# wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:43 PM BST

| | | |
|---|---|---|
| PDB ID | : | 2OM7 |
| EMDB ID: | : | EMD-1315 |
| Title | : | Structural Basis for Interaction of the Ribosome with the Switch Regions of GTP-bound Elongation Factors |
| Authors | : | Connell, S.R.; Wilson, D.N.; Rost, M.; Schueler, M.; Giesebrecht, J.; Dabrowski, M.; Mielke, T.; Fucini, P.; Spahn, C.M.T. |
| Deposited on | : | 2007-01-21 |
| Resolution | : | 7.30 Å(reported) |
| Based on PDB ID | : | 2j00, 1gix, 2j01, 1FNM, 1YL3, |

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

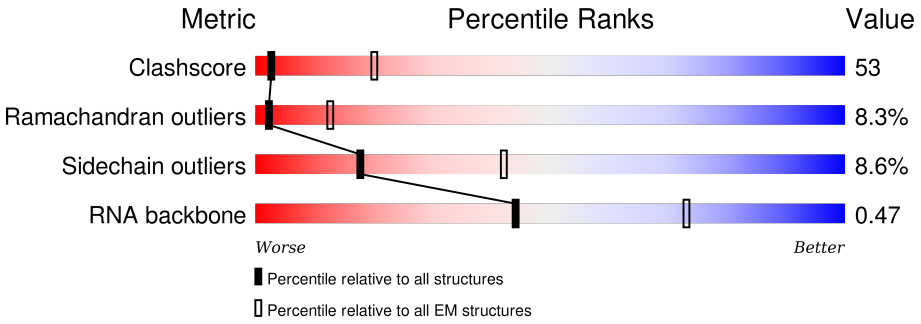
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk27241 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.30 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) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |
| RNA backbone | 3027 | 244 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 12 | 33% 67% |
| 2 | B | 28 | 7% 25% • 64% |
| 3 | C | 96 | 23% 65% 11% • |
| 4 | D | 303 | • • 96% |
| 5 | F | 29 | 14% 66% 17% • |
| 6 | G | 54 | 35% 44% 20% |
| 7 | H | 42 | 43% 38% 19% |
| 8 | I | 58 | • 34% 48% 16% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | J | 102 | 16% 29% 26% 28% |
| 10 | M | 74 | 5% 30% 42% 23% |
| 11 | E | 135 | 33% 45% 13% 7% |
| 12 | K | 229 | 38% 31% 13% 17% |
| 13 | L | 691 | 48% 42% 5% |
| 14 | N | 256 | 21% 54% 15% 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 |
|---|---|---|---|---|---|---|---|
| 10 | 5MC | M | 49 | - | - | X | - |
| 10 | 4SU | M | 8 | - | - | X | - |

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 19031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Fragment of 16S rRNA (h14).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | A | 12 | 256 | 114 | 46 | 84 | 12 | 0 | 0 |

- Molecule 2 is a RNA chain called Fragment of 16S rRNA (h15).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | B | 10 | 214 | 95 | 38 | 71 | 10 | 0 | 0 |

- Molecule 3 is a RNA chain called Fragment of 16S rRNA (h44).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | C | 96 | 2069 | 919 | 387 | 667 | 96 | 0 | 0 |

- Molecule 4 is a RNA chain called 16S ribosomal RNA (H5).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | D | 13 | 278 | 124 | 50 | 91 | 13 | 0 | 0 |

- Molecule 5 is a RNA chain called Fragment of23S rRNA (H95).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | F | 29 | 624 | 278 | 116 | 201 | 29 | 0 | 0 |

- Molecule 6 is a RNA chain called Fragment of23S rRNA (H68).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 6 | G | 54 | 1172 | 521 | 228 | 369 | 54 | 0 | 0 |

- Molecule 7 is a RNA chain called Fragment of23S rRNA (H89).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | H | 42 | Total | C | N | O | P | 0 | 0 |
| | | | 898 | 399 | 161 | 296 | 42 | | |

- Molecule 8 is a RNA chain called Fragment of23S rRNA (H42-44).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | I | 58 | Total | C | N | O | P | 0 | 0 |
| | | | 1241 | 554 | 224 | 405 | 58 | | |

- Molecule 9 is a RNA chain called Fragment of23S rRNA (H76).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | J | 73 | Total | C | N | O | P | 0 | 0 |
| | | | 1569 | 696 | 284 | 516 | 73 | | |

- Molecule 10 is a RNA chain called p/E-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | M | 74 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1570 | 702 | 269 | 524 | 74 | 1 | | |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | E | 125 | Total | C | N | O | S | 0 | 1 |
| | | | 971 | 611 | 196 | 163 | 1 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 2 | VAL | - | INSERTION | UNP P17293 |
| E | 3 | ALA | - | INSERTION | UNP P17293 |
| E | 4 | LEU | - | INSERTION | UNP P17293 |

- Molecule 12 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 12 | K | 191 | Total | C | N | O | 0 | 1 |
| | | | 1142 | 691 | 221 | 230 | | |

- Molecule 13 is a protein called Elongation factor G.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | L | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5126 | 3259 | 874 | 975 | 18 | | |

- Molecule 14 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | N | 235 | Total | C | N | O | S | 0 | 1 |
| | | | 1901 | 1213 | 342 | 341 | 5 | | |

# 3 Residue-property plots (i)

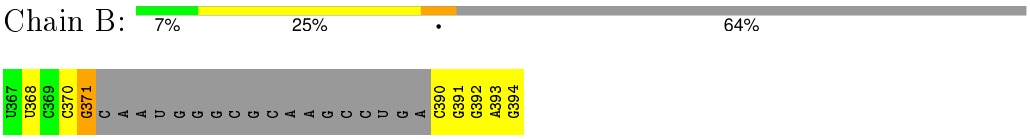
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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: Fragment of 16S rRNA (h14)

Chain A:

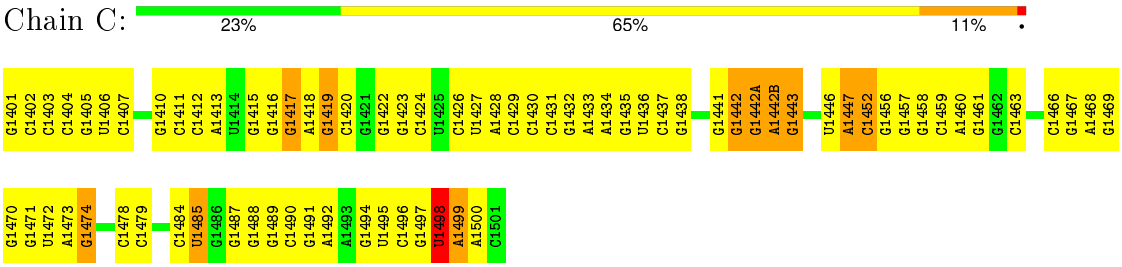

- Molecule 2: Fragment of 16S rRNA (h15)

Chain B:



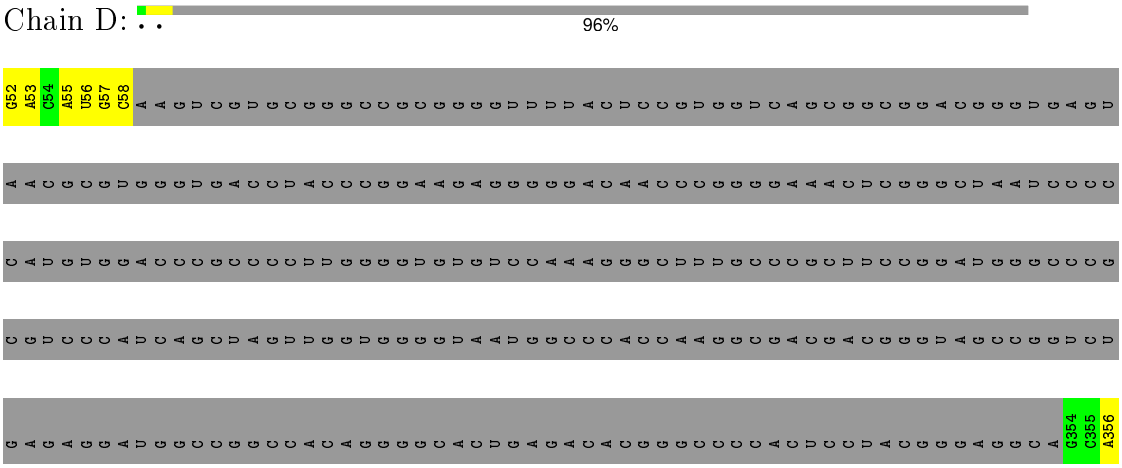

- Molecule 3: Fragment of 16S rRNA (h44)

Chain C:



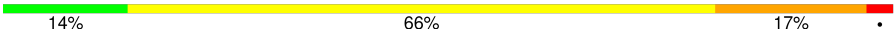

- Molecule 4: 16S ribosomal RNA (H5)

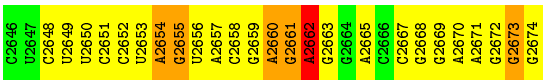
Chain D:




- Molecule 5: Fragment of23S rRNA (H95)

Chain F:




- Molecule 6: Fragment of23S rRNA (H68)

Chain G:



- Molecule 7: Fragment of23S rRNA (H89)

Chain H:



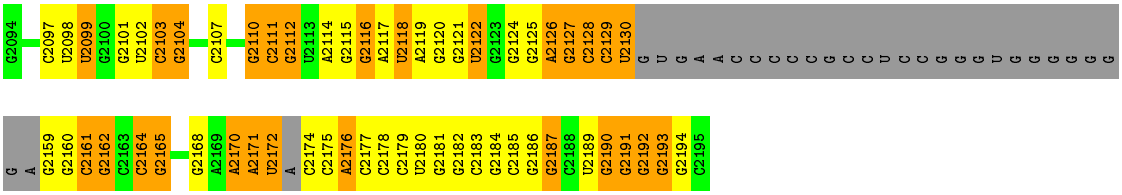
- Molecule 8: Fragment of23S rRNA (H42-44)

Chain I:



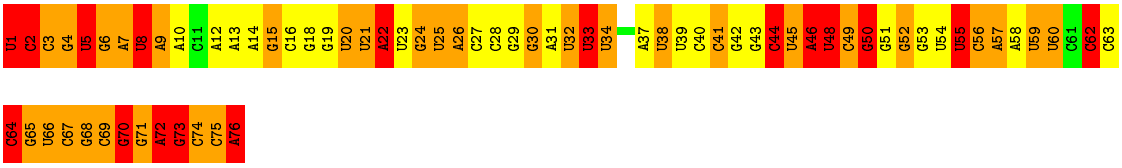
- Molecule 9: Fragment of23S rRNA (H76)

Chain J:

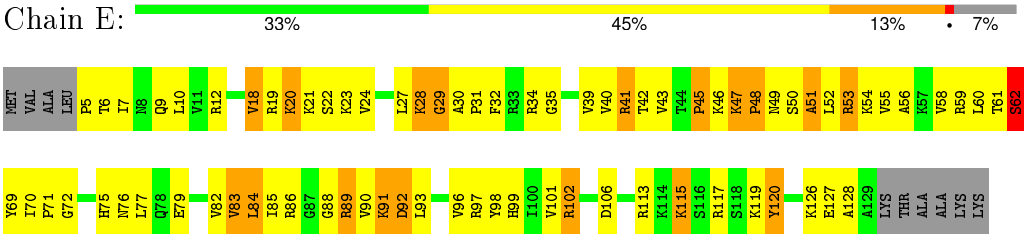

- Molecule 10: p/E-tRNA

Chain M:

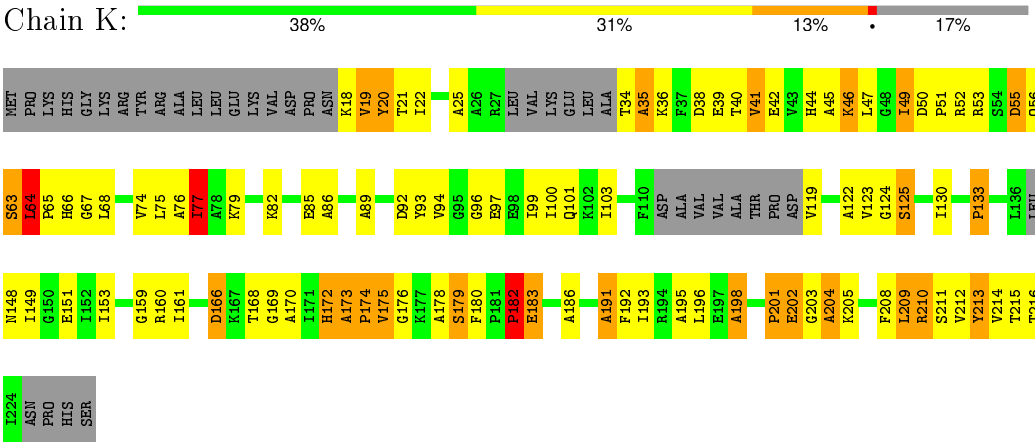
- Molecule 11: 30S ribosomal protein S12

Chain E:



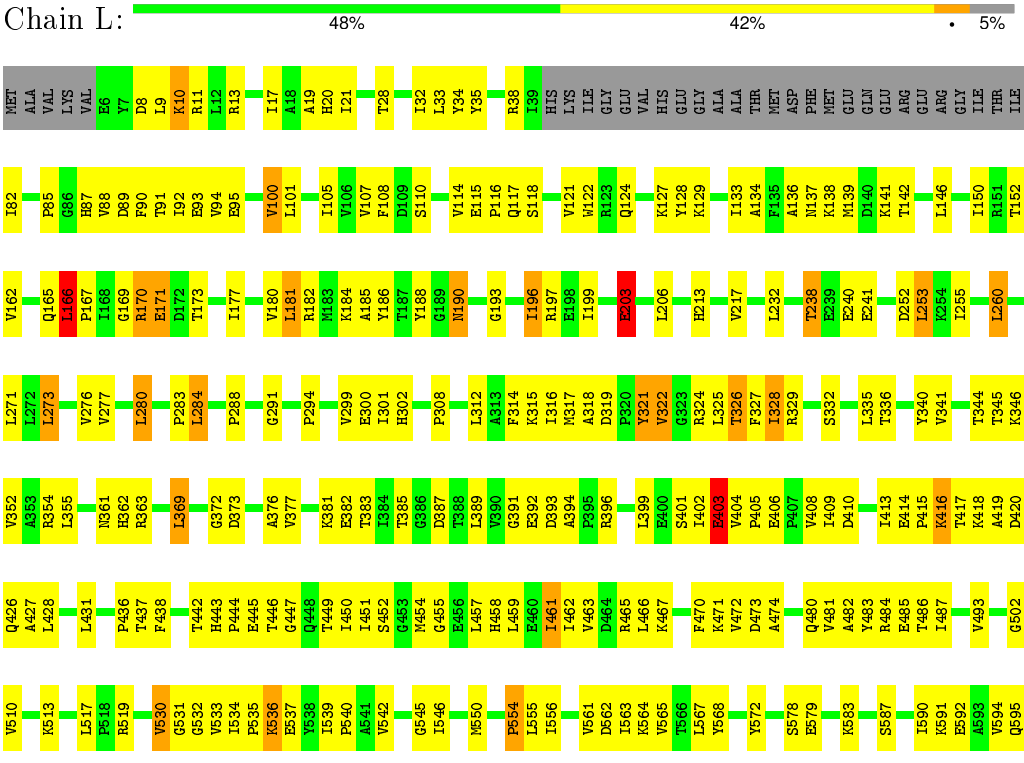

- Molecule 12: 50S ribosomal protein L1

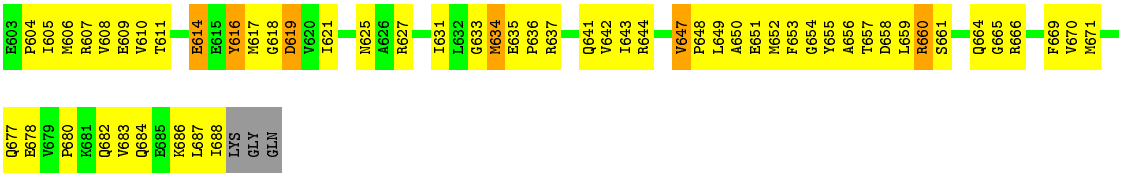
Chain K:




- Molecule 13: Elongation factor G

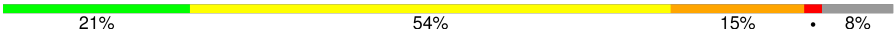
Chain L:

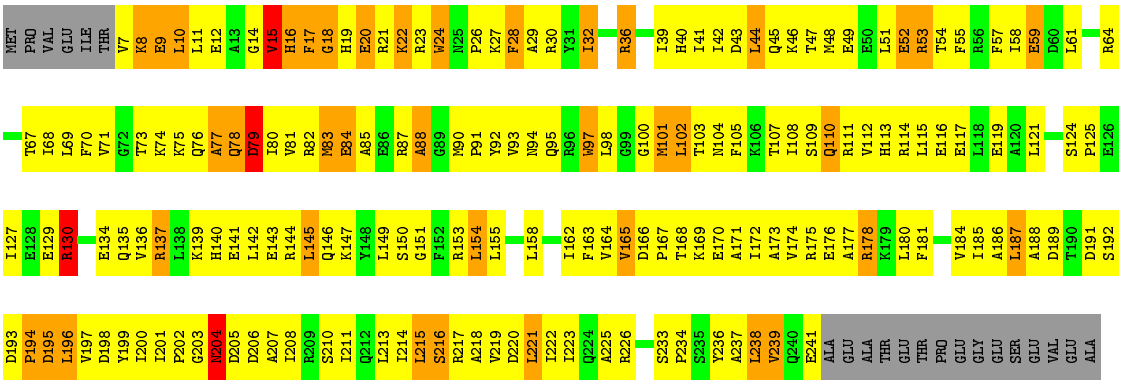





- Molecule 14: 30S ribosomal protein S2

Chain N:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | Not provided | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | Not provided | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | defocus groups | Depositor |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 19 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 39000 | Depositor |
| Image detector | Kodak SO163 film | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, 4SU, 5MC, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>2$ | RMSZ | #$\|Z\|>2$ |
| 1 | A | 0.72 | 0/285 | 0.82 | 0/442 |
| 10 | M | 2.06 | 21/1616 (1.3%) | 2.88 | 150/2512 (6.0%) |
| 11 | E | 0.53 | 0/987 | 0.74 | 0/1322 |
| 12 | K | 0.48 | 0/1145 | 0.71 | 5/1556 (0.3%) |
| 13 | L | 0.53 | 0/5219 | 0.80 | 6/7063 (0.1%) |
| 14 | N | 0.48 | 0/1936 | 0.66 | 0/2611 |
| 2 | B | 0.82 | 0/237 | 0.84 | 0/365 |
| 3 | C | 0.88 | 0/2315 | 0.89 | 1/3613 (0.0%) |
| 4 | D | 0.85 | 0/309 | 0.83 | 0/477 |
| 5 | F | 0.77 | 0/698 | 0.87 | 1/1087 (0.1%) |
| 6 | G | 0.89 | 0/1314 | 0.92 | 0/2051 |
| 7 | H | 0.78 | 0/1002 | 0.88 | 0/1561 |
| 8 | I | 1.09 | 2/1388 (0.1%) | 1.35 | 9/2162 (0.4%) |
| 9 | J | 0.68 | 0/1753 | 0.85 | 1/2735 (0.0%) |
| All | All | 0.90 | 23/20204 (0.1%) | 1.18 | 173/29557 (0.6%) |

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 |
|---|---|---|---|
| 2 | B | 0 | 1 |
| 3 | C | 0 | 7 |
| 5 | F | 1 | 0 |
| 7 | H | 0 | 1 |
| 8 | I | 0 | 5 |
| 9 | J | 1 | 0 |
| All | All | 2 | 14 |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | M | 33 | U | O3'-P | 31.01 | 1.98 | 1.61 |
| 10 | M | 15 | G | O3'-P | 23.54 | 1.89 | 1.61 |
| 10 | M | 26 | A | O3'-P | -23.25 | 1.33 | 1.61 |
| 10 | M | 24 | G | O3'-P | 19.01 | 1.83 | 1.61 |
| 10 | M | 56 | C | O3'-P | 17.65 | 1.82 | 1.61 |
| 10 | M | 25 | U | O3'-P | 16.65 | 1.81 | 1.61 |
| 10 | M | 21 | H2U | O3'-P | -13.68 | 1.44 | 1.61 |
| 10 | M | 46 | A | O3'-P | 13.44 | 1.77 | 1.61 |
| 10 | M | 76 | A | C6-N6 | -10.79 | 1.25 | 1.33 |
| 10 | M | 72 | A | O3'-P | 10.66 | 1.74 | 1.61 |
| 10 | M | 45 | U | O3'-P | -10.46 | 1.48 | 1.61 |
| 10 | M | 22 | A | N9-C4 | -10.20 | 1.31 | 1.37 |
| 10 | M | 8 | 4SU | O3'-P | -9.31 | 1.50 | 1.61 |
| 10 | M | 75 | C | O3'-P | -8.40 | 1.51 | 1.61 |
| 10 | M | 73 | G | O3'-P | -8.09 | 1.51 | 1.61 |
| 8 | I | 1083 | U | O3'-P | 7.75 | 1.70 | 1.61 |
| 8 | I | 1083 | U | C3'-O3' | 7.59 | 1.52 | 1.42 |
| 10 | M | 55 | PSU | O3'-P | 6.85 | 1.69 | 1.61 |
| 10 | M | 5 | U | C4-O4 | 5.99 | 1.28 | 1.23 |
| 10 | M | 2 | C | N3-C4 | 5.68 | 1.38 | 1.33 |
| 10 | M | 1 | U | C4-O4 | 5.47 | 1.28 | 1.23 |
| 10 | M | 60 | U | C4-O4 | 5.46 | 1.28 | 1.23 |
| 10 | M | 22 | A | C6-N1 | 5.14 | 1.39 | 1.35 |

