | 1:A:259:G:H8 | 1.81 | 0.45 |
| 1:A:458:C:H2' | 1:A:459:G:C8 | 2.52 | 0.45 |
| 1:A:491:G:O2' | 1:A:492:G:H5' | 2.16 | 0.45 |
| 1:A:716:A:N3 | 13:K:117:ASN:O | 2.50 | 0.45 |
| 1:A:1129:C:O2' | 1:A:1131:G:C8 | 2.66 | 0.45 |
| 1:A:1283:G:O2' | 1:A:1284:C:H5' | 2.17 | 0.45 |
| 1:A:1292:U:P | 9:G:41:ARG:NH2 | 2.88 | 0.45 |
| 4:B:24:TRP:CG | 4:B:25:ASN:N | 2.80 | 0.45 |
| 4:B:86:GLU:C | 4:B:88:ALA:N | 2.69 | 0.45 |
| 5:C:35:GLU:CG | 5:C:59:ARG:HH22 | 2.21 | 0.45 |
| 5:C:87:LEU:C | 5:C:89:GLU:H | 2.18 | 0.45 |
| 5:C:135:LYS:HE2 | 7:E:50:GLU:OE1 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:F:22:GLU:OE1 | 8:F:22:GLU:HA | 2.17 | 0.45 |
| 9:G:75:VAL:CG1 | 9:G:86:GLN:HB3 | 2.47 | 0.45 |
| 10:H:68:ARG:HG2 | 10:H:68:ARG:NH1 | 2.30 | 0.45 |
| 15:M:105:THR:HB | 15:M:106:ASN:H | 1.64 | 0.45 |
| 1:A:129(A):G:O2' | 1:A:130:A:OP2 | 2.35 | 0.45 |
| 1:A:484:G:O2' | 1:A:485:G:OP2 | 2.30 | 0.45 |
| 1:A:1289:A:H2' | 1:A:1290:G:H5' | 1.99 | 0.45 |
| 1:A:1320:C:H2' | 1:A:1321:C:O4' | 2.17 | 0.45 |
| 1:A:1435:G:H2' | 1:A:1436:U:H6 | 1.79 | 0.45 |
| 4:B:23:ARG:C | 4:B:23:ARG:HD3 | 2.37 | 0.45 |
| 5:C:83:ARG:C | 5:C:85:ARG:N | 2.67 | 0.45 |
| 6:D:162:LEU:HD12 | 6:D:181:MET:CE | 2.47 | 0.45 |
| 9:G:66:VAL:HG12 | 9:G:70:LYS:HE3 | 1.98 | 0.45 |
| 11:I:25:LYS:O | 11:I:60:ASP:OD1 | 2.35 | 0.45 |
| 14:L:46:LYS:HG3 | 14:L:47:LYS:N | 2.32 | 0.45 |
| 18:P:18:ARG:HD3 | 18:P:35:LYS:HD2 | 1.99 | 0.45 |
| 19:Q:97:SER:H | 19:Q:103:GLY:CA | 2.25 | 0.45 |
| 21:S:22:LEU:CD2 | 21:S:28:LYS:HD2 | 2.45 | 0.45 |
| 23:V:14:TRP:C | 23:V:16:GLY:H | 2.19 | 0.45 |
| 1:A:482:A:H2' | 1:A:483:C:O4' | 2.16 | 0.45 |
| 1:A:554:C:H2' | 1:A:555:C:H6 | 1.81 | 0.45 |
| 1:A:664:G:OP1 | 20:R:64:ARG:HD2 | 2.17 | 0.45 |
| 1:A:718:G:H5' | 1:A:719:C:OP2 | 2.17 | 0.45 |
| 1:A:963:G:HO2' | 12:J:54:PHE:HZ | 1.63 | 0.45 |
| 1:A:1278:U:H5" | 1:A:1279:A:H5' | 1.99 | 0.45 |
| 1:A:1313:U:O4 | 21:S:4:SER:HB2 | 2.16 | 0.45 |
| 1:A:1496:C:H2' | 1:A:1497:G:O4' | 2.17 | 0.45 |
| 4:B:206:ASP:CG | 4:B:207:ALA:H | 2.20 | 0.45 |
| 5:C:38:ARG:HH11 | 5:C:38:ARG:HG3 | 1.82 | 0.45 |
| 7:E:76:ILE:HG23 | 7:E:142:LEU:HD22 | 1.98 | 0.45 |
| 7:E:78:HIS:CD2 | 10:H:107:LEU:HD12 | 2.52 | 0.45 |
| 8:F:14:LEU:CA | 8:F:18:GLN:HE21 | 2.29 | 0.45 |
| 11:I:9:ARG:HG2 | 11:I:14:VAL:HA | 1.99 | 0.45 |
| 12:J:6:ILE:HD11 | 12:J:72:VAL:CG1 | 2.47 | 0.45 |
| 1:A:262:A:C6 | 1:A:263:A:C6 | 3.04 | 0.45 |
| 1:A:279:A:H5' | 1:A:281:G:H5' | 1.99 | 0.45 |
| 1:A:379:C:O2' | 1:A:380:G:H5' | 2.17 | 0.45 |
| 1:A:542:G:O2' | 1:A:543:C:H5' | 2.17 | 0.45 |
| 1:A:1143:G:H2' | 1:A:1144:G:C8 | 2.52 | 0.45 |
| 5:C:56:ASP:OD1 | 5:C:56:ASP:N | 2.49 | 0.45 |
| 6:D:35:ARG:O | 6:D:36:ARG:CB | 2.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:D:58:LEU:O | 6:D:58:LEU:HD22 | 2.16 | 0.45 |
| 8:F:86:ARG:HG2 | 8:F:86:ARG:NH1 | 2.31 | 0.45 |
| 9:G:111:ARG:NH2 | 9:G:126:ASP:OD2 | 2.49 | 0.45 |
| 11:I:8:GLY:HA3 | 11:I:79:LEU:HB3 | 1.98 | 0.45 |
| 11:I:50:LEU:C | 11:I:52:ALA:N | 2.70 | 0.45 |
| 12:J:90:LEU:H | 12:J:91:PRO:HD2 | 1.82 | 0.45 |
| 18:P:42:ARG:O | 18:P:43:LYS:C | 2.56 | 0.45 |
| 21:S:49:ILE:HD12 | 21:S:49:ILE:H | 1.81 | 0.45 |
| 1:A:101:A:O2' | 1:A:102:G:H5' | 2.18 | 0.45 |
| 1:A:116:A:H2' | 1:A:117:G:O4' | 2.17 | 0.45 |
| 1:A:299:G:H2' | 1:A:300:A:C8 | 2.52 | 0.45 |
| 1:A:428:G:O2' | 1:A:429:U:P | 2.75 | 0.45 |
| 1:A:686:U:HO2' | 1:A:687:A:H8 | 1.64 | 0.45 |
| 1:A:820:U:H4' | 1:A:821:G:OP2 | 2.17 | 0.45 |
| 1:A:982:U:H5" | 16:N:6:LEU:CD1 | 2.47 | 0.45 |
| 1:A:1014:A:H2' | 1:A:1015:A:C8 | 2.52 | 0.45 |
| 1:A:1072:G:O6 | 1:A:1102:A:N6 | 2.50 | 0.45 |
| 1:A:1372:U:OP2 | 11:I:11:LYS:HD3 | 2.17 | 0.45 |
| 8:F:10:LEU:HD12 | 8:F:59:TYR:O | 2.16 | 0.45 |
| 12:J:60:ARG:O | 12:J:61:GLU:CB | 2.65 | 0.45 |
| 16:N:3:ARG:NH2 | 16:N:6:LEU:CD1 | 2.80 | 0.45 |
| 18:P:43:LYS:HA | 18:P:48:TRP:CB | 2.47 | 0.45 |
| 22:T:68:LYS:HD2 | 22:T:68:LYS:HA | 1.69 | 0.45 |
| 1:A:252:U:H2' | 1:A:253:U:C6 | 2.51 | 0.44 |
| 1:A:394:G:H2' | 1:A:395:C:H6 | 1.82 | 0.44 |
| 1:A:828:A:H5" | 1:A:859:A:C2 | 2.53 | 0.44 |
| 1:A:1250:A:C5' | 11:I:68:GLY:N | 2.79 | 0.44 |
| 1:A:1367:C:C2 | 1:A:1368:G:C8 | 3.05 | 0.44 |
| 4:B:142:LEU:O | 4:B:143:GLU:C | 2.55 | 0.44 |
| 5:C:11:ARG:O | 5:C:14:ILE:O | 2.34 | 0.44 |
| 5:C:34:LEU:HD21 | 5:C:38:ARG:NH1 | 2.32 | 0.44 |
| 5:C:60:ALA:O | 5:C:61:ALA:HB3 | 2.17 | 0.44 |
| 6:D:117:ALA:O | 6:D:121:VAL:HG23 | 2.17 | 0.44 |
| 6:D:128:VAL:HG12 | 6:D:129:ASN:ND2 | 2.32 | 0.44 |
| 7:E:60:TYR:CE1 | 7:E:64:ARG:NH2 | 2.84 | 0.44 |
| 12:J:47:PHE:CZ | 16:N:37:PHE:HE1 | 2.35 | 0.44 |
| 15:M:16:ASP:OD1 | 15:M:16:ASP:N | 2.50 | 0.44 |
| 16:N:24:CYS:HB2 | 16:N:40:CYS:HB3 | 1.98 | 0.44 |
| 18:P:8:ARG:HB2 | 18:P:28:ARG:NH1 | 2.32 | 0.44 |
| 1:A:130:A:H1' | 1:A:263:A:O2' | 2.16 | 0.44 |
| 1:A:255:G:O6 | 1:A:266:G:O6 | 2.35 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:335:C:H2' | 1:A:336:C:H6 | 1.81 | 0.44 |
| 1:A:382:A:C2 | 1:A:383:A:C4 | 3.05 | 0.44 |
| 1:A:666:G:H5' | 1:A:726:C:H1' | 1.99 | 0.44 |
| 1:A:1053:G:O3' | 1:A:1054:C:H4' | 2.17 | 0.44 |
| 1:A:1168:A:C6 | 1:A:1169:A:C6 | 3.05 | 0.44 |
| 1:A:1176:A:O2' | 1:A:1177:G:H5' | 2.16 | 0.44 |
| 1:A:1508:G:O2' | 1:A:1509:C:H5' | 2.17 | 0.44 |
| 7:E:51:VAL:O | 7:E:54:ALA:HB3 | 2.17 | 0.44 |
| 9:G:15:ASP:O | 9:G:19:GLY:HA2 | 2.17 | 0.44 |
| 9:G:65:ALA:HB1 | 9:G:127:ALA:HB3 | 1.99 | 0.44 |
| 15:M:37:THR:O | 15:M:55:ARG:NH1 | 2.47 | 0.44 |
| 17:O:21:ASP:OD2 | 17:O:24:SER:HB3 | 2.17 | 0.44 |
| 1:A:265:G:H2' | 1:A:267:C:H5 | 1.83 | 0.44 |
| 1:A:974:A:P | 16:N:41:ARG:HH12 | 2.39 | 0.44 |
| 4:B:9:GLU:C | 4:B:10:LEU:HD23 | 2.38 | 0.44 |
| 4:B:230:VAL:CG1 | 4:B:231:GLU:N | 2.80 | 0.44 |
| 8:F:97:PHE:CB | 20:R:32:ARG:HH21 | 2.30 | 0.44 |
| 9:G:41:ARG:O | 9:G:42:ILE:C | 2.56 | 0.44 |
| 11:I:77:ILE:O | 11:I:78:LYS:C | 2.56 | 0.44 |
| 11:I:127:LYS:HA | 11:I:127:LYS:HZ2 | 1.82 | 0.44 |
| 12:J:86:MET:C | 12:J:86:MET:HE3 | 2.38 | 0.44 |
| 14:L:59:ARG:HA | 14:L:59:ARG:HE | 1.82 | 0.44 |
| 22:T:90:GLN:O | 22:T:93:GLU:HG2 | 2.17 | 0.44 |
| 1:A:46:G:H2' | 1:A:366:C:H41 | 1.82 | 0.44 |
| 1:A:216:G:H2' | 1:A:217:C:H6 | 1.81 | 0.44 |
| 1:A:673:G:H5" | 8:F:87:ARG:NH1 | 2.33 | 0.44 |
| 1:A:833:U:H2' | 1:A:834:C:C6 | 2.52 | 0.44 |
| 1:A:976:G:OP1 | 16:N:32:SER:N | 2.43 | 0.44 |
| 1:A:1223:C:OP1 | 21:S:78:ARG:NH1 | 2.51 | 0.44 |
| 1:A:1223:C:H3' | 1:A:1224:G:H5" | 1.99 | 0.44 |
| 5:C:5:ILE:H | 5:C:5:ILE:CD1 | 2.31 | 0.44 |
| 5:C:126:ARG:O | 5:C:127:ARG:CB | 2.62 | 0.44 |
| 5:C:134:ILE:HG22 | 5:C:168:ALA:CB | 2.48 | 0.44 |
| 5:C:188:LEU:HB3 | 5:C:189:ALA:H | 1.57 | 0.44 |
| 6:D:7:PRO:O | 6:D:10:ARG:HD2 | 2.18 | 0.44 |
| 6:D:146:ILE:N | 6:D:146:ILE:CD1 | 2.79 | 0.44 |
| 7:E:60:TYR:O | 7:E:64:ARG:HG2 | 2.17 | 0.44 |
| 10:H:126:LYS:C | 10:H:128:GLY:N | 2.71 | 0.44 |
| 22:T:12:ALA:C | 22:T:14:LYS:N | 2.69 | 0.44 |
| 1:A:191:G:N3 | 22:T:105:SER:HB3 | 2.32 | 0.44 |
| 1:A:528:C:N4 | 14:L:49:ASN:ND2 | 2.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:718:G:H1' | 13:K:116:HIS:HA | 1.99 | 0.44 |
| 1:A:783:C:O2' | 1:A:784:C:H5' | 2.17 | 0.44 |
| 1:A:895:G:H2' | 1:A:896:C:H6 | 1.80 | 0.44 |
| 1:A:962:C:H2' | 1:A:963:G:O4' | 2.18 | 0.44 |
| 1:A:979:C:H42 | 16:N:18:VAL:HG12 | 1.83 | 0.44 |
| 1:A:1163:C:H2' | 1:A:1164:G:C8 | 2.52 | 0.44 |
| 1:A:1316:G:N2 | 1:A:1318:A:H3' | 2.31 | 0.44 |
| 1:A:1329:A:P | 15:M:28:ALA:HB3 | 2.58 | 0.44 |
| 4:B:213:LEU:HD23 | 4:B:213:LEU:C | 2.37 | 0.44 |
| 5:C:3:ASN:O | 5:C:4:LYS:HB2 | 2.17 | 0.44 |
| 6:D:175:SER:OG | 6:D:184:LYS:HB2 | 2.17 | 0.44 |
| 7:E:51:VAL:HB | 7:E:52:PRO:CD | 2.42 | 0.44 |
| 8:F:12:PRO:HD3 | 8:F:58:GLY:HA2 | 2.00 | 0.44 |
| 12:J:65:LEU:O | 12:J:65:LEU:HG | 2.18 | 0.44 |
| 13:K:14:VAL:O | 13:K:14:VAL:HG12 | 2.18 | 0.44 |
| 13:K:34:ASP:C | 13:K:34:ASP:OD1 | 2.56 | 0.44 |
| 14:L:117:ARG:O | 14:L:119:LYS:O | 2.36 | 0.44 |
| 14:L:125:PRO:C | 14:L:127:GLU:H | 2.21 | 0.44 |
| 15:M:36:LYS:HB2 | 15:M:59:TYR:CE2 | 2.48 | 0.44 |
| 20:R:47:THR:O | 20:R:49:LYS:N | 2.50 | 0.44 |
| 22:T:13:LEU:H | 22:T:13:LEU:CD1 | 2.06 | 0.44 |
| 1:A:22:G:H2' | 1:A:23:C:C6 | 2.53 | 0.44 |
| 1:A:153:C:O2' | 1:A:154:C:H5' | 2.18 | 0.44 |
| 1:A:406:G:H2' | 1:A:407:G:C8 | 2.50 | 0.44 |
| 1:A:1123:A:H2 | 12:J:39:PRO:HG3 | 1.83 | 0.44 |
| 1:A:1191:A:H2' | 1:A:1192:C:C6 | 2.53 | 0.44 |
| 5:C:52:LEU:CD2 | 5:C:52:LEU:N | 2.80 | 0.44 |
| 7:E:19:MET:O | 7:E:20:GLN:NE2 | 2.51 | 0.44 |
| 7:E:78:HIS:HD2 | 10:H:107:LEU:HD12 | 1.82 | 0.44 |
| 7:E:80:ILE:HD12 | 7:E:80:ILE:N | 2.33 | 0.44 |
| 7:E:101:ILE:O | 7:E:120:THR:HB | 2.17 | 0.44 |
| 8:F:4:TYR:OH | 8:F:69:GLU:HA | 2.17 | 0.44 |
| 9:G:15:ASP:OD1 | 9:G:18:TYR:N | 2.45 | 0.44 |
| 12:J:6:ILE:HG13 | 12:J:6:ILE:O | 2.17 | 0.44 |
| 12:J:9:ARG:HB2 | 12:J:9:ARG:HH11 | 1.82 | 0.44 |
| 14:L:60:LEU:HD22 | 14:L:66:VAL:HG22 | 2.00 | 0.44 |
| 14:L:126:LYS:NZ | 14:L:126:LYS:C | 2.71 | 0.44 |
| 15:M:58:GLU:HA | 15:M:58:GLU:OE2 | 2.18 | 0.44 |
| 15:M:77:ASN:O | 15:M:81:LEU:HD22 | 2.18 | 0.44 |
| 20:R:53:ARG:HG3 | 20:R:63:GLN:HG2 | 1.99 | 0.44 |
| 1:A:217:C:O2' | 1:A:218:C:H5' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1027:C:H2' | 1:A:1028:C:C6 | 2.52 | 0.44 |
| 1:A:1251:A:H1' | 1:A:1369:C:O2' | 2.16 | 0.44 |
| 1:A:1347:G:H2' | 1:A:1373:G:N1 | 2.32 | 0.44 |
| 1:A:1451:A:H4' | 1:A:1452:C:OP2 | 2.18 | 0.44 |
| 14:L:46:LYS:CG | 14:L:47:LYS:N | 2.79 | 0.44 |
| 15:M:36:LYS:HD2 | 15:M:59:TYR:OH | 2.17 | 0.44 |
| 16:N:11:LYS:O | 16:N:11:LYS:HG2 | 2.16 | 0.44 |
| 16:N:16:PHE:C | 16:N:18:VAL:N | 2.70 | 0.44 |
| 1:A:157:G:C2 | 1:A:158:G:C8 | 3.06 | 0.44 |
| 1:A:877:C:O2' | 1:A:878:G:H5' | 2.18 | 0.44 |
| 1:A:1257:U:O2' | 1:A:1258:G:C8 | 2.71 | 0.44 |
| 1:A:1314:C:OP2 | 21:S:6:LYS:HD3 | 2.17 | 0.44 |
| 4:B:16:HIS:HB3 | 4:B:17:PHE:H | 1.56 | 0.44 |
| 4:B:177:ALA:O | 4:B:180:LEU:N | 2.51 | 0.44 |
| 5:C:11:ARG:O | 5:C:13:GLY:N | 2.51 | 0.44 |
| 11:I:27:THR:HG22 | 11:I:28:VAL:N | 2.33 | 0.44 |
| 11:I:65:VAL:HG21 | 11:I:73:GLN:HB3 | 2.00 | 0.44 |
| 15:M:71:ARG:HG2 | 15:M:71:ARG:HH11 | 1.82 | 0.44 |
| 20:R:43:PHE:C | 20:R:51:LEU:HD12 | 2.38 | 0.44 |
| 1:A:812:C:OP1 | 1:A:903:G:H1' | 2.18 | 0.44 |
| 1:A:938:A:C6 | 1:A:939:G:C5 | 3.06 | 0.44 |
| 1:A:1003(A):G:C2 | 1:A:1004:A:H1' | 2.52 | 0.44 |
| 1:A:1055:A:N7 | 1:A:1206:G:N1 | 2.66 | 0.44 |
| 1:A:1133:G:O2' | 1:A:1134:G:H5' | 2.18 | 0.44 |
| 1:A:1232:U:OP1 | 11:I:124:GLN:NE2 | 2.48 | 0.44 |
| 1:A:1405:G:H1' | 1:A:1519:A:O4' | 2.18 | 0.44 |
| 1:A:1460:A:H2' | 1:A:1461:G:O4' | 2.17 | 0.44 |
| 4:B:60:ASP:OD1 | 4:B:64:ARG:NH2 | 2.50 | 0.44 |
| 8:F:10:LEU:HD11 | 8:F:59:TYR:HD2 | 1.82 | 0.44 |
| 8:F:34:GLY:O | 8:F:68:PRO:HD3 | 2.18 | 0.44 |
| 11:I:8:GLY:O | 11:I:9:ARG:HG3 | 2.18 | 0.44 |
| 13:K:99:GLN:HA | 13:K:105:VAL:CG2 | 2.48 | 0.44 |
| 15:M:25:ILE:HG22 | 15:M:26:GLY:N | 2.33 | 0.44 |
| 15:M:80:ARG:O | 15:M:82:MET:N | 2.51 | 0.44 |
| 15:M:108:ARG:NH2 | 15:M:114:ARG:HA | 2.32 | 0.44 |
| 16:N:35:ARG:C | 16:N:37:PHE:N | 2.71 | 0.44 |
| 22:T:100:ILE:O | 22:T:102:GLY:N | 2.50 | 0.44 |
| 1:A:129(A):G:O2' | 1:A:190(E):U:C6 | 2.71 | 0.43 |
| 1:A:458:C:C2 | 1:A:459:G:C8 | 3.06 | 0.43 |
| 1:A:614:A:C2 | 1:A:627:G:C2 | 3.06 | 0.43 |
| 1:A:706:A:H1' | 13:K:29:ILE:HD11 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:961:U:O2' | 1:A:962:C:H5' | 2.17 | 0.43 |
| 1:A:1060:C:C5 | 5:C:2:GLY:CA | 3.01 | 0.43 |
| 9:G:141:VAL:O | 9:G:144:MET:HB2 | 2.18 | 0.43 |
| 22:T:13:LEU:O | 22:T:16:HIS:HB3 | 2.18 | 0.43 |
| 22:T:56:MET:CE | 22:T:88:VAL:HG11 | 2.48 | 0.43 |
| 1:A:190(L):U:O2' | 1:A:191:G:H5' | 2.18 | 0.43 |
| 1:A:242:C:C2' | 1:A:243:A:H5' | 2.48 | 0.43 |
| 1:A:865:A:C2 | 1:A:918:A:H4' | 2.52 | 0.43 |
| 1:A:867:G:O2' | 1:A:868:C:H5' | 2.17 | 0.43 |
| 1:A:981:U:H5' | 16:N:21:TYR:CE1 | 2.53 | 0.43 |
| 1:A:1053:G:C3' | 1:A:1054:C:C5' | 2.95 | 0.43 |
| 4:B:78:GLN:O | 4:B:78:GLN:HG2 | 2.18 | 0.43 |
| 4:B:79:ASP:HB3 | 4:B:238:LEU:HD13 | 1.99 | 0.43 |
| 12:J:14:LYS:C | 12:J:16:LEU:H | 2.20 | 0.43 |
| 13:K:43:SER:OG | 13:K:67:ASP:HB3 | 2.18 | 0.43 |
| 19:Q:59:ILE:CG2 | 19:Q:71:PHE:CD1 | 3.00 | 0.43 |
| 19:Q:97:SER:C | 19:Q:99:SER:N | 2.72 | 0.43 |
| 1:A:364:A:N6 | 14:L:28:LYS:HE2 | 2.32 | 0.43 |
| 1:A:579:G:C5' | 1:A:728:A:H1' | 2.34 | 0.43 |
| 1:A:668:G:O2' | 17:O:46:HIS:HD2 | 2.00 | 0.43 |
| 1:A:1202:G:O2' | 1:A:1203:C:H5' | 2.18 | 0.43 |
| 1:A:1287:A:H2' | 1:A:1288:A:C8 | 2.53 | 0.43 |
| 1:A:1288:A:H1' | 1:A:1352:C:O2' | 2.18 | 0.43 |
| 6:D:152:SER:O | 6:D:155:LEU:HD12 | 2.18 | 0.43 |
| 7:E:137:GLU:O | 7:E:141:GLN:HG3 | 2.18 | 0.43 |
| 8:F:2:ARG:NH1 | 8:F:69:GLU:CB | 2.81 | 0.43 |
| 8:F:35:ALA:HA | 8:F:67:MET:HB3 | 1.99 | 0.43 |
| 9:G:15:ASP:O | 9:G:19:GLY:N | 2.48 | 0.43 |
| 9:G:46:ALA:O | 9:G:50:ILE:HG13 | 2.18 | 0.43 |
| 11:I:16:ARG:CG | 11:I:64:THR:HB | 2.37 | 0.43 |
| 11:I:86:VAL:HG11 | 11:I:93:ARG:HE | 1.84 | 0.43 |
| 12:J:89:ASP:O | 12:J:90:LEU:HD12 | 2.18 | 0.43 |
| 13:K:26:ASN:O | 13:K:27:ASN:CB | 2.67 | 0.43 |
| 15:M:117:VAL:CG1 | 15:M:118:ALA:N | 2.81 | 0.43 |
| 19:Q:7:THR:O | 19:Q:23:VAL:HG13 | 2.19 | 0.43 |
| 19:Q:59:ILE:HD13 | 19:Q:59:ILE:HA | 1.77 | 0.43 |
| 1:A:686:U:C2 | 1:A:687:A:N7 | 2.86 | 0.43 |
| 1:A:1095:U:P | 1:A:1108:G:H1 | 2.41 | 0.43 |
| 1:A:1411:C:O2' | 1:A:1412:C:H5' | 2.18 | 0.43 |
| 4:B:18:GLY:HA2 | 4:B:40:HIS:O | 2.18 | 0.43 |
| 4:B:74:LYS:NZ | 4:B:206:ASP:HA | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:131:PRO:C | 4:B:133:LYS:N | 2.72 | 0.43 |
| 8:F:26:ILE:O | 8:F:30:LEU:HG | 2.19 | 0.43 |
| 12:J:47:PHE:CD1 | 12:J:47:PHE:N | 2.86 | 0.43 |
| 14:L:44:THR:HA | 14:L:45:PRO:HD3 | 1.91 | 0.43 |
| 14:L:126:LYS:CE | 14:L:126:LYS:N | 2.82 | 0.43 |
| 15:M:90:LEU:O | 15:M:93:ARG:N | 2.51 | 0.43 |
| 16:N:11:LYS:O | 16:N:12:ARG:C | 2.57 | 0.43 |
| 19:Q:13:ASP:O | 19:Q:15:MET:N | 2.52 | 0.43 |
| 19:Q:76:LEU:C | 19:Q:76:LEU:CD2 | 2.87 | 0.43 |
| 19:Q:98:LEU:O | 19:Q:98:LEU:CD1 | 2.67 | 0.43 |
| 1:A:510:A:O2' | 1:A:542:G:H1' | 2.18 | 0.43 |
| 1:A:1132:C:H2' | 1:A:1133:G:H8 | 1.84 | 0.43 |
| 4:B:16:HIS:CA | 4:B:204:ASN:HB2 | 2.46 | 0.43 |
| 5:C:148:GLY:HA3 | 5:C:172:ARG:O | 2.19 | 0.43 |
| 5:C:191:THR:HG21 | 5:C:193:TYR:CD1 | 2.54 | 0.43 |
| 6:D:162:LEU:HD12 | 6:D:181:MET:HE1 | 2.00 | 0.43 |
| 6:D:173:TRP:O | 6:D:186:LEU:HB2 | 2.18 | 0.43 |
| 7:E:36:ASP:OD2 | 7:E:40:ARG:HB2 | 2.19 | 0.43 |
| 7:E:87:SER:HB3 | 7:E:131:ILE:CD1 | 2.49 | 0.43 |
| 12:J:8:LEU:HD22 | 12:J:94:VAL:HG11 | 1.99 | 0.43 |
| 12:J:53:PRO:HA | 16:N:41:ARG:NH2 | 2.27 | 0.43 |
| 14:L:71:PRO:O | 14:L:102:ARG:CD | 2.64 | 0.43 |
| 17:O:17:ARG:NH1 | 17:O:77:ARG:NH1 | 2.67 | 0.43 |
| 19:Q:81:ARG:HE | 19:Q:81:ARG:HB2 | 1.53 | 0.43 |
| 20:R:87:ARG:HG2 | 20:R:87:ARG:NH1 | 2.32 | 0.43 |
| 1:A:81:U:H6 | 1:A:81:U:H5' | 1.83 | 0.43 |
| 1:A:709:G:O2' | 1:A:710:G:H5' | 2.19 | 0.43 |
| 1:A:1003(A):G:C2' | 1:A:1004:A:H4' | 2.43 | 0.43 |
| 1:A:1015:A:H2' | 1:A:1016:A:H8 | 1.83 | 0.43 |
| 1:A:1116:C:O2' | 1:A:1117:G:H5" | 2.18 | 0.43 |
| 1:A:1207:G:H2' | 1:A:1208:C:C6 | 2.53 | 0.43 |
| 4:B:14:GLY:O | 4:B:15:VAL:HG22 | 2.18 | 0.43 |
| 4:B:124:SER:CB | 4:B:125:PRO:CD | 2.97 | 0.43 |
| 4:B:142:LEU:O | 4:B:145:LEU:N | 2.52 | 0.43 |
| 4:B:144:ARG:HG3 | 4:B:145:LEU:H | 1.83 | 0.43 |
| 5:C:119:ARG:HG2 | 5:C:119:ARG:HH11 | 1.83 | 0.43 |
| 5:C:139:GLN:CA | 5:C:139:GLN:NE2 | 2.78 | 0.43 |
| 6:D:8:VAL:CG1 | 6:D:21:LEU:HB2 | 2.48 | 0.43 |
| 8:F:11:ASN:HA | 8:F:12:PRO:HD2 | 1.87 | 0.43 |
| 11:I:7:THR:O | 11:I:80:GLY:HA3 | 2.18 | 0.43 |
| 14:L:126:LYS:HE3 | 14:L:126:LYS:N | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:S:37:ARG:HD3 | 21:S:37:ARG:HA | 1.81 | 0.43 |
| 1:A:26:A:N6 | 1:A:558:G:H1' | 2.33 | 0.43 |
| 1:A:283:C:O2' | 1:A:284:G:H5' | 2.19 | 0.43 |
| 1:A:765:G:N2 | 1:A:812:C:O2' | 2.52 | 0.43 |
| 1:A:1003(A):G:C6 | 1:A:1004:A:N3 | 2.87 | 0.43 |
| 1:A:1294:G:O2' | 1:A:1295:G:H5' | 2.19 | 0.43 |
| 1:A:1330:U:C2' | 1:A:1331:G:H5' | 2.49 | 0.43 |
| 4:B:90:MET:HA | 4:B:91:PRO:HD3 | 1.74 | 0.43 |
| 4:B:212:GLN:O | 4:B:213:LEU:C | 2.56 | 0.43 |
| 5:C:180:ALA:O | 5:C:181:ASN:CB | 2.56 | 0.43 |
| 8:F:23:LYS:NZ | 8:F:42:GLU:OE2 | 2.48 | 0.43 |
| 10:H:51:VAL:CG1 | 10:H:52:ASP:N | 2.79 | 0.43 |
| 10:H:97:VAL:HG13 | 10:H:98:LYS:N | 2.34 | 0.43 |
| 13:K:128:ALA:O | 13:K:129:SER:HB3 | 2.17 | 0.43 |
| 14:L:89:ARG:HG2 | 14:L:97:ARG:CB | 2.48 | 0.43 |
| 15:M:21:TYR:HD1 | 15:M:21:TYR:H | 1.67 | 0.43 |
| 1:A:632:A:C2' | 1:A:633:G:H5' | 2.48 | 0.43 |
| 1:A:1036:G:H2' | 1:A:1037:C:C6 | 2.54 | 0.43 |
| 1:A:1229:A:C2 | 1:A:1230:C:C4 | 3.06 | 0.43 |
| 1:A:1270:C:O2' | 1:A:1314:C:H5' | 2.19 | 0.43 |
| 1:A:1305:G:H2' | 1:A:1331:G:N2 | 2.33 | 0.43 |
| 1:A:1346:A:O4' | 1:A:1348:U:C6 | 2.72 | 0.43 |
| 1:A:1439:C:H2' | 1:A:1440:C:H6 | 1.84 | 0.43 |
| 5:C:6:HIS:CD2 | 5:C:8:ILE:HB | 2.53 | 0.43 |
| 8:F:82:ARG:HB2 | 8:F:85:VAL:CG2 | 2.48 | 0.43 |
| 9:G:79:ARG:HG3 | 9:G:84:ASN:HB3 | 1.99 | 0.43 |
| 12:J:9:ARG:CB | 12:J:9:ARG:HH11 | 2.31 | 0.43 |
| 13:K:33:THR:HA | 13:K:39:PRO:HA | 2.00 | 0.43 |
| 15:M:96:LEU:HB3 | 15:M:97:PRO:HD2 | 2.01 | 0.43 |
| 16:N:12:ARG:HB3 | 16:N:13:THR:H | 1.58 | 0.43 |
| 19:Q:68:ARG:HG3 | 19:Q:68:ARG:O | 2.19 | 0.43 |
| 22:T:39:LYS:O | 22:T:43:LEU:HG | 2.19 | 0.43 |
| 1:A:64:G:HO2' | 1:A:65:U:P | 2.40 | 0.43 |
| 1:A:321:A:O2' | 1:A:322:C:H5' | 2.18 | 0.43 |
| 1:A:642:A:C8 | 10:H:115:SER:HA | 2.54 | 0.43 |
| 1:A:1074:G:O3' | 4:B:103:THR:CG2 | 2.66 | 0.43 |
| 1:A:1370:G:C2 | 1:A:1371:G:N7 | 2.87 | 0.43 |
| 4:B:107:THR:HA | 4:B:110:GLN:OE1 | 2.19 | 0.43 |
| 4:B:159:PRO:HB2 | 4:B:161:ALA:O | 2.19 | 0.43 |
| 6:D:64:LEU:HB2 | 6:D:198:VAL:HG11 | 2.01 | 0.43 |
| 6:D:150:GLU:C | 6:D:152:SER:H | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:F:87:ARG:NH1 | 8:F:87:ARG:CG | 2.77 | 0.43 |
| 9:G:54:THR:HG22 | 9:G:56:GLN:N | 2.24 | 0.43 |
| 11:I:45:ALA:O | 11:I:47:LEU:N | 2.51 | 0.43 |
| 11:I:107:ARG:HB3 | 11:I:107:ARG:HH11 | 1.83 | 0.43 |
| 14:L:60:LEU:HD11 | 14:L:85:ILE:HD12 | 2.01 | 0.43 |
| 16:N:16:PHE:C | 16:N:18:VAL:H | 2.21 | 0.43 |
| 16:N:44:LEU:O | 16:N:48:ALA:CB | 2.67 | 0.43 |
| 16:N:45:ARG:HH11 | 16:N:45:ARG:CG | 2.27 | 0.43 |
| 23:V:2:GLY:C | 23:V:4:GLY:N | 2.72 | 0.43 |
| 1:A:67:C:H2' | 1:A:68:G:C8 | 2.54 | 0.43 |
| 1:A:217:C:H2' | 1:A:218:C:C6 | 2.54 | 0.43 |
| 1:A:291:C:O2' | 1:A:292:G:H5' | 2.19 | 0.43 |
| 1:A:499:A:H4' | 1:A:500:G:OP1 | 2.18 | 0.43 |
| 1:A:614:A:H2' | 1:A:615:C:C6 | 2.54 | 0.43 |
| 1:A:640:A:C2' | 1:A:641:U:H5' | 2.48 | 0.43 |
| 1:A:692:U:H1' | 1:A:695:A:N7 | 2.34 | 0.43 |
| 1:A:801:U:H2' | 1:A:802:A:C8 | 2.54 | 0.43 |
| 1:A:1137:C:H4' | 1:A:1138:G:N1 | 2.33 | 0.43 |
| 1:A:1351:U:O2' | 1:A:1352:C:H5' | 2.19 | 0.43 |
| 4:B:23:ARG:O | 4:B:24:TRP:O | 2.37 | 0.43 |
| 4:B:80:ILE:CD1 | 4:B:208:ILE:HG12 | 2.48 | 0.43 |
| 4:B:97:TRP:C | 4:B:98:LEU:HD23 | 2.40 | 0.43 |
| 4:B:212:GLN:HG3 | 4:B:239:VAL:CG2 | 2.49 | 0.43 |
| 5:C:9:GLY:N | 16:N:49:HIS:O | 2.52 | 0.43 |
| 5:C:107:GLN:O | 5:C:108:ASN:CB | 2.67 | 0.43 |
| 10:H:125:ARG:HE | 10:H:125:ARG:HB2 | 1.60 | 0.43 |
| 11:I:10:ARG:C | 11:I:12:GLU:N | 2.68 | 0.43 |
| 11:I:33:PHE:C | 11:I:35:GLU:H | 2.23 | 0.43 |
| 13:K:12:ARG:O | 13:K:13:GLN:O | 2.37 | 0.43 |
| 19:Q:26:GLN:O | 19:Q:27:PHE:HB3 | 2.19 | 0.43 |
| 1:A:497:A:O2' | 1:A:498:U:OP1 | 2.28 | 0.42 |
| 1:A:519:C:H2' | 1:A:520:A:O4' | 2.18 | 0.42 |
| 1:A:831:U:O2' | 1:A:832:C:H5' | 2.19 | 0.42 |
| 1:A:1145:C:HO2' | 1:A:1146:A:P | 2.41 | 0.42 |
| 4:B:15:VAL:HB | 4:B:16:HIS:H | 1.47 | 0.42 |
| 4:B:17:PHE:CD1 | 4:B:17:PHE:C | 2.92 | 0.42 |
| 4:B:114:ARG:HH11 | 4:B:118:LEU:HG | 1.84 | 0.42 |
| 5:C:99:VAL:CG2 | 5:C:100:ALA:N | 2.82 | 0.42 |
| 7:E:77:PRO:O | 7:E:78:HIS:HB3 | 2.19 | 0.42 |
| 8:F:3:ARG:HG2 | 8:F:93:SER:OG | 2.18 | 0.42 |
| 8:F:30:LEU:HB3 | 8:F:35:ALA:CB | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:F:92:LYS:HB2 | 8:F:92:LYS:HE3 | 1.77 | 0.42 |
| 9:G:51:GLN:NE2 | 9:G:58:PRO:HD3 | 2.33 | 0.42 |
| 9:G:70:LYS:HG2 | 9:G:96:GLN:O | 2.19 | 0.42 |
| 13:K:70:LYS:O | 13:K:73:MET:N | 2.52 | 0.42 |
| 15:M:117:VAL:HG12 | 15:M:118:ALA:N | 2.33 | 0.42 |
| 16:N:33:VAL:O | 16:N:33:VAL:HG13 | 2.19 | 0.42 |
| 19:Q:97:SER:O | 19:Q:102:GLY:N | 2.51 | 0.42 |
| 1:A:444:C:H2' | 1:A:445:G:C8 | 2.51 | 0.42 |
| 1:A:542:G:H2' | 1:A:543:C:C6 | 2.50 | 0.42 |
| 1:A:851:G:H2' | 1:A:852:G:H8 | 1.83 | 0.42 |
| 1:A:865:A:H2 | 1:A:918:A:H4' | 1.84 | 0.42 |
| 1:A:881:G:P | 14:L:12:ARG:HH22 | 2.42 | 0.42 |
| 1:A:983:A:HO2' | 1:A:1049:U:HO2' | 1.66 | 0.42 |
| 1:A:1301:U:O2' | 1:A:1302:U:P | 2.77 | 0.42 |
| 4:B:23:ARG:HH11 | 4:B:24:TRP:CA | 2.33 | 0.42 |
| 5:C:108:ASN:ND2 | 5:C:110:ASN:HB2 | 2.32 | 0.42 |
| 7:E:16:THR:HG22 | 7:E:27:ARG:O | 2.18 | 0.42 |
| 9:G:81:GLY:C | 9:G:83:ALA:H | 2.22 | 0.42 |
| 10:H:31:PHE:O | 10:H:35:ILE:HG13 | 2.19 | 0.42 |
| 11:I:31:GLN:HG2 | 11:I:35:GLU:HG2 | 2.00 | 0.42 |
| 14:L:89:ARG:NH2 | 14:L:97:ARG:HE | 2.18 | 0.42 |
| 14:L:110:VAL:O | 14:L:113:ARG:HB2 | 2.19 | 0.42 |
| 17:O:77:ARG:O | 17:O:81:LEU:N | 2.43 | 0.42 |
| 1:A:369:C:O2' | 1:A:370:C:H5' | 2.19 | 0.42 |
| 1:A:730:G:N3 | 1:A:765:G:H4' | 2.34 | 0.42 |
| 1:A:1227:A:H2' | 1:A:1228:C:O5' | 2.19 | 0.42 |
| 1:A:1339:A:H2' | 1:A:1340:A:O4' | 2.19 | 0.42 |
| 1:A:1368:G:HO2' | 1:A:1369:C:H5' | 1.83 | 0.42 |
| 6:D:31:CYS:O | 6:D:31:CYS:SG | 2.77 | 0.42 |
| 7:E:76:ILE:HG23 | 7:E:77:PRO:CD | 2.42 | 0.42 |
| 8:F:91:VAL:HG13 | 20:R:72:ARG:HH22 | 1.83 | 0.42 |
| 12:J:45:ARG:HB2 | 12:J:65:LEU:HB3 | 2.02 | 0.42 |
| 14:L:89:ARG:HA | 14:L:97:ARG:HA | 2.00 | 0.42 |
| 17:O:67:LEU:HD11 | 17:O:87:ILE:HD13 | 2.00 | 0.42 |
| 21:S:42:PRO:HD3 | 21:S:67:VAL:CG1 | 2.49 | 0.42 |
| 1:A:425:G:O2' | 1:A:426:G:H5' | 2.19 | 0.42 |
| 1:A:528:C:H5' | 1:A:535:A:N6 | 2.34 | 0.42 |
| 1:A:1118:C:H1' | 1:A:1179:A:N9 | 2.34 | 0.42 |
| 1:A:1145:C:O2' | 1:A:1146:A:C8 | 2.72 | 0.42 |
| 1:A:1465:C:O2' | 1:A:1466:C:H5' | 2.19 | 0.42 |
| 4:B:101:MET:HE2 | 4:B:108:ILE:HG21 | 1.98 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:164:VAL:O | 4:B:186:ALA:HA | 2.19 | 0.42 |
| 9:G:121:ALA:O | 9:G:125:MET:HG3 | 2.19 | 0.42 |
| 10:H:36:LEU:HA | 10:H:39:LEU:HD23 | 2.01 | 0.42 |
| 13:K:40:ILE:HG23 | 13:K:75:TYR:CD2 | 2.55 | 0.42 |
| 15:M:34:LEU:CD1 | 15:M:41:PRO:HA | 2.40 | 0.42 |
| 20:R:26:LEU:HD22 | 20:R:39:VAL:HG23 | 2.01 | 0.42 |
| 1:A:247:G:OP2 | 19:Q:99:SER:HB2 | 2.20 | 0.42 |
| 1:A:264:U:H4' | 19:Q:63:ARG:HD3 | 2.02 | 0.42 |
| 1:A:437:U:C5' | 6:D:155:LEU:HD22 | 2.47 | 0.42 |
| 1:A:635:G:O2' | 1:A:636:U:H5' | 2.19 | 0.42 |
| 1:A:669:U:H2' | 1:A:670:G:C8 | 2.55 | 0.42 |
| 1:A:794:A:C5 | 1:A:795:C:C4 | 3.07 | 0.42 |
| 1:A:1004:A:N7 | 1:A:1036:G:O6 | 2.53 | 0.42 |
| 1:A:1229:A:H2' | 1:A:1230:C:H6 | 1.84 | 0.42 |
| 1:A:1407:C:O2' | 1:A:1408:A:H5' | 2.20 | 0.42 |
| 1:A:1429:C:H2' | 1:A:1430:C:C6 | 2.55 | 0.42 |
| 4:B:78:GLN:O | 4:B:94:ASN:ND2 | 2.52 | 0.42 |
| 5:C:175:LEU:HD21 | 5:C:201:TYR:CD2 | 2.54 | 0.42 |
| 6:D:150:GLU:C | 6:D:152:SER:N | 2.73 | 0.42 |
| 7:E:12:LEU:HD22 | 7:E:13:ILE:N | 2.34 | 0.42 |
| 10:H:104:ARG:NH2 | 10:H:138:TRP:CZ3 | 2.88 | 0.42 |
| 11:I:51:ARG:HG3 | 11:I:56:LEU:HD12 | 2.00 | 0.42 |
| 11:I:117:HIS:O | 11:I:118:LYS:HG3 | 2.20 | 0.42 |
| 23:V:3:LYS:HB3 | 23:V:14:TRP:CG | 2.54 | 0.42 |
| 1:A:992:U:O2' | 1:A:993:G:P | 2.78 | 0.42 |
| 1:A:1109:C:P | 5:C:176:HIS:CD2 | 3.12 | 0.42 |
| 1:A:1117:G:N2 | 1:A:1180:A:H1' | 2.34 | 0.42 |
| 1:A:1130:A:OP2 | 1:A:1131:G:OP2 | 2.37 | 0.42 |
| 1:A:1251:A:H5' | 11:I:12:GLU:OE1 | 2.20 | 0.42 |
| 1:A:1459:C:O2' | 1:A:1460:A:H5' | 2.19 | 0.42 |
| 1:A:1487:G:O2' | 1:A:1488:G:H5' | 2.19 | 0.42 |
| 1:A:1514:C:O2' | 1:A:1515:C:H5' | 2.19 | 0.42 |
| 5:C:132:ARG:O | 5:C:133:ALA:C | 2.58 | 0.42 |
| 9:G:16:LEU:H | 9:G:16:LEU:CD2 | 2.33 | 0.42 |
| 13:K:18:ARG:NH1 | 13:K:35:PRO:O | 2.52 | 0.42 |
| 13:K:82:VAL:HG23 | 13:K:105:VAL:HG13 | 2.01 | 0.42 |
| 15:M:84:ILE:O | 15:M:85:GLY:C | 2.58 | 0.42 |
| 17:O:34:LEU:O | 17:O:38:ARG:HG2 | 2.20 | 0.42 |
| 19:Q:60:ILE:HD13 | 19:Q:61:GLU:H | 1.85 | 0.42 |
| 21:S:20:LEU:HA | 21:S:23:ASN:HD22 | 1.83 | 0.42 |
| 22:T:57:ARG:CB | 22:T:57:ARG:HH11 | 2.32 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:270:A:H2' | 1:A:271:C:H6 | 1.84 | 0.42 |
| 1:A:394:G:H2' | 1:A:395:C:C6 | 2.54 | 0.42 |
| 1:A:542:G:H5' | 6:D:41:GLY:HA3 | 2.01 | 0.42 |
| 1:A:558:G:H2' | 1:A:559:A:H2 | 1.84 | 0.42 |
| 1:A:644:G:C5 | 1:A:645:C:C5 | 3.08 | 0.42 |
| 1:A:815:A:H4' | 1:A:817:C:C5 | 2.55 | 0.42 |
| 1:A:1089:G:O2' | 1:A:1090:U:H5' | 2.19 | 0.42 |
| 1:A:1091:U:C2 | 1:A:1093:A:OP2 | 2.72 | 0.42 |
| 1:A:1102:A:H2' | 1:A:1103:C:C6 | 2.55 | 0.42 |
| 1:A:1207:G:HO2' | 1:A:1208:C:H5' | 1.84 | 0.42 |
| 4:B:79:ASP:C | 4:B:81:VAL:H | 2.23 | 0.42 |
| 4:B:177:ALA:CB | 4:B:184:VAL:HG22 | 2.50 | 0.42 |
| 4:B:178:ARG:NH1 | 10:H:71:GLY:O | 2.53 | 0.42 |
| 4:B:206:ASP:O | 4:B:207:ALA:HB3 | 2.20 | 0.42 |
| 5:C:101:LEU:O | 5:C:101:LEU:CD2 | 2.67 | 0.42 |
| 6:D:13:ARG:HD3 | 6:D:36:ARG:O | 2.18 | 0.42 |
| 7:E:93:PRO:HG2 | 10:H:105:ARG:NH2 | 2.34 | 0.42 |
| 10:H:119:LEU:CD1 | 10:H:124:ALA:HA | 2.49 | 0.42 |
| 15:M:6:GLY:O | 15:M:7:VAL:CG2 | 2.67 | 0.42 |
| 15:M:66:LEU:O | 15:M:67:GLU:O | 2.37 | 0.42 |
| 1:A:533:A:O2' | 1:A:535:A:OP2 | 2.21 | 0.42 |
| 1:A:579:G:H5' | 1:A:728:A:C1' | 2.33 | 0.42 |
| 1:A:1069:C:O2' | 1:A:1192:C:H1' | 2.19 | 0.42 |
| 1:A:1226:C:H4' | 21:S:80:TYR:CZ | 2.55 | 0.42 |
| 7:E:43:LEU:O | 7:E:62:ALA:HA | 2.19 | 0.42 |
| 13:K:20:TYR:O | 13:K:30:VAL:HA | 2.19 | 0.42 |
| 14:L:89:ARG:NH2 | 14:L:97:ARG:NH2 | 2.65 | 0.42 |
| 15:M:2:ALA:O | 15:M:4:ILE:HG13 | 2.20 | 0.42 |
| 22:T:101:GLY:C | 22:T:103:GLY:N | 2.71 | 0.42 |
| 23:V:2:GLY:O | 23:V:4:GLY:N | 2.53 | 0.42 |
| 1:A:154:C:O2' | 1:A:155:C:H5' | 2.20 | 0.42 |
| 1:A:185:A:N3 | 22:T:81:LYS:NZ | 2.55 | 0.42 |
| 1:A:190(B):C:H2' | 1:A:190(C):C:O4' | 2.20 | 0.42 |
| 1:A:310:G:H2' | 1:A:311:C:H6 | 1.84 | 0.42 |
| 1:A:807:A:H2' | 1:A:808:C:H6 | 1.82 | 0.42 |
| 1:A:951:G:O2' | 1:A:952:U:H5' | 2.20 | 0.42 |
| 1:A:1187:G:P | 11:I:113:LYS:HE2 | 2.60 | 0.42 |
| 5:C:35:GLU:CG | 5:C:59:ARG:NH2 | 2.77 | 0.42 |
| 6:D:17:VAL:CG1 | 6:D:18:LYS:N | 2.83 | 0.42 |
| 6:D:30:LYS:C | 6:D:32:ALA:N | 2.72 | 0.42 |
| 6:D:61:LYS:HD3 | 6:D:206:PHE:CD2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:F:60:PHE:CZ | 20:R:78:LEU:HD21 | 2.55 | 0.42 |
| 9:G:75:VAL:HG11 | 9:G:86:GLN:HB3 | 2.01 | 0.42 |
| 14:L:42:THR:OG1 | 14:L:52:LEU:HB3 | 2.20 | 0.42 |
| 14:L:98:TYR:CD1 | 14:L:98:TYR:N | 2.87 | 0.42 |
| 15:M:21:TYR:N | 15:M:21:TYR:CD1 | 2.88 | 0.42 |
| 1:A:169:C:O2' | 1:A:170:U:H5' | 2.19 | 0.42 |
| 1:A:474:G:H2' | 1:A:475:G:H8 | 1.85 | 0.42 |
| 1:A:489:C:H2' | 1:A:490:G:H8 | 1.85 | 0.42 |
| 1:A:603:U:H2' | 1:A:604:G:C8 | 2.55 | 0.42 |
| 1:A:718:G:H4' | 13:K:117:ASN:HD21 | 1.84 | 0.42 |
| 1:A:814:A:N7 | 1:A:816:A:C4 | 2.87 | 0.42 |
| 1:A:933:G:OP2 | 9:G:3:ARG:HB3 | 2.20 | 0.42 |
| 1:A:1014:A:H2 | 1:A:1219:U:H1' | 1.80 | 0.42 |
| 1:A:1060:C:N4 | 5:C:2:GLY:N | 2.67 | 0.42 |
| 1:A:1061:G:C6 | 1:A:1062:U:N3 | 2.88 | 0.42 |
| 1:A:1079:G:O3' | 7:E:14:ARG:NH2 | 2.53 | 0.42 |
| 1:A:1165:C:C2' | 1:A:1166:G:H5' | 2.50 | 0.42 |
| 1:A:1347:G:C5 | 11:I:107:ARG:NH1 | 2.70 | 0.42 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.68 | 0.42 |
| 4:B:64:ARG:CB | 4:B:64:ARG:HH11 | 2.33 | 0.42 |
| 4:B:101:MET:HE3 | 4:B:108:ILE:HG21 | 2.01 | 0.42 |
| 8:F:1:MET:CE | 8:F:1:MET:N | 2.82 | 0.42 |
| 11:I:97:LYS:C | 11:I:99:LEU:N | 2.73 | 0.42 |
| 13:K:69:ALA:CB | 13:K:101:SER:HB2 | 2.50 | 0.42 |
| 14:L:78:GLN:O | 14:L:80:HIS:N | 2.52 | 0.42 |
| 1:A:417:C:O2' | 1:A:418:C:H5' | 2.20 | 0.41 |
| 1:A:791:G:C6 | 1:A:792:A:N7 | 2.87 | 0.41 |
| 1:A:1018:C:O2' | 1:A:1019:C:H5' | 2.20 | 0.41 |
| 1:A:1030:C:H2' | 1:A:1030(A):G:O4' | 2.19 | 0.41 |
| 1:A:1161:C:H2' | 1:A:1162:C:C6 | 2.55 | 0.41 |
| 1:A:1256:A:H61 | 1:A:1278:U:C1' | 2.33 | 0.41 |
| 1:A:1281:U:C6 | 1:A:1281:U:C3' | 3.02 | 0.41 |
| 1:A:1364:U:O2' | 1:A:1365:G:H5' | 2.20 | 0.41 |
| 7:E:26:PHE:H | 7:E:26:PHE:HD1 | 1.62 | 0.41 |
| 9:G:49:ILE:C | 9:G:51:GLN:H | 2.23 | 0.41 |
| 9:G:89:MET:HB2 | 9:G:155:ARG:NH1 | 2.34 | 0.41 |
| 11:I:107:ARG:HH11 | 11:I:107:ARG:CB | 2.32 | 0.41 |
| 12:J:44:VAL:HA | 12:J:66:ARG:HA | 2.02 | 0.41 |
| 20:R:32:ARG:HE | 20:R:32:ARG:HB2 | 1.61 | 0.41 |
| 1:A:58:C:O2' | 1:A:59:A:H5' | 2.20 | 0.41 |
| 1:A:166:G:H2' | 1:A:167:G:H8 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:433:C:H2' | 1:A:434:U:C6 | 2.55 | 0.41 |
| 1:A:490:G:O2' | 1:A:491:G:H5' | 2.20 | 0.41 |
| 1:A:632:A:H2' | 1:A:633:G:H5' | 2.01 | 0.41 |
| 1:A:1223:C:P | 1:A:1224:G:H3' | 2.60 | 0.41 |
| 1:A:1355:G:O2' | 1:A:1356:G:H5' | 2.20 | 0.41 |
| 1:A:1365:G:O2' | 1:A:1366:C:H5' | 2.19 | 0.41 |
| 5:C:112:SER:CB | 5:C:115:LEU:HD12 | 2.48 | 0.41 |
| 5:C:191:THR:HG22 | 5:C:192:THR:N | 2.35 | 0.41 |
| 6:D:64:LEU:C | 6:D:64:LEU:HD13 | 2.41 | 0.41 |
| 11:I:95:LYS:C | 11:I:98:PRO:HD2 | 2.40 | 0.41 |
| 14:L:60:LEU:HB2 | 14:L:64:TYR:O | 2.20 | 0.41 |
| 15:M:23:TYR:HB3 | 15:M:67:GLU:HA | 2.02 | 0.41 |
| 15:M:91:ARG:HH22 | 15:M:103:THR:HG21 | 1.85 | 0.41 |
| 19:Q:70:ARG:NH1 | 19:Q:70:ARG:CG | 2.83 | 0.41 |
| 20:R:47:THR:C | 20:R:49:LYS:H | 2.24 | 0.41 |
| 21:S:80:TYR:O | 21:S:81:ARG:C | 2.59 | 0.41 |
| 1:A:132:C:O3' | 22:T:74:LYS:CE | 2.62 | 0.41 |
| 1:A:363:A:O2' | 1:A:364:A:H5' | 2.19 | 0.41 |
| 1:A:645:C:H2' | 1:A:646:U:C6 | 2.55 | 0.41 |
| 1:A:926:G:H3' | 1:A:1505:G:H21 | 1.85 | 0.41 |
| 1:A:1072:G:C5 | 1:A:1073:U:C4 | 3.08 | 0.41 |
| 1:A:1125:U:H3 | 12:J:5:ARG:CZ | 2.33 | 0.41 |
| 4:B:7:VAL:HG23 | 4:B:7:VAL:O | 2.20 | 0.41 |
| 5:C:65:ALA:O | 5:C:66:VAL:HB | 2.19 | 0.41 |
| 5:C:97:LYS:O | 5:C:98:ASN:C | 2.59 | 0.41 |
| 6:D:7:PRO:CB | 6:D:10:ARG:HD2 | 2.49 | 0.41 |
| 6:D:76:ARG:HA | 6:D:76:ARG:HD2 | 1.87 | 0.41 |
| 7:E:107:ARG:O | 7:E:108:ALA:C | 2.58 | 0.41 |
| 8:F:10:LEU:HD12 | 8:F:10:LEU:H | 1.85 | 0.41 |
| 9:G:30:ILE:HD13 | 9:G:120:ILE:HD13 | 2.01 | 0.41 |
| 9:G:90:GLU:H | 9:G:155:ARG:NH1 | 2.17 | 0.41 |
| 12:J:6:ILE:HG13 | 12:J:72:VAL:HB | 2.02 | 0.41 |
| 13:K:69:ALA:O | 13:K:70:LYS:C | 2.57 | 0.41 |
| 15:M:20:THR:C | 15:M:22:ILE:N | 2.74 | 0.41 |
| 20:R:37:VAL:HG22 | 20:R:78:LEU:HB3 | 2.02 | 0.41 |
| 22:T:43:LEU:CD1 | 22:T:55:ILE:HD12 | 2.51 | 0.41 |
| 22:T:89:ARG:NH2 | 22:T:106:ALA:HA | 2.35 | 0.41 |
| 1:A:19:C:H2' | 1:A:20:U:C6 | 2.50 | 0.41 |
| 1:A:50:A:N6 | 1:A:361:G:H4' | 2.35 | 0.41 |
| 1:A:124:G:C5 | 1:A:125:U:C4 | 3.08 | 0.41 |
| 1:A:250:A:O5' | 1:A:250:A:H8 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:302:G:N3 | 1:A:556:C:H4' | 2.35 | 0.41 |
| 1:A:533:A:C5 | 1:A:536:C:C4 | 3.08 | 0.41 |
| 1:A:838:G:N2 | 1:A:849:C:C2 | 2.89 | 0.41 |
| 1:A:1091:U:O2 | 1:A:1093:A:H8 | 2.01 | 0.41 |
| 1:A:1312:G:N7 | 21:S:3:ARG:O | 2.54 | 0.41 |
| 1:A:1320:C:H5 | 21:S:37:ARG:CZ | 2.33 | 0.41 |
| 1:A:1419:G:H2' | 1:A:1420:C:C6 | 2.55 | 0.41 |
| 2:Y:31:C:H1' | 2:Y:40:G:N2 | 2.35 | 0.41 |
| 4:B:95:GLN:OE1 | 4:B:95:GLN:HA | 2.21 | 0.41 |
| 5:C:64:VAL:CB | 5:C:99:VAL:HB | 2.38 | 0.41 |
| 7:E:152:ARG:HA | 10:H:64:LYS:HZ3 | 1.85 | 0.41 |
| 8:F:30:LEU:HD11 | 8:F:63:TYR:CD1 | 2.56 | 0.41 |
| 8:F:91:VAL:CG1 | 8:F:92:LYS:N | 2.82 | 0.41 |
| 8:F:101:ALA:HB2 | 20:R:28:GLU:HB2 | 2.02 | 0.41 |
| 9:G:111:ARG:HB3 | 9:G:113:GLU:OE2 | 2.19 | 0.41 |
| 9:G:140:ASP:OD1 | 9:G:143:ARG:NH1 | 2.54 | 0.41 |
| 12:J:39:PRO:O | 12:J:69:ASN:O | 2.38 | 0.41 |
| 12:J:48:THR:OG1 | 12:J:62:HIS:CD2 | 2.74 | 0.41 |
| 12:J:80:LYS:HA | 12:J:83:GLU:HB2 | 2.02 | 0.41 |
| 15:M:20:THR:O | 15:M:22:ILE:N | 2.52 | 0.41 |
| 15:M:81:LEU:HA | 15:M:84:ILE:HD11 | 2.02 | 0.41 |
| 21:S:19:VAL:CG1 | 21:S:20:LEU:N | 2.83 | 0.41 |
| 1:A:123:C:OP1 | 1:A:312:C:H5' | 2.21 | 0.41 |
| 1:A:344:A:H5" | 1:A:345:C:C5 | 2.55 | 0.41 |
| 1:A:373:A:C2 | 1:A:482:A:C6 | 3.07 | 0.41 |
| 1:A:767:A:H2' | 1:A:768:A:O4' | 2.20 | 0.41 |
| 1:A:998:G:O2' | 1:A:999:C:H5' | 2.21 | 0.41 |
| 1:A:1182:G:HO2' | 1:A:1183:A:P | 2.37 | 0.41 |
| 1:A:1216:G:OP1 | 16:N:3:ARG:HG2 | 2.20 | 0.41 |
| 1:A:1249:C:H4' | 11:I:36:TYR:OH | 2.21 | 0.41 |
| 1:A:1355:G:H2' | 1:A:1356:G:C8 | 2.55 | 0.41 |
| 4:B:122:PHE:O | 4:B:123:ALA:HB2 | 2.20 | 0.41 |
| 4:B:231:GLU:CD | 4:B:231:GLU:H | 2.22 | 0.41 |
| 5:C:123:GLN:HB3 | 5:C:128:PHE:HB2 | 2.02 | 0.41 |
| 5:C:187:ALA:HB3 | 5:C:198:VAL:HB | 2.03 | 0.41 |
| 6:D:17:VAL:HG12 | 6:D:18:LYS:N | 2.35 | 0.41 |
| 6:D:24:GLU:C | 6:D:26:CYS:H | 2.23 | 0.41 |
| 6:D:149:ALA:O | 6:D:150:GLU:C | 2.59 | 0.41 |
| 7:E:18:ARG:HG2 | 7:E:19:MET:N | 2.36 | 0.41 |
| 8:F:37:VAL:HA | 8:F:65:VAL:HG12 | 2.02 | 0.41 |
| 9:G:65:ALA:HB1 | 9:G:127:ALA:CB | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:I:84:ALA:HA | 11:I:87:GLN:HB3 | 2.02 | 0.41 |
| 12:J:8:LEU:HD12 | 12:J:20:ALA:HB2 | 2.03 | 0.41 |
| 16:N:3:ARG:O | 16:N:5:ALA:N | 2.54 | 0.41 |
| 16:N:45:ARG:NH1 | 16:N:45:ARG:CG | 2.83 | 0.41 |
| 18:P:26:ARG:HD2 | 18:P:31:LYS:O | 2.20 | 0.41 |
| 1:A:17:U:H4' | 1:A:1080:A:O4' | 2.21 | 0.41 |
| 1:A:284:G:O2' | 1:A:285:G:H5' | 2.21 | 0.41 |
| 1:A:582:U:H2' | 1:A:583:A:C8 | 2.56 | 0.41 |
| 1:A:723:U:H2' | 1:A:723:U:O2 | 2.19 | 0.41 |
| 1:A:961:U:H2' | 1:A:962:C:C5' | 2.51 | 0.41 |
| 1:A:1327:C:O2' | 1:A:1328:C:H5' | 2.21 | 0.41 |
| 1:A:1381:U:HO2' | 1:A:1382:C:H5' | 1.85 | 0.41 |
| 4:B:69:LEU:HD12 | 4:B:155:LEU:CD1 | 2.51 | 0.41 |
| 4:B:114:ARG:NH1 | 4:B:118:LEU:HD21 | 2.36 | 0.41 |
| 4:B:239:VAL:O | 4:B:239:VAL:CG1 | 2.65 | 0.41 |
| 5:C:141:VAL:HG11 | 5:C:202:ILE:HG23 | 2.01 | 0.41 |
| 5:C:147:LYS:HE3 | 5:C:203:PHE:CZ | 2.56 | 0.41 |
| 6:D:19:LEU:HD22 | 6:D:67:ILE:HG13 | 2.02 | 0.41 |
| 6:D:31:CYS:C | 6:D:33:MET:H | 2.24 | 0.41 |
| 7:E:76:ILE:N | 7:E:76:ILE:HD12 | 2.34 | 0.41 |
| 7:E:99:GLY:O | 7:E:117:ASP:HA | 2.21 | 0.41 |
| 7:E:126:ARG:NH1 | 7:E:126:ARG:HG3 | 2.36 | 0.41 |
| 8:F:75:LEU:HD13 | 8:F:75:LEU:C | 2.41 | 0.41 |
| 20:R:36:ASN:CG | 20:R:39:VAL:HG12 | 2.41 | 0.41 |
| 1:A:1054:C:O2' | 1:A:1055:A:C5' | 2.69 | 0.41 |
| 4:B:59:GLU:CG | 4:B:60:ASP:N | 2.83 | 0.41 |
| 5:C:85:ARG:HD2 | 5:C:85:ARG:O | 2.21 | 0.41 |
| 6:D:98:GLU:CG | 6:D:189:PRO:HG3 | 2.51 | 0.41 |
| 8:F:62:TRP:CD1 | 20:R:35:ARG:CZ | 3.04 | 0.41 |
| 10:H:29:SER:O | 10:H:30:ARG:C | 2.59 | 0.41 |
| 17:O:36:ILE:CG1 | 17:O:59:MET:HE3 | 2.50 | 0.41 |
| 17:O:70:LEU:C | 17:O:72:ARG:N | 2.73 | 0.41 |
| 21:S:18:LYS:O | 21:S:22:LEU:HG | 2.21 | 0.41 |
| 22:T:56:MET:HE2 | 22:T:88:VAL:CB | 2.48 | 0.41 |
| 1:A:479:C:H2' | 1:A:480:U:O4' | 2.21 | 0.41 |
| 1:A:557:G:H2' | 1:A:558:G:C8 | 2.56 | 0.41 |
| 1:A:718:G:C5' | 1:A:719:C:OP2 | 2.69 | 0.41 |
| 1:A:1029:C:H2' | 1:A:1030:C:C6 | 2.54 | 0.41 |
| 1:A:1121:U:O2' | 1:A:1122:U:H5' | 2.20 | 0.41 |
| 1:A:1278:U:H5' | 1:A:1279:A:O4' | 2.21 | 0.41 |
| 1:A:1349:A:H2' | 1:A:1350:A:C8 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1405:G:H1' | 1:A:1519:A:C4' | 2.50 | 0.41 |
| 4:B:151:GLY:C | 4:B:153:ARG:H | 2.24 | 0.41 |
| 4:B:155:LEU:HA | 4:B:155:LEU:HD23 | 1.86 | 0.41 |
| 5:C:83:ARG:HE | 5:C:87:LEU:CD1 | 2.33 | 0.41 |
| 6:D:62:GLN:NE2 | 6:D:65:ARG:HH12 | 2.18 | 0.41 |
| 8:F:67:MET:HE1 | 8:F:75:LEU:HB2 | 2.02 | 0.41 |
| 10:H:51:VAL:HG21 | 10:H:60:ARG:NH1 | 2.35 | 0.41 |
| 12:J:49:VAL:O | 12:J:60:ARG:C | 2.59 | 0.41 |
| 15:M:4:ILE:HG23 | 15:M:57:ARG:HA | 2.02 | 0.41 |
| 19:Q:102:GLY:O | 19:Q:103:GLY:O | 2.38 | 0.41 |
| 21:S:14:HIS:O | 21:S:18:LYS:HB2 | 2.21 | 0.41 |
| 21:S:16:LEU:C | 21:S:18:LYS:N | 2.72 | 0.41 |
| 1:A:50:A:H4' | 1:A:51:A:H5' | 2.02 | 0.41 |
| 1:A:136:C:H2' | 1:A:137:C:H6 | 1.86 | 0.41 |
| 1:A:304:U:O2' | 1:A:305:G:H5' | 2.20 | 0.41 |
| 1:A:404:U:H2' | 1:A:405:U:H6 | 1.86 | 0.41 |
| 1:A:586:C:O3' | 10:H:89:PRO:HB2 | 2.21 | 0.41 |
| 1:A:619:U:O2 | 6:D:133:VAL:HA | 2.20 | 0.41 |
| 1:A:682:G:O2' | 1:A:683:G:H5' | 2.21 | 0.41 |
| 1:A:916:G:H2' | 1:A:917:G:H8 | 1.86 | 0.41 |
| 1:A:934:C:C4 | 1:A:1345:U:C5 | 3.09 | 0.41 |
| 1:A:1068:G:OP2 | 1:A:1068:G:H8 | 2.02 | 0.41 |
| 1:A:1126:U:C2 | 1:A:1127:G:C8 | 3.08 | 0.41 |
| 1:A:1153:C:C2 | 1:A:1154:G:C8 | 3.09 | 0.41 |
| 1:A:1441:G:H1' | 1:A:1460:A:N6 | 2.36 | 0.41 |
| 2:Y:30:C:H6 | 2:Y:30:C:O5' | 2.03 | 0.41 |
| 4:B:17:PHE:O | 4:B:18:GLY:O | 2.39 | 0.41 |
| 4:B:80:ILE:HD11 | 4:B:208:ILE:CG2 | 2.43 | 0.41 |
| 4:B:82:ARG:HG3 | 4:B:83:MET:N | 2.36 | 0.41 |
| 4:B:118:LEU:HB3 | 4:B:142:LEU:HG | 2.03 | 0.41 |
| 7:E:5:ASP:CG | 7:E:6:PHE:N | 2.72 | 0.41 |
| 7:E:150:ARG:HG3 | 7:E:150:ARG:NH1 | 2.36 | 0.41 |
| 10:H:51:VAL:CG1 | 10:H:52:ASP:H | 2.33 | 0.41 |
| 10:H:51:VAL:CG2 | 10:H:60:ARG:HG2 | 2.51 | 0.41 |
| 11:I:97:LYS:N | 11:I:98:PRO:CD | 2.83 | 0.41 |
| 12:J:39:PRO:HA | 12:J:70:ARG:HH11 | 1.84 | 0.41 |
| 12:J:79:ARG:HG2 | 12:J:79:ARG:HH11 | 1.85 | 0.41 |
| 12:J:81:THR:C | 12:J:83:GLU:N | 2.73 | 0.41 |
| 14:L:88:GLY:H | 14:L:98:TYR:HA | 1.85 | 0.41 |
| 15:M:82:MET:CE | 15:M:92:HIS:HB3 | 2.50 | 0.41 |
| 15:M:105:THR:O | 15:M:106:ASN:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:O:36:ILE:HA | 17:O:59:MET:CE | 2.51 | 0.41 |
| 18:P:20:VAL:HG12 | 18:P:21:VAL:O | 2.20 | 0.41 |
| 19:Q:63:ARG:HG2 | 19:Q:64:PRO:HD2 | 2.03 | 0.41 |
| 21:S:74:PHE:CD1 | 21:S:74:PHE:N | 2.89 | 0.41 |
| 1:A:166:G:O2' | 1:A:167:G:H5' | 2.20 | 0.41 |
| 1:A:272:C:O2' | 1:A:273:A:H5' | 2.21 | 0.41 |
| 1:A:645:C:H2' | 1:A:646:U:H6 | 1.85 | 0.41 |
| 1:A:678:U:H2' | 1:A:679:C:C6 | 2.56 | 0.41 |
| 1:A:855:G:H2' | 1:A:856:C:C6 | 2.56 | 0.41 |
| 1:A:947:G:H2' | 1:A:948:C:O4' | 2.21 | 0.41 |
| 1:A:1154:G:H2' | 1:A:1155:G:C8 | 2.47 | 0.41 |
| 1:A:1288:A:C6 | 1:A:1289:A:C5 | 3.09 | 0.41 |
| 1:A:1300:G:C2' | 1:A:1301:U:OP2 | 2.68 | 0.41 |
| 1:A:1494:G:O2' | 1:A:1495:U:H5' | 2.21 | 0.41 |
| 4:B:64:ARG:NH1 | 4:B:64:ARG:HB2 | 2.36 | 0.41 |
| 4:B:228:GLY:O | 4:B:229:VAL:C | 2.59 | 0.41 |
| 12:J:24:VAL:HG12 | 12:J:28:ARG:NE | 2.36 | 0.41 |
| 12:J:49:VAL:CG1 | 16:N:41:ARG:HD2 | 2.46 | 0.41 |
| 13:K:99:GLN:HG2 | 13:K:105:VAL:HG21 | 2.03 | 0.41 |
| 14:L:126:LYS:C | 14:L:126:LYS:HZ2 | 2.24 | 0.41 |
| 15:M:15:VAL:HG23 | 15:M:43:THR:O | 2.21 | 0.41 |
| 16:N:11:LYS:HE3 | 16:N:11:LYS:HB2 | 1.90 | 0.41 |
| 18:P:63:GLY:O | 18:P:64:ALA:C | 2.59 | 0.41 |
| 1:A:90:U:H2' | 1:A:91:C:C6 | 2.56 | 0.40 |
| 1:A:180:U:C2' | 1:A:181:G:H5' | 2.50 | 0.40 |
| 1:A:204:U:H5' | 1:A:216:G:O4' | 2.21 | 0.40 |
| 1:A:523:A:H61 | 14:L:53:ARG:NH1 | 2.20 | 0.40 |
| 1:A:983:A:C2 | 1:A:984:C:C6 | 3.09 | 0.40 |
| 1:A:1010:G:O2' | 1:A:1011:G:H5' | 2.21 | 0.40 |
| 1:A:1082:G:O2' | 1:A:1083:U:H5' | 2.21 | 0.40 |
| 1:A:1278:U:H4' | 1:A:1279:A:H5' | 1.99 | 0.40 |
| 4:B:230:VAL:HG13 | 4:B:231:GLU:OE2 | 2.21 | 0.40 |
| 5:C:14:ILE:O | 5:C:15:THR:C | 2.60 | 0.40 |
| 6:D:8:VAL:O | 6:D:10:ARG:N | 2.54 | 0.40 |
| 6:D:149:ALA:O | 6:D:152:SER:N | 2.38 | 0.40 |
| 9:G:122:HIS:HD2 | 9:G:125:MET:HE1 | 1.84 | 0.40 |
| 15:M:63:THR:HG23 | 15:M:64:TRP:N | 2.35 | 0.40 |
| 16:N:44:LEU:O | 16:N:48:ALA:HB2 | 2.21 | 0.40 |
| 19:Q:103:GLY:O | 19:Q:104:LYS:HD3 | 2.20 | 0.40 |
| 22:T:43:LEU:HD12 | 22:T:52:ALA:HA | 2.03 | 0.40 |
| 1:A:67:C:O2' | 1:A:171:A:H1' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:130:A:C8 | 19:Q:63:ARG:HG3 | 2.56 | 0.40 |
| 1:A:421:U:C5' | 1:A:422:C:OP2 | 2.65 | 0.40 |
| 1:A:560:U:O2' | 1:A:561:U:OP2 | 2.30 | 0.40 |
| 1:A:739:C:O2' | 17:O:42:HIS:ND1 | 2.46 | 0.40 |
| 1:A:751:U:H4' | 17:O:24:SER:HA | 2.02 | 0.40 |
| 1:A:972:C:O2' | 12:J:55:LYS:HA | 2.22 | 0.40 |
| 1:A:1002:G:N1 | 1:A:1003:G:C6 | 2.89 | 0.40 |
| 1:A:1125:U:O4 | 12:J:5:ARG:HG2 | 2.22 | 0.40 |
| 1:A:1145:C:O2' | 1:A:1146:A:O5' | 2.32 | 0.40 |
| 1:A:1442:G:C6 | 1:A:1446:A:N6 | 2.88 | 0.40 |
| 4:B:18:GLY:CA | 4:B:41:ILE:HA | 2.50 | 0.40 |
| 4:B:124:SER:O | 4:B:127:ILE:HG13 | 2.20 | 0.40 |
| 5:C:147:LYS:HE2 | 5:C:205:GLY:CA | 2.52 | 0.40 |
| 5:C:150:LYS:HB2 | 5:C:169:ALA:HB1 | 2.02 | 0.40 |
| 7:E:102:ALA:HB2 | 7:E:120:THR:HB | 2.03 | 0.40 |
| 7:E:102:ALA:CB | 7:E:120:THR:HG21 | 2.51 | 0.40 |
| 7:E:126:ARG:HG3 | 7:E:126:ARG:HH11 | 1.86 | 0.40 |
| 8:F:23:LYS:HE2 | 8:F:23:LYS:HB3 | 1.97 | 0.40 |
| 8:F:75:LEU:HD13 | 8:F:75:LEU:O | 2.21 | 0.40 |
| 10:H:65:TYR:HA | 10:H:79:VAL:HG23 | 2.03 | 0.40 |
| 14:L:89:ARG:HG2 | 14:L:97:ARG:HB3 | 2.02 | 0.40 |
| 15:M:25:ILE:HD11 | 15:M:60:VAL:HG13 | 2.03 | 0.40 |
| 16:N:37:PHE:C | 16:N:39:LEU:N | 2.75 | 0.40 |
| 18:P:43:LYS:HG2 | 18:P:48:TRP:CE2 | 2.56 | 0.40 |
| 22:T:63:ILE:HD13 | 22:T:80:ARG:HB2 | 2.04 | 0.40 |
| 22:T:100:ILE:O | 22:T:100:ILE:HG22 | 2.21 | 0.40 |
| 1:A:141:A:H2' | 1:A:142:G:O4' | 2.22 | 0.40 |
| 1:A:1112:C:O2 | 5:C:179:ARG:HB2 | 2.21 | 0.40 |
| 1:A:1286:A:H2' | 1:A:1287:A:O5' | 2.21 | 0.40 |
| 4:B:72:GLY:HA3 | 4:B:81:VAL:HG21 | 2.04 | 0.40 |
| 4:B:97:TRP:CH2 | 4:B:176:GLU:CD | 2.93 | 0.40 |
| 9:G:110:GLN:OE1 | 9:G:110:GLN:HA | 2.21 | 0.40 |
| 9:G:139:GLU:O | 9:G:143:ARG:HG3 | 2.22 | 0.40 |
| 10:H:25:ASP:N | 10:H:25:ASP:OD1 | 2.54 | 0.40 |
| 12:J:16:LEU:O | 12:J:17:ASP:C | 2.60 | 0.40 |
| 12:J:23:ILE:CG2 | 12:J:72:VAL:HG11 | 2.51 | 0.40 |
| 15:M:91:ARG:HA | 15:M:91:ARG:HD2 | 1.97 | 0.40 |
| 1:A:154:C:H2' | 1:A:155:C:H6 | 1.87 | 0.40 |
| 1:A:224:C:H2' | 1:A:225:C:H6 | 1.87 | 0.40 |
| 1:A:426:G:H2' | 1:A:427:U:C6 | 2.57 | 0.40 |
| 1:A:582:U:C2 | 1:A:760:G:C6 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:757:U:O2' | 1:A:879:C:H1' | 2.22 | 0.40 |
| 1:A:812:C:O2' | 1:A:813:U:OP2 | 2.19 | 0.40 |
| 1:A:942:G:H2' | 1:A:943:U:C6 | 2.57 | 0.40 |
| 1:A:1065:U:O2' | 1:A:1066:C:OP2 | 2.30 | 0.40 |
| 1:A:1342:C:O3' | 11:I:125:TYR:CE2 | 2.74 | 0.40 |
| 1:A:1524:C:OP1 | 13:K:120:ARG:NH1 | 2.54 | 0.40 |
| 4:B:14:GLY:C | 4:B:15:VAL:CG2 | 2.90 | 0.40 |
| 4:B:91:PRO:HG2 | 4:B:155:LEU:HG | 2.03 | 0.40 |
| 4:B:112:VAL:C | 4:B:114:ARG:N | 2.73 | 0.40 |
| 4:B:140:HIS:O | 4:B:141:GLU:C | 2.58 | 0.40 |
| 5:C:123:GLN:NE2 | 5:C:140:ARG:HH22 | 2.20 | 0.40 |
| 5:C:153:VAL:HG12 | 5:C:154:SER:N | 2.36 | 0.40 |
| 5:C:154:SER:OG | 5:C:155:GLY:N | 2.53 | 0.40 |
| 9:G:51:GLN:O | 9:G:53:LYS:N | 2.54 | 0.40 |
| 9:G:115:ARG:HB3 | 9:G:118:VAL:CG2 | 2.52 | 0.40 |
| 10:H:75:ARG:HA | 10:H:76:PRO:HD3 | 1.77 | 0.40 |
| 14:L:46:LYS:HE3 | 14:L:47:LYS:HB2 | 2.03 | 0.40 |
| 15:M:59:TYR:O | 15:M:62:ASN:O | 2.38 | 0.40 |
| 15:M:81:LEU:HA | 15:M:84:ILE:HG12 | 2.03 | 0.40 |
| 17:O:85:LEU:HD23 | 17:O:85:LEU:HA | 1.86 | 0.40 |
| 21:S:22:LEU:HD13 | 21:S:28:LYS:HB3 | 2.02 | 0.40 |
| 1:A:373:A:C1' | 1:A:481:G:O2' | 2.69 | 0.40 |
| 1:A:620:C:H2' | 1:A:621:A:O4' | 2.21 | 0.40 |
| 1:A:665:A:N3 | 1:A:732:C:H2' | 2.36 | 0.40 |
| 1:A:1169:A:H2' | 1:A:1171:G:O4' | 2.22 | 0.40 |
| 1:A:1191:A:H2' | 1:A:1192:C:H6 | 1.85 | 0.40 |
| 8:F:42:GLU:HG3 | 8:F:61:LEU:HD23 | 2.03 | 0.40 |
| 9:G:95:ARG:HG2 | 9:G:99:LEU:CD1 | 2.52 | 0.40 |
| 12:J:25:GLU:C | 12:J:27:ALA:H | 2.25 | 0.40 |
| 14:L:123:LYS:H | 14:L:123:LYS:HG2 | 1.66 | 0.40 |
| 21:S:32:LYS:O | 21:S:32:LYS:HG3 | 2.22 | 0.40 |
| 22:T:14:LYS:O | 22:T:18:GLN:HG3 | 2.21 | 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 |
|---|---|---|---|---|---|---|
| 4 | B | 232/256 (91%) | 159 (68%) | 49 (21%) | 24 (10%) | 0 2 |
| 5 | C | 204/239 (85%) | 128 (63%) | 44 (22%) | 32 (16%) | 0 1 |
| 6 | D | 206/208 (99%) | 170 (82%) | 25 (12%) | 11 (5%) | 2 11 |
| 7 | E | 148/161 (92%) | 132 (89%) | 15 (10%) | 1 (1%) | 22 60 |
| 8 | F | 99/101 (98%) | 80 (81%) | 16 (16%) | 3 (3%) | 4 24 |
| 9 | G | 153/155 (99%) | 121 (79%) | 28 (18%) | 4 (3%) | 5 27 |
| 10 | H | 136/138 (99%) | 117 (86%) | 17 (12%) | 2 (2%) | 10 42 |
| 11 | I | 125/128 (98%) | 91 (73%) | 24 (19%) | 10 (8%) | 1 4 |
| 12 | J | 96/104 (92%) | 58 (60%) | 21 (22%) | 17 (18%) | 0 0 |
| 13 | K | 117/129 (91%) | 95 (81%) | 13 (11%) | 9 (8%) | 1 5 |
| 14 | L | 122/135 (90%) | 99 (81%) | 16 (13%) | 7 (6%) | 1 10 |
| 15 | M | 116/126 (92%) | 83 (72%) | 21 (18%) | 12 (10%) | 0 2 |
| 16 | N | 58/60 (97%) | 33 (57%) | 15 (26%) | 10 (17%) | 0 0 |
| 17 | O | 86/88 (98%) | 78 (91%) | 6 (7%) | 2 (2%) | 6 30 |
| 18 | P | 81/88 (92%) | 64 (79%) | 13 (16%) | 4 (5%) | 2 13 |
| 19 | Q | 102/104 (98%) | 85 (83%) | 10 (10%) | 7 (7%) | 1 6 |
| 20 | R | 71/88 (81%) | 62 (87%) | 5 (7%) | 4 (6%) | 2 10 |
| 21 | S | 78/92 (85%) | 57 (73%) | 15 (19%) | 6 (8%) | 1 5 |
| 22 | T | 97/106 (92%) | 73 (75%) | 15 (16%) | 9 (9%) | 0 3 |
| 23 | V | 22/26 (85%) | 15 (68%) | 6 (27%) | 1 (4%) | 2 14 |
| All | All | 2349/2532 (93%) | 1800 (77%) | 374 (16%) | 175 (7%) | 1 5 |

All (175) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | B | 15 | VAL |
| 4 | B | 17 | PHE |
| 4 | B | 21 | ARG |
| 4 | B | 23 | ARG |
| 4 | B | 24 | TRP |
| 4 | B | 123 | ALA |
| 4 | B | 142 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | B | 143 | GLU |
| 4 | B | 190 | THR |
| 4 | B | 229 | VAL |
| 4 | B | 232 | PRO |
| 5 | C | 15 | THR |
| 5 | C | 16 | ARG |
| 5 | C | 26 | LYS |
| 5 | C | 82 | GLU |
| 5 | C | 84 | ILE |
| 5 | C | 98 | ASN |
| 5 | C | 100 | ALA |
| 5 | C | 101 | LEU |
| 5 | C | 156 | ARG |
| 5 | C | 187 | ALA |
| 5 | C | 189 | ALA |
| 6 | D | 36 | ARG |
| 7 | E | 16 | THR |
| 8 | F | 36 | ARG |
| 10 | H | 91 | ARG |
| 11 | I | 41 | VAL |
| 11 | I | 127 | LYS |
| 12 | J | 34 | VAL |
| 12 | J | 61 | GLU |
| 12 | J | 79 | ARG |
| 13 | K | 13 | GLN |
| 13 | K | 127 | LYS |
| 14 | L | 27 | LEU |
| 14 | L | 28 | LYS |
| 14 | L | 47 | LYS |
| 15 | M | 6 | GLY |
| 15 | M | 23 | TYR |
| 15 | M | 24 | GLY |
| 15 | M | 27 | LYS |
| 15 | M | 67 | GLU |
| 15 | M | 86 | CYS |
| 16 | N | 22 | THR |
| 17 | O | 88 | ARG |
| 18 | P | 52 | ASP |
| 18 | P | 64 | ALA |
| 19 | Q | 14 | LYS |
| 19 | Q | 80 | GLY |
| 19 | Q | 81 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | Q | 96 | GLN |
| 20 | R | 19 | LYS |
| 20 | R | 87 | ARG |
| 21 | S | 5 | LEU |
| 22 | T | 9 | ASN |
| 22 | T | 11 | SER |
| 4 | B | 8 | LYS |
| 4 | B | 18 | GLY |
| 4 | B | 95 | GLN |
| 4 | B | 195 | ASP |
| 4 | B | 228 | GLY |
| 5 | C | 66 | VAL |
| 5 | C | 127 | ARG |
| 5 | C | 154 | SER |
| 5 | C | 171 | GLY |
| 5 | C | 179 | ARG |
| 6 | D | 31 | CYS |
| 6 | D | 44 | GLY |
| 8 | F | 35 | ALA |
| 9 | G | 4 | ARG |
| 9 | G | 80 | VAL |
| 10 | H | 105 | ARG |
| 11 | I | 11 | LYS |
| 11 | I | 46 | ALA |
| 11 | I | 55 | ALA |
| 11 | I | 58 | ARG |
| 11 | I | 78 | LYS |
| 12 | J | 27 | ALA |
| 12 | J | 30 | SER |
| 12 | J | 32 | ALA |
| 12 | J | 54 | PHE |
| 12 | J | 55 | LYS |
| 12 | J | 72 | VAL |
| 13 | K | 90 | GLY |
| 14 | L | 79 | GLU |
| 14 | L | 116 | SER |
| 15 | M | 63 | THR |
| 15 | M | 106 | ASN |
| 16 | N | 15 | LYS |
| 16 | N | 36 | PHE |
| 16 | N | 56 | VAL |
| 18 | P | 10 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | Q | 103 | GLY |
| 20 | R | 48 | GLY |
| 22 | T | 74 | LYS |
| 22 | T | 96 | GLY |
| 22 | T | 102 | GLY |
| 4 | B | 20 | GLU |
| 4 | B | 74 | LYS |
| 5 | C | 102 | ASN |
| 5 | C | 181 | ASN |
| 5 | C | 205 | GLY |
| 6 | D | 4 | TYR |
| 6 | D | 42 | GLN |
| 12 | J | 65 | LEU |
| 12 | J | 90 | LEU |
| 12 | J | 99 | LYS |
| 13 | K | 15 | ALA |
| 13 | K | 27 | ASN |
| 13 | K | 117 | ASN |
| 14 | L | 48 | PRO |
| 14 | L | 126 | LYS |
| 15 | M | 3 | ARG |
| 15 | M | 21 | TYR |
| 16 | N | 12 | ARG |
| 16 | N | 14 | PRO |
| 19 | Q | 68 | ARG |
| 19 | Q | 98 | LEU |
| 21 | S | 6 | LYS |
| 21 | S | 32 | LYS |
| 22 | T | 73 | HIS |
| 22 | T | 103 | GLY |
| 23 | V | 9 | ARG |
| 4 | B | 9 | GLU |
| 4 | B | 16 | HIS |
| 4 | B | 39 | ILE |
| 4 | B | 90 | MET |
| 5 | C | 12 | LEU |
| 5 | C | 108 | ASN |
| 5 | C | 146 | ALA |
| 5 | C | 188 | LEU |
| 6 | D | 5 | ILE |
| 6 | D | 7 | PRO |
| 6 | D | 9 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | D | 88 | VAL |
| 8 | F | 98 | LEU |
| 9 | G | 41 | ARG |
| 11 | I | 105 | ASP |
| 12 | J | 39 | PRO |
| 12 | J | 40 | LEU |
| 12 | J | 73 | ASP |
| 12 | J | 86 | MET |
| 15 | M | 4 | ILE |
| 16 | N | 26 | ARG |
| 20 | R | 38 | GLU |
| 21 | S | 17 | GLU |
| 21 | S | 30 | LEU |
| 5 | C | 4 | LYS |
| 5 | C | 14 | ILE |
| 5 | C | 29 | TYR |
| 11 | I | 121 | ARG |
| 13 | K | 69 | ALA |
| 16 | N | 4 | LYS |
| 17 | O | 75 | PRO |
| 22 | T | 94 | ALA |
| 4 | B | 130 | ARG |
| 5 | C | 53 | ALA |
| 5 | C | 168 | ALA |
| 6 | D | 91 | SER |
| 11 | I | 12 | GLU |
| 13 | K | 70 | LYS |
| 16 | N | 23 | ARG |
| 21 | S | 9 | VAL |
| 22 | T | 97 | ALA |
| 6 | D | 87 | GLY |
| 12 | J | 4 | ILE |
| 18 | P | 51 | VAL |
| 4 | B | 227 | GLY |
| 5 | C | 81 | GLY |
| 15 | M | 97 | PRO |
| 5 | C | 55 | VAL |
| 5 | C | 57 | ILE |
| 9 | G | 42 | ILE |
| 13 | K | 48 | ILE |
| 16 | N | 25 | VAL |
| 5 | C | 13 | GLY |