All (173) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | M | 25 | U | P-O3'-C3' | 31.25 | 157.21 | 119.70 |
| 10 | M | 75 | C | P-O3'-C3' | -29.62 | 84.16 | 119.70 |
| 10 | M | 8 | 4SU | O3'-P-O5' | -27.02 | 52.65 | 104.00 |
| 8 | I | 1084 | A | O5'-P-OP2 | -26.83 | 78.50 | 110.70 |
| 10 | M | 24 | G | P-O3'-C3' | -24.75 | 90.00 | 119.70 |
| 10 | M | 15 | G | P-O3'-C3' | 24.42 | 149.00 | 119.70 |
| 10 | M | 31 | A | OP2-P-O3' | 23.42 | 156.73 | 105.20 |
| 10 | M | 40 | C | OP2-P-O3' | 21.49 | 152.47 | 105.20 |
| 10 | M | 15 | G | O3'-P-O5' | 21.41 | 144.68 | 104.00 |
| 10 | M | 31 | A | O3'-P-O5' | -19.13 | 67.66 | 104.00 |
| 13 | L | 600 | VAL | O-C-N | -19.01 | 92.28 | 122.70 |
| 10 | M | 40 | C | O3'-P-O5' | -17.77 | 70.24 | 104.00 |
| 10 | M | 44 | C | O3'-P-O5' | 17.76 | 137.75 | 104.00 |
| 10 | M | 72 | A | P-O3'-C3' | 16.16 | 139.09 | 119.70 |
| 10 | M | 16 | C | P-O3'-C3' | 15.60 | 138.42 | 119.70 |
| 10 | M | 8 | 4SU | OP1-P-O3' | 15.56 | 139.43 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | L | 600 | VAL | CA-C-N | 14.33 | 148.72 | 117.20 |
| 10 | M | 29 | G | OP1-P-O3' | -13.86 | 74.70 | 105.20 |
| 10 | M | 33 | U | P-O3'-C3' | 13.37 | 135.74 | 119.70 |
| 10 | M | 32 | U | OP1-P-O3' | -13.35 | 75.84 | 105.20 |
| 10 | M | 8 | 4SU | P-O3'-C3' | -13.09 | 104.00 | 119.70 |
| 13 | L | 600 | VAL | C-N-CA | 12.94 | 154.06 | 121.70 |
| 10 | M | 75 | C | O3'-P-O5' | 11.84 | 126.49 | 104.00 |
| 10 | M | 32 | U | O4'-C1'-N1 | 11.52 | 117.42 | 108.20 |
| 10 | M | 44 | C | P-O3'-C3' | -11.41 | 106.01 | 119.70 |
| 10 | M | 5 | U | C2-N3-C4 | -11.30 | 120.22 | 127.00 |
| 10 | M | 1 | U | P-O3'-C3' | 11.28 | 133.23 | 119.70 |
| 10 | M | 46 | A | OP1-P-O3' | 10.93 | 129.24 | 105.20 |
| 10 | M | 31 | A | OP1-P-O3' | -10.74 | 81.56 | 105.20 |
| 10 | M | 56 | C | P-O3'-C3' | -10.54 | 107.05 | 119.70 |
| 10 | M | 40 | C | OP1-P-O3' | -9.96 | 83.29 | 105.20 |
| 10 | M | 33 | U | OP1-P-O3' | 9.74 | 126.62 | 105.20 |
| 10 | M | 75 | C | OP1-P-O3' | -9.47 | 84.38 | 105.20 |
| 10 | M | 21 | H2U | P-O3'-C3' | 9.20 | 130.74 | 119.70 |
| 10 | M | 42 | G | OP1-P-O3' | -9.19 | 84.99 | 105.20 |
| 10 | M | 29 | G | O3'-P-O5' | 9.02 | 121.14 | 104.00 |
| 10 | M | 74 | C | P-O3'-C3' | -8.99 | 108.91 | 119.70 |
| 10 | M | 27 | C | OP1-P-O3' | -8.97 | 85.47 | 105.20 |
| 10 | M | 66 | U | N3-C4-C5 | 8.96 | 119.97 | 114.60 |
| 10 | M | 48 | U | C2-N3-C4 | -8.90 | 121.66 | 127.00 |
| 10 | M | 32 | U | O3'-P-O5' | 8.87 | 120.85 | 104.00 |
| 10 | M | 62 | C | O4'-C1'-N1 | 8.66 | 115.13 | 108.20 |
| 3 | C | 1498 | U | C2'-C3'-O3' | 8.54 | 128.28 | 109.50 |
| 10 | M | 46 | A | OP2-P-O3' | -8.49 | 86.51 | 105.20 |
| 10 | M | 5 | U | N1-C2-N3 | 8.39 | 119.93 | 114.90 |
| 10 | M | 5 | U | N3-C4-C5 | 8.26 | 119.56 | 114.60 |
| 10 | M | 1 | U | C2-N3-C4 | -8.21 | 122.08 | 127.00 |
| 10 | M | 46 | A | P-O3'-C3' | -8.21 | 109.85 | 119.70 |
| 10 | M | 29 | G | OP2-P-O3' | 8.19 | 123.21 | 105.20 |
| 10 | M | 59 | U | C2-N3-C4 | -8.16 | 122.10 | 127.00 |
| 10 | M | 64 | C | O4'-C1'-N1 | 8.15 | 114.72 | 108.20 |
| 10 | M | 28 | C | OP1-P-O3' | -8.12 | 87.34 | 105.20 |
| 10 | M | 27 | C | OP2-P-O3' | 7.99 | 122.78 | 105.20 |
| 10 | M | 75 | C | P-O5'-C5' | -7.86 | 108.32 | 120.90 |
| 10 | M | 1 | U | N3-C4-C5 | 7.82 | 119.29 | 114.60 |
| 10 | M | 44 | C | OP1-P-O3' | -7.81 | 88.01 | 105.20 |
| 10 | M | 15 | G | OP2-P-O3' | -7.79 | 88.06 | 105.20 |
| 10 | M | 30 | G | O4'-C1'-N9 | 7.70 | 114.36 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | I | 1084 | A | O5'-P-OP1 | 7.67 | 119.91 | 110.70 |
| 9 | J | 2191 | G | C2'-C3'-O3' | 7.67 | 126.37 | 109.50 |
| 10 | M | 15 | G | OP1-P-O3' | -7.64 | 88.39 | 105.20 |
| 8 | I | 1059 | G | N9-C1'-C2' | -7.59 | 103.65 | 112.00 |
| 10 | M | 59 | U | N3-C4-C5 | 7.57 | 119.14 | 114.60 |
| 10 | M | 33 | U | OP2-P-O3' | -7.56 | 88.57 | 105.20 |
| 5 | F | 2662 | A | N9-C1'-C2' | 7.56 | 123.82 | 114.00 |
| 8 | I | 1084 | A | C5'-C4'-C3' | -7.50 | 104.00 | 116.00 |
| 10 | M | 57 | A | P-O3'-C3' | 7.42 | 128.60 | 119.70 |
| 10 | M | 40 | C | O4'-C1'-N1 | 7.41 | 114.13 | 108.20 |
| 10 | M | 73 | G | C5-C6-N1 | 7.39 | 115.19 | 111.50 |
| 10 | M | 41 | C | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 10 | M | 70 | G | C5-C6-N1 | 7.33 | 115.16 | 111.50 |
| 10 | M | 25 | U | OP1-P-O3' | 7.29 | 121.23 | 105.20 |
| 10 | M | 21 | H2U | O3'-P-O5' | 7.09 | 117.46 | 104.00 |
| 10 | M | 2 | C | N3-C4-C5 | -7.03 | 119.09 | 121.90 |
| 8 | I | 1085 | A | N9-C1'-C2' | 6.90 | 122.97 | 114.00 |
| 10 | M | 42 | G | O4'-C1'-N9 | 6.87 | 113.69 | 108.20 |
| 10 | M | 3 | C | N3-C4-C5 | -6.82 | 119.17 | 121.90 |
| 10 | M | 62 | C | N1-C1'-C2' | -6.82 | 104.50 | 112.00 |
| 10 | M | 48 | U | N3-C4-C5 | 6.80 | 118.68 | 114.60 |
| 10 | M | 69 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 10 | M | 60 | U | N3-C4-C5 | 6.74 | 118.65 | 114.60 |
| 10 | M | 75 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 10 | M | 57 | A | N1-C2-N3 | -6.71 | 125.95 | 129.30 |
| 10 | M | 5 | U | P-O3'-C3' | 6.70 | 127.74 | 119.70 |
| 10 | M | 26 | A | O3'-P-O5' | 6.68 | 116.70 | 104.00 |
| 10 | M | 41 | C | OP2-P-O3' | 6.68 | 119.90 | 105.20 |
| 10 | M | 30 | G | C1'-O4'-C4' | -6.65 | 104.58 | 109.90 |
| 10 | M | 76 | A | N1-C2-N3 | -6.64 | 125.98 | 129.30 |
| 10 | M | 39 | U | OP2-P-O3' | 6.62 | 119.77 | 105.20 |
| 10 | M | 60 | U | C2-N3-C4 | -6.58 | 123.05 | 127.00 |
| 10 | M | 4 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 10 | M | 73 | G | O4'-C1'-N9 | 6.49 | 113.39 | 108.20 |
| 10 | M | 32 | U | N1-C1'-C2' | -6.46 | 104.89 | 112.00 |
| 10 | M | 66 | U | C2-N3-C4 | -6.42 | 123.15 | 127.00 |
| 10 | M | 73 | G | C6-N1-C2 | -6.41 | 121.25 | 125.10 |
| 10 | M | 64 | C | P-O3'-C3' | -6.39 | 112.03 | 119.70 |
| 10 | M | 66 | U | OP1-P-OP2 | -6.37 | 110.04 | 119.60 |
| 10 | M | 58 | A | N1-C2-N3 | -6.37 | 126.11 | 129.30 |
| 10 | M | 69 | C | N3-C4-C5 | -6.36 | 119.36 | 121.90 |
| 10 | M | 48 | U | N1-C2-N3 | 6.32 | 118.69 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | M | 67 | C | N3-C4-C5 | -6.31 | 119.38 | 121.90 |
| 10 | M | 29 | G | C5'-C4'-C3' | -6.31 | 105.91 | 116.00 |
| 10 | M | 42 | G | C1'-O4'-C4' | -6.28 | 104.87 | 109.90 |
| 10 | M | 60 | U | P-O3'-C3' | -6.25 | 112.20 | 119.70 |
| 10 | M | 70 | G | C6-N1-C2 | -6.23 | 121.36 | 125.10 |
| 10 | M | 26 | A | O4'-C1'-N9 | 6.22 | 113.18 | 108.20 |
| 12 | K | 174 | PRO | N-CA-CB | 6.18 | 110.71 | 103.30 |
| 10 | M | 50 | G | C5-C6-N1 | 6.17 | 114.59 | 111.50 |
| 10 | M | 42 | G | O3'-P-O5' | 6.17 | 115.72 | 104.00 |
| 10 | M | 76 | A | C5-C6-N1 | -6.15 | 114.62 | 117.70 |
| 10 | M | 2 | C | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 10 | M | 25 | U | O3'-P-O5' | -6.14 | 92.33 | 104.00 |
| 10 | M | 63 | C | OP1-P-OP2 | -6.12 | 110.42 | 119.60 |
| 10 | M | 74 | C | O5'-P-OP1 | 6.09 | 118.00 | 110.70 |
| 10 | M | 7 | A | O4'-C1'-N9 | 6.07 | 113.06 | 108.20 |
| 10 | M | 32 | U | C5'-C4'-O4' | 6.04 | 116.35 | 109.10 |
| 10 | M | 33 | U | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 10 | M | 4 | G | C5-C6-N1 | 6.02 | 114.51 | 111.50 |
| 10 | M | 57 | A | OP1-P-OP2 | -6.02 | 110.57 | 119.60 |
| 10 | M | 51 | G | C5-C6-N1 | 5.99 | 114.49 | 111.50 |
| 10 | M | 7 | A | N1-C2-N3 | -5.96 | 126.32 | 129.30 |
| 8 | I | 1083 | U | O3'-P-O5' | 5.95 | 115.30 | 104.00 |
| 8 | I | 1105 | U | N1-C1'-C2' | 5.95 | 121.73 | 114.00 |
| 10 | M | 28 | C | O3'-P-O5' | 5.85 | 115.11 | 104.00 |
| 10 | M | 62 | C | OP1-P-OP2 | -5.82 | 110.86 | 119.60 |
| 10 | M | 48 | U | OP1-P-OP2 | -5.81 | 110.88 | 119.60 |
| 13 | L | 530 | VAL | N-CA-C | 5.80 | 126.67 | 111.00 |
| 10 | M | 64 | C | OP1-P-OP2 | -5.77 | 110.94 | 119.60 |
| 10 | M | 6 | G | P-O3'-C3' | -5.74 | 112.81 | 119.70 |
| 10 | M | 1 | U | N1-C2-N3 | 5.72 | 118.33 | 114.90 |
| 10 | M | 76 | A | C6-N1-C2 | 5.68 | 122.01 | 118.60 |
| 10 | M | 71 | G | C5-C6-N1 | 5.65 | 114.32 | 111.50 |
| 10 | M | 6 | G | OP1-P-OP2 | -5.62 | 111.16 | 119.60 |
| 10 | M | 64 | C | N1-C1'-C2' | -5.60 | 105.84 | 112.00 |
| 10 | M | 64 | C | N3-C4-C5 | -5.58 | 119.67 | 121.90 |
| 10 | M | 66 | U | C5-C4-O4 | -5.54 | 122.58 | 125.90 |
| 12 | K | 133 | PRO | N-CA-CB | 5.54 | 109.95 | 103.30 |
| 10 | M | 42 | G | OP2-P-O3' | 5.53 | 117.36 | 105.20 |
| 10 | M | 60 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 10 | M | 63 | C | O5'-P-OP2 | 5.47 | 117.27 | 110.70 |
| 10 | M | 41 | C | P-O5'-C5' | 5.47 | 129.65 | 120.90 |
| 10 | M | 74 | C | OP1-P-OP2 | -5.45 | 111.43 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | M | 72 | A | OP1-P-OP2 | -5.42 | 111.46 | 119.60 |
| 10 | M | 70 | G | OP1-P-OP2 | -5.42 | 111.47 | 119.60 |
| 10 | M | 67 | C | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 10 | M | 72 | A | N1-C2-N3 | -5.41 | 126.59 | 129.30 |
| 8 | I | 1104 | C | C5'-C4'-C3' | 5.40 | 124.64 | 116.00 |
| 10 | M | 67 | C | C2-N3-C4 | 5.39 | 122.59 | 119.90 |
| 10 | M | 62 | C | C2-N3-C4 | 5.38 | 122.59 | 119.90 |
| 10 | M | 51 | G | C6-N1-C2 | -5.38 | 121.87 | 125.10 |
| 10 | M | 59 | U | OP1-P-OP2 | -5.38 | 111.53 | 119.60 |
| 10 | M | 32 | U | OP2-P-O3' | 5.36 | 116.99 | 105.20 |
| 10 | M | 75 | C | C2-N3-C4 | 5.35 | 122.57 | 119.90 |
| 12 | K | 220 | PRO | N-CA-CB | 5.34 | 109.71 | 103.30 |
| 10 | M | 72 | A | OP2-P-O3' | -5.32 | 93.49 | 105.20 |
| 10 | M | 70 | G | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |
| 8 | I | 1083 | U | OP2-P-O3' | 5.30 | 116.86 | 105.20 |
| 10 | M | 73 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |
| 10 | M | 68 | G | OP1-P-OP2 | -5.29 | 111.67 | 119.60 |
| 12 | K | 201 | PRO | N-CA-CB | 5.28 | 109.64 | 103.30 |
| 10 | M | 2 | C | OP1-P-OP2 | -5.27 | 111.69 | 119.60 |
| 10 | M | 5 | U | O4'-C1'-N1 | 5.22 | 112.37 | 108.20 |
| 10 | M | 39 | U | OP1-P-O3' | -5.19 | 93.78 | 105.20 |
| 10 | M | 52 | G | OP1-P-OP2 | -5.19 | 111.81 | 119.60 |
| 10 | M | 66 | U | C4-C5-C6 | -5.18 | 116.59 | 119.70 |
| 12 | K | 182 | PRO | N-CA-CB | 5.18 | 109.51 | 103.30 |
| 10 | M | 38 | U | O4'-C1'-N1 | 5.09 | 112.28 | 108.20 |
| 13 | L | 532 | GLY | N-CA-C | -5.09 | 100.37 | 113.10 |
| 10 | M | 1 | U | OP1-P-OP2 | -5.09 | 111.97 | 119.60 |
| 13 | L | 166 | LEU | CA-CB-CG | 5.08 | 126.97 | 115.30 |
| 10 | M | 59 | U | N1-C2-N3 | 5.07 | 117.94 | 114.90 |
| 10 | M | 50 | G | O5'-C5'-C4' | -5.03 | 102.15 | 111.70 |
| 10 | M | 65 | G | OP1-P-OP2 | -5.00 | 112.09 | 119.60 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 5 | F | 2662 | A | C1' |
| 9 | J | 2191 | G | C3' |

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 371 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | C | 1407 | C | Sidechain |
| 3 | C | 1417 | G | Sidechain |
| 3 | C | 1418 | A | Sidechain |
| 3 | C | 1434 | A | Sidechain |
| 3 | C | 1463 | C | Sidechain |
| 3 | C | 1474 | G | Sidechain |
| 3 | C | 1485 | U | Sidechain |
| 7 | H | 2464 | C | Sidechain |
| 8 | I | 1059 | G | Sidechain |
| 8 | I | 1091 | G | Sidechain |
| 8 | I | 1092 | C | Sidechain |
| 8 | I | 1093 | G | Sidechain |
| 8 | I | 1101 | U | 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 | 256 | 0 | 131 | 5 | 0 |
| 2 | B | 214 | 0 | 110 | 24 | 0 |
| 3 | C | 2069 | 0 | 1046 | 86 | 0 |
| 4 | D | 278 | 0 | 141 | 28 | 0 |
| 5 | F | 624 | 0 | 314 | 85 | 0 |
| 6 | G | 1172 | 0 | 591 | 46 | 0 |
| 7 | H | 898 | 0 | 456 | 21 | 0 |
| 8 | I | 1241 | 0 | 625 | 313 | 0 |
| 9 | J | 1569 | 0 | 790 | 79 | 0 |
| 10 | M | 1570 | 0 | 800 | 112 | 0 |
| 11 | E | 971 | 0 | 1057 | 106 | 0 |
| 12 | K | 1142 | 0 | 865 | 113 | 0 |
| 13 | L | 5126 | 0 | 5163 | 628 | 0 |
| 14 | N | 1901 | 0 | 1951 | 251 | 0 |
| All | All | 19031 | 0 | 14040 | 1734 | 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 53.

All (1734) 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) |
|---|---|---|---|
| 4:D:55:A:C2 | 13:L:322:VAL:HG12 | 1.22 | 1.75 |
| 13:L:556:ILE:CD1 | 13:L:601:ILE:HD13 | 1.28 | 1.64 |
| 13:L:408:VAL:CG1 | 13:L:669:PHE:HE1 | 1.12 | 1.57 |
| 5:F:2661:G:N1 | 13:L:20:HIS:CE1 | 1.72 | 1.54 |
| 2:B:368:U:C5 | 13:L:354:ARG:CD | 1.92 | 1.52 |
| 2:B:368:U:C5 | 13:L:354:ARG:HD2 | 1.00 | 1.51 |
| 5:F:2662:A:H61 | 13:L:21:ILE:CD1 | 1.22 | 1.49 |
| 13:L:594:VAL:CG1 | 13:L:599:PRO:HB3 | 1.38 | 1.49 |
| 13:L:484:ARG:HB3 | 13:L:606:MET:CG | 1.41 | 1.48 |
| 13:L:484:ARG:NE | 13:L:649:LEU:CD1 | 1.73 | 1.47 |
| 13:L:408:VAL:CG1 | 13:L:669:PHE:CE1 | 1.95 | 1.47 |
| 4:D:55:A:H2 | 13:L:322:VAL:CG1 | 1.24 | 1.45 |
| 13:L:484:ARG:HH21 | 13:L:671:MET:CE | 1.26 | 1.45 |
| 13:L:484:ARG:CA | 13:L:649:LEU:HA | 1.48 | 1.41 |
| 9:J:2168:G:N2 | 10:M:56:C:N3 | 1.63 | 1.41 |
| 8:I:1095:A:C5' | 13:L:617:MET:HB3 | 1.45 | 1.40 |
| 13:L:484:ARG:HB3 | 13:L:606:MET:CB | 1.49 | 1.39 |
| 13:L:408:VAL:HG12 | 13:L:669:PHE:CE1 | 1.54 | 1.39 |
| 5:F:2662:A:C6 | 13:L:21:ILE:HG12 | 1.57 | 1.39 |
| 5:F:2662:A:N1 | 13:L:21:ILE:HG12 | 1.31 | 1.39 |
| 5:F:2660:A:C2' | 13:L:660:ARG:HG3 | 1.52 | 1.39 |
| 4:D:55:A:C2 | 13:L:322:VAL:CG1 | 1.97 | 1.37 |
| 13:L:484:ARG:HA | 13:L:649:LEU:CA | 1.53 | 1.34 |
| 5:F:2662:A:N6 | 13:L:21:ILE:HD11 | 1.36 | 1.33 |
| 5:F:2661:G:N1 | 13:L:20:HIS:HE1 | 0.86 | 1.32 |
| 13:L:406:GLU:HG3 | 13:L:669:PHE:O | 1.24 | 1.31 |
| 13:L:484:ARG:NE | 13:L:649:LEU:HD12 | 0.98 | 1.31 |
| 5:F:2662:A:N6 | 13:L:21:ILE:CG1 | 1.94 | 1.30 |
| 13:L:406:GLU:OE2 | 13:L:671:MET:N | 1.61 | 1.29 |
| 8:I:1067:A:O2' | 13:L:634:MET:N | 1.61 | 1.29 |
| 13:L:486:THR:HG22 | 13:L:600:VAL:CG1 | 1.62 | 1.28 |
| 10:M:75:C:C2' | 10:M:76:A:H5' | 1.59 | 1.28 |
| 4:D:55:A:H1' | 13:L:321:TYR:CA | 1.36 | 1.28 |
| 13:L:485:GLU:N | 13:L:649:LEU:N | 1.61 | 1.28 |
| 10:M:75:C:H2' | 10:M:76:A:C5' | 1.62 | 1.28 |
| 5:F:2660:A:H2' | 13:L:660:ARG:CG | 1.62 | 1.27 |
| 5:F:2662:A:N6 | 13:L:21:ILE:CD1 | 1.92 | 1.27 |
| 13:L:406:GLU:OE2 | 13:L:670:VAL:CA | 1.82 | 1.26 |
| 13:L:485:GLU:CA | 13:L:647:VAL:O | 1.83 | 1.25 |
| 13:L:556:ILE:CG1 | 13:L:601:ILE:HD13 | 1.66 | 1.25 |
| 13:L:484:ARG:C | 13:L:648:PRO:C | 1.84 | 1.25 |
| 13:L:556:ILE:HG12 | 13:L:601:ILE:CD1 | 1.66 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1095:A:H5' | 13:L:617:MET:CB | 1.45 | 1.24 |
| 13:L:127:LYS:NZ | 13:L:402:ILE:HG13 | 1.47 | 1.24 |
| 5:F:2662:A:H61 | 13:L:21:ILE:CG1 | 1.50 | 1.24 |
| 13:L:484:ARG:O | 13:L:647:VAL:HG22 | 1.22 | 1.24 |
| 13:L:556:ILE:HD11 | 13:L:601:ILE:CG2 | 1.66 | 1.23 |
| 13:L:594:VAL:CG1 | 13:L:599:PRO:CB | 2.14 | 1.23 |
| 5:F:2662:A:C6 | 13:L:21:ILE:CG1 | 2.21 | 1.23 |
| 13:L:485:GLU:HB2 | 13:L:604:PRO:O | 1.38 | 1.22 |
| 5:F:2661:G:C2 | 13:L:20:HIS:HE1 | 1.59 | 1.21 |
| 10:M:33:U:O3' | 10:M:34:U:P | 1.98 | 1.21 |
| 13:L:485:GLU:HB3 | 13:L:605:ILE:CD1 | 1.69 | 1.20 |
| 13:L:127:LYS:CE | 13:L:402:ILE:HG13 | 1.68 | 1.20 |
| 8:I:1095:A:C2 | 13:L:614:GLU:OE1 | 1.94 | 1.20 |
| 13:L:406:GLU:CG | 13:L:670:VAL:HA | 1.72 | 1.19 |
| 13:L:484:ARG:NH2 | 13:L:671:MET:CE | 2.04 | 1.19 |
| 13:L:594:VAL:HG13 | 13:L:599:PRO:CB | 1.72 | 1.18 |
| 8:I:1095:A:N1 | 13:L:614:GLU:OE1 | 1.75 | 1.18 |
| 13:L:484:ARG:NH2 | 13:L:671:MET:HE1 | 1.58 | 1.18 |
| 5:F:2662:A:N1 | 13:L:21:ILE:CG1 | 2.05 | 1.18 |
| 13:L:486:THR:N | 13:L:600:VAL:O | 1.76 | 1.17 |
| 13:L:124:GLN:HE22 | 13:L:401:SER:CB | 1.57 | 1.17 |
| 13:L:556:ILE:CG1 | 13:L:601:ILE:CD1 | 2.21 | 1.17 |
| 13:L:556:ILE:CD1 | 13:L:601:ILE:CD1 | 2.24 | 1.16 |
| 13:L:485:GLU:HB3 | 13:L:605:ILE:HD13 | 1.16 | 1.16 |
| 13:L:408:VAL:HG12 | 13:L:669:PHE:CZ | 1.78 | 1.16 |
| 13:L:484:ARG:CD | 13:L:606:MET:HG3 | 1.75 | 1.16 |
| 2:B:368:U:H5 | 13:L:354:ARG:CD | 1.39 | 1.16 |
| 13:L:406:GLU:CD | 13:L:670:VAL:HA | 1.67 | 1.15 |
| 13:L:555:LEU:O | 13:L:688:ILE:HG23 | 1.47 | 1.15 |
| 8:I:1095:A:OP1 | 13:L:617:MET:CB | 1.95 | 1.15 |
| 13:L:406:GLU:OE2 | 13:L:670:VAL:C | 1.83 | 1.14 |
| 9:J:2175:C:H2' | 9:J:2176:A:H5" | 1.28 | 1.14 |
| 8:I:1054:A:N6 | 8:I:1105:U:H3 | 1.46 | 1.14 |
| 13:L:484:ARG:CB | 13:L:606:MET:HB2 | 1.79 | 1.13 |
| 8:I:1085:A:H1' | 8:I:1086:A:C4' | 1.78 | 1.13 |
| 13:L:484:ARG:O | 13:L:647:VAL:C | 1.86 | 1.13 |
| 13:L:484:ARG:O | 13:L:647:VAL:CG2 | 1.95 | 1.13 |
| 13:L:485:GLU:N | 13:L:647:VAL:O | 1.81 | 1.13 |
| 8:I:1085:A:H1' | 8:I:1086:A:H4' | 1.13 | 1.13 |
| 8:I:1095:A:P | 13:L:617:MET:HB3 | 1.88 | 1.13 |
| 13:L:556:ILE:HG22 | 13:L:688:ILE:CA | 1.77 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:408:VAL:HG11 | 13:L:669:PHE:HE1 | 1.00 | 1.13 |
| 13:L:92:ILE:HG21 | 13:L:436:PRO:HD2 | 1.28 | 1.13 |
| 13:L:484:ARG:HE | 13:L:649:LEU:CD1 | 1.46 | 1.12 |
| 13:L:556:ILE:HG22 | 13:L:688:ILE:HA | 1.18 | 1.12 |
| 5:F:2660:A:C1' | 13:L:660:ARG:HG3 | 1.79 | 1.11 |
| 13:L:406:GLU:CG | 13:L:669:PHE:O | 1.96 | 1.11 |
| 2:B:368:U:C4 | 13:L:354:ARG:HD2 | 1.85 | 1.11 |
| 8:I:1095:A:OP1 | 13:L:617:MET:HB2 | 1.49 | 1.11 |
| 13:L:484:ARG:CB | 13:L:606:MET:CG | 2.28 | 1.11 |
| 3:C:1441:G:H5" | 3:C:1442:G:H5" | 1.24 | 1.10 |
| 13:L:485:GLU:CB | 13:L:605:ILE:HD13 | 1.82 | 1.09 |
| 3:C:1494:G:O4' | 13:L:502:GLY:HA2 | 1.46 | 1.09 |
| 13:L:555:LEU:O | 13:L:688:ILE:HG12 | 1.51 | 1.08 |
| 13:L:484:ARG:HB3 | 13:L:606:MET:HG3 | 1.34 | 1.08 |
| 5:F:2660:A:C2' | 13:L:660:ARG:CG | 2.22 | 1.08 |
| 9:J:2128:C:H2' | 9:J:2129:C:H5" | 1.29 | 1.08 |
| 5:F:2660:A:H2' | 13:L:660:ARG:CD | 1.74 | 1.08 |
| 5:F:2660:A:C1' | 13:L:665:GLY:N | 2.17 | 1.08 |
| 8:I:1061:U:H4' | 8:I:1070:A:C1' | 1.83 | 1.08 |
| 13:L:484:ARG:HB3 | 13:L:606:MET:HB2 | 1.21 | 1.08 |
| 9:J:2168:G:N2 | 10:M:56:C:C4 | 2.22 | 1.08 |
| 13:L:406:GLU:OE2 | 13:L:670:VAL:HA | 1.45 | 1.07 |
| 10:M:64:C:H5' | 12:K:53:ARG:HH21 | 0.91 | 1.06 |
| 14:N:22:LYS:HA | 14:N:22:LYS:NZ | 1.69 | 1.06 |
| 12:K:58:VAL:HG21 | 12:K:166:ASP:H | 0.97 | 1.06 |
| 13:L:484:ARG:HH21 | 13:L:671:MET:HE1 | 0.92 | 1.06 |
| 10:M:64:C:H5' | 12:K:53:ARG:NH2 | 1.70 | 1.06 |
| 13:L:484:ARG:HD3 | 13:L:606:MET:HG3 | 1.10 | 1.05 |
| 8:I:1095:A:C5' | 13:L:617:MET:CB | 2.18 | 1.05 |
| 14:N:22:LYS:HZ3 | 14:N:22:LYS:HA | 1.03 | 1.05 |
| 10:M:73:G:O2' | 10:M:74:C:H5' | 1.57 | 1.04 |
| 13:L:484:ARG:C | 13:L:647:VAL:O | 1.96 | 1.04 |
| 13:L:484:ARG:CB | 13:L:606:MET:CB | 2.34 | 1.04 |
| 8:I:1095:A:O5' | 13:L:617:MET:HB3 | 1.55 | 1.04 |
| 6:G:1884:A:H2' | 6:G:1885:A:H5" | 1.40 | 1.04 |
| 13:L:127:LYS:NZ | 13:L:402:ILE:CG1 | 2.14 | 1.03 |
| 13:L:484:ARG:HG2 | 13:L:652:MET:HG3 | 1.40 | 1.03 |
| 5:F:2661:G:C2 | 13:L:20:HIS:CE1 | 2.40 | 1.02 |
| 4:D:55:A:C1' | 13:L:321:TYR:CA | 2.29 | 1.02 |
| 13:L:556:ILE:HD13 | 13:L:601:ILE:CD1 | 1.88 | 1.02 |
| 5:F:2660:A:H1' | 13:L:665:GLY:CA | 1.90 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1067:A:N7 | 13:L:631:ILE:O | 1.93 | 1.02 |
| 3:C:1494:G:O4' | 13:L:502:GLY:CA | 2.04 | 1.02 |
| 10:M:64:C:C5' | 12:K:53:ARG:HH21 | 1.72 | 1.02 |
| 13:L:482:ALA:N | 13:L:655:TYR:H | 1.51 | 1.01 |
| 13:L:556:ILE:CD1 | 13:L:601:ILE:HG21 | 1.89 | 1.01 |
| 13:L:484:ARG:CB | 13:L:606:MET:HG3 | 1.87 | 1.01 |
| 13:L:486:THR:CG2 | 13:L:600:VAL:HG12 | 1.90 | 1.01 |
| 13:L:486:THR:HG22 | 13:L:600:VAL:HG12 | 1.38 | 1.01 |
| 5:F:2660:A:H1' | 13:L:665:GLY:N | 1.76 | 1.00 |
| 8:I:1061:U:H4' | 8:I:1070:A:H1' | 1.38 | 1.00 |
| 11:E:46:LYS:HG2 | 11:E:47:LYS:H | 1.19 | 1.00 |
| 4:D:55:A:H1' | 13:L:321:TYR:HA | 1.04 | 1.00 |
| 9:J:2129:C:H2' | 9:J:2130:U:H4' | 1.38 | 1.00 |
| 5:F:2660:A:H2' | 13:L:660:ARG:HG3 | 1.12 | 0.99 |
| 10:M:8:4SU:C4' | 10:M:49:5MC:H5' | 1.92 | 0.99 |
| 13:L:484:ARG:HD3 | 13:L:606:MET:CG | 1.92 | 0.99 |
| 13:L:556:ILE:HD13 | 13:L:601:ILE:HD13 | 1.01 | 0.99 |
| 13:L:406:GLU:HG3 | 13:L:670:VAL:HA | 1.34 | 0.99 |
| 8:I:1063:G:N2 | 8:I:1075:C:N3 | 2.11 | 0.99 |
| 6:G:1879:C:H2' | 6:G:1880:C:H5" | 1.41 | 0.99 |
| 13:L:556:ILE:HD11 | 13:L:601:ILE:HG21 | 1.02 | 0.98 |
| 5:F:2660:A:C1' | 13:L:665:GLY:CA | 2.41 | 0.98 |
| 9:J:2103:C:H3' | 9:J:2104:G:H5" | 1.41 | 0.98 |
| 13:L:486:THR:O | 13:L:600:VAL:N | 1.95 | 0.98 |
| 12:K:58:VAL:HG21 | 12:K:166:ASP:N | 1.78 | 0.98 |
| 13:L:482:ALA:HA | 13:L:653:PHE:HA | 1.45 | 0.98 |
| 8:I:1065:U:C3' | 8:I:1066:U:H5" | 1.93 | 0.98 |
| 7:H:2464:C:HO2' | 7:H:2465:C:H6 | 1.02 | 0.98 |
| 13:L:485:GLU:C | 13:L:605:ILE:HG23 | 1.84 | 0.98 |
| 5:F:2660:A:O4' | 13:L:665:GLY:N | 1.97 | 0.97 |
| 14:N:185:ILE:HG22 | 14:N:199:TYR:HB2 | 1.45 | 0.97 |
| 13:L:594:VAL:HG12 | 13:L:599:PRO:CB | 1.85 | 0.97 |
| 5:F:2662:A:C6 | 13:L:21:ILE:CD1 | 2.45 | 0.97 |
| 13:L:594:VAL:HG12 | 13:L:599:PRO:HB3 | 1.34 | 0.97 |
| 8:I:1085:A:O2' | 8:I:1086:A:O4' | 1.81 | 0.97 |
| 8:I:1061:U:C4' | 8:I:1070:A:H1' | 1.94 | 0.97 |
| 13:L:486:THR:CG2 | 13:L:600:VAL:CG1 | 2.41 | 0.97 |
| 12:K:168:THR:HA | 12:K:173:ALA:HB2 | 1.45 | 0.97 |
| 13:L:484:ARG:C | 13:L:649:LEU:N | 2.05 | 0.97 |
| 13:L:124:GLN:NE2 | 13:L:401:SER:OG | 1.98 | 0.97 |
| 12:K:46:LYS:HA | 12:K:46:LYS:HE2 | 1.46 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:J:2175:C:C2' | 9:J:2176:A:H5" | 1.95 | 0.96 |
| 13:L:482:ALA:H | 13:L:655:TYR:H | 1.10 | 0.96 |
| 13:L:410:ASP:OD1 | 13:L:653:PHE:HD1 | 1.47 | 0.95 |
| 8:I:1061:U:H3' | 8:I:1061:U:OP2 | 1.66 | 0.95 |
| 11:E:59:ARG:HH21 | 13:L:418:LYS:HE3 | 1.31 | 0.95 |
| 13:L:556:ILE:HG12 | 13:L:601:ILE:CG1 | 1.96 | 0.94 |
| 8:I:1087:G:H21 | 8:I:1103:A:H2' | 1.32 | 0.94 |
| 13:L:484:ARG:CZ | 13:L:649:LEU:CD1 | 2.46 | 0.94 |
| 13:L:409:ILE:HD13 | 13:L:654:GLY:HA2 | 1.50 | 0.94 |
| 13:L:142:THR:HA | 13:L:171:GLU:HG2 | 1.50 | 0.94 |
| 11:E:47:LYS:HB3 | 11:E:48:PRO:HD3 | 1.48 | 0.94 |
| 8:I:1057:A:H61 | 8:I:1081:U:H3 | 1.11 | 0.94 |
| 8:I:1102:C:H1' | 8:I:1103:A:C8 | 2.04 | 0.93 |
| 9:J:2128:C:C2' | 9:J:2129:C:H5" | 1.99 | 0.93 |
| 13:L:484:ARG:CD | 13:L:649:LEU:HD12 | 1.97 | 0.93 |
| 5:F:2662:A:N1 | 13:L:21:ILE:CD1 | 2.32 | 0.92 |
| 13:L:555:LEU:O | 13:L:688:ILE:CG2 | 2.16 | 0.92 |
| 8:I:1069:A:H4' | 8:I:1070:A:C5' | 1.98 | 0.92 |
| 10:M:8:4SU:C5' | 10:M:49:5MC:H5' | 1.98 | 0.92 |
| 14:N:18:GLY:H | 14:N:42:ILE:HG22 | 1.32 | 0.92 |
| 13:L:594:VAL:HG13 | 13:L:599:PRO:HB3 | 0.95 | 0.92 |
| 8:I:1065:U:H3' | 8:I:1066:U:H5" | 1.49 | 0.92 |
| 5:F:2662:A:N6 | 13:L:21:ILE:HG13 | 1.82 | 0.92 |
| 9:J:2168:G:N2 | 10:M:56:C:C2 | 2.38 | 0.92 |
| 11:E:6:THR:H | 11:E:9:GLN:HE21 | 1.12 | 0.92 |
| 10:M:37:A:O3' | 10:M:38:U:P | 2.27 | 0.92 |
| 11:E:32:PHE:HB3 | 11:E:84:LEU:HD21 | 1.50 | 0.92 |
| 4:D:55:A:C1' | 13:L:321:TYR:HA | 1.91 | 0.91 |
| 13:L:556:ILE:HG22 | 13:L:688:ILE:N | 1.85 | 0.91 |
| 13:L:486:THR:HG22 | 13:L:600:VAL:HG11 | 1.53 | 0.91 |
| 13:L:409:ILE:HA | 13:L:654:GLY:HA2 | 1.50 | 0.91 |
| 5:F:2656:U:H4' | 13:L:141:LYS:HZ2 | 1.35 | 0.91 |
| 8:I:1064:C:H2' | 8:I:1065:U:H6 | 1.36 | 0.90 |
| 8:I:1081:U:H2' | 8:I:1082:U:C5 | 2.06 | 0.90 |
| 8:I:1095:A:P | 13:L:617:MET:CB | 2.55 | 0.90 |
| 3:C:1442:G:H5' | 3:C:1442:G:C8 | 2.06 | 0.90 |
| 5:F:2660:A:H1' | 13:L:665:GLY:HA2 | 1.50 | 0.90 |
| 13:L:410:ASP:OD1 | 13:L:653:PHE:CD1 | 2.23 | 0.90 |
| 8:I:1054:A:N1 | 8:I:1105:U:O2 | 2.05 | 0.90 |
| 13:L:127:LYS:HZ3 | 13:L:402:ILE:CG1 | 1.81 | 0.90 |
| 13:L:484:ARG:CG | 13:L:606:MET:HG3 | 2.02 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1087:G:H21 | 8:I:1103:A:C2' | 1.85 | 0.89 |
| 13:L:484:ARG:CD | 13:L:649:LEU:CD1 | 2.50 | 0.89 |
| 10:M:8:4SU:O2' | 10:M:46:A:H1' | 1.71 | 0.89 |
| 13:L:406:GLU:HG3 | 13:L:669:PHE:C | 1.92 | 0.89 |
| 10:M:66:U:H2' | 10:M:67:C:C6 | 2.08 | 0.89 |
| 13:L:406:GLU:HG3 | 13:L:670:VAL:CA | 2.03 | 0.89 |
| 8:I:1058:G:O2' | 8:I:1059:G:H5' | 1.73 | 0.89 |
| 8:I:1064:C:H2' | 8:I:1065:U:C6 | 2.08 | 0.89 |
| 13:L:519:ARG:HG2 | 13:L:677:GLN:HE22 | 1.35 | 0.88 |
| 13:L:485:GLU:C | 13:L:647:VAL:O | 2.11 | 0.88 |
| 2:B:368:U:C4 | 13:L:354:ARG:NH1 | 2.41 | 0.88 |
| 9:J:2175:C:H1' | 12:K:215:THR:HA | 1.52 | 0.88 |
| 13:L:89:ASP:HB3 | 13:L:454:MET:SD | 2.14 | 0.88 |
| 13:L:486:THR:HG21 | 13:L:678:GLU:CD | 1.94 | 0.88 |
| 5:F:2662:A:C6 | 13:L:21:ILE:HD11 | 2.07 | 0.88 |
| 8:I:1063:G:N1 | 8:I:1075:C:N4 | 2.22 | 0.88 |
| 13:L:137:ASN:HD21 | 13:L:263:ALA:H | 1.19 | 0.88 |
| 13:L:484:ARG:NH2 | 13:L:671:MET:HE3 | 1.79 | 0.88 |
| 8:I:1069:A:C4' | 8:I:1070:A:H5" | 2.03 | 0.87 |
| 8:I:1069:A:H4' | 8:I:1070:A:H5" | 1.54 | 0.87 |
| 10:M:8:4SU:H5" | 10:M:49:5MC:H5' | 1.55 | 0.87 |
| 13:L:555:LEU:O | 13:L:688:ILE:CG1 | 2.21 | 0.87 |
| 6:G:1879:C:C2' | 6:G:1880:C:H5" | 2.03 | 0.87 |
| 13:L:484:ARG:CZ | 13:L:649:LEU:HD12 | 2.02 | 0.87 |
| 10:M:73:G:C2' | 10:M:74:C:H5' | 2.04 | 0.87 |
| 13:L:556:ILE:HG23 | 13:L:601:ILE:HD11 | 1.55 | 0.87 |
| 13:L:127:LYS:HD2 | 13:L:401:SER:HA | 1.53 | 0.87 |
| 5:F:2662:A:H61 | 13:L:21:ILE:HD11 | 0.94 | 0.87 |
| 14:N:48:MET:HA | 14:N:51:LEU:HD12 | 1.56 | 0.87 |
| 6:G:1884:A:C2' | 6:G:1885:A:H5" | 2.05 | 0.87 |
| 14:N:137:ARG:HH11 | 14:N:137:ARG:HA | 1.38 | 0.87 |
| 13:L:484:ARG:O | 13:L:648:PRO:N | 2.07 | 0.86 |
| 12:K:49:ILE:H | 12:K:49:ILE:HD12 | 1.39 | 0.86 |
| 13:L:483:TYR:O | 13:L:649:LEU:O | 1.94 | 0.86 |
| 8:I:1054:A:H2' | 8:I:1055:G:C8 | 2.09 | 0.86 |
| 5:F:2660:A:C2' | 13:L:660:ARG:CD | 2.46 | 0.86 |
| 4:D:55:A:C2 | 13:L:322:VAL:HG13 | 2.08 | 0.86 |
| 11:E:18:VAL:HG23 | 11:E:19:ARG:H | 1.41 | 0.86 |
| 10:M:19:G:H4' | 10:M:20:H2U:OP1 | 1.74 | 0.85 |
| 13:L:555:LEU:C | 13:L:688:ILE:HG12 | 1.96 | 0.85 |
| 13:L:556:ILE:CG2 | 13:L:688:ILE:N | 2.39 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:M:69:C:H2' | 10:M:70:G:C8 | 2.11 | 0.85 |
| 5:F:2659:G:O3' | 13:L:664:GLN:OE1 | 1.89 | 0.85 |
| 13:L:482:ALA:N | 13:L:655:TYR:N | 2.25 | 0.84 |
| 14:N:187:LEU:HD23 | 14:N:201:ILE:HG22 | 1.57 | 0.84 |
| 11:E:41:ARG:HB3 | 11:E:41:ARG:HH11 | 1.40 | 0.84 |
| 13:L:92:ILE:HG21 | 13:L:436:PRO:CD | 2.07 | 0.84 |
| 6:G:1840:G:H1 | 6:G:1902:C:H42 | 1.24 | 0.84 |
| 14:N:51:LEU:HD23 | 14:N:201:ILE:HD12 | 1.58 | 0.84 |
| 5:F:2660:A:H1' | 13:L:665:GLY:H | 1.40 | 0.84 |
| 11:E:60:LEU:HD21 | 11:E:66:VAL:HG22 | 1.57 | 0.84 |