### 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 |
|---|---|---|---|---|---|
| 4 | B | 202/220 (92%) | 175 (87%) | 27 (13%) | 4 17 |
| 5 | C | 160/188 (85%) | 144 (90%) | 16 (10%) | 7 29 |
| 6 | D | 180/180 (100%) | 167 (93%) | 13 (7%) | 14 45 |
| 7 | E | 115/122 (94%) | 99 (86%) | 16 (14%) | 3 16 |
| 8 | F | 90/90 (100%) | 80 (89%) | 10 (11%) | 6 25 |
| 9 | G | 126/126 (100%) | 120 (95%) | 6 (5%) | 25 62 |
| 10 | H | 119/119 (100%) | 106 (89%) | 13 (11%) | 6 25 |
| 11 | I | 98/99 (99%) | 87 (89%) | 11 (11%) | 6 24 |
| 12 | J | 87/91 (96%) | 79 (91%) | 8 (9%) | 9 34 |
| 13 | K | 90/99 (91%) | 83 (92%) | 7 (8%) | 12 42 |
| 14 | L | 104/111 (94%) | 94 (90%) | 10 (10%) | 8 32 |
| 15 | M | 94/101 (93%) | 83 (88%) | 11 (12%) | 5 22 |
| 16 | N | 49/49 (100%) | 43 (88%) | 6 (12%) | 5 21 |
| 17 | O | 79/79 (100%) | 73 (92%) | 6 (8%) | 13 43 |
| 18 | P | 72/74 (97%) | 68 (94%) | 4 (6%) | 21 56 |
| 19 | Q | 96/96 (100%) | 87 (91%) | 9 (9%) | 8 32 |
| 20 | R | 64/77 (83%) | 61 (95%) | 3 (5%) | 26 63 |
| 21 | S | 71/79 (90%) | 62 (87%) | 9 (13%) | 4 19 |
| 22 | T | 76/82 (93%) | 70 (92%) | 6 (8%) | 12 41 |
| 23 | V | 19/21 (90%) | 19 (100%) | 0 | 100 100 |
| All | All | 1991/2103 (95%) | 1800 (90%) | 191 (10%) | 8 32 |