| 13:L:409:ILE:HD13 | 13:L:654:GLY:CA | 2.06 | 0.84 |
| 5:F:2661:G:N2 | 13:L:20:HIS:CE1 | 2.46 | 0.84 |
| 10:M:14:A:H2' | 10:M:15:G:C8 | 2.13 | 0.84 |
| 13:L:415:PRO:HG3 | 13:L:421:GLN:HG2 | 1.60 | 0.84 |
| 13:L:556:ILE:HG12 | 13:L:601:ILE:HG12 | 1.60 | 0.84 |
| 10:M:1:U:H2' | 10:M:2:C:H6 | 1.43 | 0.84 |
| 5:F:2656:U:H4' | 13:L:141:LYS:NZ | 1.91 | 0.84 |
| 13:L:484:ARG:O | 13:L:648:PRO:C | 2.15 | 0.83 |
| 10:M:52:G:H1 | 10:M:62:C:H42 | 1.25 | 0.83 |
| 9:J:2189:U:H3' | 9:J:2190:G:H5" | 1.60 | 0.83 |
| 6:G:1846:G:H5' | 6:G:1847:A:OP2 | 1.78 | 0.83 |
| 12:K:49:ILE:HG22 | 12:K:50:ASP:H | 1.43 | 0.83 |
| 12:K:44:HIS:CD2 | 12:K:175:VAL:HA | 2.14 | 0.83 |
| 9:J:2189:U:C3' | 9:J:2190:G:H5" | 2.09 | 0.83 |
| 13:L:556:ILE:CG2 | 13:L:688:ILE:HA | 2.07 | 0.82 |
| 10:M:64:C:C5' | 12:K:53:ARG:NH2 | 2.34 | 0.82 |
| 13:L:165:GLN:HE21 | 13:L:260:LEU:H | 1.24 | 0.82 |
| 8:I:1063:G:C2 | 8:I:1075:C:N3 | 2.47 | 0.82 |
| 13:L:484:ARG:CZ | 13:L:649:LEU:HD11 | 2.09 | 0.82 |
| 8:I:1061:U:C5' | 8:I:1070:A:H4' | 2.09 | 0.82 |
| 13:L:124:GLN:NE2 | 13:L:401:SER:CB | 2.41 | 0.82 |
| 4:D:55:A:N3 | 13:L:322:VAL:CG1 | 2.42 | 0.82 |
| 13:L:481:VAL:HG11 | 13:L:658:ASP:OD1 | 1.79 | 0.82 |
| 13:L:238:THR:HG22 | 13:L:241:GLU:H | 1.45 | 0.82 |
| 5:F:2660:A:O2' | 13:L:660:ARG:HD2 | 1.80 | 0.81 |
| 8:I:1063:G:O6 | 8:I:1069:A:O3' | 1.96 | 0.81 |
| 13:L:482:ALA:HA | 13:L:653:PHE:CA | 2.07 | 0.81 |
| 8:I:1067:A:O2' | 13:L:633:GLY:C | 2.07 | 0.81 |
| 13:L:486:THR:CG2 | 13:L:678:GLU:CD | 2.48 | 0.81 |
| 13:L:556:ILE:HG12 | 13:L:601:ILE:HD11 | 1.61 | 0.81 |
| 12:K:18:LYS:HD2 | 12:K:19:VAL:HG23 | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:M:8:4SU:H4' | 10:M:49:5MC:H5' | 1.61 | 0.81 |
| 10:M:66:U:H2' | 10:M:67:C:H6 | 1.43 | 0.81 |
| 10:M:69:C:H2' | 10:M:70:G:H8 | 1.44 | 0.81 |
| 14:N:67:THR:HG21 | 14:N:155:LEU:HG | 1.62 | 0.81 |
| 12:K:58:VAL:CG2 | 12:K:166:ASP:H | 1.87 | 0.81 |
| 13:L:413:ILE:HD13 | 13:L:451:ILE:HD11 | 1.63 | 0.81 |
| 13:L:406:GLU:CB | 13:L:669:PHE:O | 2.28 | 0.80 |
| 13:L:485:GLU:C | 13:L:605:ILE:CG2 | 2.42 | 0.80 |
| 13:L:408:VAL:O | 13:L:655:TYR:N | 2.14 | 0.80 |
| 3:C:1468:A:H2' | 3:C:1469:G:O4' | 1.80 | 0.80 |
| 14:N:44:LEU:HD12 | 14:N:44:LEU:H | 1.46 | 0.80 |
| 11:E:24:VAL:HG13 | 11:E:98:TYR:CE2 | 2.16 | 0.80 |
| 13:L:484:ARG:C | 13:L:648:PRO:O | 2.19 | 0.80 |
| 13:L:484:ARG:CG | 13:L:652:MET:HG3 | 2.03 | 0.80 |
| 2:B:368:U:H5 | 13:L:354:ARG:CG | 1.94 | 0.79 |
| 3:C:1497:G:O2' | 3:C:1498:U:H5' | 1.82 | 0.79 |
| 10:M:1:U:H2' | 10:M:2:C:C6 | 2.16 | 0.79 |
| 13:L:316:ILE:HD12 | 13:L:324:ARG:HH21 | 1.46 | 0.79 |
| 13:L:531:GLY:H | 13:L:533:VAL:HG23 | 1.48 | 0.79 |
| 8:I:1066:U:O2' | 8:I:1067:A:H3' | 1.82 | 0.79 |
| 13:L:165:GLN:HE21 | 13:L:260:LEU:HD13 | 1.46 | 0.79 |
| 2:B:368:U:OP1 | 13:L:351:ARG:NE | 2.16 | 0.79 |
| 8:I:1057:A:N6 | 8:I:1081:U:H3 | 1.80 | 0.78 |
| 3:C:1442:G:H2' | 3:C:1442(A):G:H5" | 1.65 | 0.78 |
| 14:N:36:ARG:HB2 | 14:N:41:ILE:HD11 | 1.64 | 0.78 |
| 4:D:55:A:N3 | 13:L:322:VAL:HG13 | 1.99 | 0.78 |
| 13:L:484:ARG:C | 13:L:647:VAL:C | 2.40 | 0.78 |
| 13:L:165:GLN:NE2 | 13:L:260:LEU:H | 1.82 | 0.78 |
| 14:N:84:GLU:HB3 | 14:N:219:VAL:HG21 | 1.66 | 0.78 |
| 3:C:1490:C:O2' | 3:C:1491:G:H5' | 1.83 | 0.78 |
| 13:L:486:THR:O | 13:L:600:VAL:HG12 | 1.84 | 0.77 |
| 8:I:1067:A:N3 | 13:L:634:MET:CE | 2.47 | 0.77 |
| 11:E:46:LYS:CG | 11:E:47:LYS:H | 1.97 | 0.77 |
| 13:L:127:LYS:CD | 13:L:401:SER:HA | 2.14 | 0.77 |
| 8:I:1089:G:O5' | 8:I:1089:G:H8 | 1.67 | 0.77 |
| 11:E:89:ARG:NH1 | 11:E:89:ARG:HB2 | 2.00 | 0.77 |
| 7:H:2468:G:H22 | 7:H:2481:G:H2' | 1.48 | 0.77 |
| 12:K:64:LEU:HD13 | 12:K:65:PRO:HD2 | 1.64 | 0.77 |
| 14:N:20:GLU:HG3 | 14:N:191:ASP:HB2 | 1.65 | 0.77 |
| 13:L:484:ARG:HH21 | 13:L:671:MET:HE3 | 1.25 | 0.76 |
| 13:L:556:ILE:CG2 | 13:L:601:ILE:HD11 | 2.15 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:408:VAL:HG13 | 13:L:669:PHE:CE1 | 2.17 | 0.76 |
| 6:G:1887:C:C3' | 6:G:1888:G:H5" | 2.16 | 0.76 |
| 5:F:2660:A:N9 | 13:L:660:ARG:HG3 | 2.00 | 0.76 |
| 14:N:201:ILE:HG21 | 14:N:214:ILE:HG21 | 1.67 | 0.76 |
| 11:E:59:ARG:NH2 | 13:L:418:LYS:HE3 | 2.00 | 0.76 |
| 10:M:3:C:O2' | 10:M:4:G:H5' | 1.84 | 0.76 |
| 9:J:2180:U:H2' | 9:J:2181:G:C8 | 2.20 | 0.76 |
| 10:M:24:G:C6 | 10:M:25:U:C4 | 2.73 | 0.76 |
| 13:L:484:ARG:HB2 | 13:L:606:MET:HB2 | 1.67 | 0.76 |
| 14:N:19:HIS:O | 14:N:39:ILE:HG23 | 1.84 | 0.76 |
| 3:C:1422:G:H2' | 3:C:1423:G:H8 | 1.51 | 0.75 |
| 14:N:158:LEU:H | 14:N:158:LEU:HD12 | 1.51 | 0.75 |
| 8:I:1069:A:H4' | 8:I:1070:A:O5' | 1.83 | 0.75 |
| 8:I:1067:A:HO2' | 13:L:634:MET:N | 1.81 | 0.75 |
| 3:C:1458:G:H2' | 3:C:1459:C:H6 | 1.51 | 0.75 |
| 13:L:519:ARG:HG2 | 13:L:677:GLN:NE2 | 2.00 | 0.75 |
| 8:I:1061:U:H3' | 8:I:1061:U:P | 2.26 | 0.75 |
| 8:I:1085:A:C1' | 8:I:1086:A:H4' | 2.07 | 0.75 |
| 3:C:1443:G:N2 | 3:C:1460:A:H1' | 2.02 | 0.75 |
| 5:F:2661:G:H22 | 13:L:20:HIS:CE1 | 2.05 | 0.75 |
| 13:L:556:ILE:CG2 | 13:L:688:ILE:CA | 2.61 | 0.75 |
| 12:K:44:HIS:HD2 | 12:K:175:VAL:HA | 1.49 | 0.75 |
| 7:H:2468:G:N2 | 7:H:2481:G:H2' | 2.00 | 0.75 |
| 9:J:2110:G:H1 | 9:J:2179:C:H42 | 1.32 | 0.75 |
| 8:I:1056:G:O6 | 8:I:1101:U:H3' | 1.86 | 0.74 |
| 13:L:127:LYS:HZ1 | 13:L:402:ILE:HG13 | 1.44 | 0.74 |
| 8:I:1068:G:H4' | 8:I:1096:A:H1' | 1.69 | 0.74 |
| 1:A:349:A:O2' | 1:A:350:G:H5' | 1.87 | 0.74 |
| 13:L:545:GLY:HA2 | 13:L:583:LYS:HE3 | 1.69 | 0.74 |
| 8:I:1061:U:H4' | 8:I:1070:A:O4' | 1.86 | 0.74 |
| 14:N:36:ARG:H | 14:N:41:ILE:HD13 | 1.52 | 0.74 |
| 14:N:204:ASN:HD21 | 14:N:207:ALA:N | 1.85 | 0.74 |
| 10:M:8:4SU:H5" | 10:M:49:5MC:C5' | 2.17 | 0.74 |
| 13:L:408:VAL:HG11 | 13:L:669:PHE:CE1 | 1.90 | 0.74 |
| 14:N:97:TRP:CH2 | 14:N:173:ALA:HA | 2.23 | 0.74 |
| 13:L:321:TYR:O | 13:L:322:VAL:HG13 | 1.88 | 0.74 |
| 14:N:178:ARG:HB2 | 14:N:178:ARG:HH11 | 1.53 | 0.74 |
| 8:I:1086:A:OP1 | 8:I:1104:C:H4' | 1.86 | 0.74 |
| 6:G:1879:C:C3' | 6:G:1880:C:H5" | 2.18 | 0.74 |
| 13:L:406:GLU:HB2 | 13:L:669:PHE:O | 1.87 | 0.73 |
| 9:J:2168:G:C2 | 10:M:56:C:N3 | 2.55 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1067:A:C5 | 13:L:631:ILE:C | 2.61 | 0.73 |
| 6:G:1899:G:N2 | 6:G:1902:C:H41 | 1.86 | 0.73 |
| 13:L:621:ILE:HD11 | 13:L:643:ILE:HD13 | 1.69 | 0.73 |
| 14:N:10:LEU:HD23 | 14:N:10:LEU:H | 1.53 | 0.73 |
| 8:I:1095:A:P | 13:L:618:GLY:H | 2.12 | 0.73 |
| 13:L:13:ARG:HH11 | 13:L:277:VAL:HA | 1.53 | 0.73 |
| 8:I:1084:A:N1 | 8:I:1085:A:N1 | 2.36 | 0.73 |
| 3:C:1494:G:O3' | 13:L:503:GLY:HA2 | 1.87 | 0.73 |
| 6:G:1899:G:H22 | 6:G:1902:C:H41 | 1.35 | 0.73 |
| 13:L:321:TYR:O | 13:L:322:VAL:HG22 | 1.89 | 0.73 |
| 14:N:88:ALA:HB2 | 14:N:219:VAL:HG13 | 1.71 | 0.73 |
| 13:L:484:ARG:HB3 | 13:L:606:MET:HG2 | 1.60 | 0.73 |
| 13:L:166:LEU:HD22 | 13:L:180:VAL:HG11 | 1.70 | 0.73 |
| 13:L:536:LYS:HD2 | 13:L:537:GLU:N | 2.04 | 0.73 |
| 13:L:484:ARG:O | 13:L:648:PRO:O | 2.07 | 0.72 |
| 8:I:1095:A:OP1 | 13:L:617:MET:N | 2.22 | 0.72 |
| 10:M:68:G:O2' | 10:M:69:C:H5' | 1.89 | 0.72 |
| 8:I:1083:U:H6 | 8:I:1083:U:OP2 | 1.72 | 0.72 |
| 14:N:7:VAL:O | 14:N:11:LEU:HG | 1.88 | 0.72 |
| 12:K:45:ALA:CB | 12:K:210:ARG:HA | 2.19 | 0.72 |
| 14:N:69:LEU:HB3 | 14:N:162:ILE:HG22 | 1.70 | 0.72 |
| 13:L:169:GLY:HA3 | 13:L:173:THR:O | 1.90 | 0.72 |
| 14:N:67:THR:C | 14:N:68:ILE:HD12 | 2.09 | 0.72 |
| 14:N:77:ALA:HB2 | 14:N:211:ILE:HD13 | 1.69 | 0.72 |
| 13:L:484:ARG:CA | 13:L:649:LEU:CA | 2.30 | 0.72 |
| 8:I:1073:A:N7 | 8:I:1074:G:C5 | 2.57 | 0.72 |
| 8:I:1086:A:H3' | 8:I:1087:G:H5' | 1.72 | 0.72 |
| 13:L:486:THR:HG21 | 13:L:678:GLU:OE1 | 1.88 | 0.72 |
| 14:N:204:ASN:HD21 | 14:N:207:ALA:H | 1.36 | 0.72 |
| 14:N:178:ARG:HH22 | 14:N:196:LEU:C | 1.93 | 0.71 |
| 8:I:1095:A:H5" | 13:L:618:GLY:N | 2.04 | 0.71 |
| 11:E:115:LYS:O | 11:E:117:ARG:HG3 | 1.90 | 0.71 |
| 14:N:74:LYS:NZ | 14:N:76:GLN:HB2 | 2.06 | 0.71 |
| 8:I:1087:G:N2 | 8:I:1103:A:H2' | 2.04 | 0.71 |
| 11:E:47:LYS:CB | 11:E:48:PRO:HD3 | 2.20 | 0.71 |
| 3:C:1435:G:H2' | 3:C:1436:U:C6 | 2.26 | 0.71 |
| 8:I:1066:U:O2 | 8:I:1068:G:H3' | 1.90 | 0.71 |
| 13:L:482:ALA:CA | 13:L:653:PHE:CA | 2.67 | 0.71 |
| 8:I:1087:G:H2' | 8:I:1103:A:H2 | 1.55 | 0.71 |
| 10:M:24:G:C5 | 10:M:25:U:C5 | 2.79 | 0.71 |
| 13:L:467:LYS:O | 13:L:471:LYS:HA | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:1428:A:H2' | 3:C:1429:C:C6 | 2.26 | 0.70 |
| 12:K:49:ILE:HG22 | 12:K:50:ASP:N | 2.06 | 0.70 |
| 5:F:2660:A:C1' | 13:L:665:GLY:H | 1.96 | 0.70 |
| 10:M:67:C:H2' | 10:M:68:G:H8 | 1.55 | 0.70 |
| 6:G:1887:C:H3' | 6:G:1888:G:H5" | 1.73 | 0.70 |
| 13:L:536:LYS:HD2 | 13:L:537:GLU:H | 1.56 | 0.70 |
| 5:F:2661:G:C6 | 13:L:20:HIS:CE1 | 2.77 | 0.70 |
| 13:L:405:PRO:HB2 | 13:L:454:MET:HG2 | 1.72 | 0.70 |
| 7:H:2461:C:H2' | 7:H:2462:U:C6 | 2.27 | 0.70 |
| 6:G:1899:G:H22 | 6:G:1902:C:N4 | 1.89 | 0.70 |
| 10:M:22:A:H8 | 10:M:22:A:H5' | 1.54 | 0.70 |
| 13:L:424:LEU:HD13 | 13:L:472:VAL:HG11 | 1.74 | 0.70 |
| 8:I:1087:G:H21 | 8:I:1103:A:C3' | 2.04 | 0.70 |
| 3:C:1442(A):G:H3' | 3:C:1442(B):A:H5" | 1.71 | 0.70 |
| 13:L:114:VAL:HG12 | 13:L:152:THR:OG1 | 1.91 | 0.70 |
| 14:N:233:SER:HB2 | 14:N:234:PRO:HD2 | 1.74 | 0.70 |
| 8:I:1080:C:H2' | 8:I:1081:U:O4' | 1.90 | 0.70 |
| 14:N:18:GLY:H | 14:N:42:ILE:CG2 | 2.02 | 0.70 |
| 10:M:22:A:H2' | 10:M:23:U:H5' | 1.74 | 0.70 |
| 5:F:2672:G:H2' | 5:F:2673:G:H5" | 1.73 | 0.70 |
| 8:I:1065:U:C2' | 8:I:1066:U:H5" | 2.21 | 0.70 |
| 8:I:1067:A:C5 | 13:L:631:ILE:O | 2.45 | 0.70 |
| 14:N:30:ARG:HH21 | 14:N:194:PRO:CG | 2.04 | 0.70 |
| 13:L:485:GLU:HB3 | 13:L:605:ILE:HD12 | 1.73 | 0.69 |
| 8:I:1063:G:C6 | 8:I:1075:C:N4 | 2.59 | 0.69 |
| 9:J:2178:C:H4' | 12:K:46:LYS:NZ | 2.07 | 0.69 |
| 2:B:368:U:OP2 | 13:L:351:ARG:HG3 | 1.92 | 0.69 |
| 14:N:218:ALA:O | 14:N:222:ILE:HG13 | 1.93 | 0.69 |
| 10:M:25:U:H2' | 10:M:26:A:C8 | 2.27 | 0.69 |
| 2:B:368:U:P | 13:L:351:ARG:HE | 2.13 | 0.69 |
| 13:L:482:ALA:CA | 13:L:653:PHE:HA | 2.18 | 0.69 |
| 8:I:1058:G:O2' | 8:I:1059:G:C5' | 2.40 | 0.69 |
| 8:I:1086:A:C3' | 8:I:1087:G:H5' | 2.23 | 0.69 |
| 14:N:21:ARG:HB3 | 14:N:39:ILE:HA | 1.75 | 0.69 |
| 13:L:555:LEU:HB3 | 13:L:688:ILE:HD11 | 1.74 | 0.69 |
| 5:F:2660:A:O4' | 13:L:664:GLN:C | 2.30 | 0.69 |
| 2:B:368:U:OP2 | 13:L:351:ARG:CG | 2.41 | 0.69 |
| 11:E:6:THR:OG1 | 11:E:9:GLN:HG3 | 1.93 | 0.69 |
| 11:E:24:VAL:HG12 | 11:E:24:VAL:O | 1.91 | 0.69 |
| 11:E:24:VAL:HG13 | 11:E:98:TYR:HE2 | 1.54 | 0.69 |
| 14:N:121:LEU:HD23 | 14:N:121:LEU:O | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:556:ILE:HG21 | 13:L:687:LEU:CB | 2.22 | 0.69 |
| 11:E:58:VAL:O | 11:E:65:GLU:HA | 1.93 | 0.69 |
| 12:K:82:LYS:NZ | 12:K:151:GLU:HA | 2.08 | 0.69 |
| 8:I:1053:C:O2' | 8:I:1054:A:H5' | 1.92 | 0.68 |
| 10:M:37:A:C3' | 10:M:38:U:P | 2.80 | 0.68 |
| 9:J:2180:U:H2' | 9:J:2181:G:H8 | 1.55 | 0.68 |
| 13:L:556:ILE:HD11 | 13:L:601:ILE:HG23 | 1.73 | 0.68 |
| 8:I:1092:C:H3' | 8:I:1092:C:C6 | 2.28 | 0.68 |
| 13:L:556:ILE:HG21 | 13:L:687:LEU:HB2 | 1.75 | 0.68 |
| 13:L:482:ALA:H | 13:L:655:TYR:N | 1.89 | 0.68 |
| 13:L:481:VAL:HG23 | 13:L:655:TYR:HB2 | 1.74 | 0.68 |
| 8:I:1091:G:N1 | 8:I:1101:U:C4 | 2.62 | 0.68 |
| 8:I:1087:G:N2 | 8:I:1103:A:C2' | 2.55 | 0.68 |
| 11:E:92:ASP:O | 11:E:93:LEU:HD23 | 1.93 | 0.68 |
| 8:I:1102:C:O2' | 8:I:1103:A:O5' | 2.12 | 0.68 |
| 14:N:36:ARG:H | 14:N:41:ILE:CD1 | 2.06 | 0.68 |
| 11:E:41:ARG:CB | 11:E:41:ARG:HH11 | 2.06 | 0.68 |
| 13:L:607:ARG:HH22 | 13:L:644:ARG:HE | 1.40 | 0.68 |
| 9:J:2121:G:H2' | 9:J:2122:U:C6 | 2.28 | 0.68 |
| 9:J:2168:G:N2 | 10:M:19:G:H1 | 1.91 | 0.67 |
| 8:I:1102:C:C1' | 8:I:1103:A:C8 | 2.78 | 0.67 |
| 13:L:92:ILE:CG2 | 13:L:436:PRO:HD2 | 2.16 | 0.67 |
| 11:E:41:ARG:CG | 11:E:42:THR:H | 2.05 | 0.67 |
| 9:J:2127:G:H2' | 9:J:2128:C:C6 | 2.29 | 0.67 |
| 13:L:539:ILE:O | 13:L:542:VAL:HG12 | 1.94 | 0.67 |
| 13:L:484:ARG:CZ | 13:L:671:MET:CE | 2.66 | 0.67 |
| 8:I:1061:U:H5" | 8:I:1070:A:H4' | 1.75 | 0.67 |
| 14:N:163:PHE:HA | 14:N:185:ILE:HG13 | 1.76 | 0.67 |
| 13:L:594:VAL:CG1 | 13:L:599:PRO:HB2 | 2.18 | 0.67 |
| 8:I:1060:U:H5" | 8:I:1061:U:O4 | 1.93 | 0.67 |
| 8:I:1102:C:C2' | 8:I:1103:A:H8 | 2.08 | 0.67 |
| 14:N:102:LEU:CD1 | 14:N:102:LEU:H | 2.07 | 0.67 |
| 13:L:627:ARG:HH21 | 13:L:655:TYR:HD1 | 1.43 | 0.67 |
| 13:L:238:THR:HG23 | 13:L:240:GLU:OE2 | 1.94 | 0.67 |
| 13:L:484:ARG:C | 13:L:647:VAL:HG22 | 2.12 | 0.67 |
| 8:I:1087:G:H2' | 8:I:1089:G:H4' | 1.77 | 0.67 |
| 3:C:1460:A:H2' | 3:C:1461:G:O4' | 1.95 | 0.67 |
| 8:I:1063:G:H2' | 8:I:1064:C:C6 | 2.30 | 0.67 |
| 8:I:1057:A:C8 | 8:I:1085:A:N1 | 2.63 | 0.67 |
| 10:M:37:A:H3' | 10:M:38:U:P | 2.35 | 0.67 |
| 12:K:51:PRO:HG3 | 12:K:204:ALA:HB3 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:18:GLY:N | 14:N:42:ILE:HG22 | 2.08 | 0.67 |
| 9:J:2182:G:H2' | 9:J:2183:C:H6 | 1.60 | 0.67 |
| 8:I:1071:G:C8 | 8:I:1089:G:C6 | 2.82 | 0.66 |
| 13:L:142:THR:HA | 13:L:171:GLU:CG | 2.22 | 0.66 |
| 10:M:52:G:H1 | 10:M:62:C:N4 | 1.93 | 0.66 |
| 13:L:485:GLU:CB | 13:L:605:ILE:CD1 | 2.54 | 0.66 |
| 11:E:46:LYS:HG2 | 11:E:47:LYS:N | 2.03 | 0.66 |
| 12:K:191:ALA:O | 12:K:195:ALA:HB3 | 1.95 | 0.66 |
| 13:L:637:ARG:HG3 | 13:L:637:ARG:HH11 | 1.60 | 0.66 |
| 13:L:556:ILE:CG2 | 13:L:687:LEU:C | 2.63 | 0.66 |
| 13:L:555:LEU:O | 13:L:688:ILE:CB | 2.43 | 0.66 |
| 13:L:91:THR:HG21 | 13:L:403:GLU:O | 1.95 | 0.66 |
| 3:C:1458:G:H2' | 3:C:1459:C:C6 | 2.31 | 0.66 |
| 13:L:519:ARG:NE | 13:L:678:GLU:HG3 | 2.10 | 0.66 |
| 3:C:1441:G:C5' | 3:C:1442:G:H5" | 2.16 | 0.66 |
| 13:L:546:ILE:O | 13:L:550:MET:HG3 | 1.95 | 0.66 |
| 1:A:340:U:O2' | 1:A:341:C:H5' | 1.96 | 0.66 |
| 5:F:2660:A:O2' | 13:L:665:GLY:HA2 | 1.96 | 0.66 |
| 3:C:1442(A):G:C3' | 3:C:1442(B):A:H5" | 2.26 | 0.66 |
| 2:B:368:U:C5 | 13:L:354:ARG:NE | 2.64 | 0.66 |
| 8:I:1068:G:N1 | 8:I:1073:A:C2 | 2.64 | 0.66 |
| 5:F:2660:A:C4' | 13:L:665:GLY:HA3 | 2.26 | 0.66 |
| 8:I:1074:G:O2' | 8:I:1075:C:H5' | 1.96 | 0.66 |
| 8:I:1102:C:H1' | 8:I:1103:A:N7 | 2.11 | 0.66 |
| 13:L:13:ARG:NH1 | 13:L:277:VAL:O | 2.29 | 0.66 |
| 5:F:2660:A:O4' | 13:L:665:GLY:CA | 2.43 | 0.65 |