All (191) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | B | 8 | LYS |
| 4 | B | 10 | LEU |
| 4 | B | 15 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | B | 23 | ARG |
| 4 | B | 24 | TRP |
| 4 | B | 25 | ASN |
| 4 | B | 82 | ARG |
| 4 | B | 87 | ARG |
| 4 | B | 90 | MET |
| 4 | B | 98 | LEU |
| 4 | B | 117 | GLU |
| 4 | B | 121 | LEU |
| 4 | B | 129 | GLU |
| 4 | B | 141 | GLU |
| 4 | B | 156 | LYS |
| 4 | B | 162 | ILE |
| 4 | B | 163 | PHE |
| 4 | B | 165 | VAL |
| 4 | B | 169 | LYS |
| 4 | B | 170 | GLU |
| 4 | B | 178 | ARG |
| 4 | B | 187 | LEU |
| 4 | B | 204 | ASN |
| 4 | B | 208 | ILE |
| 4 | B | 231 | GLU |
| 4 | B | 232 | PRO |
| 4 | B | 236 | TYR |
| 5 | C | 3 | ASN |
| 5 | C | 5 | ILE |
| 5 | C | 14 | ILE |
| 5 | C | 26 | LYS |
| 5 | C | 35 | GLU |
| 5 | C | 44 | GLU |
| 5 | C | 52 | LEU |
| 5 | C | 56 | ASP |
| 5 | C | 99 | VAL |
| 5 | C | 139 | GLN |
| 5 | C | 162 | GLN |
| 5 | C | 166 | GLU |
| 5 | C | 167 | TRP |
| 5 | C | 184 | TYR |
| 5 | C | 188 | LEU |
| 5 | C | 204 | LEU |
| 6 | D | 9 | CYS |
| 6 | D | 15 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | D | 33 | MET |
| 6 | D | 36 | ARG |
| 6 | D | 57 | ARG |
| 6 | D | 58 | LEU |
| 6 | D | 72 | GLU |
| 6 | D | 96 | LEU |
| 6 | D | 122 | ARG |
| 6 | D | 127 | THR |
| 6 | D | 157 | LEU |
| 6 | D | 192 | GLU |
| 6 | D | 193 | ASP |
| 7 | E | 12 | LEU |
| 7 | E | 15 | ARG |
| 7 | E | 25 | ARG |
| 7 | E | 26 | PHE |
| 7 | E | 31 | LEU |
| 7 | E | 33 | VAL |
| 7 | E | 41 | VAL |
| 7 | E | 43 | LEU |
| 7 | E | 53 | LEU |
| 7 | E | 73 | ASN |
| 7 | E | 79 | GLU |
| 7 | E | 80 | ILE |
| 7 | E | 89 | ILE |
| 7 | E | 120 | THR |
| 7 | E | 144 | THR |
| 7 | E | 150 | ARG |
| 8 | F | 1 | MET |
| 8 | F | 10 | LEU |
| 8 | F | 24 | GLU |
| 8 | F | 55 | ASP |
| 8 | F | 63 | TYR |
| 8 | F | 69 | GLU |
| 8 | F | 74 | ASP |
| 8 | F | 86 | ARG |
| 8 | F | 89 | MET |
| 8 | F | 95 | GLU |
| 9 | G | 11 | GLN |
| 9 | G | 37 | ASN |
| 9 | G | 38 | LEU |
| 9 | G | 84 | ASN |
| 9 | G | 149 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | G | 156 | TRP |
| 10 | H | 24 | THR |
| 10 | H | 26 | VAL |
| 10 | H | 52 | ASP |
| 10 | H | 63 | LEU |
| 10 | H | 81 | HIS |
| 10 | H | 84 | ARG |
| 10 | H | 85 | ARG |
| 10 | H | 91 | ARG |
| 10 | H | 92 | ARG |
| 10 | H | 112 | LEU |
| 10 | H | 125 | ARG |
| 10 | H | 127 | LEU |
| 10 | H | 133 | LEU |
| 11 | I | 2 | GLU |
| 11 | I | 16 | ARG |
| 11 | I | 38 | GLN |
| 11 | I | 41 | VAL |
| 11 | I | 58 | ARG |
| 11 | I | 65 | VAL |
| 11 | I | 75 | ASP |
| 11 | I | 79 | LEU |
| 11 | I | 92 | TYR |
| 11 | I | 111 | ARG |
| 11 | I | 121 | ARG |
| 12 | J | 29 | ARG |
| 12 | J | 45 | ARG |
| 12 | J | 57 | LYS |
| 12 | J | 60 | ARG |
| 12 | J | 66 | ARG |
| 12 | J | 73 | ASP |
| 12 | J | 83 | GLU |
| 12 | J | 89 | ASP |
| 13 | K | 24 | SER |
| 13 | K | 29 | ILE |
| 13 | K | 30 | VAL |
| 13 | K | 35 | PRO |
| 13 | K | 54 | ARG |
| 13 | K | 57 | THR |
| 13 | K | 73 | MET |
| 14 | L | 33 | ARG |
| 14 | L | 41 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | L | 48 | PRO |
| 14 | L | 53 | ARG |
| 14 | L | 59 | ARG |
| 14 | L | 60 | LEU |
| 14 | L | 79 | GLU |
| 14 | L | 113 | ARG |
| 14 | L | 114 | LYS |
| 14 | L | 126 | LYS |
| 15 | M | 40 | ASN |
| 15 | M | 44 | ARG |
| 15 | M | 56 | LEU |
| 15 | M | 59 | TYR |
| 15 | M | 70 | LEU |
| 15 | M | 81 | LEU |
| 15 | M | 102 | ARG |
| 15 | M | 105 | THR |
| 15 | M | 106 | ASN |
| 15 | M | 110 | ARG |
| 15 | M | 115 | LYS |
| 16 | N | 12 | ARG |
| 16 | N | 14 | PRO |
| 16 | N | 22 | THR |
| 16 | N | 31 | ARG |
| 16 | N | 41 | ARG |
| 16 | N | 44 | LEU |
| 17 | O | 10 | LYS |
| 17 | O | 31 | LEU |
| 17 | O | 34 | LEU |
| 17 | O | 39 | LEU |
| 17 | O | 70 | LEU |
| 17 | O | 81 | LEU |
| 18 | P | 2 | VAL |
| 18 | P | 8 | ARG |
| 18 | P | 53 | VAL |
| 18 | P | 62 | VAL |
| 19 | Q | 9 | VAL |
| 19 | Q | 38 | ARG |
| 19 | Q | 48 | GLU |
| 19 | Q | 53 | LEU |
| 19 | Q | 60 | ILE |
| 19 | Q | 68 | ARG |
| 19 | Q | 74 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | Q | 76 | LEU |
| 19 | Q | 101 | ARG |
| 20 | R | 36 | ASN |
| 20 | R | 54 | ARG |
| 20 | R | 55 | ARG |
| 21 | S | 5 | LEU |
| 21 | S | 7 | LYS |
| 21 | S | 12 | ASP |
| 21 | S | 15 | LEU |
| 21 | S | 36 | ARG |
| 21 | S | 61 | TYR |
| 21 | S | 62 | ILE |
| 21 | S | 65 | ASN |
| 21 | S | 81 | ARG |
| 22 | T | 13 | LEU |
| 22 | T | 42 | GLN |
| 22 | T | 57 | ARG |
| 22 | T | 73 | HIS |
| 22 | T | 75 | ASN |
| 22 | T | 84 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | B | 19 | HIS |
| 4 | B | 25 | ASN |
| 4 | B | 40 | HIS |
| 4 | B | 94 | ASN |
| 4 | B | 204 | ASN |
| 4 | B | 212 | GLN |
| 4 | B | 240 | GLN |
| 5 | C | 3 | ASN |
| 5 | C | 6 | HIS |
| 5 | C | 37 | GLN |
| 5 | C | 107 | GLN |
| 5 | C | 108 | ASN |
| 5 | C | 110 | ASN |
| 5 | C | 123 | GLN |
| 5 | C | 139 | GLN |
| 5 | C | 170 | GLN |
| 5 | C | 176 | HIS |
| 5 | C | 181 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | D | 42 | GLN |
| 6 | D | 62 | GLN |
| 6 | D | 123 | HIS |
| 6 | D | 161 | ASN |
| 7 | E | 20 | GLN |
| 7 | E | 73 | ASN |
| 8 | F | 18 | GLN |
| 8 | F | 32 | ASN |
| 8 | F | 57 | GLN |
| 8 | F | 73 | ASN |
| 8 | F | 94 | GLN |
| 8 | F | 100 | ASN |
| 9 | G | 37 | ASN |
| 9 | G | 51 | GLN |
| 9 | G | 56 | GLN |
| 9 | G | 64 | GLN |
| 9 | G | 68 | ASN |
| 9 | G | 96 | GLN |
| 9 | G | 106 | GLN |
| 9 | G | 122 | HIS |
| 11 | I | 31 | GLN |
| 11 | I | 73 | GLN |
| 12 | J | 62 | HIS |
| 12 | J | 78 | ASN |
| 13 | K | 38 | ASN |
| 13 | K | 93 | GLN |
| 13 | K | 117 | ASN |
| 14 | L | 49 | ASN |
| 14 | L | 75 | HIS |
| 15 | M | 40 | ASN |
| 17 | O | 37 | ASN |
| 17 | O | 46 | HIS |
| 18 | P | 16 | HIS |
| 19 | Q | 16 | GLN |
| 20 | R | 36 | ASN |
| 21 | S | 14 | HIS |
| 21 | S | 23 | ASN |
| 21 | S | 47 | HIS |
| 21 | S | 56 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A | 1511/1522 (99%) | 211 (13%) | 69 (4%) |
| 2 | Y | 14/17 (82%) | 1 (7%) | 0 |
| 3 | Z | 3/6 (50%) | 0 | 0 |
| All | All | 1528/1545 (98%) | 212 (13%) | 69 (4%) |