| 7:H:2455:G:H2' | 7:H:2456:C:C6 | 2.30 | 0.65 |
| 9:J:2177:C:O2' | 12:K:46:LYS:HE3 | 1.96 | 0.65 |
| 12:K:47:LEU:HD21 | 12:K:172:HIS:CB | 2.26 | 0.65 |
| 13:L:484:ARG:CA | 13:L:649:LEU:N | 2.57 | 0.65 |
| 9:J:2178:C:H4' | 12:K:46:LYS:HZ3 | 1.61 | 0.65 |
| 9:J:2181:G:H2' | 9:J:2182:G:H8 | 1.61 | 0.65 |
| 8:I:1062:G:N3 | 8:I:1062:G:H2' | 2.11 | 0.65 |
| 11:E:27:LEU:O | 11:E:29:GLY:N | 2.29 | 0.65 |
| 13:L:423:LYS:HG3 | 13:L:472:VAL:HG22 | 1.76 | 0.65 |
| 10:M:54:5MU:C2' | 10:M:55:PSU:H5" | 2.25 | 0.65 |
| 4:D:55:A:C2 | 13:L:322:VAL:HA | 2.32 | 0.65 |
| 8:I:1071:G:OP2 | 8:I:1071:G:H8 | 1.79 | 0.65 |
| 8:I:1062:G:O6 | 8:I:1077:A:C5 | 2.50 | 0.65 |
| 12:K:41:VAL:HB | 12:K:178:ALA:HB3 | 1.79 | 0.65 |
| 14:N:135:GLN:O | 14:N:139:LYS:HB2 | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:1426:C:O2' | 3:C:1427:U:H5' | 1.95 | 0.65 |
| 13:L:345:THR:O | 13:L:346:LYS:HG3 | 1.97 | 0.65 |
| 9:J:2129:C:H2' | 9:J:2130:U:C4' | 2.21 | 0.65 |
| 14:N:75:LYS:HG2 | 14:N:78:GLN:NE2 | 2.12 | 0.65 |
| 13:L:606:MET:HE3 | 13:L:671:MET:HG2 | 1.78 | 0.65 |
| 11:E:28:LYS:O | 11:E:29:GLY:C | 2.34 | 0.65 |
| 5:F:2653:U:C5' | 5:F:2654:A:H5" | 2.26 | 0.65 |
| 9:J:2175:C:C3' | 9:J:2176:A:H5" | 2.27 | 0.65 |
| 13:L:110:SER:HB3 | 13:L:139:MET:CE | 2.26 | 0.65 |
| 13:L:517:LEU:HD13 | 13:L:564:LYS:HB2 | 1.79 | 0.65 |
| 14:N:23:ARG:HG3 | 14:N:23:ARG:HH11 | 1.62 | 0.65 |
| 13:L:556:ILE:HG23 | 13:L:688:ILE:HG12 | 1.79 | 0.64 |
| 8:I:1071:G:H2' | 8:I:1072:C:C5' | 2.27 | 0.64 |
| 8:I:1085:A:O2' | 8:I:1086:A:C4' | 2.46 | 0.64 |
| 8:I:1095:A:O4' | 13:L:617:MET:HG3 | 1.97 | 0.64 |
| 8:I:1091:G:H1 | 8:I:1100:C:N4 | 1.96 | 0.64 |
| 3:C:1435:G:H2' | 3:C:1436:U:H6 | 1.61 | 0.64 |
| 13:L:9:LEU:HD13 | 13:L:284:LEU:HD13 | 1.80 | 0.64 |
| 12:K:76:ALA:HB3 | 12:K:94:VAL:CG1 | 2.27 | 0.64 |
| 8:I:1063:G:N2 | 8:I:1076:C:C6 | 2.66 | 0.64 |
| 8:I:1054:A:N6 | 8:I:1104:C:N4 | 2.45 | 0.64 |
| 8:I:1107:G:O2' | 8:I:1108:U:H5' | 1.98 | 0.64 |
| 14:N:21:ARG:CB | 14:N:39:ILE:HA | 2.27 | 0.64 |
| 5:F:2672:G:C2' | 5:F:2673:G:H5" | 2.28 | 0.64 |
| 11:E:75:HIS:CD2 | 11:E:77:LEU:H | 2.15 | 0.64 |
| 8:I:1061:U:C4' | 8:I:1070:A:C1' | 2.63 | 0.64 |
| 8:I:1071:G:H2' | 8:I:1072:C:H5' | 1.80 | 0.64 |
| 8:I:1069:A:C2 | 8:I:1096:A:H5' | 2.33 | 0.64 |
| 11:E:6:THR:N | 11:E:9:GLN:HE21 | 1.92 | 0.64 |
| 8:I:1052:C:O2' | 8:I:1053:C:H5' | 1.97 | 0.64 |
| 11:E:102:ARG:HG2 | 11:E:102:ARG:HH11 | 1.61 | 0.64 |
| 13:L:422:GLU:O | 13:L:426:GLN:HG2 | 1.98 | 0.64 |
| 8:I:1067:A:C6 | 8:I:1068:G:O6 | 2.50 | 0.64 |
| 8:I:1087:G:N2 | 8:I:1103:A:H3' | 2.13 | 0.64 |
| 12:K:56:GLN:O | 12:K:57:ASN:HB2 | 1.96 | 0.64 |
| 6:G:1844:C:O2' | 6:G:1845:G:H5' | 1.97 | 0.64 |
| 13:L:519:ARG:CZ | 13:L:678:GLU:HG3 | 2.28 | 0.64 |
| 8:I:1070:A:N6 | 8:I:1096:A:C2 | 2.66 | 0.64 |
| 8:I:1063:G:N7 | 8:I:1070:A:P | 2.71 | 0.64 |
| 14:N:144:ARG:HG3 | 14:N:145:LEU:N | 2.13 | 0.64 |
| 1:A:341:C:O2' | 1:A:342:C:H5' | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1091:G:N2 | 8:I:1101:U:C6 | 2.66 | 0.64 |
| 14:N:165:VAL:HG23 | 14:N:166:ASP:H | 1.61 | 0.64 |
| 13:L:486:THR:CG2 | 13:L:600:VAL:HG11 | 2.21 | 0.63 |
| 8:I:1063:G:H2' | 8:I:1064:C:H6 | 1.62 | 0.63 |
| 14:N:97:TRP:HZ2 | 14:N:102:LEU:HD13 | 1.62 | 0.63 |
| 14:N:114:ARG:HA | 14:N:117:GLU:HG3 | 1.81 | 0.63 |
| 8:I:1092:C:N4 | 8:I:1093:G:C4 | 2.67 | 0.63 |
| 14:N:115:LEU:HD23 | 14:N:153:ARG:CZ | 2.29 | 0.63 |
| 6:G:1842:G:H2' | 6:G:1843:C:C6 | 2.33 | 0.63 |
| 14:N:101:MET:HA | 14:N:108:ILE:HG13 | 1.81 | 0.63 |
| 8:I:1081:U:H2' | 8:I:1082:U:C4 | 2.33 | 0.63 |
| 6:G:1887:C:H2' | 6:G:1888:G:H5" | 1.80 | 0.63 |
| 8:I:1060:U:H5" | 8:I:1061:U:C4 | 2.32 | 0.63 |
| 10:M:1:U:O2' | 10:M:2:C:H5' | 1.98 | 0.63 |
| 8:I:1064:C:C2' | 8:I:1065:U:H6 | 2.12 | 0.63 |
| 13:L:114:VAL:HG12 | 13:L:152:THR:CB | 2.27 | 0.63 |
| 13:L:513:LYS:HG3 | 13:L:568:TYR:CE1 | 2.33 | 0.63 |
| 9:J:2116:G:H5' | 9:J:2117:A:OP2 | 1.98 | 0.63 |
| 13:L:600:VAL:CG2 | 13:L:684:GLN:OE1 | 2.47 | 0.63 |
| 5:F:2662:A:H61 | 13:L:21:ILE:HG13 | 1.46 | 0.63 |
| 8:I:1091:G:N2 | 8:I:1100:C:N3 | 2.45 | 0.63 |
| 13:L:288:PRO:HG2 | 13:L:300:GLU:HG2 | 1.81 | 0.63 |
| 13:L:556:ILE:CG2 | 13:L:601:ILE:CD1 | 2.77 | 0.63 |
| 14:N:44:LEU:HA | 14:N:47:THR:OG1 | 1.99 | 0.63 |
| 3:C:1431:C:H2' | 3:C:1432:G:H5' | 1.81 | 0.63 |
| 13:L:166:LEU:HD22 | 13:L:180:VAL:CG1 | 2.29 | 0.63 |
| 14:N:42:ILE:HD11 | 14:N:202:PRO:HB2 | 1.80 | 0.63 |
| 13:L:484:ARG:HG2 | 13:L:652:MET:CG | 2.23 | 0.62 |
| 8:I:1057:A:N3 | 8:I:1058:G:C8 | 2.67 | 0.62 |
| 8:I:1057:A:N1 | 8:I:1082:U:O4 | 2.32 | 0.62 |
| 13:L:92:ILE:HG23 | 13:L:93:GLU:N | 2.13 | 0.62 |
| 13:L:316:ILE:HD13 | 13:L:326:THR:HB | 1.80 | 0.62 |
| 13:L:484:ARG:HD3 | 13:L:649:LEU:HD13 | 1.79 | 0.62 |
| 13:L:95:GLU:HB3 | 13:L:128:TYR:OH | 1.99 | 0.62 |
| 11:E:91:LYS:O | 11:E:92:ASP:HB2 | 1.97 | 0.62 |
| 6:G:1847:A:H3' | 6:G:1848:A:H5' | 1.81 | 0.62 |
| 12:K:18:LYS:HB3 | 12:K:22:ILE:HD11 | 1.81 | 0.62 |
| 3:C:1401:G:H2' | 3:C:1402:C:O4' | 1.98 | 0.62 |
| 14:N:169:LYS:HD2 | 14:N:170:GLU:OE2 | 1.99 | 0.62 |
| 12:K:85:GLU:HB3 | 12:K:153:ILE:CB | 2.28 | 0.62 |
| 6:G:1899:G:O2' | 6:G:1900:A:H5" | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:K:18:LYS:O | 12:K:20:TYR:N | 2.32 | 0.62 |
| 12:K:45:ALA:HB2 | 12:K:210:ARG:HA | 1.80 | 0.62 |
| 11:E:119:LYS:C | 11:E:120:TYR:HD1 | 2.02 | 0.62 |
| 5:F:2658:C:H2' | 5:F:2658:C:O2 | 1.99 | 0.62 |
| 9:J:2162:G:H5' | 9:J:2171:A:H5" | 1.81 | 0.62 |
| 12:K:74:VAL:HA | 12:K:119:VAL:CB | 2.30 | 0.62 |
| 8:I:1087:G:N2 | 8:I:1103:A:C3' | 2.63 | 0.62 |
| 10:M:73:G:N2 | 10:M:74:C:H1' | 2.14 | 0.62 |
| 10:M:67:C:H2' | 10:M:68:G:C8 | 2.34 | 0.62 |
| 12:K:50:ASP:CG | 12:K:55:ASP:HA | 2.20 | 0.62 |
| 14:N:41:ILE:HD12 | 14:N:41:ILE:N | 2.14 | 0.62 |
| 13:L:408:VAL:O | 13:L:656:ALA:N | 2.32 | 0.62 |
| 13:L:413:ILE:HD13 | 13:L:451:ILE:CD1 | 2.29 | 0.62 |
| 11:E:88:GLY:H | 11:E:98:TYR:HA | 1.65 | 0.62 |
| 13:L:607:ARG:NH2 | 13:L:644:ARG:HE | 1.97 | 0.62 |
| 14:N:167:PRO:HG2 | 14:N:168:THR:H | 1.65 | 0.62 |
| 13:L:408:VAL:O | 13:L:654:GLY:C | 2.38 | 0.62 |
| 9:J:2168:G:N1 | 10:M:19:G:N1 | 2.47 | 0.62 |
| 8:I:1064:C:C2' | 8:I:1065:U:C6 | 2.82 | 0.62 |
| 12:K:21:THR:O | 12:K:22:ILE:HD13 | 2.00 | 0.62 |
| 2:B:392:G:H2' | 2:B:393:A:H8 | 1.65 | 0.62 |
| 13:L:556:ILE:HG22 | 13:L:687:LEU:C | 2.20 | 0.62 |
| 13:L:455:GLY:HA2 | 13:L:657:THR:HG22 | 1.82 | 0.62 |
| 8:I:1061:U:O4' | 8:I:1070:A:H1' | 1.99 | 0.62 |
| 8:I:1066:U:H2' | 8:I:1067:A:H5" | 1.81 | 0.62 |
| 13:L:20:HIS:HD2 | 13:L:117:GLN:H | 1.46 | 0.61 |
| 12:K:76:ALA:HB3 | 12:K:94:VAL:HG13 | 1.82 | 0.61 |
| 13:L:484:ARG:HD3 | 13:L:606:MET:CE | 2.30 | 0.61 |
| 5:F:2660:A:C1' | 13:L:660:ARG:CG | 2.68 | 0.61 |
| 14:N:92:TYR:CE2 | 14:N:151:GLY:HA3 | 2.35 | 0.61 |
| 13:L:462:ILE:O | 13:L:466:LEU:HD13 | 2.00 | 0.61 |
| 13:L:137:ASN:ND2 | 13:L:263:ALA:H | 1.95 | 0.61 |
| 12:K:34:THR:O | 12:K:35:ALA:CB | 2.48 | 0.61 |
| 3:C:1431:C:C2' | 3:C:1432:G:H5' | 2.30 | 0.61 |
| 13:L:19:ALA:HB2 | 13:L:107:VAL:HB | 1.82 | 0.61 |
| 5:F:2672:G:C3' | 5:F:2673:G:H5" | 2.31 | 0.61 |
| 8:I:1078:U:H5" | 8:I:1079:C:OP1 | 2.00 | 0.61 |
| 8:I:1092:C:C3' | 8:I:1092:C:C6 | 2.84 | 0.61 |
| 13:L:105:ILE:HG12 | 13:L:133:ILE:HD11 | 1.82 | 0.61 |
| 13:L:129:LYS:HB3 | 13:L:253:LEU:HD21 | 1.83 | 0.61 |
| 8:I:1069:A:N6 | 8:I:1073:A:C4 | 2.69 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1095:A:OP1 | 13:L:617:MET:CA | 2.48 | 0.61 |
| 8:I:1106:G:C6 | 8:I:1107:G:C6 | 2.89 | 0.61 |
| 12:K:22:ILE:CG2 | 12:K:25:ALA:HB2 | 2.30 | 0.61 |
| 3:C:1412:C:H2' | 3:C:1413:A:C8 | 2.36 | 0.61 |
| 11:E:82:VAL:HB | 11:E:106:ASP:OD1 | 2.01 | 0.61 |
| 13:L:445:GLU:HG3 | 13:L:446:THR:H | 1.66 | 0.61 |
| 8:I:1091:G:C2 | 8:I:1101:U:C2 | 2.89 | 0.61 |
| 14:N:36:ARG:HB2 | 14:N:41:ILE:CD1 | 2.30 | 0.61 |
| 10:M:22:A:C2' | 10:M:23:U:H5' | 2.31 | 0.61 |
| 13:L:481:VAL:CG2 | 13:L:655:TYR:CA | 2.78 | 0.60 |
| 13:L:481:VAL:CG2 | 13:L:655:TYR:HA | 2.26 | 0.60 |
| 11:E:47:LYS:HB3 | 11:E:48:PRO:CD | 2.25 | 0.60 |
| 13:L:181:LEU:HD12 | 13:L:181:LEU:O | 2.01 | 0.60 |
| 13:L:556:ILE:HG23 | 13:L:688:ILE:CG1 | 2.30 | 0.60 |
| 12:K:191:ALA:O | 12:K:193:ILE:N | 2.34 | 0.60 |
| 13:L:127:LYS:HE2 | 13:L:402:ILE:HG13 | 1.76 | 0.60 |
| 8:I:1059:G:OP2 | 8:I:1061:U:O4 | 2.19 | 0.60 |
| 8:I:1095:A:O5' | 13:L:617:MET:CB | 2.36 | 0.60 |
| 10:M:64:C:C4' | 12:K:53:ARG:NH2 | 2.64 | 0.60 |
| 11:E:45:PRO:HD3 | 11:E:51:ALA:O | 2.01 | 0.60 |
| 11:E:89:ARG:HH11 | 11:E:89:ARG:HB2 | 1.65 | 0.60 |
| 3:C:1456:G:H2' | 3:C:1457:G:O4' | 2.00 | 0.60 |
| 2:B:368:U:C5 | 13:L:354:ARG:CG | 2.74 | 0.60 |
| 10:M:8:4SU:O2' | 10:M:46:A:C1' | 2.48 | 0.60 |
| 12:K:47:LEU:HD23 | 12:K:47:LEU:N | 2.15 | 0.60 |
| 12:K:49:ILE:CD1 | 12:K:49:ILE:H | 2.12 | 0.60 |
| 3:C:1442(A):G:H3' | 3:C:1442(B):A:C5' | 2.30 | 0.60 |
| 13:L:621:ILE:CD1 | 13:L:643:ILE:HD13 | 2.31 | 0.60 |
| 8:I:1077:A:H2' | 8:I:1078:U:O4' | 2.02 | 0.60 |
| 8:I:1056:G:C2 | 8:I:1102:C:N4 | 2.70 | 0.60 |
| 14:N:219:VAL:HA | 14:N:222:ILE:HD12 | 1.83 | 0.60 |
| 9:J:2186:G:H2' | 9:J:2187:G:H5" | 1.84 | 0.60 |
| 8:I:1067:A:N3 | 13:L:634:MET:HE1 | 2.15 | 0.60 |
| 13:L:213:HIS:O | 13:L:217:VAL:HG23 | 2.02 | 0.60 |
| 9:J:2182:G:H2' | 9:J:2183:C:C6 | 2.35 | 0.60 |
| 12:K:77:ILE:HG21 | 12:K:122:ALA:C | 2.22 | 0.60 |
| 13:L:682:GLN:HG3 | 13:L:686:LYS:HE3 | 1.84 | 0.60 |
| 12:K:89:ALA:HB2 | 12:K:153:ILE:HA | 1.83 | 0.59 |
| 13:L:486:THR:HG21 | 13:L:678:GLU:CG | 2.32 | 0.59 |
| 14:N:115:LEU:HD13 | 14:N:145:LEU:HD12 | 1.83 | 0.59 |
| 14:N:187:LEU:HA | 14:N:201:ILE:HB | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:F:2653:U:H5' | 5:F:2654:A:H5" | 1.81 | 0.59 |
| 13:L:427:ALA:HB1 | 13:L:470:PHE:CD2 | 2.37 | 0.59 |
| 13:L:600:VAL:HG22 | 13:L:684:GLN:OE1 | 2.03 | 0.59 |
| 8:I:1102:C:HO2' | 8:I:1103:A:H8 | 1.50 | 0.59 |
| 10:M:73:G:N2 | 10:M:74:C:C1' | 2.64 | 0.59 |
| 11:E:23:LYS:O | 11:E:24:VAL:HG23 | 2.02 | 0.59 |
| 14:N:103:THR:HA | 14:N:180:LEU:HD11 | 1.84 | 0.59 |
| 14:N:141:GLU:O | 14:N:145:LEU:HB2 | 2.02 | 0.59 |
| 10:M:73:G:C2' | 10:M:74:C:C5' | 2.79 | 0.59 |
| 14:N:197:VAL:CG1 | 14:N:200:ILE:HG12 | 2.33 | 0.59 |
| 4:D:55:A:H1' | 13:L:321:TYR:C | 2.19 | 0.59 |
| 2:B:368:U:O2 | 4:D:356:A:H2 | 1.86 | 0.59 |
| 9:J:2168:G:H22 | 10:M:56:C:N4 | 2.00 | 0.59 |
| 8:I:1087:G:H2' | 8:I:1103:A:C2 | 2.36 | 0.59 |
| 12:K:191:ALA:C | 12:K:193:ILE:H | 2.06 | 0.59 |
| 13:L:294:PRO:HD3 | 13:L:396:ARG:O | 2.02 | 0.59 |
| 13:L:486:THR:O | 13:L:600:VAL:CG1 | 2.51 | 0.59 |
| 13:L:20:HIS:CD2 | 13:L:117:GLN:HB2 | 2.38 | 0.59 |
| 8:I:1065:U:H3' | 8:I:1066:U:C5' | 2.28 | 0.59 |
| 5:F:2657:A:H1' | 5:F:2665:A:N6 | 2.18 | 0.59 |
| 14:N:194:PRO:HG2 | 14:N:195:ASP:H | 1.68 | 0.59 |
| 3:C:1437:C:O2' | 3:C:1438:G:H5' | 2.03 | 0.59 |
| 4:D:55:A:N3 | 13:L:322:VAL:N | 2.50 | 0.59 |
| 13:L:481:VAL:HG11 | 13:L:658:ASP:CG | 2.22 | 0.59 |
| 5:F:2660:A:O2' | 13:L:660:ARG:CD | 2.45 | 0.59 |
| 12:K:46:LYS:CE | 12:K:46:LYS:HA | 2.27 | 0.59 |
| 11:E:60:LEU:HD22 | 11:E:60:LEU:N | 2.18 | 0.59 |
| 14:N:171:ALA:O | 14:N:174:VAL:HB | 2.03 | 0.59 |
| 8:I:1063:G:N2 | 8:I:1075:C:C2 | 2.71 | 0.59 |
| 11:E:45:PRO:HB3 | 11:E:49:ASN:HB2 | 1.84 | 0.59 |
| 6:G:1887:C:C2' | 6:G:1888:G:H5" | 2.33 | 0.59 |
| 12:K:77:ILE:O | 12:K:77:ILE:HD13 | 2.02 | 0.59 |
| 9:J:2175:C:H2' | 9:J:2176:A:C5' | 2.19 | 0.58 |
| 6:G:1840:G:H1 | 6:G:1902:C:N4 | 1.97 | 0.58 |
| 12:K:77:ILE:HD12 | 12:K:123:VAL:N | 2.18 | 0.58 |
| 14:N:59:GLU:HB2 | 14:N:221:LEU:HD11 | 1.85 | 0.58 |
| 6:G:1884:A:C3' | 6:G:1885:A:H5" | 2.34 | 0.58 |
| 10:M:55:PSU:H2' | 10:M:57:A:OP2 | 2.03 | 0.58 |
| 11:E:53:ARG:HH11 | 11:E:53:ARG:HG2 | 1.67 | 0.58 |
| 3:C:1484:C:H2' | 3:C:1485:U:H6 | 1.69 | 0.58 |
| 8:I:1054:A:C2' | 8:I:1055:G:C8 | 2.83 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1063:G:N2 | 8:I:1076:C:N1 | 2.51 | 0.58 |
| 7:H:2463:C:O2' | 7:H:2464:C:H5' | 2.02 | 0.58 |
| 13:L:405:PRO:HG3 | 13:L:437:THR:HB | 1.83 | 0.58 |
| 14:N:167:PRO:O | 14:N:171:ALA:N | 2.37 | 0.58 |
| 3:C:1410:G:H2' | 3:C:1411:C:C6 | 2.39 | 0.58 |
| 13:L:35:TYR:OH | 13:L:193:GLY:HA3 | 2.03 | 0.58 |
| 9:J:2098:U:H2' | 9:J:2099:U:C6 | 2.39 | 0.58 |
| 8:I:1083:U:OP2 | 8:I:1083:U:C6 | 2.53 | 0.58 |
| 14:N:236:TYR:HA | 14:N:239:VAL:HG23 | 1.86 | 0.58 |
| 13:L:556:ILE:HG21 | 13:L:687:LEU:C | 2.24 | 0.58 |
| 13:L:484:ARG:HD3 | 13:L:649:LEU:CD1 | 2.31 | 0.58 |
| 12:K:49:ILE:CG2 | 12:K:50:ASP:H | 2.16 | 0.58 |
| 10:M:75:C:H2' | 10:M:76:A:H5' | 0.70 | 0.58 |
| 10:M:8:4SU:HO2' | 10:M:46:A:H1' | 1.69 | 0.58 |
| 14:N:22:LYS:HZ3 | 14:N:22:LYS:CA | 1.96 | 0.58 |
| 14:N:32:ILE:HA | 14:N:42:ILE:HA | 1.85 | 0.58 |
| 14:N:43:ASP:OD2 | 14:N:46:LYS:HB2 | 2.03 | 0.58 |
| 11:E:84:LEU:HD23 | 11:E:85:ILE:N | 2.19 | 0.58 |
| 8:I:1095:A:C5' | 13:L:618:GLY:N | 2.67 | 0.58 |
| 13:L:619:ASP:OD2 | 13:L:619:ASP:N | 2.36 | 0.58 |
| 8:I:1054:A:H2' | 8:I:1055:G:N7 | 2.18 | 0.58 |
| 8:I:1065:U:H2' | 8:I:1066:U:H5" | 1.85 | 0.58 |
| 8:I:1066:U:C2 | 8:I:1069:A:OP2 | 2.57 | 0.58 |
| 8:I:1068:G:N1 | 8:I:1073:A:H2 | 2.01 | 0.58 |
| 10:M:73:G:H2' | 10:M:74:C:H5' | 1.82 | 0.58 |
| 11:E:32:PHE:HB3 | 11:E:84:LEU:CD2 | 2.28 | 0.58 |
| 10:M:25:U:O4 | 10:M:26:A:N6 | 2.36 | 0.58 |
| 13:L:542:VAL:O | 13:L:546:ILE:HG13 | 2.04 | 0.58 |
| 11:E:120:TYR:N | 11:E:120:TYR:HD1 | 2.02 | 0.58 |
| 10:M:19:G:C4' | 10:M:20:H2U:OP1 | 2.42 | 0.58 |
| 8:I:1071:G:OP2 | 8:I:1071:G:C8 | 2.57 | 0.58 |
| 6:G:1899:G:N2 | 6:G:1902:C:N4 | 2.49 | 0.58 |
| 13:L:238:THR:HG22 | 13:L:241:GLU:N | 2.17 | 0.58 |
| 3:C:1404:C:H2' | 3:C:1405:G:C8 | 2.39 | 0.58 |
| 13:L:409:ILE:HG13 | 13:L:455:GLY:HA2 | 1.85 | 0.57 |
| 4:D:358:U:OP1 | 13:L:381:LYS:HE3 | 2.04 | 0.57 |
| 12:K:40:THR:HG21 | 12:K:215:THR:CB | 2.34 | 0.57 |
| 9:J:2103:C:H3' | 9:J:2104:G:C5' | 2.25 | 0.57 |
| 9:J:2103:C:C3' | 9:J:2104:G:H5" | 2.25 | 0.57 |
| 9:J:2181:G:H2' | 9:J:2182:G:C8 | 2.38 | 0.57 |
| 9:J:2098:U:H2' | 9:J:2099:U:H6 | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:47:THR:HG23 | 14:N:202:PRO:HG2 | 1.85 | 0.57 |
| 11:E:18:VAL:HG23 | 11:E:19:ARG:N | 2.15 | 0.57 |
| 10:M:25:U:H2' | 10:M:26:A:H8 | 1.70 | 0.57 |
| 7:H:2491:U:O2' | 7:H:2492:U:H5' | 2.04 | 0.57 |
| 14:N:165:VAL:HG23 | 14:N:166:ASP:N | 2.19 | 0.57 |
| 11:E:102:ARG:CG | 11:E:102:ARG:HH11 | 2.16 | 0.57 |
| 12:K:97:GLU:HA | 12:K:100:ILE:HG12 | 1.85 | 0.57 |
| 5:F:2662:A:H2' | 13:L:457:LEU:HD13 | 1.87 | 0.57 |
| 8:I:1097:U:H2' | 8:I:1098:A:O5' | 2.04 | 0.57 |
| 14:N:91:PRO:HG3 | 14:N:154:LEU:HD12 | 1.85 | 0.57 |
| 10:M:10:A:C6 | 10:M:26:A:C2 | 2.93 | 0.57 |
| 14:N:113:HIS:O | 14:N:117:GLU:HG2 | 2.05 | 0.57 |
| 14:N:185:ILE:HG22 | 14:N:199:TYR:CB | 2.26 | 0.57 |
| 11:E:89:ARG:NE | 11:E:91:LYS:HE2 | 2.19 | 0.57 |
| 11:E:32:PHE:CB | 11:E:84:LEU:HD21 | 2.29 | 0.57 |
| 3:C:1497:G:C2' | 3:C:1498:U:H5' | 2.33 | 0.57 |
| 13:L:445:GLU:HG3 | 13:L:446:THR:N | 2.18 | 0.57 |
| 13:L:408:VAL:CG1 | 13:L:669:PHE:CZ | 2.58 | 0.57 |
| 12:K:49:ILE:HD12 | 12:K:49:ILE:N | 2.13 | 0.57 |
| 13:L:17:ILE:N | 13:L:17:ILE:HD12 | 2.19 | 0.57 |
| 12:K:39:GLU:HG2 | 12:K:180:PHE:CB | 2.35 | 0.57 |
| 8:I:1073:A:N7 | 8:I:1074:G:C6 | 2.72 | 0.57 |
| 8:I:1058:G:N1 | 8:I:1081:U:C2 | 2.72 | 0.57 |
| 8:I:1102:C:O2' | 8:I:1103:A:H8 | 1.88 | 0.57 |
| 9:J:2186:G:C2' | 9:J:2187:G:H5" | 2.35 | 0.57 |
| 8:I:1082:U:H3' | 8:I:1083:U:C6 | 2.39 | 0.57 |
| 12:K:50:ASP:OD1 | 12:K:55:ASP:HA | 2.05 | 0.57 |
| 13:L:114:VAL:HG12 | 13:L:152:THR:HB | 1.87 | 0.57 |
| 12:K:89:ALA:HB2 | 12:K:153:ILE:CB | 2.34 | 0.57 |
| 2:B:390:C:H2' | 2:B:391:G:C8 | 2.40 | 0.57 |
| 13:L:506:GLN:NE2 | 13:L:578:SER:OG | 2.38 | 0.57 |
| 14:N:100:GLY:O | 14:N:104:ASN:N | 2.38 | 0.57 |
| 8:I:1082:U:H6 | 8:I:1082:U:O5' | 1.88 | 0.57 |
| 14:N:134:GLU:HA | 14:N:137:ARG:HB2 | 1.86 | 0.57 |
| 11:E:18:VAL:O | 11:E:19:ARG:HB3 | 2.03 | 0.57 |
| 8:I:1078:U:C2 | 8:I:1088:A:H1' | 2.40 | 0.57 |
| 11:E:119:LYS:C | 11:E:120:TYR:CD1 | 2.78 | 0.57 |
| 13:L:600:VAL:HA | 13:L:684:GLN:NE2 | 2.20 | 0.57 |
| 8:I:1066:U:C2' | 8:I:1067:A:H5" | 2.35 | 0.57 |
| 8:I:1086:A:H3' | 8:I:1087:G:C5' | 2.35 | 0.57 |
| 8:I:1102:C:H2' | 8:I:1102:C:O2 | 2.03 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:158:LEU:HD12 | 14:N:158:LEU:N | 2.20 | 0.56 |
| 14:N:193:ASP:OD2 | 14:N:196:LEU:HD11 | 2.04 | 0.56 |
| 13:L:684:GLN:O | 13:L:688:ILE:HG13 | 2.04 | 0.56 |
| 13:L:554:PRO:HG3 | 13:L:599:PRO:HG3 | 1.86 | 0.56 |
| 8:I:1052:C:C2 | 8:I:1053:C:C5 | 2.92 | 0.56 |
| 14:N:70:PHE:CE2 | 14:N:163:PHE:HD1 | 2.23 | 0.56 |
| 6:G:1847:A:H3' | 6:G:1848:A:C5' | 2.34 | 0.56 |
| 14:N:236:TYR:HA | 14:N:239:VAL:CG2 | 2.36 | 0.56 |
| 13:L:486:THR:O | 13:L:600:VAL:CB | 2.52 | 0.56 |
| 8:I:1065:U:N3 | 8:I:1066:U:C6 | 2.73 | 0.56 |
| 8:I:1056:G:N2 | 8:I:1104:C:N4 | 2.53 | 0.56 |
| 10:M:62:C:H2' | 10:M:62:C:O2 | 2.05 | 0.56 |
| 14:N:75:LYS:HA | 14:N:78:GLN:HG3 | 1.87 | 0.56 |
| 11:E:70:ILE:N | 11:E:70:ILE:HD12 | 2.20 | 0.56 |
| 11:E:39:VAL:HG12 | 11:E:40:VAL:N | 2.20 | 0.56 |
| 8:I:1087:G:C2 | 8:I:1103:A:C4 | 2.93 | 0.56 |
| 14:N:32:ILE:HD13 | 14:N:40:HIS:HB3 | 1.88 | 0.56 |
| 9:J:2189:U:C2' | 9:J:2190:G:H5" | 2.36 | 0.56 |
| 13:L:391:GLY:O | 13:L:392:GLU:HB3 | 2.05 | 0.56 |
| 14:N:112:VAL:HG22 | 14:N:149:LEU:HD13 | 1.88 | 0.56 |
| 12:K:41:VAL:HB | 12:K:178:ALA:CB | 2.36 | 0.56 |
| 5:F:2660:A:H4' | 13:L:665:GLY:HA3 | 1.88 | 0.56 |
| 5:F:2662:A:N1 | 13:L:21:ILE:HD13 | 2.17 | 0.56 |
| 8:I:1068:G:C6 | 8:I:1073:A:C2 | 2.93 | 0.56 |
| 13:L:404:VAL:HG13 | 13:L:405:PRO:HD2 | 1.86 | 0.56 |
| 14:N:144:ARG:HA | 14:N:147:LYS:HB3 | 1.86 | 0.56 |
| 10:M:22:A:H2' | 10:M:23:U:C5' | 2.36 | 0.56 |
| 8:I:1057:A:C2 | 8:I:1058:G:C8 | 2.93 | 0.56 |
| 14:N:69:LEU:HD13 | 14:N:91:PRO:HB2 | 1.87 | 0.56 |
| 11:E:60:LEU:N | 11:E:64:TYR:O | 2.34 | 0.56 |
| 12:K:75:LEU:HD23 | 12:K:76:ALA:N | 2.21 | 0.56 |
| 11:E:120:TYR:CD1 | 11:E:120:TYR:N | 2.73 | 0.56 |
| 2:B:390:C:H2' | 2:B:391:G:H8 | 1.70 | 0.56 |
| 14:N:14:GLY:O | 14:N:15:VAL:HG13 | 2.04 | 0.56 |
| 13:L:647:VAL:HG21 | 13:L:652:MET:SD | 2.46 | 0.56 |
| 14:N:87:ARG:O | 14:N:87:ARG:HD2 | 2.06 | 0.56 |
| 14:N:23:ARG:HG2 | 14:N:23:ARG:O | 2.06 | 0.56 |
| 13:L:329:ARG:HH21 | 13:L:372:GLY:HA2 | 1.71 | 0.56 |
| 11:E:21:LYS:N | 11:E:21:LYS:HD2 | 2.21 | 0.56 |
| 14:N:142:LEU:HD23 | 14:N:142:LEU:C | 2.26 | 0.56 |
| 8:I:1092:C:N4 | 8:I:1093:G:N3 | 2.53 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:M:14:A:N6 | 10:M:46:A:C2 | 2.74 | 0.55 |
| 3:C:1422:G:H2' | 3:C:1423:G:C8 | 2.38 | 0.55 |
| 3:C:1410:G:H2' | 3:C:1411:C:H6 | 1.70 | 0.55 |
| 14:N:24:TRP:HD1 | 14:N:24:TRP:H | 1.54 | 0.55 |
| 13:L:188:TYR:CE1 | 13:L:196:ILE:HG12 | 2.41 | 0.55 |
| 8:I:1082:U:H3' | 8:I:1082:U:C6 | 2.41 | 0.55 |
| 8:I:1087:G:C5 | 8:I:1103:A:C6 | 2.95 | 0.55 |
| 13:L:316:ILE:CD1 | 13:L:326:THR:HB | 2.37 | 0.55 |
| 13:L:409:ILE:HD13 | 13:L:654:GLY:C | 2.27 | 0.55 |
| 8:I:1074:G:C5 | 8:I:1075:C:H5 | 2.25 | 0.55 |
| 8:I:1058:G:C6 | 8:I:1081:U:C2 | 2.94 | 0.55 |
| 10:M:50:G:O6 | 10:M:65:G:C6 | 2.59 | 0.55 |
| 10:M:70:G:H2' | 10:M:71:G:H8 | 1.70 | 0.55 |
| 11:E:27:LEU:HD22 | 11:E:27:LEU:N | 2.22 | 0.55 |
| 9:J:2102:U:C5 | 9:J:2187:G:O6 | 2.59 | 0.55 |
| 4:D:55:A:C2 | 13:L:322:VAL:CA | 2.88 | 0.55 |
| 8:I:1085:A:O2' | 8:I:1086:A:C5' | 2.54 | 0.55 |
| 9:J:2175:C:H1' | 12:K:215:THR:CA | 2.33 | 0.55 |
| 3:C:1441:G:H5" | 3:C:1442:G:C5' | 2.17 | 0.55 |
| 14:N:114:ARG:O | 14:N:117:GLU:HB2 | 2.07 | 0.55 |
| 11:E:119:LYS:O | 11:E:120:TYR:HB2 | 2.07 | 0.55 |
| 14:N:142:LEU:HD23 | 14:N:142:LEU:O | 2.07 | 0.55 |
| 13:L:190:ASN:HD22 | 13:L:190:ASN:C | 2.09 | 0.55 |
| 11:E:82:VAL:O | 11:E:106:ASP:HB2 | 2.07 | 0.55 |
| 10:M:69:C:C2 | 10:M:70:G:N7 | 2.74 | 0.55 |
| 8:I:1077:A:N7 | 8:I:1078:U:N3 | 2.55 | 0.55 |
| 9:J:2184:G:H2' | 9:J:2185:C:C6 | 2.42 | 0.55 |
| 13:L:486:THR:CA | 13:L:600:VAL:HG12 | 2.36 | 0.55 |
| 13:L:594:VAL:HG12 | 13:L:599:PRO:CG | 2.37 | 0.55 |
| 8:I:1068:G:C2 | 8:I:1069:A:N6 | 2.72 | 0.55 |
| 8:I:1070:A:N6 | 8:I:1096:A:H2 | 2.04 | 0.55 |
| 8:I:1107:G:C2' | 8:I:1108:U:H5' | 2.37 | 0.55 |
| 11:E:90:VAL:HG12 | 11:E:90:VAL:O | 2.07 | 0.55 |
| 11:E:41:ARG:HG2 | 11:E:42:THR:H | 1.72 | 0.55 |
| 4:D:55:A:C2 | 13:L:322:VAL:CB | 2.87 | 0.55 |
| 8:I:1054:A:H61 | 8:I:1105:U:H3 | 0.68 | 0.55 |
| 8:I:1084:A:C2 | 8:I:1085:A:C2 | 2.94 | 0.55 |
| 12:K:46:LYS:HB2 | 12:K:209:LEU:CB | 2.37 | 0.55 |
| 12:K:89:ALA:HB2 | 12:K:153:ILE:CA | 2.36 | 0.55 |
| 13:L:602:LEU:HD23 | 13:L:678:GLU:HA | 1.88 | 0.54 |
| 8:I:1064:C:H3' | 8:I:1065:U:C5 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:1442:G:C2' | 3:C:1442(A):G:H5" | 2.36 | 0.54 |
| 14:N:19:HIS:CE1 | 14:N:206:ASP:HB2 | 2.42 | 0.54 |
| 8:I:1070:A:C8 | 8:I:1097:U:O5' | 2.59 | 0.54 |
| 13:L:124:GLN:HE22 | 13:L:401:SER:HB3 | 1.61 | 0.54 |
| 11:E:126:LYS:HE2 | 11:E:128:ALA:H | 1.72 | 0.54 |
| 13:L:449:THR:O | 13:L:450:ILE:HD13 | 2.07 | 0.54 |
| 13:L:519:ARG:HD2 | 13:L:677:GLN:HA | 1.89 | 0.54 |
| 8:I:1072:C:H2' | 8:I:1093:G:O6 | 2.08 | 0.54 |
| 13:L:415:PRO:CG | 13:L:421:GLN:HG2 | 2.35 | 0.54 |
| 14:N:194:PRO:O | 14:N:196:LEU:N | 2.39 | 0.54 |
| 12:K:212:VAL:O | 12:K:213:TYR:CB | 2.55 | 0.54 |
| 13:L:648:PRO:HG2 | 13:L:651:GLU:CG | 2.37 | 0.54 |
| 8:I:1070:A:H8 | 8:I:1097:U:O5' | 1.90 | 0.54 |
| 12:K:39:GLU:HA | 12:K:180:PHE:HA | 1.89 | 0.54 |
| 9:J:2111:C:H1' | 9:J:2118:U:H1' | 1.89 | 0.54 |
| 13:L:363:ARG:HH11 | 13:L:363:ARG:HG3 | 1.71 | 0.54 |
| 5:F:2662:A:O2' | 13:L:457:LEU:CD1 | 2.56 | 0.54 |
| 14:N:188:ALA:O | 14:N:202:PRO:HA | 2.07 | 0.54 |
| 13:L:137:ASN:ND2 | 13:L:138:LYS:H | 2.06 | 0.54 |
| 10:M:53:G:N3 | 10:M:53:G:H2' | 2.23 | 0.54 |
| 8:I:1077:A:C8 | 8:I:1078:U:C4 | 2.96 | 0.54 |
| 13:L:481:VAL:HG23 | 13:L:655:TYR:CA | 2.37 | 0.54 |
| 8:I:1061:U:H5' | 8:I:1070:A:H4' | 1.86 | 0.54 |
| 7:H:2469:A:H2 | 7:H:2481:G:H21 | 1.55 | 0.54 |
| 14:N:158:LEU:H | 14:N:158:LEU:CD1 | 2.20 | 0.54 |
| 14:N:97:TRP:HH2 | 14:N:176:GLU:CD | 2.11 | 0.54 |
| 13:L:406:GLU:HG3 | 13:L:670:VAL:N | 2.22 | 0.54 |
| 9:J:2168:G:C2 | 10:M:56:C:C2 | 2.94 | 0.54 |
| 14:N:102:LEU:N | 14:N:102:LEU:HD12 | 2.23 | 0.54 |
| 13:L:110:SER:HB3 | 13:L:139:MET:HE3 | 1.88 | 0.54 |
| 9:J:2101:G:C6 | 9:J:2102:U:C5 | 2.96 | 0.54 |
| 11:E:34:ARG:HG2 | 11:E:35:GLY:N | 2.23 | 0.54 |
| 9:J:2189:U:H2' | 9:J:2190:G:H5" | 1.90 | 0.54 |
| 4:D:55:A:C4' | 13:L:321:TYR:HB3 | 2.27 | 0.54 |
| 13:L:481:VAL:HG23 | 13:L:655:TYR:CB | 2.37 | 0.54 |
| 13:L:483:TYR:C | 13:L:649:LEU:O | 2.45 | 0.54 |
| 8:I:1052:C:C2 | 8:I:1053:C:H5 | 2.26 | 0.54 |
| 8:I:1063:G:N2 | 8:I:1076:C:C2 | 2.76 | 0.54 |
| 13:L:625:ASN:HD21 | 13:L:631:ILE:HD13 | 1.73 | 0.54 |
| 11:E:50:SER:O | 11:E:51:ALA:HB2 | 2.08 | 0.54 |
| 13:L:238:THR:HB | 13:L:241:GLU:OE1 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:115:GLU:HB3 | 13:L:116:PRO:HD2 | 1.90 | 0.54 |
| 8:I:1053:C:C2' | 8:I:1054:A:H5' | 2.37 | 0.53 |
| 8:I:1080:C:O2' | 8:I:1081:U:H5' | 2.08 | 0.53 |
| 14:N:163:PHE:HA | 14:N:185:ILE:O | 2.07 | 0.53 |
| 14:N:70:PHE:O | 14:N:92:TYR:HA | 2.08 | 0.53 |
| 7:H:2485:G:O2' | 7:H:2486:G:H5' | 2.08 | 0.53 |
| 13:L:555:LEU:HB3 | 13:L:688:ILE:CD1 | 2.39 | 0.53 |
| 4:D:358:U:H2' | 4:D:359:U:C6 | 2.43 | 0.53 |
| 8:I:1061:U:H2' | 8:I:1061:U:O2 | 2.08 | 0.53 |
| 7:H:2461:C:H2' | 7:H:2462:U:H6 | 1.69 | 0.53 |
| 11:E:89:ARG:HE | 11:E:91:LYS:HE2 | 1.74 | 0.53 |
| 12:K:18:LYS:HD3 | 12:K:19:VAL:H | 1.74 | 0.53 |
| 12:K:82:LYS:HZ2 | 12:K:151:GLU:HA | 1.71 | 0.53 |
| 13:L:101:LEU:HD12 | 13:L:101:LEU:C | 2.28 | 0.53 |
| 13:L:519:ARG:CG | 13:L:677:GLN:NE2 | 2.69 | 0.53 |
| 8:I:1099:G:H2' | 8:I:1100:C:H6 | 1.74 | 0.53 |
| 13:L:127:LYS:HZ3 | 13:L:402:ILE:HG12 | 1.69 | 0.53 |
| 13:L:417:THR:C | 13:L:419:ALA:H | 2.10 | 0.53 |
| 13:L:417:THR:O | 13:L:419:ALA:N | 2.39 | 0.53 |
| 14:N:102:LEU:N | 14:N:102:LEU:CD1 | 2.69 | 0.53 |
| 5:F:2660:A:C1' | 13:L:665:GLY:HA2 | 2.19 | 0.53 |
| 13:L:165:GLN:NE2 | 13:L:260:LEU:HD13 | 2.21 | 0.53 |
| 3:C:1431:C:H2' | 3:C:1432:G:C5' | 2.38 | 0.53 |
| 14:N:74:LYS:HZ1 | 14:N:76:GLN:HB2 | 1.74 | 0.53 |
| 14:N:121:LEU:O | 14:N:127:ILE:HD11 | 2.08 | 0.53 |
| 13:L:408:VAL:HG12 | 13:L:669:PHE:HZ | 1.63 | 0.53 |
| 10:M:75:C:C2 | 10:M:76:A:H4' | 2.44 | 0.53 |
| 14:N:213:LEU:HD23 | 14:N:213:LEU:C | 2.29 | 0.53 |
| 11:E:71:PRO:HD2 | 11:E:102:ARG:NH1 | 2.23 | 0.53 |
| 13:L:486:THR:N | 13:L:600:VAL:HG12 | 2.24 | 0.53 |
| 2:B:368:U:OP2 | 13:L:351:ARG:HG2 | 2.09 | 0.53 |
| 14:N:54:THR:HG23 | 14:N:199:TYR:HB3 | 1.91 | 0.53 |
| 11:E:41:ARG:CB | 11:E:41:ARG:NH1 | 2.72 | 0.53 |
| 14:N:194:PRO:O | 14:N:195:ASP:C | 2.47 | 0.53 |
| 13:L:484:ARG:O | 13:L:648:PRO:CA | 2.54 | 0.53 |
| 8:I:1059:G:N7 | 8:I:1060:U:O4' | 2.42 | 0.53 |
| 9:J:2178:C:O5' | 12:K:46:LYS:HD2 | 2.09 | 0.53 |
| 5:F:2668:G:O2' | 5:F:2669:G:H5' | 2.09 | 0.53 |
| 11:E:34:ARG:HG2 | 11:E:35:GLY:H | 1.72 | 0.53 |
| 6:G:1876:A:H2' | 6:G:1877:A:C8 | 2.44 | 0.53 |
| 5:F:2649:U:H2' | 5:F:2650:U:C6 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:130:ARG:HA | 14:N:130:ARG:HE | 1.74 | 0.53 |
| 13:L:32:ILE:HG23 | 13:L:273:LEU:HD11 | 1.89 | 0.53 |
| 8:I:1057:A:C2 | 8:I:1058:G:C5 | 2.98 | 0.52 |
| 14:N:68:ILE:N | 14:N:68:ILE:HD12 | 2.24 | 0.52 |
| 14:N:216:SER:O | 14:N:218:ALA:N | 2.43 | 0.52 |
| 3:C:1458:G:O2' | 3:C:1459:C:H5' | 2.08 | 0.52 |
| 3:C:1405:G:O2' | 3:C:1406:U:H5' | 2.08 | 0.52 |
| 13:L:182:ARG:HB2 | 13:L:184:LYS:HD2 | 1.91 | 0.52 |
| 13:L:425:SER:HA | 13:L:428:LEU:HD12 | 1.90 | 0.52 |
| 4:D:55:A:N3 | 13:L:321:TYR:C | 2.62 | 0.52 |
| 12:K:22:ILE:HG22 | 12:K:25:ALA:HB2 | 1.90 | 0.52 |
| 5:F:2673:G:O2' | 5:F:2674:G:H5' | 2.08 | 0.52 |
| 13:L:308:PRO:HB2 | 13:L:394:ALA:HB1 | 1.91 | 0.52 |
| 5:F:2660:A:O2' | 13:L:660:ARG:CG | 2.57 | 0.52 |
| 4:D:356:A:H2' | 4:D:357:G:H8 | 1.74 | 0.52 |
| 4:D:357:G:C2 | 4:D:358:U:C5 | 2.98 | 0.52 |
| 8:I:1095:A:C8 | 8:I:1096:A:H8 | 2.28 | 0.52 |
| 11:E:41:ARG:CG | 11:E:42:THR:N | 2.72 | 0.52 |
| 14:N:30:ARG:HH21 | 14:N:194:PRO:HG2 | 1.74 | 0.52 |
| 12:K:89:ALA:CB | 12:K:153:ILE:HA | 2.39 | 0.52 |
| 13:L:118:SER:O | 13:L:121:VAL:HG22 | 2.10 | 0.52 |
| 13:L:170:ARG:HG2 | 13:L:170:ARG:HH11 | 1.74 | 0.52 |
| 13:L:484:ARG:CZ | 13:L:671:MET:HE3 | 2.08 | 0.52 |
| 8:I:1057:A:C4 | 8:I:1058:G:C8 | 2.97 | 0.52 |
| 14:N:112:VAL:O | 14:N:115:LEU:HB3 | 2.09 | 0.52 |
| 10:M:69:C:N3 | 10:M:70:G:N7 | 2.57 | 0.52 |
| 13:L:550:MET:SD | 13:L:563:ILE:HD11 | 2.49 | 0.52 |
| 2:B:392:G:H2' | 2:B:393:A:C8 | 2.44 | 0.52 |
| 13:L:483:TYR:OH | 13:L:627:ARG:CZ | 2.56 | 0.52 |
| 8:I:1095:A:C8 | 8:I:1096:A:C8 | 2.97 | 0.52 |
| 8:I:1106:G:C6 | 8:I:1107:G:O6 | 2.63 | 0.52 |
| 10:M:7:A:C8 | 10:M:49:5MC:HM52 | 2.45 | 0.52 |
| 12:K:168:THR:CA | 12:K:173:ALA:HB2 | 2.31 | 0.52 |
| 10:M:65:G:O2' | 10:M:66:U:H5' | 2.08 | 0.52 |
| 13:L:546:ILE:HG23 | 13:L:590:ILE:HG12 | 1.92 | 0.52 |
| 8:I:1072:C:H2' | 8:I:1093:G:C6 | 2.44 | 0.52 |
| 11:E:86:ARG:HB2 | 11:E:101:VAL:HG22 | 1.91 | 0.52 |
| 14:N:68:ILE:H | 14:N:90:MET:HE2 | 1.73 | 0.52 |
| 12:K:64:LEU:HD13 | 12:K:65:PRO:CD | 2.37 | 0.52 |
| 4:D:52:G:O2' | 4:D:53:A:H5' | 2.10 | 0.52 |
| 8:I:1067:A:N3 | 13:L:634:MET:HE2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1102:C:C2' | 8:I:1103:A:O5' | 2.57 | 0.52 |
| 14:N:109:SER:O | 14:N:112:VAL:N | 2.43 | 0.52 |
| 13:L:114:VAL:CG1 | 13:L:152:THR:HB | 2.39 | 0.52 |
| 13:L:636:PRO:HD3 | 13:L:641:GLN:HE22 | 1.75 | 0.52 |
| 13:L:160:ARG:HD3 | 13:L:255:ILE:HG22 | 1.92 | 0.52 |
| 8:I:1091:G:N1 | 8:I:1100:C:N4 | 2.57 | 0.52 |
| 8:I:1094:U:C5 | 8:I:1096:A:OP2 | 2.63 | 0.52 |
| 14:N:162:ILE:O | 14:N:185:ILE:HG12 | 2.09 | 0.52 |
| 14:N:178:ARG:HH22 | 14:N:196:LEU:CA | 2.22 | 0.52 |
| 14:N:124:SER:OG | 14:N:125:PRO:HD2 | 2.09 | 0.52 |
| 6:G:1865:G:H5' | 6:G:1866:C:OP2 | 2.10 | 0.52 |
| 10:M:71:G:H2' | 10:M:72:A:H8 | 1.75 | 0.52 |
| 14:N:15:VAL:H | 14:N:16:HIS:CE1 | 2.27 | 0.52 |
| 13:L:115:GLU:HB3 | 13:L:116:PRO:CD | 2.39 | 0.52 |
| 13:L:486:THR:C | 13:L:600:VAL:HG12 | 2.30 | 0.52 |
| 8:I:1084:A:N3 | 8:I:1084:A:H2' | 2.24 | 0.52 |
| 3:C:1457:G:C2 | 3:C:1458:G:C8 | 2.98 | 0.52 |
| 10:M:22:A:H5' | 10:M:22:A:C8 | 2.42 | 0.52 |