All (212) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 8 | A |
| 1 | A | 9 | G |
| 1 | A | 32 | A |
| 1 | A | 39 | G |
| 1 | A | 48 | C |
| 1 | A | 49 | U |
| 1 | A | 51 | A |
| 1 | A | 52 | G |
| 1 | A | 61 | G |
| 1 | A | 65 | U |
| 1 | A | 81 | U |
| 1 | A | 82 | U |
| 1 | A | 101 | A |
| 1 | A | 116 | A |
| 1 | A | 120 | A |
| 1 | A | 121 | C |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 163 | C |
| 1 | A | 181 | G |
| 1 | A | 182 | U |
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 202 | U |
| 1 | A | 203 | U |
| 1 | A | 204 | U |
| 1 | A | 216 | G |
| 1 | A | 244 | U |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 252 | U |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 280 | C |
| 1 | A | 282 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 289 | G |
| 1 | A | 316 | G |
| 1 | A | 321 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 332 | G |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 350 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 366 | C |
| 1 | A | 367 | U |
| 1 | A | 373 | A |
| 1 | A | 397 | A |
| 1 | A | 398 | C |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 421 | U |
| 1 | A | 422 | C |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 439 | A |
| 1 | A | 452 | A |
| 1 | A | 461 | C |
| 1 | A | 462 | G |
| 1 | A | 481 | G |
| 1 | A | 482 | A |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 486 | U |
| 1 | A | 497 | A |
| 1 | A | 498 | U |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 518 | C |
| 1 | A | 527 | G |
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 534 | U |
| 1 | A | 547 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 561 | U |
| 1 | A | 562 | C |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 575 | G |
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 653 | A |
| 1 | A | 665 | A |
| 1 | A | 688 | G |
| 1 | A | 701 | C |
| 1 | A | 702 | A |
| 1 | A | 703 | G |
| 1 | A | 718 | G |
| 1 | A | 721 | G |
| 1 | A | 723 | U |
| 1 | A | 724 | G |
| 1 | A | 731 | G |
| 1 | A | 748 | C |
| 1 | A | 755 | G |
| 1 | A | 777 | A |
| 1 | A | 781 | A |
| 1 | A | 782 | A |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 813 | U |
| 1 | A | 815 | A |
| 1 | A | 817 | C |
| 1 | A | 828 | A |
| 1 | A | 839 | U |
| 1 | A | 840 | C |
| 1 | A | 841 | U |
| 1 | A | 914 | A |
| 1 | A | 926 | G |
| 1 | A | 927 | G |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 945 | G |
| 1 | A | 960 | U |
| 1 | A | 965 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 966 | G |
| 1 | A | 968 | A |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 994 | A |
| 1 | A | 1004 | A |
| 1 | A | 1005 | A |
| 1 | A | 1026 | G |
| 1 | A | 1031 | G |
| 1 | A | 1050 | G |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1068 | G |
| 1 | A | 1085 | U |
| 1 | A | 1086 | U |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1101 | A |
| 1 | A | 1102 | A |
| 1 | A | 1117 | G |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |
| 1 | A | 1129 | C |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1136 | U |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1139 | G |
| 1 | A | 1145 | C |
| 1 | A | 1146 | A |
| 1 | A | 1152 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1159 | U |
| 1 | A | 1160 | G |
| 1 | A | 1183 | A |
| 1 | A | 1184 | G |
| 1 | A | 1191 | A |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1202 | G |
| 1 | A | 1212 | U |
| 1 | A | 1214 | C |
| 1 | A | 1224 | G |
| 1 | A | 1225 | A |
| 1 | A | 1250 | A |
| 1 | A | 1257 | U |
| 1 | A | 1279 | A |
| 1 | A | 1280 | A |
| 1 | A | 1281 | U |
| 1 | A | 1282 | C |
| 1 | A | 1285 | A |
| 1 | A | 1286 | A |
| 1 | A | 1287 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1303 | C |
| 1 | A | 1305 | G |
| 1 | A | 1338 | G |
| 1 | A | 1346 | A |
| 1 | A | 1347 | G |
| 1 | A | 1348 | U |
| 1 | A | 1379 | G |
| 1 | A | 1398 | A |
| 1 | A | 1442 | G |
| 1 | A | 1443 | G |
| 1 | A | 1446 | A |
| 1 | A | 1447 | G |
| 1 | A | 1452 | C |
| 1 | A | 1487 | G |
| 1 | A | 1492 | A |
| 1 | A | 1497 | G |
| 1 | A | 1499 | A |
| 1 | A | 1502 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1517 | G |
| 1 | A | 1520 | G |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 2 | Y | 34 | G |

All (69) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 7 | G |
| 1 | A | 48 | C |
| 1 | A | 51 | A |
| 1 | A | 60 | A |
| 1 | A | 64 | G |
| 1 | A | 81 | U |
| 1 | A | 115 | G |
| 1 | A | 119 | A |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |
| 1 | A | 202 | U |
| 1 | A | 204 | U |
| 1 | A | 243 | A |
| 1 | A | 250 | A |
| 1 | A | 251 | G |
| 1 | A | 266 | G |
| 1 | A | 279 | A |
| 1 | A | 281 | G |
| 1 | A | 328 | C |
| 1 | A | 344 | A |
| 1 | A | 350 | G |
| 1 | A | 353 | A |
| 1 | A | 366 | C |
| 1 | A | 372 | C |
| 1 | A | 421 | U |
| 1 | A | 428 | G |
| 1 | A | 438 | G |
| 1 | A | 484 | G |
| 1 | A | 485 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 496 | A |
| 1 | A | 497 | A |
| 1 | A | 509 | A |
| 1 | A | 533 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 575 | G |
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 722 | A |
| 1 | A | 793 | U |
| 1 | A | 812 | C |
| 1 | A | 913 | A |
| 1 | A | 965 | A |
| 1 | A | 975 | A |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 1049 | U |
| 1 | A | 1065 | U |
| 1 | A | 1067 | A |
| 1 | A | 1085 | U |
| 1 | A | 1101 | A |
| 1 | A | 1145 | C |
| 1 | A | 1182 | G |
| 1 | A | 1183 | A |
| 1 | A | 1190 | G |
| 1 | A | 1201 | A |
| 1 | A | 1224 | G |
| 1 | A | 1281 | U |
| 1 | A | 1285 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1346 | A |
| 1 | A | 1347 | G |
| 1 | A | 1451 | A |
| 1 | A | 1498 | U |
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1528 | U |

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

1 non-standard protein/DNA/RNA residue is 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 | $\#\|Z\| > 2$ |
| 2 | PSU | Y | 38 | 2 | 18,21,22 | 1.81 | 2 (11%) | 22,30,33 | 1.41 | 3 (13%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | PSU | Y | 38 | 2 | - | 0/7/25/26 | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Y | 38 | PSU | C2-N1 | 6.01 | 1.44 | 1.36 |
| 2 | Y | 38 | PSU | C6-N1 | 3.20 | 1.41 | 1.36 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Y | 38 | PSU | C6-C5-C4 | 3.74 | 120.81 | 118.20 |
| 2 | Y | 38 | PSU | O2-C2-N1 | 3.51 | 126.66 | 122.79 |
| 2 | Y | 38 | PSU | O4'-C1'-C2' | 2.10 | 108.11 | 105.14 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | Y | 38 | PSU | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 161 ligands modelled in this entry, 160 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 24 | PAR | A | 1545 | - | 45,45,45 | 1.74 | 12 (26%) | 64,67,67 | 1.12 | 5 (7%) |

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 |
|---|---|---|---|---|---|---|---|
| 24 | PAR | A | 1545 | - | - | 4/18/94/94 | 0/4/4/4 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | A | 1545 | PAR | C64-C54 | 5.74 | 1.59 | 1.52 |
| 24 | A | 1545 | PAR | O54-C14 | 3.99 | 1.52 | 1.41 |
| 24 | A | 1545 | PAR | O33-C14 | 2.73 | 1.49 | 1.41 |
| 24 | A | 1545 | PAR | C31-C21 | 2.47 | 1.56 | 1.53 |
| 24 | A | 1545 | PAR | C11-C21 | 2.39 | 1.57 | 1.52 |
| 24 | A | 1545 | PAR | C41-C51 | 2.27 | 1.57 | 1.53 |
| 24 | A | 1545 | PAR | O44-C44 | 2.19 | 1.48 | 1.43 |
| 24 | A | 1545 | PAR | O51-C11 | 2.18 | 1.47 | 1.41 |
| 24 | A | 1545 | PAR | C52-C42 | 2.16 | 1.56 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | A | 1545 | PAR | C44-C54 | 2.15 | 1.57 | 1.53 |
| 24 | A | 1545 | PAR | C44-C34 | 2.12 | 1.57 | 1.52 |
| 24 | A | 1545 | PAR | O33-C33 | 2.11 | 1.49 | 1.43 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A | 1545 | PAR | O54-C54-C64 | 3.47 | 112.47 | 106.01 |
| 24 | A | 1545 | PAR | O52-C13-C23 | 3.12 | 114.42 | 107.96 |
| 24 | A | 1545 | PAR | C14-O54-C54 | 2.87 | 119.32 | 113.69 |
| 24 | A | 1545 | PAR | O11-C11-C21 | 2.16 | 111.93 | 108.22 |
| 24 | A | 1545 | PAR | C22-C32-C42 | 2.02 | 114.63 | 109.53 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | A | 1545 | PAR | C24-C14-O33-C33 |
| 24 | A | 1545 | PAR | C33-C43-C53-O53 |
| 24 | A | 1545 | PAR | O54-C54-C64-N64 |
| 24 | A | 1545 | PAR | C23-C33-O33-C14 |

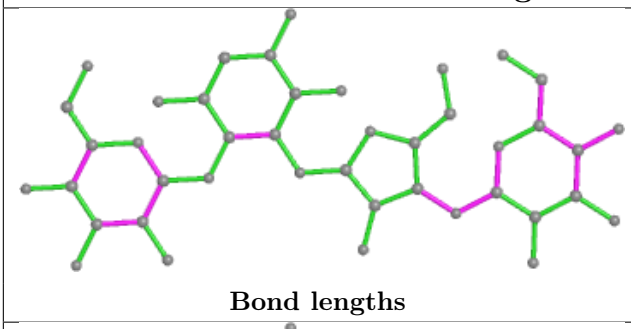
There are no ring outliers.