| 13:L:391:GLY:C | 13:L:393:ASP:H | 2.13 | 0.52 |
| 9:J:2193:G:H5' | 9:J:2193:G:H8 | 1.74 | 0.52 |
| 8:I:1089:G:O5' | 8:I:1089:G:C8 | 2.57 | 0.51 |
| 13:L:127:LYS:CE | 13:L:402:ILE:CG1 | 2.63 | 0.51 |
| 9:J:2127:G:N1 | 9:J:2161:C:H1' | 2.25 | 0.51 |
| 6:G:1880:C:H5' | 6:G:1880:C:H6 | 1.74 | 0.51 |
| 14:N:215:LEU:O | 14:N:218:ALA:HB3 | 2.10 | 0.51 |
| 13:L:486:THR:HG21 | 13:L:678:GLU:HG2 | 1.91 | 0.51 |
| 9:J:2168:G:C2 | 10:M:19:G:N1 | 2.77 | 0.51 |
| 11:E:83:VAL:HG13 | 11:E:84:LEU:N | 2.24 | 0.51 |
| 8:I:1091:G:N1 | 8:I:1101:U:N3 | 2.58 | 0.51 |
| 14:N:144:ARG:HG3 | 14:N:145:LEU:H | 1.75 | 0.51 |
| 14:N:166:ASP:HB2 | 14:N:205:ASP:OD2 | 2.10 | 0.51 |
| 14:N:88:ALA:HB2 | 14:N:219:VAL:CG1 | 2.39 | 0.51 |
| 9:J:2115:G:H5' | 9:J:2116:G:OP2 | 2.11 | 0.51 |
| 11:E:113:ARG:HH11 | 11:E:113:ARG:HG2 | 1.75 | 0.51 |
| 11:E:69:TYR:C | 11:E:70:ILE:HD12 | 2.30 | 0.51 |
| 11:E:22:SER:C | 11:E:24:VAL:H | 2.13 | 0.51 |
| 10:M:25:U:C2 | 10:M:26:A:C8 | 2.98 | 0.51 |
| 13:L:8:ASP:OD1 | 13:L:10:LYS:HE2 | 2.10 | 0.51 |
| 7:H:2464:C:O2' | 7:H:2465:C:H6 | 1.80 | 0.51 |
| 11:E:41:ARG:HG2 | 11:E:42:THR:N | 2.26 | 0.51 |
| 7:H:2467:C:H2' | 7:H:2468:G:O4' | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:J:2186:G:C3' | 9:J:2187:G:H5" | 2.41 | 0.51 |
| 13:L:519:ARG:HA | 13:L:519:ARG:HH11 | 1.75 | 0.51 |
| 8:I:1086:A:C2' | 8:I:1087:G:H5' | 2.41 | 0.51 |
| 13:L:85:PRO:HG2 | 13:L:94:VAL:CG2 | 2.40 | 0.51 |
| 10:M:25:U:N3 | 10:M:26:A:C5 | 2.79 | 0.51 |
| 3:C:1443:G:H22 | 3:C:1460:A:H1' | 1.75 | 0.51 |
| 14:N:168:THR:HG21 | 14:N:192:SER:HA | 1.92 | 0.51 |
| 8:I:1063:G:C4 | 8:I:1064:C:C5 | 2.99 | 0.51 |
| 10:M:69:C:C2 | 10:M:70:G:C8 | 2.99 | 0.51 |
| 10:M:53:G:C2 | 10:M:62:C:C2 | 2.99 | 0.51 |
| 7:H:2481:G:HO2' | 7:H:2482:G:P | 2.34 | 0.51 |
| 1:A:348:G:O2' | 1:A:349:A:H5' | 2.10 | 0.51 |
| 12:K:75:LEU:HD23 | 12:K:75:LEU:C | 2.32 | 0.51 |
| 11:E:52:LEU:O | 11:E:54:LYS:HD2 | 2.11 | 0.51 |
| 8:I:1068:G:C4 | 8:I:1069:A:N6 | 2.79 | 0.51 |
| 13:L:90:PHE:O | 13:L:94:VAL:HG23 | 2.11 | 0.51 |
| 13:L:414:GLU:C | 13:L:474:ALA:HB1 | 2.30 | 0.51 |
| 14:N:208:ILE:HA | 14:N:211:ILE:HD12 | 1.93 | 0.51 |
| 13:L:519:ARG:CZ | 13:L:678:GLU:CG | 2.89 | 0.50 |
| 8:I:1087:G:N3 | 8:I:1103:A:C4 | 2.80 | 0.50 |
| 13:L:127:LYS:CD | 13:L:401:SER:CA | 2.88 | 0.50 |
| 11:E:62:SER:O | 11:E:64:TYR:HD1 | 1.93 | 0.50 |
| 12:K:82:LYS:HZ1 | 12:K:151:GLU:HA | 1.75 | 0.50 |
| 2:B:390:C:H6 | 2:B:390:C:O5' | 1.93 | 0.50 |
| 14:N:184:VAL:O | 14:N:198:ASP:HB2 | 2.11 | 0.50 |
| 8:I:1061:U:H4' | 8:I:1070:A:C4' | 2.41 | 0.50 |
| 8:I:1087:G:C4 | 8:I:1103:A:C2 | 2.99 | 0.50 |
| 5:F:2660:A:O2' | 13:L:665:GLY:CA | 2.58 | 0.50 |
| 14:N:144:ARG:O | 14:N:147:LYS:HB3 | 2.11 | 0.50 |
| 11:E:61:THR:OG1 | 11:E:62:SER:N | 2.45 | 0.50 |
| 8:I:1062:G:C6 | 8:I:1077:A:C4 | 2.99 | 0.50 |
| 13:L:335:LEU:HD11 | 13:L:341:VAL:HG11 | 1.94 | 0.50 |
| 8:I:1071:G:C2' | 8:I:1072:C:H5' | 2.41 | 0.50 |
| 8:I:1085:A:HO2' | 8:I:1086:A:C4' | 2.09 | 0.50 |
| 8:I:1097:U:H2' | 8:I:1098:A:C5' | 2.41 | 0.50 |
| 8:I:1102:C:C1' | 8:I:1103:A:H8 | 2.22 | 0.50 |
| 13:L:87:HIS:HB3 | 13:L:90:PHE:CE1 | 2.47 | 0.50 |
| 5:F:2656:U:C4 | 5:F:2657:A:H2 | 2.30 | 0.50 |
| 9:J:2111:C:H5' | 9:J:2112:G:OP1 | 2.11 | 0.50 |
| 14:N:97:TRP:CH2 | 14:N:176:GLU:OE2 | 2.65 | 0.50 |
| 3:C:1436:U:O2' | 3:C:1437:C:H5' | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:34:TYR:CZ | 13:L:38:ARG:HD3 | 2.47 | 0.50 |
| 13:L:519:ARG:HD3 | 13:L:562:ASP:OD1 | 2.12 | 0.50 |
| 8:I:1086:A:H2' | 8:I:1087:G:H5' | 1.94 | 0.50 |
| 13:L:85:PRO:HG2 | 13:L:94:VAL:N | 2.27 | 0.50 |
| 14:N:19:HIS:HD2 | 14:N:189:ASP:OD2 | 1.95 | 0.50 |
| 9:J:2107:C:H42 | 9:J:2182:G:H1 | 1.60 | 0.50 |
| 14:N:19:HIS:HE1 | 14:N:206:ASP:HB2 | 1.76 | 0.50 |
| 8:I:1063:G:N7 | 8:I:1070:A:OP2 | 2.45 | 0.50 |
| 8:I:1082:U:C3' | 8:I:1082:U:C6 | 2.94 | 0.50 |
| 11:E:90:VAL:O | 11:E:92:ASP:N | 2.45 | 0.50 |
| 3:C:1433:A:C6 | 3:C:1468:A:C4 | 3.00 | 0.50 |
| 3:C:1459:C:O2' | 3:C:1460:A:H5' | 2.11 | 0.50 |
| 13:L:431:LEU:HD11 | 13:L:465:ARG:HD3 | 1.93 | 0.50 |
| 8:I:1053:C:O2 | 8:I:1053:C:H2' | 2.11 | 0.50 |
| 8:I:1057:A:N1 | 8:I:1058:G:C5 | 2.80 | 0.50 |
| 12:K:46:LYS:HB2 | 12:K:208:PHE:O | 2.12 | 0.50 |
| 11:E:89:ARG:HA | 11:E:97:ARG:HA | 1.93 | 0.50 |
| 14:N:84:GLU:OE1 | 14:N:216:SER:HA | 2.12 | 0.50 |
| 14:N:98:LEU:O | 14:N:101:MET:HG3 | 2.11 | 0.50 |
| 9:J:2164:C:H5" | 9:J:2165:G:N7 | 2.27 | 0.50 |
| 14:N:73:THR:HG22 | 14:N:95:GLN:O | 2.12 | 0.50 |
| 5:F:2662:A:O2' | 13:L:457:LEU:HD11 | 2.11 | 0.49 |
| 14:N:213:LEU:HD22 | 14:N:214:ILE:HD13 | 1.94 | 0.49 |
| 14:N:178:ARG:NH2 | 14:N:196:LEU:HA | 2.27 | 0.49 |
| 2:B:368:U:C6 | 13:L:354:ARG:CD | 2.80 | 0.49 |
| 8:I:1054:A:N1 | 8:I:1105:U:C2 | 2.77 | 0.49 |
| 14:N:194:PRO:O | 14:N:197:VAL:N | 2.45 | 0.49 |
| 13:L:534:ILE:HD12 | 13:L:567:LEU:HD11 | 1.94 | 0.49 |
| 8:I:1095:A:O4' | 13:L:617:MET:CG | 2.60 | 0.49 |
| 14:N:164:VAL:CG1 | 14:N:165:VAL:N | 2.75 | 0.49 |
| 14:N:216:SER:C | 14:N:218:ALA:H | 2.16 | 0.49 |
| 13:L:13:ARG:HH11 | 13:L:277:VAL:CA | 2.24 | 0.49 |
| 3:C:1436:U:H2' | 3:C:1437:C:H6 | 1.77 | 0.49 |
| 9:J:2162:G:H5' | 9:J:2171:A:C5' | 2.42 | 0.49 |
| 13:L:449:THR:C | 13:L:450:ILE:HD13 | 2.33 | 0.49 |
| 11:E:55:VAL:HG12 | 11:E:56:ALA:N | 2.27 | 0.49 |
| 12:K:20:TYR:CG | 12:K:21:THR:N | 2.80 | 0.49 |
| 14:N:55:PHE:HE1 | 14:N:218:ALA:HA | 1.78 | 0.49 |
| 14:N:28:PHE:O | 14:N:28:PHE:CD1 | 2.66 | 0.49 |
| 14:N:149:LEU:O | 14:N:153:ARG:HG3 | 2.13 | 0.49 |
| 14:N:84:GLU:HB3 | 14:N:219:VAL:CG2 | 2.39 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:607:ARG:NH2 | 13:L:644:ARG:HH21 | 2.11 | 0.49 |
| 13:L:122:TRP:CD2 | 13:L:157:LEU:HD13 | 2.48 | 0.49 |
| 13:L:658:ASP:O | 13:L:661:SER:HB3 | 2.12 | 0.49 |
| 8:I:1071:G:H2' | 8:I:1072:C:H5" | 1.94 | 0.49 |
| 10:M:73:G:N3 | 10:M:73:G:H2' | 2.27 | 0.49 |
| 8:I:1064:C:H3' | 8:I:1065:U:H5 | 1.75 | 0.49 |
| 8:I:1065:U:C3' | 8:I:1066:U:C5' | 2.80 | 0.49 |
| 14:N:185:ILE:HG22 | 14:N:199:TYR:CD1 | 2.48 | 0.49 |
| 14:N:187:LEU:O | 14:N:187:LEU:HD13 | 2.12 | 0.49 |
| 12:K:49:ILE:CG2 | 12:K:50:ASP:N | 2.75 | 0.49 |
| 14:N:75:LYS:C | 14:N:77:ALA:H | 2.16 | 0.49 |
| 13:L:536:LYS:HD2 | 13:L:537:GLU:HG3 | 1.95 | 0.49 |
| 11:E:53:ARG:NH1 | 11:E:53:ARG:HG2 | 2.27 | 0.49 |
| 8:I:1083:U:H5" | 8:I:1083:U:C6 | 2.48 | 0.49 |
| 8:I:1087:G:O6 | 8:I:1102:C:N3 | 2.46 | 0.49 |
| 7:H:2469:A:H3' | 7:H:2470:G:O4' | 2.12 | 0.49 |
| 14:N:178:ARG:CB | 14:N:178:ARG:HH11 | 2.23 | 0.49 |
| 8:I:1064:C:C4 | 8:I:1075:C:N4 | 2.80 | 0.49 |
| 8:I:1069:A:O2' | 8:I:1070:A:H5" | 2.13 | 0.49 |
| 13:L:417:THR:O | 13:L:418:LYS:HB2 | 2.13 | 0.49 |
| 13:L:454:MET:H | 13:L:458:HIS:HD2 | 1.59 | 0.49 |
| 14:N:24:TRP:CZ3 | 14:N:26:PRO:HA | 2.48 | 0.49 |
| 9:J:2184:G:H2' | 9:J:2185:C:H6 | 1.76 | 0.49 |
| 14:N:107:THR:HG23 | 14:N:110:GLN:OE1 | 2.12 | 0.49 |
| 13:L:328:ILE:O | 13:L:328:ILE:HD13 | 2.12 | 0.49 |
| 12:K:99:ILE:HG22 | 12:K:99:ILE:O | 2.13 | 0.49 |
| 3:C:1478:C:O2' | 3:C:1479:C:H5' | 2.13 | 0.49 |
| 13:L:409:ILE:HD11 | 13:L:657:THR:H | 1.77 | 0.49 |
| 13:L:485:GLU:HB2 | 13:L:605:ILE:HD13 | 1.83 | 0.49 |
| 5:F:2660:A:H3' | 5:F:2661:G:O4' | 2.12 | 0.49 |
| 11:E:45:PRO:HG2 | 11:E:51:ALA:N | 2.28 | 0.49 |
| 14:N:80:ILE:HG13 | 14:N:81:VAL:H | 1.78 | 0.49 |
| 13:L:484:ARG:HD3 | 13:L:606:MET:SD | 2.53 | 0.48 |
| 13:L:485:GLU:CB | 13:L:605:ILE:HA | 2.37 | 0.48 |
| 2:B:368:U:H5 | 13:L:354:ARG:HD2 | 0.68 | 0.48 |
| 8:I:1054:A:C5 | 8:I:1055:G:O6 | 2.66 | 0.48 |
| 8:I:1054:A:N6 | 8:I:1104:C:H42 | 2.11 | 0.48 |
| 3:C:1404:C:H6 | 3:C:1404:C:O5' | 1.95 | 0.48 |
| 13:L:484:ARG:CD | 13:L:649:LEU:HD13 | 2.33 | 0.48 |
| 10:M:73:G:H2' | 10:M:74:C:C5' | 2.42 | 0.48 |
| 10:M:1:U:O2' | 10:M:2:C:C5' | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:1473:A:H2' | 3:C:1474:G:C8 | 2.47 | 0.48 |
| 11:E:20:LYS:H | 11:E:20:LYS:HD3 | 1.77 | 0.48 |
| 8:I:1057:A:N1 | 8:I:1081:U:O2 | 2.46 | 0.48 |
| 8:I:1085:A:C1' | 8:I:1086:A:C4' | 2.72 | 0.48 |
| 13:L:85:PRO:HG2 | 13:L:94:VAL:CA | 2.43 | 0.48 |
| 10:M:50:G:C6 | 10:M:65:G:C6 | 3.01 | 0.48 |
| 14:N:83:MET:O | 14:N:85:ALA:N | 2.47 | 0.48 |
| 3:C:1442:G:H5' | 3:C:1442:G:N9 | 2.27 | 0.48 |
| 14:N:162:ILE:HG13 | 14:N:162:ILE:O | 2.13 | 0.48 |
| 3:C:1470:G:O2' | 3:C:1471:G:H5' | 2.13 | 0.48 |
| 13:L:312:LEU:HD23 | 13:L:399:LEU:HB2 | 1.96 | 0.48 |
| 14:N:12:GLU:C | 14:N:14:GLY:N | 2.67 | 0.48 |
| 10:M:50:G:C6 | 10:M:65:G:N1 | 2.81 | 0.48 |
| 6:G:1848:A:C4 | 6:G:1849:G:C8 | 3.01 | 0.48 |
| 3:C:1495:U:H2' | 3:C:1496:C:H6 | 1.78 | 0.48 |
| 13:L:443:HIS:HB3 | 13:L:446:THR:OG1 | 2.13 | 0.48 |
| 6:G:1866:C:H2' | 6:G:1876:A:O4' | 2.12 | 0.48 |
| 13:L:291:GLY:O | 13:L:299:VAL:N | 2.45 | 0.48 |
| 13:L:587:SER:O | 13:L:591:LYS:HG2 | 2.14 | 0.48 |
| 10:M:59:U:C5 | 10:M:60:U:C4 | 3.02 | 0.48 |
| 13:L:146:LEU:O | 13:L:150:ILE:HG12 | 2.14 | 0.48 |
| 13:L:486:THR:CG2 | 13:L:678:GLU:CG | 2.91 | 0.48 |
| 13:L:481:VAL:HG21 | 13:L:627:ARG:HH21 | 1.77 | 0.48 |
| 13:L:127:LYS:HE3 | 13:L:402:ILE:HG13 | 1.80 | 0.48 |
| 9:J:2127:G:H2' | 9:J:2128:C:N1 | 2.28 | 0.48 |
| 8:I:1082:U:C5 | 8:I:1083:U:C5 | 3.02 | 0.48 |
| 9:J:2160:G:H3' | 9:J:2161:C:H5" | 1.95 | 0.48 |
| 14:N:197:VAL:HG12 | 14:N:200:ILE:HG12 | 1.95 | 0.48 |
| 14:N:8:LYS:O | 14:N:9:GLU:C | 2.51 | 0.48 |
| 6:G:1842:G:H2' | 6:G:1843:C:H6 | 1.79 | 0.48 |
| 13:L:607:ARG:HH21 | 13:L:644:ARG:HH21 | 1.60 | 0.48 |
| 13:L:110:SER:CB | 13:L:139:MET:HE2 | 2.44 | 0.48 |
| 8:I:1057:A:C8 | 8:I:1085:A:C6 | 3.01 | 0.48 |
| 3:C:1484:C:H2' | 3:C:1485:U:C6 | 2.48 | 0.48 |
| 14:N:129:GLU:O | 14:N:130:ARG:HB2 | 2.14 | 0.48 |
| 3:C:1431:C:H42 | 3:C:1469:G:H1 | 1.60 | 0.48 |
| 14:N:41:ILE:CD1 | 14:N:41:ILE:N | 2.77 | 0.48 |
| 10:M:24:G:C6 | 10:M:25:U:C5 | 3.02 | 0.48 |
| 14:N:124:SER:O | 14:N:127:ILE:HG12 | 2.14 | 0.48 |
| 13:L:486:THR:CG2 | 13:L:678:GLU:HG2 | 2.44 | 0.47 |
| 8:I:1071:G:C2' | 8:I:1072:C:C5' | 2.91 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:K:208:PHE:O | 12:K:209:LEU:CB | 2.62 | 0.47 |
| 14:N:49:GLU:O | 14:N:52:GLU:HB3 | 2.14 | 0.47 |
| 11:E:58:VAL:O | 11:E:60:LEU:HD22 | 2.13 | 0.47 |
| 13:L:510:VAL:HG11 | 13:L:542:VAL:HG21 | 1.96 | 0.47 |
| 5:F:2651:C:O2' | 5:F:2652:C:H5' | 2.13 | 0.47 |
| 8:I:1091:G:N2 | 8:I:1101:U:N1 | 2.61 | 0.47 |
| 13:L:85:PRO:HG3 | 13:L:93:GLU:HB3 | 1.95 | 0.47 |
| 13:L:92:ILE:CG2 | 13:L:93:GLU:N | 2.77 | 0.47 |
| 14:N:22:LYS:H | 14:N:40:HIS:CE1 | 2.32 | 0.47 |
| 5:F:2656:U:C4' | 13:L:141:LYS:HZ2 | 2.15 | 0.47 |
| 6:G:1899:G:N2 | 6:G:1902:C:C5 | 2.82 | 0.47 |
| 11:E:102:ARG:CG | 11:E:102:ARG:NH1 | 2.74 | 0.47 |
| 3:C:1411:C:O2' | 3:C:1412:C:H5' | 2.14 | 0.47 |
| 12:K:77:ILE:HG21 | 12:K:122:ALA:CA | 2.43 | 0.47 |
| 14:N:172:ILE:N | 14:N:172:ILE:HD12 | 2.30 | 0.47 |
| 8:I:1058:G:C2' | 8:I:1059:G:O5' | 2.62 | 0.47 |
| 8:I:1071:G:C5 | 8:I:1089:G:C2 | 3.02 | 0.47 |
| 5:F:2671:A:H2' | 5:F:2672:G:H8 | 1.79 | 0.47 |
| 14:N:100:GLY:O | 14:N:104:ASN:HB3 | 2.15 | 0.47 |
| 5:F:2648:C:O2' | 5:F:2649:U:H5' | 2.14 | 0.47 |
| 6:G:1854:A:H3' | 6:G:1855:G:H8 | 1.80 | 0.47 |
| 3:C:1466:C:H2' | 3:C:1467:G:H5' | 1.95 | 0.47 |
| 8:I:1054:A:C6 | 8:I:1055:G:O6 | 2.66 | 0.47 |
| 6:G:1848:A:C5 | 6:G:1849:G:C8 | 3.02 | 0.47 |
| 13:L:344:THR:C | 13:L:346:LYS:H | 2.18 | 0.47 |
| 13:L:122:TRP:CE3 | 13:L:157:LEU:HD13 | 2.49 | 0.47 |
| 8:I:1059:G:N7 | 8:I:1060:U:C1' | 2.78 | 0.47 |
| 8:I:1067:A:HO2' | 13:L:634:MET:CG | 2.20 | 0.47 |
| 14:N:204:ASN:ND2 | 14:N:204:ASN:C | 2.68 | 0.47 |
| 14:N:102:LEU:HD13 | 14:N:102:LEU:H | 1.76 | 0.47 |
| 14:N:23:ARG:HG3 | 14:N:23:ARG:NH1 | 2.27 | 0.47 |
| 14:N:238:LEU:HD23 | 14:N:238:LEU:N | 2.29 | 0.47 |
| 13:L:361:ASN:O | 13:L:362:HIS:HB3 | 2.15 | 0.47 |
| 14:N:43:ASP:OD1 | 14:N:45:GLN:HB3 | 2.15 | 0.47 |
| 14:N:239:VAL:HG12 | 14:N:239:VAL:O | 2.15 | 0.47 |
| 12:K:62:VAL:O | 12:K:63:SER:C | 2.53 | 0.47 |
| 13:L:483:TYR:HB2 | 13:L:651:GLU:N | 2.03 | 0.47 |
| 13:L:631:ILE:HD12 | 13:L:631:ILE:N | 2.30 | 0.47 |
| 11:E:60:LEU:HD22 | 11:E:60:LEU:H | 1.79 | 0.47 |
| 3:C:1436:U:H2' | 3:C:1437:C:C6 | 2.49 | 0.47 |
| 3:C:1402:C:H2' | 3:C:1403:C:H6 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:61:LEU:HA | 14:N:64:ARG:HG2 | 1.95 | 0.47 |
| 9:J:2192:G:C2 | 9:J:2193:G:C8 | 3.02 | 0.47 |
| 3:C:1466:C:C2' | 3:C:1467:G:H5' | 2.44 | 0.47 |
| 10:M:12:A:O2' | 10:M:13:A:H5' | 2.15 | 0.47 |
| 13:L:556:ILE:CG1 | 13:L:601:ILE:CG1 | 2.77 | 0.47 |
| 13:L:519:ARG:CG | 13:L:677:GLN:HE22 | 2.15 | 0.47 |
| 5:F:2662:A:C2' | 13:L:457:LEU:HD13 | 2.44 | 0.47 |
| 8:I:1092:C:H3' | 8:I:1092:C:H6 | 1.80 | 0.47 |
| 13:L:318:ALA:HA | 13:L:324:ARG:HA | 1.96 | 0.47 |
| 2:B:394:G:HO2' | 13:L:340:TYR:HH | 1.63 | 0.47 |
| 13:L:363:ARG:HG3 | 13:L:363:ARG:NH1 | 2.30 | 0.47 |
| 13:L:487:ILE:HG22 | 13:L:599:PRO:N | 2.30 | 0.47 |
| 8:I:1066:U:N3 | 8:I:1069:A:OP1 | 2.48 | 0.47 |
| 12:K:40:THR:O | 12:K:40:THR:HG23 | 2.15 | 0.47 |
| 14:N:92:TYR:CE2 | 14:N:151:GLY:CA | 2.98 | 0.47 |
| 3:C:1423:G:O2' | 3:C:1424:C:H5' | 2.15 | 0.47 |
| 13:L:166:LEU:CD2 | 13:L:180:VAL:HG11 | 2.41 | 0.47 |
| 13:L:556:ILE:CD1 | 13:L:601:ILE:CG2 | 2.60 | 0.47 |
| 8:I:1063:G:C2 | 8:I:1075:C:C4 | 3.02 | 0.47 |
| 13:L:9:LEU:O | 13:L:11:ARG:N | 2.48 | 0.47 |
| 11:E:71:PRO:HD2 | 11:E:102:ARG:HH11 | 1.78 | 0.47 |
| 9:J:2162:G:OP2 | 9:J:2162:G:H3' | 2.14 | 0.47 |
| 10:M:43:G:H2' | 10:M:44:C:O4' | 2.15 | 0.47 |
| 14:N:19:HIS:CD2 | 14:N:205:ASP:OD1 | 2.68 | 0.46 |
| 13:L:181:LEU:HD12 | 13:L:181:LEU:C | 2.35 | 0.46 |
| 14:N:27:LYS:C | 14:N:29:ALA:H | 2.19 | 0.46 |
| 13:L:408:VAL:O | 13:L:654:GLY:CA | 2.62 | 0.46 |
| 8:I:1069:A:C3' | 8:I:1070:A:H5" | 2.46 | 0.46 |
| 6:G:1878:G:H2' | 6:G:1879:C:C6 | 2.49 | 0.46 |
| 5:F:2656:U:C5' | 13:L:141:LYS:HZ1 | 2.28 | 0.46 |
| 13:L:114:VAL:O | 13:L:114:VAL:HG13 | 2.16 | 0.46 |
| 9:J:2114:A:N3 | 9:J:2114:A:H2' | 2.30 | 0.46 |
| 13:L:89:ASP:O | 13:L:91:THR:N | 2.42 | 0.46 |
| 8:I:1097:U:C2' | 8:I:1098:A:O5' | 2.64 | 0.46 |
| 14:N:187:LEU:HA | 14:N:201:ILE:O | 2.15 | 0.46 |