1 monomer is involved in 2 short contacts:

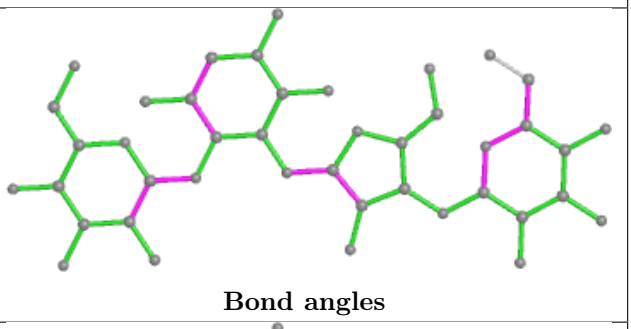
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | A | 1545 | PAR | 2 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

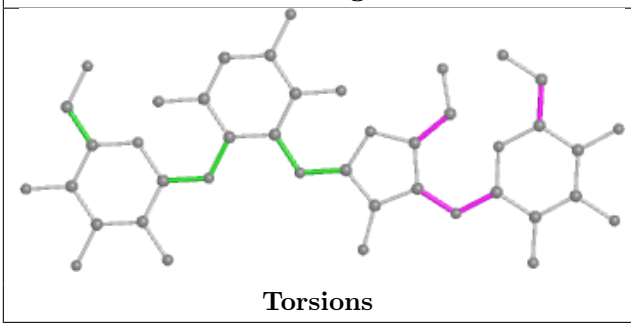
**Ligand PAR A 1545**



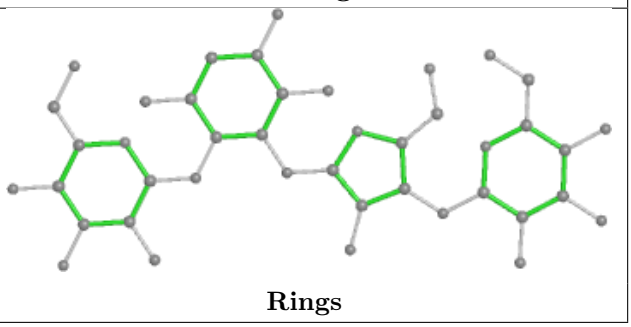
Bond lengths



Bond angles



Torsions



Rings

## 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 | 1513/1522 (99%) | 1.13 | 168 (11%) 5 1 | 25, 57, 134, 201 | 0 |
| 2 | Y | 14/17 (82%) | 0.95 | 0 100 100 | 60, 113, 163, 179 | 0 |
| 3 | Z | 4/6 (66%) | 1.20 | 1 (25%) 0 0 | 65, 69, 85, 179 | 0 |
| 4 | B | 234/256 (91%) | 0.15 | 11 (4%) 31 11 | 38, 96, 154, 190 | 0 |
| 5 | C | 206/239 (86%) | 0.36 | 9 (4%) 34 13 | 44, 83, 144, 182 | 0 |
| 6 | D | 208/208 (100%) | 0.13 | 7 (3%) 45 19 | 39, 64, 115, 166 | 0 |
| 7 | E | 150/161 (93%) | 0.03 | 1 (0%) 87 69 | 27, 50, 86, 155 | 0 |
| 8 | F | 101/101 (100%) | 0.40 | 4 (3%) 38 15 | 51, 87, 132, 156 | 0 |
| 9 | G | 155/155 (100%) | -0.05 | 1 (0%) 89 72 | 38, 70, 130, 175 | 0 |
| 10 | H | 138/138 (100%) | -0.03 | 2 (1%) 75 49 | 25, 46, 90, 127 | 0 |
| 11 | I | 127/128 (99%) | 0.61 | 13 (10%) 6 2 | 39, 86, 135, 161 | 0 |
| 12 | J | 98/104 (94%) | 1.45 | 29 (29%) 0 0 | 42, 110, 178, 201 | 0 |
| 13 | K | 119/129 (92%) | 0.17 | 2 (1%) 70 41 | 27, 61, 104, 180 | 0 |
| 14 | L | 124/135 (91%) | 0.14 | 1 (0%) 86 65 | 22, 61, 114, 166 | 0 |
| 15 | M | 118/126 (93%) | 0.17 | 5 (4%) 36 14 | 41, 73, 119, 146 | 0 |
| 16 | N | 60/60 (100%) | 0.73 | 8 (13%) 3 1 | 49, 80, 123, 174 | 0 |
| 17 | O | 88/88 (100%) | 0.39 | 4 (4%) 33 12 | 34, 60, 109, 178 | 0 |
| 18 | P | 83/88 (94%) | 0.05 | 1 (1%) 79 54 | 28, 48, 70, 146 | 0 |
| 19 | Q | 104/104 (100%) | 0.48 | 8 (7%) 13 4 | 28, 48, 149, 201 | 0 |
| 20 | R | 73/88 (82%) | 0.32 | 2 (2%) 54 26 | 41, 70, 152, 186 | 0 |
| 21 | S | 80/92 (86%) | 0.95 | 13 (16%) 1 0 | 53, 101, 164, 180 | 0 |
| 22 | T | 99/106 (93%) | -0.00 | 1 (1%) 82 59 | 30, 55, 105, 159 | 0 |
| 23 | V | 24/26 (92%) | 0.42 | 2 (8%) 11 3 | 42, 64, 114, 151 | 0 |
| All | All | 3920/4077 (96%) | 0.62 | 293 (7%) 14 4 | 22, 65, 141, 201 | 0 |

All (293) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 19 | Q | 102 | GLY | 10.0 |
| 1 | A | 1534 | A | 8.5 |
| 19 | Q | 105 | ALA | 8.0 |
| 19 | Q | 104 | LYS | 7.8 |
| 21 | S | 3 | ARG | 7.7 |
| 1 | A | 1129 | C | 7.6 |
| 1 | A | 1540 | U | 7.5 |
| 1 | A | 1541 | U | 6.9 |
| 19 | Q | 103 | GLY | 5.7 |
| 1 | A | 1144 | G | 5.6 |
| 1 | A | 1034 | G | 5.5 |
| 1 | A | 1024 | G | 5.5 |
| 12 | J | 72 | VAL | 5.5 |
| 6 | D | 23 | GLY | 5.1 |
| 1 | A | 1006 | C | 4.9 |
| 1 | A | 1004 | A | 4.9 |
| 1 | A | 1025 | U | 4.8 |
| 1 | A | 993 | G | 4.7 |
| 1 | A | 1277 | C | 4.6 |
| 10 | H | 1 | MET | 4.6 |
| 1 | A | 1539 | C | 4.5 |
| 12 | J | 10 | GLY | 4.4 |
| 1 | A | 1027 | C | 4.4 |
| 1 | A | 1030(A) | G | 4.4 |
| 16 | N | 6 | LEU | 4.4 |
| 16 | N | 3 | ARG | 4.3 |
| 12 | J | 37 | PRO | 4.3 |
| 11 | I | 17 | VAL | 4.2 |
| 11 | I | 15 | ALA | 4.2 |
| 1 | A | 992 | U | 4.2 |
| 12 | J | 36 | GLY | 4.2 |
| 1 | A | 1003(A) | G | 4.1 |
| 1 | A | 1221 | G | 4.1 |
| 1 | A | 1030(B) | C | 4.1 |
| 1 | A | 1001 | A | 4.0 |
| 1 | A | 1276 | G | 3.9 |
| 17 | O | 22 | THR | 3.9 |
| 19 | Q | 96 | GLN | 3.9 |
| 1 | A | 1421 | G | 3.9 |
| 6 | D | 2 | GLY | 3.8 |
| 21 | S | 4 | SER | 3.8 |
| 23 | V | 6 | ARG | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 1023 | G | 3.7 |
| 21 | S | 27 | GLU | 3.7 |
| 12 | J | 70 | ARG | 3.7 |
| 1 | A | 841 | U | 3.7 |
| 5 | C | 63 | ASN | 3.7 |
| 16 | N | 18 | VAL | 3.7 |
| 12 | J | 93 | GLY | 3.7 |
| 1 | A | 1022 | G | 3.6 |
| 12 | J | 74 | ILE | 3.6 |
| 1 | A | 1124 | G | 3.6 |
| 1 | A | 1174 | G | 3.6 |
| 1 | A | 1029 | C | 3.6 |
| 1 | A | 1019 | C | 3.5 |
| 13 | K | 128 | ALA | 3.5 |
| 1 | A | 438 | G | 3.5 |
| 1 | A | 1131 | G | 3.5 |
| 1 | A | 1283 | G | 3.5 |
| 11 | I | 102 | LEU | 3.5 |
| 11 | I | 19 | LEU | 3.5 |
| 16 | N | 30 | ALA | 3.4 |
| 1 | A | 1002 | G | 3.4 |
| 1 | A | 1128 | C | 3.4 |
| 1 | A | 1282 | C | 3.4 |
| 1 | A | 1011 | G | 3.4 |
| 12 | J | 31 | GLY | 3.4 |
| 1 | A | 266 | G | 3.4 |
| 1 | A | 1182 | G | 3.4 |
| 6 | D | 3 | ARG | 3.3 |
| 12 | J | 34 | VAL | 3.3 |
| 1 | A | 1278 | U | 3.3 |
| 1 | A | 437 | U | 3.3 |
| 12 | J | 78 | ASN | 3.3 |
| 1 | A | 1135 | U | 3.3 |
| 21 | S | 26 | GLY | 3.3 |
| 1 | A | 978 | A | 3.3 |
| 1 | A | 1010 | G | 3.2 |
| 1 | A | 1255 | G | 3.2 |
| 1 | A | 1220 | G | 3.2 |
| 1 | A | 1140 | C | 3.2 |
| 19 | Q | 97 | SER | 3.2 |
| 1 | A | 1005 | A | 3.1 |
| 1 | A | 723 | U | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 959 | A | 3.1 |
| 1 | A | 410 | G | 3.1 |
| 1 | A | 530 | G | 3.1 |
| 1 | A | 1137 | C | 3.1 |
| 1 | A | 1287 | A | 3.1 |
| 1 | A | 1017 | G | 3.1 |
| 1 | A | 1269 | A | 3.1 |
| 1 | A | 413 | G | 3.1 |
| 1 | A | 1268 | A | 3.1 |
| 21 | S | 53 | ASN | 3.0 |
| 11 | I | 7 | THR | 3.0 |
| 18 | P | 83 | GLU | 3.0 |
| 11 | I | 128 | ARG | 3.0 |
| 1 | A | 1139 | G | 3.0 |
| 12 | J | 89 | ASP | 3.0 |
| 1 | A | 1030(C) | G | 3.0 |
| 20 | R | 25 | THR | 3.0 |
| 15 | M | 106 | ASN | 3.0 |
| 1 | A | 1467 | G | 3.0 |
| 12 | J | 38 | ILE | 3.0 |
| 17 | O | 23 | GLY | 2.9 |
| 1 | A | 160 | A | 2.9 |
| 12 | J | 79 | ARG | 2.9 |
| 21 | S | 54 | GLY | 2.9 |
| 1 | A | 1035 | A | 2.9 |
| 21 | S | 14 | HIS | 2.9 |
| 1 | A | 426 | G | 2.9 |
| 4 | B | 238 | LEU | 2.9 |
| 1 | A | 1143 | G | 2.9 |
| 1 | A | 1222 | G | 2.9 |
| 1 | A | 161 | A | 2.9 |
| 21 | S | 37 | ARG | 2.8 |
| 1 | A | 1016 | A | 2.8 |
| 1 | A | 1041 | A | 2.8 |
| 4 | B | 19 | HIS | 2.8 |
| 1 | A | 1127 | G | 2.8 |
| 1 | A | 1146 | A | 2.8 |
| 1 | A | 1133 | G | 2.8 |
| 21 | S | 34 | TRP | 2.8 |
| 12 | J | 27 | ALA | 2.8 |
| 17 | O | 89 | GLY | 2.8 |
| 1 | A | 1200 | C | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 1181 | G | 2.8 |
| 5 | C | 76 | VAL | 2.8 |
| 1 | A | 1026 | G | 2.8 |
| 1 | A | 1503 | A | 2.7 |
| 11 | I | 18 | PHE | 2.7 |
| 12 | J | 7 | LYS | 2.7 |
| 16 | N | 60 | SER | 2.7 |
| 1 | A | 1145 | C | 2.7 |
| 1 | A | 548 | G | 2.7 |
| 4 | B | 16 | HIS | 2.7 |
| 5 | C | 78 | GLY | 2.7 |
| 1 | A | 1003 | G | 2.7 |
| 12 | J | 80 | LYS | 2.7 |
| 16 | N | 32 | SER | 2.7 |
| 1 | A | 1030 | C | 2.7 |
| 1 | A | 1279 | A | 2.7 |
| 1 | A | 427 | U | 2.7 |
| 1 | A | 1048 | G | 2.7 |
| 14 | L | 28 | LYS | 2.7 |
| 4 | B | 35 | GLU | 2.7 |
| 1 | A | 1141 | C | 2.7 |
| 1 | A | 1147 | C | 2.7 |
| 11 | I | 65 | VAL | 2.6 |
| 12 | J | 85 | LEU | 2.6 |
| 19 | Q | 101 | ARG | 2.6 |
| 4 | B | 122 | PHE | 2.6 |
| 1 | A | 428 | G | 2.6 |
| 11 | I | 70 | LYS | 2.6 |
| 1 | A | 1000 | U | 2.6 |
| 1 | A | 1248 | A | 2.6 |
| 1 | A | 1007 | C | 2.6 |
| 1 | A | 1313 | U | 2.6 |
| 23 | V | 24 | ARG | 2.6 |
| 1 | A | 991 | U | 2.6 |
| 1 | A | 750 | G | 2.6 |
| 1 | A | 1130 | A | 2.6 |
| 17 | O | 39 | LEU | 2.6 |
| 21 | S | 2 | PRO | 2.6 |
| 1 | A | 1134 | G | 2.6 |
| 1 | A | 1260 | C | 2.6 |
| 1 | A | 1014 | A | 2.5 |
| 1 | A | 1442 | G | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 15 | M | 7 | VAL | 2.5 |
| 16 | N | 61 | TRP | 2.5 |
| 1 | A | 1013 | G | 2.5 |
| 12 | J | 75 | ILE | 2.5 |
| 22 | T | 103 | GLY | 2.5 |
| 1 | A | 532 | A | 2.5 |
| 7 | E | 5 | ASP | 2.5 |
| 1 | A | 406 | G | 2.5 |
| 5 | C | 21 | ARG | 2.5 |
| 12 | J | 8 | LEU | 2.5 |
| 1 | A | 989 | C | 2.5 |
| 12 | J | 24 | VAL | 2.5 |
| 8 | F | 75 | LEU | 2.5 |
| 1 | A | 1288 | A | 2.5 |
| 1 | A | 1020 | U | 2.5 |
| 12 | J | 81 | THR | 2.5 |
| 11 | I | 92 | TYR | 2.5 |
| 1 | A | 1482 | G | 2.4 |
| 12 | J | 35 | SER | 2.4 |
| 12 | J | 56 | HIS | 2.4 |
| 1 | A | 1213 | A | 2.4 |
| 1 | A | 1474 | G | 2.4 |
| 12 | J | 6 | ILE | 2.4 |
| 15 | M | 81 | LEU | 2.4 |
| 1 | A | 411 | A | 2.4 |
| 1 | A | 255 | G | 2.4 |
| 1 | A | 758 | G | 2.4 |
| 20 | R | 17 | SER | 2.4 |
| 15 | M | 9 | ILE | 2.3 |
| 1 | A | 1159 | U | 2.3 |
| 1 | A | 960 | U | 2.3 |
| 12 | J | 76 | ASN | 2.3 |
| 1 | A | 481 | G | 2.3 |
| 1 | A | 701 | C | 2.3 |
| 1 | A | 1030(D) | A | 2.3 |
| 1 | A | 159 | G | 2.3 |
| 1 | A | 1219 | U | 2.3 |
| 1 | A | 371 | G | 2.3 |
| 1 | A | 494 | G | 2.3 |
| 1 | A | 1053 | G | 2.3 |
| 1 | A | 1318 | A | 2.3 |
| 21 | S | 52 | TYR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 11 | I | 11 | LYS | 2.3 |
| 16 | N | 29 | ARG | 2.3 |
| 1 | A | 1323 | G | 2.3 |
| 1 | A | 1355 | G | 2.3 |
| 8 | F | 64 | GLN | 2.3 |
| 12 | J | 28 | ARG | 2.3 |
| 1 | A | 373 | A | 2.3 |
| 1 | A | 1371 | G | 2.3 |
| 11 | I | 111 | ARG | 2.3 |
| 4 | B | 18 | GLY | 2.3 |
| 9 | G | 2 | ALA | 2.3 |
| 12 | J | 54 | PHE | 2.2 |
| 1 | A | 409 | G | 2.2 |
| 1 | A | 1171 | G | 2.2 |
| 6 | D | 32 | ALA | 2.2 |
| 19 | Q | 16 | GLN | 2.2 |
| 1 | A | 439 | A | 2.2 |
| 1 | A | 1334 | G | 2.2 |
| 5 | C | 178 | LEU | 2.2 |
| 1 | A | 1198 | G | 2.2 |
| 21 | S | 49 | ILE | 2.2 |
| 1 | A | 1178 | G | 2.2 |
| 1 | A | 1259 | C | 2.2 |
| 1 | A | 1370 | G | 2.2 |
| 6 | D | 25 | ARG | 2.2 |
| 12 | J | 71 | LEU | 2.2 |
| 1 | A | 1175 | G | 2.2 |
| 13 | K | 42 | TRP | 2.2 |
| 5 | C | 23 | TYR | 2.2 |
| 6 | D | 9 | CYS | 2.2 |
| 1 | A | 837 | G | 2.2 |
| 5 | C | 77 | ILE | 2.2 |
| 1 | A | 1361(A) | C | 2.2 |
| 4 | B | 131 | PRO | 2.2 |
| 1 | A | 1046 | A | 2.2 |
| 10 | H | 2 | LEU | 2.1 |
| 4 | B | 235 | SER | 2.1 |
| 1 | A | 251 | G | 2.1 |
| 1 | A | 254 | G | 2.1 |
| 1 | A | 975 | A | 2.1 |
| 1 | A | 1349 | A | 2.1 |
| 1 | A | 840 | C | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 1028 | C | 2.1 |
| 1 | A | 264 | U | 2.1 |
| 1 | A | 797 | C | 2.1 |
| 1 | A | 1132 | C | 2.1 |
| 5 | C | 59 | ARG | 2.1 |
| 1 | A | 529 | G | 2.1 |
| 1 | A | 1015 | A | 2.1 |
| 1 | A | 1033 | G | 2.1 |
| 1 | A | 1363 | A | 2.1 |
| 1 | A | 1441 | G | 2.1 |
| 6 | D | 21 | LEU | 2.1 |
| 15 | M | 88 | ARG | 2.1 |
| 5 | C | 95 | THR | 2.1 |
| 8 | F | 65 | VAL | 2.1 |
| 1 | A | 1018 | C | 2.1 |
| 4 | B | 121 | LEU | 2.1 |
| 3 | Z | 4 | U | 2.1 |
| 1 | A | 418 | C | 2.1 |
| 1 | A | 1037 | C | 2.1 |
| 1 | A | 1038 | C | 2.1 |
| 1 | A | 666 | G | 2.1 |
| 1 | A | 1036 | G | 2.1 |
| 8 | F | 101 | ALA | 2.1 |
| 1 | A | 1285 | A | 2.1 |
| 4 | B | 81 | VAL | 2.0 |
| 11 | I | 85 | LEU | 2.0 |
| 1 | A | 497 | A | 2.0 |
| 1 | A | 984 | C | 2.0 |
| 1 | A | 1249 | C | 2.0 |
| 1 | A | 657 | G | 2.0 |
| 1 | A | 1475 | G | 2.0 |
| 1 | A | 253 | U | 2.0 |
| 1 | A | 492 | G | 2.0 |
| 1 | A | 581 | G | 2.0 |
| 1 | A | 1271 | G | 2.0 |
| 1 | A | 1304 | G | 2.0 |
| 1 | A | 1422 | G | 2.0 |
| 21 | S | 28 | LYS | 2.0 |
| 1 | A | 1067 | A | 2.0 |
| 4 | B | 118 | LEU | 2.0 |
| 12 | J | 29 | ARG | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | PSU | Y | 38 | 20/21 | 0.92 | 0.18 | 24,24,24,24 | 0 |

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 25 | MG | A | 1647 | 1/1 | 0.28 | 0.28 | 24,24,24,24 | 1 |
| 25 | MG | A | 1618 | 1/1 | 0.42 | 0.73 | 24,24,24,24 | 1 |
| 25 | MG | A | 1572 | 1/1 | 0.49 | 0.68 | 24,24,24,24 | 1 |
| 25 | MG | A | 441 | 1/1 | 0.54 | 0.21 | 24,24,24,24 | 1 |
| 25 | MG | A | 1655 | 1/1 | 0.56 | 0.40 | 24,24,24,24 | 1 |
| 25 | MG | A | 1641 | 1/1 | 0.59 | 0.58 | 24,24,24,24 | 1 |
| 25 | MG | A | 1675 | 1/1 | 0.59 | 0.42 | 24,24,24,24 | 1 |
| 25 | MG | A | 1610 | 1/1 | 0.61 | 0.16 | 24,24,24,24 | 0 |
| 25 | MG | A | 1617 | 1/1 | 0.63 | 0.45 | 24,24,24,24 | 1 |
| 25 | MG | A | 464 | 1/1 | 0.63 | 0.26 | 24,24,24,24 | 1 |
| 25 | MG | A | 1645 | 1/1 | 0.63 | 0.74 | 24,24,24,24 | 1 |
| 25 | MG | A | 1609 | 1/1 | 0.67 | 0.17 | 24,24,24,24 | 1 |
| 25 | MG | A | 1615 | 1/1 | 0.70 | 0.73 | 24,24,24,24 | 1 |
| 25 | MG | A | 1678 | 1/1 | 0.70 | 0.48 | 24,24,24,24 | 1 |
| 25 | MG | A | 1616 | 1/1 | 0.71 | 0.30 | 24,24,24,24 | 1 |
| 25 | MG | A | 1579 | 1/1 | 0.73 | 0.34 | 24,24,24,24 | 1 |
| 25 | MG | A | 1624 | 1/1 | 0.73 | 0.41 | 24,24,24,24 | 1 |
| 25 | MG | A | 1663 | 1/1 | 0.74 | 0.39 | 24,24,24,24 | 1 |
| 25 | MG | A | 1668 | 1/1 | 0.74 | 0.18 | 24,24,24,24 | 1 |
| 25 | MG | A | 1555 | 1/1 | 0.76 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1605 | 1/1 | 0.77 | 0.17 | 24,24,24,24 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 25 | MG | A | 1644 | 1/1 | 0.77 | 0.69 | 24,24,24,24 | 1 |
| 25 | MG | A | 1625 | 1/1 | 0.77 | 0.21 | 24,24,24,24 | 1 |
| 25 | MG | A | 1646 | 1/1 | 0.77 | 0.22 | 24,24,24,24 | 0 |
| 25 | MG | A | 1567 | 1/1 | 0.78 | 0.49 | 24,24,24,24 | 1 |
| 25 | MG | A | 1673 | 1/1 | 0.78 | 0.37 | 24,24,24,24 | 1 |
| 25 | MG | A | 1619 | 1/1 | 0.78 | 0.49 | 24,24,24,24 | 1 |
| 25 | MG | A | 1635 | 1/1 | 0.78 | 0.28 | 24,24,24,24 | 1 |
| 25 | MG | A | 1680 | 1/1 | 0.78 | 0.64 | 24,24,24,24 | 1 |
| 25 | MG | A | 465 | 1/1 | 0.79 | 0.21 | 24,24,24,24 | 1 |
| 25 | MG | A | 1620 | 1/1 | 0.79 | 0.24 | 24,24,24,24 | 1 |
| 25 | MG | A | 1632 | 1/1 | 0.79 | 0.60 | 24,24,24,24 | 1 |
| 25 | MG | A | 493 | 1/1 | 0.79 | 0.27 | 24,24,24,24 | 1 |
| 25 | MG | A | 1549 | 1/1 | 0.80 | 0.67 | 24,24,24,24 | 1 |
| 25 | MG | A | 1607 | 1/1 | 0.80 | 0.37 | 24,24,24,24 | 1 |
| 25 | MG | A | 1585 | 1/1 | 0.80 | 0.49 | 24,24,24,24 | 1 |
| 25 | MG | A | 1575 | 1/1 | 0.81 | 0.16 | 24,24,24,24 | 1 |
| 25 | MG | A | 1659 | 1/1 | 0.81 | 0.35 | 24,24,24,24 | 1 |
| 25 | MG | A | 1603 | 1/1 | 0.81 | 0.30 | 24,24,24,24 | 1 |
| 25 | MG | A | 1643 | 1/1 | 0.81 | 0.17 | 24,24,24,24 | 1 |
| 25 | MG | A | 71 | 1/1 | 0.81 | 0.52 | 24,24,24,24 | 1 |
| 25 | MG | A | 466 | 1/1 | 0.81 | 0.54 | 24,24,24,24 | 1 |
| 25 | MG | J | 449 | 1/1 | 0.81 | 0.24 | 24,24,24,24 | 1 |
| 25 | MG | A | 1666 | 1/1 | 0.82 | 0.34 | 24,24,24,24 | 1 |
| 25 | MG | A | 1636 | 1/1 | 0.82 | 0.58 | 24,24,24,24 | 1 |
| 25 | MG | A | 1628 | 1/1 | 0.82 | 0.19 | 24,24,24,24 | 0 |
| 25 | MG | A | 1649 | 1/1 | 0.82 | 0.24 | 24,24,24,24 | 1 |
| 25 | MG | A | 1648 | 1/1 | 0.83 | 0.19 | 24,24,24,24 | 1 |
| 25 | MG | Y | 500 | 1/1 | 0.83 | 0.35 | 24,24,24,24 | 1 |
| 25 | MG | A | 1681 | 1/1 | 0.83 | 0.72 | 24,24,24,24 | 1 |
| 25 | MG | A | 1630 | 1/1 | 0.84 | 0.28 | 24,24,24,24 | 1 |
| 25 | MG | A | 1664 | 1/1 | 0.84 | 0.84 | 24,24,24,24 | 1 |
| 25 | MG | A | 1621 | 1/1 | 0.84 | 0.54 | 24,24,24,24 | 1 |
| 25 | MG | A | 1623 | 1/1 | 0.85 | 0.22 | 24,24,24,24 | 1 |
| 25 | MG | A | 1614 | 1/1 | 0.85 | 0.15 | 24,24,24,24 | 1 |
| 25 | MG | A | 1573 | 1/1 | 0.86 | 0.19 | 24,24,24,24 | 1 |
| 25 | MG | A | 1640 | 1/1 | 0.86 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1650 | 1/1 | 0.86 | 1.81 | 24,24,24,24 | 1 |
| 25 | MG | A | 1563 | 1/1 | 0.86 | 0.27 | 24,24,24,24 | 0 |
| 25 | MG | A | 1662 | 1/1 | 0.87 | 0.56 | 24,24,24,24 | 1 |
| 25 | MG | A | 1661 | 1/1 | 0.87 | 0.49 | 24,24,24,24 | 1 |
| 25 | MG | A | 1590 | 1/1 | 0.88 | 0.50 | 24,24,24,24 | 1 |
| 25 | MG | A | 1674 | 1/1 | 0.88 | 0.18 | 24,24,24,24 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 25 | MG | A | 1631 | 1/1 | 0.88 | 0.22 | 24,24,24,24 | 1 |
| 25 | MG | A | 210 | 1/1 | 0.88 | 0.18 | 24,24,24,24 | 1 |
| 25 | MG | A | 1551 | 1/1 | 0.88 | 0.16 | 24,24,24,24 | 1 |
| 25 | MG | A | 1604 | 1/1 | 0.88 | 0.18 | 24,24,24,24 | 1 |
| 25 | MG | A | 1637 | 1/1 | 0.88 | 0.18 | 24,24,24,24 | 0 |
| 25 | MG | A | 1547 | 1/1 | 0.88 | 0.30 | 24,24,24,24 | 0 |
| 25 | MG | D | 215 | 1/1 | 0.88 | 0.25 | 24,24,24,24 | 1 |
| 25 | MG | A | 1671 | 1/1 | 0.88 | 0.29 | 24,24,24,24 | 1 |
| 25 | MG | A | 1633 | 1/1 | 0.89 | 0.21 | 24,24,24,24 | 1 |
| 25 | MG | A | 214 | 1/1 | 0.89 | 0.30 | 24,24,24,24 | 1 |
| 25 | MG | A | 1658 | 1/1 | 0.89 | 0.22 | 24,24,24,24 | 1 |
| 25 | MG | A | 1582 | 1/1 | 0.90 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1565 | 1/1 | 0.90 | 0.24 | 24,24,24,24 | 0 |
| 25 | MG | A | 1560 | 1/1 | 0.90 | 0.48 | 24,24,24,24 | 0 |
| 25 | MG | A | 1562 | 1/1 | 0.90 | 0.18 | 24,24,24,24 | 1 |
| 25 | MG | A | 467 | 1/1 | 0.90 | 0.20 | 24,24,24,24 | 1 |
| 25 | MG | A | 471 | 1/1 | 0.90 | 0.41 | 24,24,24,24 | 1 |
| 25 | MG | A | 213 | 1/1 | 0.90 | 0.49 | 24,24,24,24 | 1 |
| 25 | MG | A | 1581 | 1/1 | 0.90 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1629 | 1/1 | 0.90 | 0.64 | 24,24,24,24 | 1 |
| 25 | MG | A | 1639 | 1/1 | 0.90 | 0.14 | 24,24,24,24 | 0 |
| 25 | MG | A | 1548 | 1/1 | 0.91 | 0.18 | 24,24,24,24 | 0 |
| 25 | MG | A | 470 | 1/1 | 0.91 | 0.27 | 24,24,24,24 | 1 |
| 25 | MG | A | 1638 | 1/1 | 0.91 | 0.52 | 24,24,24,24 | 1 |
| 25 | MG | A | 1654 | 1/1 | 0.91 | 0.38 | 24,24,24,24 | 1 |
| 25 | MG | A | 1584 | 1/1 | 0.91 | 0.25 | 24,24,24,24 | 1 |
| 25 | MG | A | 1676 | 1/1 | 0.91 | 0.20 | 24,24,24,24 | 1 |
| 25 | MG | E | 468 | 1/1 | 0.91 | 0.23 | 24,24,24,24 | 1 |
| 25 | MG | A | 1677 | 1/1 | 0.91 | 0.22 | 24,24,24,24 | 1 |
| 24 | PAR | A | 1545 | 42/42 | 0.92 | 0.25 | 24,24,24,24 | 0 |
| 25 | MG | A | 1665 | 1/1 | 0.92 | 0.51 | 24,24,24,24 | 1 |
| 25 | MG | A | 1596 | 1/1 | 0.92 | 0.34 | 24,24,24,24 | 0 |
| 25 | MG | A | 1642 | 1/1 | 0.92 | 0.14 | 24,24,24,24 | 1 |
| 25 | MG | A | 1597 | 1/1 | 0.92 | 0.26 | 24,24,24,24 | 0 |
| 25 | MG | A | 1602 | 1/1 | 0.92 | 0.21 | 24,24,24,24 | 1 |
| 25 | MG | A | 1571 | 1/1 | 0.93 | 0.25 | 24,24,24,24 | 1 |
| 25 | MG | A | 211 | 1/1 | 0.93 | 0.25 | 24,24,24,24 | 0 |
| 25 | MG | A | 1586 | 1/1 | 0.93 | 0.10 | 24,24,24,24 | 0 |
| 25 | MG | A | 473 | 1/1 | 0.93 | 0.14 | 24,24,24,24 | 1 |
| 25 | MG | A | 1574 | 1/1 | 0.93 | 0.16 | 24,24,24,24 | 0 |
| 25 | MG | A | 1679 | 1/1 | 0.93 | 0.62 | 24,24,24,24 | 1 |
| 25 | MG | A | 1612 | 1/1 | 0.93 | 0.45 | 24,24,24,24 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 25 | MG | A | 1592 | 1/1 | 0.93 | 0.37 | 24,24,24,24 | 1 |
| 25 | MG | A | 1667 | 1/1 | 0.93 | 0.24 | 24,24,24,24 | 1 |
| 25 | MG | A | 1569 | 1/1 | 0.93 | 0.65 | 24,24,24,24 | 1 |
| 25 | MG | A | 1669 | 1/1 | 0.93 | 0.12 | 24,24,24,24 | 1 |
| 25 | MG | A | 1653 | 1/1 | 0.93 | 0.31 | 24,24,24,24 | 1 |
| 25 | MG | A | 1576 | 1/1 | 0.93 | 0.16 | 24,24,24,24 | 1 |
| 25 | MG | A | 1600 | 1/1 | 0.94 | 0.33 | 24,24,24,24 | 0 |
| 25 | MG | A | 1606 | 1/1 | 0.94 | 0.27 | 24,24,24,24 | 0 |
| 25 | MG | A | 1552 | 1/1 | 0.94 | 0.27 | 24,24,24,24 | 0 |
| 25 | MG | A | 87 | 1/1 | 0.94 | 0.26 | 24,24,24,24 | 1 |
| 25 | MG | A | 1591 | 1/1 | 0.94 | 0.21 | 24,24,24,24 | 1 |
| 25 | MG | A | 1611 | 1/1 | 0.94 | 0.40 | 24,24,24,24 | 1 |
| 25 | MG | A | 1556 | 1/1 | 0.94 | 0.24 | 24,24,24,24 | 0 |
| 25 | MG | A | 469 | 1/1 | 0.94 | 0.20 | 24,24,24,24 | 1 |
| 25 | MG | A | 1651 | 1/1 | 0.94 | 0.45 | 24,24,24,24 | 1 |
| 25 | MG | A | 1626 | 1/1 | 0.94 | 0.41 | 24,24,24,24 | 0 |
| 25 | MG | A | 1601 | 1/1 | 0.94 | 0.40 | 24,24,24,24 | 0 |
| 25 | MG | A | 1568 | 1/1 | 0.94 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1656 | 1/1 | 0.94 | 0.21 | 24,24,24,24 | 0 |
| 25 | MG | A | 1577 | 1/1 | 0.94 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1599 | 1/1 | 0.94 | 0.18 | 24,24,24,24 | 0 |
| 25 | MG | A | 1660 | 1/1 | 0.94 | 0.26 | 24,24,24,24 | 0 |
| 25 | MG | A | 1652 | 1/1 | 0.95 | 0.29 | 24,24,24,24 | 0 |
| 25 | MG | A | 1557 | 1/1 | 0.95 | 0.28 | 24,24,24,24 | 0 |
| 25 | MG | A | 1595 | 1/1 | 0.95 | 0.09 | 24,24,24,24 | 0 |
| 25 | MG | A | 1587 | 1/1 | 0.95 | 0.26 | 24,24,24,24 | 0 |
| 25 | MG | A | 1553 | 1/1 | 0.96 | 0.19 | 24,24,24,24 | 0 |
| 25 | MG | A | 1672 | 1/1 | 0.96 | 0.58 | 24,24,24,24 | 1 |
| 25 | MG | A | 1561 | 1/1 | 0.96 | 0.28 | 24,24,24,24 | 0 |
| 25 | MG | A | 1583 | 1/1 | 0.96 | 0.35 | 24,24,24,24 | 1 |
| 25 | MG | A | 1550 | 1/1 | 0.96 | 0.38 | 24,24,24,24 | 0 |
| 25 | MG | A | 1566 | 1/1 | 0.96 | 0.34 | 24,24,24,24 | 0 |
| 25 | MG | A | 1613 | 1/1 | 0.96 | 0.39 | 24,24,24,24 | 1 |
| 25 | MG | A | 1627 | 1/1 | 0.96 | 0.29 | 24,24,24,24 | 1 |
| 25 | MG | A | 1608 | 1/1 | 0.97 | 0.14 | 24,24,24,24 | 1 |
| 25 | MG | A | 1588 | 1/1 | 0.97 | 0.24 | 24,24,24,24 | 0 |
| 25 | MG | A | 1589 | 1/1 | 0.97 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1657 | 1/1 | 0.97 | 0.12 | 24,24,24,24 | 1 |
| 25 | MG | A | 1598 | 1/1 | 0.97 | 0.09 | 24,24,24,24 | 1 |
| 25 | MG | A | 1558 | 1/1 | 0.97 | 0.25 | 24,24,24,24 | 0 |
| 25 | MG | A | 1559 | 1/1 | 0.97 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1564 | 1/1 | 0.97 | 0.52 | 24,24,24,24 | 1 |

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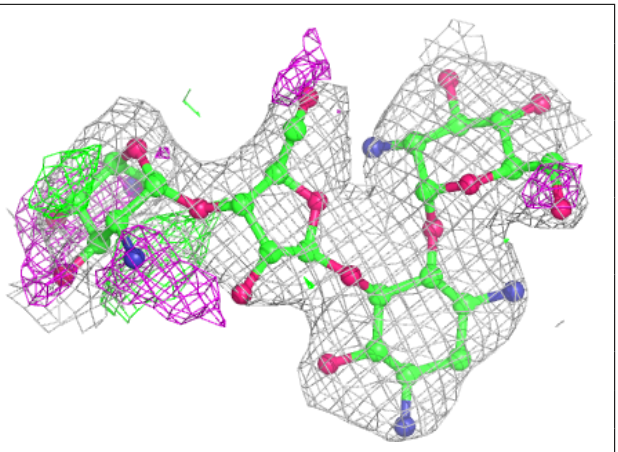
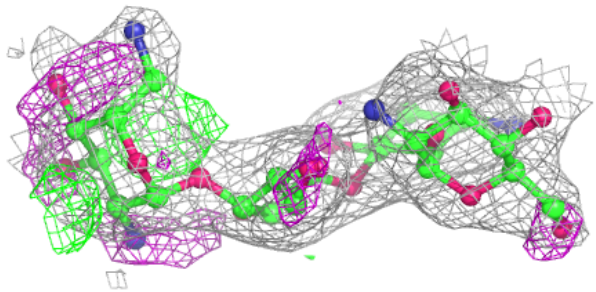
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 25 | MG | A | 1594 | 1/1 | 0.97 | 0.26 | 24,24,24,24 | 0 |
| 25 | MG | A | 1570 | 1/1 | 0.97 | 0.37 | 24,24,24,24 | 1 |
| 25 | MG | A | 1593 | 1/1 | 0.98 | 0.20 | 24,24,24,24 | 0 |
| 25 | MG | A | 1578 | 1/1 | 0.98 | 0.20 | 24,24,24,24 | 0 |
| 25 | MG | A | 1634 | 1/1 | 0.98 | 0.25 | 24,24,24,24 | 1 |
| 25 | MG | A | 86 | 1/1 | 0.98 | 0.24 | 24,24,24,24 | 0 |
| 25 | MG | A | 1580 | 1/1 | 0.98 | 0.20 | 24,24,24,24 | 1 |
| 25 | MG | A | 1554 | 1/1 | 0.98 | 0.23 | 24,24,24,24 | 0 |
| 25 | MG | A | 1546 | 1/1 | 0.98 | 0.19 | 24,24,24,24 | 0 |
| 25 | MG | M | 475 | 1/1 | 0.98 | 0.17 | 24,24,24,24 | 1 |
| 26 | ZN | D | 306 | 1/1 | 0.98 | 0.32 | 24,24,24,24 | 1 |
| 25 | MG | A | 1622 | 1/1 | 0.99 | 0.56 | 24,24,24,24 | 1 |
| 25 | MG | A | 1670 | 1/1 | 0.99 | 0.27 | 24,24,24,24 | 1 |
| 26 | ZN | N | 307 | 1/1 | 0.99 | 0.19 | 24,24,24,24 | 1 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around PAR A 1545:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)





## 6.5 Other polymers (i)

There are no such residues in this entry.