| 13:L:415:PRO:HA | 13:L:474:ALA:HB2 | 1.98 | 0.46 |
| 14:N:216:SER:C | 14:N:218:ALA:N | 2.68 | 0.46 |
| 5:F:2658:C:C2' | 5:F:2658:C:O2 | 2.63 | 0.46 |
| 12:K:68:LEU:CD2 | 12:K:179:SER:HA | 2.46 | 0.46 |
| 13:L:264:LEU:HD23 | 13:L:264:LEU:O | 2.15 | 0.46 |
| 13:L:600:VAL:HG11 | 13:L:678:GLU:OE2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:627:ARG:NH2 | 13:L:655:TYR:HD1 | 2.13 | 0.46 |
| 8:I:1057:A:C2 | 8:I:1058:G:N7 | 2.83 | 0.46 |
| 3:C:1496:C:H2' | 3:C:1497:G:C8 | 2.51 | 0.46 |
| 14:N:98:LEU:HB2 | 14:N:101:MET:HE2 | 1.98 | 0.46 |
| 13:L:319:ASP:HB2 | 13:L:325:LEU:HD12 | 1.98 | 0.46 |
| 9:J:2124:G:C2' | 9:J:2125:G:H5' | 2.45 | 0.46 |
| 12:K:183:GLU:CB | 12:K:186:ALA:HB3 | 2.45 | 0.46 |
| 13:L:555:LEU:HD13 | 13:L:684:GLN:HG2 | 1.26 | 0.46 |
| 8:I:1071:G:C3' | 8:I:1072:C:H5' | 2.44 | 0.46 |
| 12:K:18:LYS:CD | 12:K:19:VAL:HG23 | 2.41 | 0.46 |
| 13:L:196:ILE:HD13 | 13:L:197:ARG:N | 2.31 | 0.46 |
| 13:L:636:PRO:HD3 | 13:L:641:GLN:NE2 | 2.30 | 0.46 |
| 3:C:1416:G:H2' | 3:C:1417:G:O4' | 2.15 | 0.46 |
| 11:E:7:ILE:O | 11:E:10:LEU:N | 2.49 | 0.46 |
| 13:L:95:GLU:CD | 13:L:402:ILE:HA | 2.36 | 0.46 |
| 11:E:60:LEU:HD23 | 11:E:64:TYR:HB3 | 1.98 | 0.46 |
| 3:C:1430:C:O2' | 3:C:1431:C:H5' | 2.16 | 0.46 |
| 3:C:1469:G:H2' | 3:C:1470:G:H8 | 1.81 | 0.46 |
| 8:I:1078:U:C5' | 8:I:1079:C:OP1 | 2.63 | 0.46 |
| 13:L:139:MET:HA | 13:L:139:MET:HE2 | 1.98 | 0.46 |
| 8:I:1053:C:C2 | 8:I:1106:G:N2 | 2.77 | 0.46 |
| 8:I:1105:U:HO2' | 8:I:1106:G:P | 2.38 | 0.46 |
| 11:E:86:ARG:HB2 | 11:E:101:VAL:CG2 | 2.45 | 0.46 |
| 8:I:1077:A:H3' | 8:I:1078:U:C6 | 2.50 | 0.46 |
| 4:D:55:A:H2 | 13:L:322:VAL:HG12 | 0.42 | 0.46 |
| 5:F:2660:A:O4' | 13:L:665:GLY:HA3 | 2.09 | 0.46 |
| 14:N:153:ARG:O | 14:N:154:LEU:C | 2.54 | 0.46 |
| 10:M:70:G:H2' | 10:M:71:G:C8 | 2.50 | 0.46 |
| 11:E:42:THR:O | 11:E:42:THR:HG23 | 2.15 | 0.46 |
| 12:K:191:ALA:C | 12:K:193:ILE:N | 2.69 | 0.46 |
| 14:N:175:ARG:O | 14:N:176:GLU:C | 2.55 | 0.46 |
| 14:N:178:ARG:HH22 | 14:N:196:LEU:HA | 1.81 | 0.46 |
| 6:G:1860:G:H2' | 6:G:1861:G:H8 | 1.81 | 0.46 |
| 7:H:2464:C:O2' | 7:H:2465:C:P | 2.74 | 0.46 |
| 13:L:403:GLU:HG2 | 13:L:404:VAL:N | 2.31 | 0.46 |
| 14:N:155:LEU:N | 14:N:155:LEU:HD22 | 2.31 | 0.46 |
| 14:N:80:ILE:HG13 | 14:N:81:VAL:N | 2.30 | 0.46 |
| 14:N:204:ASN:HD22 | 14:N:204:ASN:C | 2.19 | 0.46 |
| 5:F:2653:U:C3' | 5:F:2654:A:H5" | 2.46 | 0.46 |
| 13:L:609:GLU:HB2 | 13:L:670:VAL:CG2 | 2.46 | 0.45 |
| 8:I:1097:U:C2 | 8:I:1098:A:O4' | 2.69 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:M:4:G:C2' | 10:M:5:U:O5' | 2.64 | 0.45 |
| 12:K:41:VAL:O | 12:K:178:ALA:HB3 | 2.16 | 0.45 |
| 13:L:110:SER:OG | 13:L:136:ALA:HB1 | 2.16 | 0.45 |
| 14:N:239:VAL:O | 14:N:241:GLU:N | 2.49 | 0.45 |
| 3:C:1488:G:O2' | 3:C:1489:G:H5' | 2.16 | 0.45 |
| 8:I:1074:G:C4 | 8:I:1075:C:H5 | 2.34 | 0.45 |
| 9:J:2176:A:H2' | 9:J:2177:C:C6 | 2.52 | 0.45 |
| 14:N:189:ASP:OD1 | 14:N:205:ASP:HB3 | 2.16 | 0.45 |
| 14:N:67:THR:HA | 14:N:90:MET:HE1 | 1.97 | 0.45 |
| 11:E:119:LYS:O | 11:E:120:TYR:CB | 2.64 | 0.45 |
| 13:L:484:ARG:HA | 13:L:649:LEU:HA | 0.62 | 0.45 |
| 4:D:358:U:H2' | 4:D:359:U:H6 | 1.80 | 0.45 |
| 8:I:1057:A:H2 | 8:I:1082:U:H3 | 1.63 | 0.45 |
| 8:I:1087:G:N9 | 8:I:1103:A:C2 | 2.84 | 0.45 |
| 14:N:91:PRO:CG | 14:N:154:LEU:HD12 | 2.46 | 0.45 |
| 11:E:88:GLY:O | 11:E:99:HIS:ND1 | 2.48 | 0.45 |
| 14:N:78:GLN:HB3 | 14:N:94:ASN:HD21 | 1.80 | 0.45 |
| 14:N:97:TRP:CZ3 | 14:N:173:ALA:HA | 2.51 | 0.45 |
| 13:L:345:THR:HG22 | 13:L:345:THR:O | 2.17 | 0.45 |
| 13:L:288:PRO:HB2 | 13:L:301:ILE:O | 2.16 | 0.45 |
| 2:B:393:A:C2 | 2:B:394:G:C8 | 3.04 | 0.45 |
| 12:K:77:ILE:HD12 | 12:K:123:VAL:H | 1.80 | 0.45 |
| 14:N:220:ASP:O | 14:N:223:ILE:N | 2.49 | 0.45 |
| 13:L:487:ILE:CG2 | 13:L:594:VAL:HA | 2.46 | 0.45 |
| 13:L:595:GLN:HA | 13:L:599:PRO:HG3 | 1.99 | 0.45 |
| 10:M:46:A:H2' | 10:M:48:U:C4' | 2.47 | 0.45 |
| 6:G:1843:C:O2' | 6:G:1844:C:H5' | 2.17 | 0.45 |
| 9:J:2170:A:O2' | 9:J:2171:A:C8 | 2.66 | 0.45 |
| 12:K:67:GLY:O | 12:K:68:LEU:HB2 | 2.17 | 0.45 |
| 8:I:1056:G:H21 | 8:I:1104:C:N4 | 2.15 | 0.45 |
| 8:I:1063:G:C2 | 8:I:1075:C:N4 | 2.85 | 0.45 |
| 8:I:1096:A:N7 | 8:I:1097:U:C6 | 2.85 | 0.45 |
| 8:I:1075:C:H2' | 8:I:1075:C:O2 | 2.15 | 0.45 |
| 12:K:47:LEU:HD21 | 12:K:172:HIS:CA | 2.46 | 0.45 |
| 7:H:2464:C:O2' | 7:H:2465:C:O5' | 2.35 | 0.45 |
| 5:F:2656:U:C5' | 13:L:141:LYS:NZ | 2.80 | 0.45 |
| 5:F:2656:U:C4' | 13:L:141:LYS:NZ | 2.73 | 0.45 |
| 10:M:24:G:C4 | 10:M:25:U:C5 | 3.05 | 0.45 |
| 10:M:22:A:H2' | 10:M:23:U:O4' | 2.16 | 0.45 |
| 3:C:1484:C:O2' | 3:C:1485:U:H5' | 2.17 | 0.45 |
| 14:N:16:HIS:HB3 | 14:N:210:SER:CB | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:M:75:C:C2' | 10:M:76:A:C5' | 2.41 | 0.45 |
| 13:L:458:HIS:CE1 | 13:L:462:ILE:HD11 | 2.51 | 0.45 |
| 3:C:1437:C:H2' | 3:C:1438:G:H8 | 1.80 | 0.45 |
| 12:K:34:THR:O | 12:K:35:ALA:HB2 | 2.17 | 0.45 |
| 4:D:55:A:N3 | 13:L:322:VAL:CA | 2.79 | 0.45 |
| 8:I:1072:C:H42 | 8:I:1100:C:H41 | 1.65 | 0.45 |
| 8:I:1068:G:C2 | 8:I:1073:A:C2 | 3.05 | 0.45 |
| 14:N:19:HIS:CG | 14:N:20:GLU:H | 2.34 | 0.45 |
| 14:N:39:ILE:CG2 | 14:N:40:HIS:N | 2.79 | 0.45 |
| 14:N:52:GLU:O | 14:N:54:THR:N | 2.50 | 0.45 |
| 12:K:51:PRO:HB3 | 12:K:203:GLY:C | 2.37 | 0.45 |
| 13:L:413:ILE:CD1 | 13:L:451:ILE:HD11 | 2.40 | 0.45 |
| 14:N:219:VAL:O | 14:N:222:ILE:HB | 2.16 | 0.45 |
| 4:D:57:G:O2' | 4:D:58:C:H5' | 2.17 | 0.45 |
| 13:L:92:ILE:HG23 | 13:L:93:GLU:H | 1.79 | 0.45 |
| 13:L:418:LYS:HA | 13:L:421:GLN:CB | 2.47 | 0.45 |
| 10:M:50:G:C6 | 10:M:65:G:C2 | 3.05 | 0.45 |
| 13:L:616:TYR:HA | 13:L:619:ASP:OD1 | 2.17 | 0.45 |
| 13:L:485:GLU:C | 13:L:605:ILE:CD1 | 2.85 | 0.45 |
| 12:K:51:PRO:HB2 | 12:K:202:GLU:CB | 2.46 | 0.45 |
| 3:C:1431:C:O2' | 3:C:1432:G:H5' | 2.17 | 0.45 |
| 14:N:198:ASP:N | 14:N:198:ASP:OD2 | 2.47 | 0.45 |
| 13:L:461:ILE:O | 13:L:465:ARG:HB2 | 2.17 | 0.45 |
| 13:L:493:VAL:HG11 | 13:L:592:GLU:HG3 | 1.99 | 0.45 |
| 13:L:483:TYR:HB3 | 13:L:651:GLU:HB2 | 1.97 | 0.44 |
| 8:I:1063:G:N7 | 8:I:1070:A:OP1 | 2.50 | 0.44 |
| 8:I:1069:A:H2 | 8:I:1096:A:H5' | 1.78 | 0.44 |
| 8:I:1064:C:N4 | 8:I:1075:C:N4 | 2.65 | 0.44 |
| 11:E:89:ARG:NH2 | 11:E:91:LYS:HD3 | 2.32 | 0.44 |
| 3:C:1471:G:O2' | 3:C:1472:U:H5' | 2.17 | 0.44 |
| 12:K:64:LEU:HD12 | 12:K:66:HIS:HB2 | 1.98 | 0.44 |
| 11:E:75:HIS:CG | 11:E:76:ASN:N | 2.81 | 0.44 |
| 13:L:485:GLU:OE2 | 13:L:650:ALA:HB3 | 2.17 | 0.44 |
| 14:N:74:LYS:HG3 | 14:N:77:ALA:HB3 | 1.99 | 0.44 |
| 8:I:1062:G:O6 | 8:I:1077:A:C4 | 2.70 | 0.44 |
| 8:I:1078:U:N3 | 8:I:1088:A:O2' | 2.45 | 0.44 |
| 11:E:21:LYS:HD2 | 11:E:21:LYS:H | 1.83 | 0.44 |
| 13:L:680:PRO:HD2 | 13:L:683:VAL:HG21 | 2.00 | 0.44 |
| 13:L:481:VAL:HB | 13:L:655:TYR:HA | 1.37 | 0.44 |
| 8:I:1057:A:C8 | 8:I:1085:A:C2 | 3.05 | 0.44 |
| 14:N:211:ILE:O | 14:N:215:LEU:HB2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:28:THR:O | 13:L:32:ILE:HG13 | 2.17 | 0.44 |
| 13:L:530:VAL:CG1 | 13:L:530:VAL:O | 2.62 | 0.44 |
| 13:L:481:VAL:HG21 | 13:L:627:ARG:NH2 | 2.31 | 0.44 |
| 14:N:46:LYS:O | 14:N:47:THR:C | 2.55 | 0.44 |
| 13:L:280:LEU:HA | 13:L:280:LEU:HD12 | 1.75 | 0.44 |
| 14:N:101:MET:O | 14:N:105:PHE:N | 2.50 | 0.44 |
| 9:J:2192:G:H2' | 9:J:2193:G:H5" | 1.99 | 0.44 |
| 13:L:82:ILE:HG12 | 13:L:100:VAL:HG12 | 1.99 | 0.44 |
| 7:H:2476:A:N3 | 7:H:2476:A:H3' | 2.32 | 0.44 |
| 8:I:1106:G:O6 | 8:I:1107:G:O6 | 2.35 | 0.44 |
| 10:M:7:A:N7 | 10:M:49:5MC:HM52 | 2.31 | 0.44 |
| 9:J:2103:C:H5' | 9:J:2104:G:OP2 | 2.17 | 0.44 |
| 11:E:5:PRO:HA | 11:E:9:GLN:NE2 | 2.33 | 0.44 |
| 11:E:58:VAL:N | 11:E:66:VAL:O | 2.49 | 0.44 |
| 13:L:238:THR:HG22 | 13:L:241:GLU:HG3 | 1.98 | 0.44 |
| 6:G:1851:U:C2' | 6:G:1852:C:H5' | 2.48 | 0.44 |
| 4:D:55:A:C6 | 4:D:56:U:C2 | 3.06 | 0.44 |
| 13:L:600:VAL:HG11 | 13:L:678:GLU:HB3 | 1.99 | 0.44 |
| 13:L:486:THR:CG2 | 13:L:678:GLU:OE1 | 2.62 | 0.44 |
| 10:M:62:C:O2 | 10:M:62:C:C2' | 2.63 | 0.44 |
| 11:E:22:SER:C | 11:E:24:VAL:N | 2.70 | 0.44 |
| 14:N:77:ALA:HB2 | 14:N:211:ILE:CD1 | 2.45 | 0.44 |
| 14:N:59:GLU:C | 14:N:61:LEU:H | 2.20 | 0.44 |
| 13:L:406:GLU:O | 13:L:408:VAL:HG13 | 2.17 | 0.44 |
| 8:I:1063:G:N1 | 8:I:1075:C:C4 | 2.84 | 0.44 |
| 3:C:1472:U:O2' | 3:C:1473:A:H5' | 2.18 | 0.44 |
| 3:C:1423:G:H2' | 3:C:1424:C:H6 | 1.83 | 0.44 |
| 14:N:114:ARG:HA | 14:N:117:GLU:CG | 2.46 | 0.44 |
| 12:K:180:PHE:O | 12:K:182:PRO:N | 2.51 | 0.44 |
| 13:L:438:PHE:HB2 | 13:L:452:SER:O | 2.17 | 0.44 |
| 13:L:20:HIS:CD2 | 13:L:117:GLN:H | 2.31 | 0.44 |
| 8:I:1067:A:N6 | 13:L:631:ILE:H | 2.16 | 0.44 |
| 9:J:2175:C:C1' | 12:K:215:THR:HA | 2.37 | 0.44 |
| 14:N:97:TRP:CH2 | 14:N:176:GLU:CD | 2.91 | 0.44 |
| 13:L:114:VAL:HG22 | 13:L:114:VAL:O | 2.17 | 0.44 |
| 10:M:54:5MU:H2' | 10:M:55:PSU:H5" | 1.98 | 0.44 |
| 3:C:1401:G:C2 | 3:C:1402:C:H1' | 2.53 | 0.44 |
| 3:C:1412:C:H2' | 3:C:1413:A:H8 | 1.79 | 0.44 |
| 12:K:97:GLU:CA | 12:K:100:ILE:HG12 | 2.46 | 0.44 |
| 13:L:507:TYR:C | 13:L:507:TYR:CD1 | 2.91 | 0.44 |
| 13:L:409:ILE:O | 13:L:452:SER:HA | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:487:ILE:HA | 13:L:599:PRO:HA | 2.00 | 0.44 |
| 8:I:1071:G:O5' | 8:I:1089:G:O6 | 2.36 | 0.44 |
| 10:M:73:G:N2 | 10:M:74:C:O4' | 2.51 | 0.44 |
| 14:N:189:ASP:N | 14:N:189:ASP:OD1 | 2.49 | 0.44 |
| 14:N:68:ILE:H | 14:N:90:MET:CE | 2.29 | 0.44 |
| 3:C:1452:C:H4' | 3:C:1456:G:C5' | 2.47 | 0.44 |
| 8:I:1090:U:OP2 | 8:I:1090:U:H6 | 2.01 | 0.44 |
| 14:N:17:PHE:N | 14:N:17:PHE:CD2 | 2.85 | 0.43 |
| 14:N:71:VAL:HG13 | 14:N:93:VAL:HB | 1.99 | 0.43 |
| 6:G:1844:C:C2' | 6:G:1845:G:H5' | 2.47 | 0.43 |
| 14:N:116:GLU:HA | 14:N:119:GLU:CB | 2.48 | 0.43 |
| 13:L:269:VAL:O | 13:L:273:LEU:HD22 | 2.18 | 0.43 |
| 9:J:2124:G:O2' | 9:J:2125:G:H5' | 2.18 | 0.43 |
| 8:I:1059:G:O6 | 8:I:1060:U:H1' | 2.17 | 0.43 |
| 5:F:2653:U:H5' | 5:F:2654:A:C5' | 2.45 | 0.43 |
| 3:C:1488:G:H2' | 3:C:1489:G:H8 | 1.83 | 0.43 |
| 13:L:348:ARG:HH21 | 13:L:350:GLU:HA | 1.83 | 0.43 |
| 13:L:608:VAL:HG12 | 13:L:610:VAL:HG23 | 2.01 | 0.43 |
| 14:N:68:ILE:N | 14:N:68:ILE:CD1 | 2.81 | 0.43 |
| 13:L:637:ARG:HG3 | 13:L:637:ARG:NH1 | 2.29 | 0.43 |
| 9:J:2193:G:C4 | 9:J:2194:G:C8 | 3.06 | 0.43 |
| 12:K:68:LEU:HD22 | 12:K:179:SER:HA | 1.99 | 0.43 |
| 7:H:2472:G:H2' | 7:H:2475:C:H42 | 1.83 | 0.43 |
| 3:C:1446:U:O2' | 3:C:1447:A:H3' | 2.19 | 0.43 |
| 13:L:409:ILE:CD1 | 13:L:657:THR:H | 2.32 | 0.43 |
| 13:L:606:MET:HB3 | 13:L:671:MET:HG3 | 1.99 | 0.43 |
| 8:I:1053:C:H2' | 8:I:1054:A:O4' | 2.18 | 0.43 |
| 8:I:1082:U:H3' | 8:I:1083:U:H6 | 1.82 | 0.43 |
| 8:I:1095:A:OP2 | 13:L:618:GLY:N | 2.43 | 0.43 |
| 14:N:42:ILE:CD1 | 14:N:202:PRO:HB2 | 2.47 | 0.43 |
| 13:L:409:ILE:HD11 | 13:L:657:THR:N | 2.29 | 0.43 |
| 14:N:21:ARG:HB2 | 14:N:39:ILE:HA | 1.99 | 0.43 |
| 13:L:345:THR:C | 13:L:346:LYS:HG3 | 2.39 | 0.43 |
| 14:N:12:GLU:O | 14:N:14:GLY:N | 2.52 | 0.43 |
| 8:I:1085:A:C2' | 8:I:1086:A:O4' | 2.66 | 0.43 |
| 8:I:1095:A:P | 13:L:617:MET:HB2 | 2.44 | 0.43 |
| 9:J:2126:A:O2' | 9:J:2127:G:P | 2.76 | 0.43 |
| 14:N:19:HIS:CD2 | 14:N:20:GLU:HG2 | 2.53 | 0.43 |
| 13:L:186:TYR:HB3 | 13:L:196:ILE:HD11 | 2.00 | 0.43 |
| 3:C:1415:G:H2' | 3:C:1416:G:H8 | 1.84 | 0.43 |
| 13:L:348:ARG:HH11 | 13:L:382:GLU:HG3 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:N:79:ASP:O | 14:N:82:ARG:HB3 | 2.19 | 0.43 |
| 12:K:196:LEU:C | 12:K:198:ALA:N | 2.71 | 0.43 |
| 8:I:1073:A:OP2 | 8:I:1094:U:O4 | 2.36 | 0.43 |
| 13:L:85:PRO:HG2 | 13:L:94:VAL:HA | 2.00 | 0.43 |
| 14:N:46:LYS:HA | 14:N:49:GLU:OE1 | 2.18 | 0.43 |
| 14:N:52:GLU:O | 14:N:53:ARG:C | 2.57 | 0.43 |
| 6:G:1863:G:H2' | 6:G:1864:U:O4' | 2.19 | 0.43 |
| 8:I:1066:U:HO2' | 8:I:1068:G:H8 | 1.61 | 0.43 |
| 14:N:54:THR:O | 14:N:57:PHE:HB3 | 2.18 | 0.43 |
| 6:G:1885:A:C8 | 6:G:1885:A:H5' | 2.54 | 0.43 |
| 13:L:417:THR:C | 13:L:419:ALA:N | 2.72 | 0.43 |
| 6:G:1899:G:H21 | 6:G:1902:C:H5 | 1.64 | 0.43 |
| 9:J:2189:U:H3' | 9:J:2190:G:C5' | 2.39 | 0.43 |
| 8:I:1077:A:C5 | 8:I:1078:U:C2 | 3.06 | 0.43 |
| 12:K:38:ASP:O | 12:K:180:PHE:HA | 2.19 | 0.43 |
| 13:L:519:ARG:HA | 13:L:519:ARG:NH1 | 2.33 | 0.43 |
| 14:N:30:ARG:HG2 | 14:N:30:ARG:H | 1.67 | 0.43 |
| 13:L:8:ASP:O | 13:L:9:LEU:C | 2.57 | 0.43 |
| 13:L:308:PRO:HB2 | 13:L:394:ALA:CB | 2.49 | 0.43 |
| 3:C:1446:U:H4' | 3:C:1447:A:N7 | 2.33 | 0.43 |
| 10:M:9:A:N6 | 10:M:46:A:C2 | 2.87 | 0.43 |
| 12:K:18:LYS:HD3 | 12:K:19:VAL:N | 2.32 | 0.43 |
| 3:C:1495:U:H2' | 3:C:1496:C:C6 | 2.53 | 0.43 |
| 13:L:324:ARG:NH2 | 13:L:383:THR:O | 2.51 | 0.43 |
| 8:I:1078:U:O2 | 8:I:1088:A:H4' | 2.18 | 0.43 |
| 13:L:252:ASP:O | 13:L:253:LEU:HB2 | 2.18 | 0.43 |
| 13:L:355:LEU:HD13 | 13:L:369:LEU:HD22 | 2.00 | 0.43 |
| 3:C:1499:A:C4 | 3:C:1500:A:C8 | 3.07 | 0.43 |
| 14:N:111:ARG:HG2 | 14:N:111:ARG:HH11 | 1.84 | 0.42 |
| 14:N:144:ARG:O | 14:N:147:LYS:N | 2.52 | 0.42 |
| 13:L:546:ILE:HD13 | 13:L:565:VAL:HG11 | 2.01 | 0.42 |
| 6:G:1854:A:H3' | 6:G:1855:G:C8 | 2.54 | 0.42 |
| 5:F:2662:A:O2' | 13:L:457:LEU:HD13 | 2.19 | 0.42 |
| 8:I:1052:C:O2 | 8:I:1053:C:C6 | 2.72 | 0.42 |
| 8:I:1068:G:C6 | 8:I:1073:A:H2 | 2.34 | 0.42 |
| 8:I:1082:U:C5 | 8:I:1083:U:C4 | 3.07 | 0.42 |
| 8:I:1084:A:N1 | 8:I:1085:A:C2 | 2.87 | 0.42 |
| 14:N:71:VAL:HB | 14:N:164:VAL:HG22 | 2.01 | 0.42 |
| 12:K:49:ILE:O | 12:K:51:PRO:HD3 | 2.19 | 0.42 |
| 13:L:539:ILE:N | 13:L:540:PRO:HD2 | 2.34 | 0.42 |
| 14:N:221:LEU:HD13 | 14:N:221:LEU:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:486:THR:C | 13:L:600:VAL:H | 2.21 | 0.42 |
| 8:I:1094:U:N3 | 8:I:1096:A:H5" | 2.34 | 0.42 |
| 9:J:2178:C:C5' | 12:K:46:LYS:HD2 | 2.50 | 0.42 |
| 13:L:414:GLU:O | 13:L:474:ALA:HB1 | 2.19 | 0.42 |
| 10:M:65:G:H2' | 10:M:66:U:C6 | 2.54 | 0.42 |
| 12:K:20:TYR:N | 12:K:20:TYR:CD1 | 2.88 | 0.42 |
| 9:J:2124:G:H2' | 9:J:2125:G:O4' | 2.19 | 0.42 |
| 13:L:409:ILE:HG12 | 13:L:656:ALA:HB3 | 2.01 | 0.42 |
| 8:I:1106:G:H2' | 8:I:1107:G:C8 | 2.54 | 0.42 |
| 14:N:17:PHE:HD2 | 14:N:17:PHE:N | 2.16 | 0.42 |
| 12:K:19:VAL:HB | 12:K:20:TYR:HD1 | 1.85 | 0.42 |
| 13:L:276:VAL:O | 13:L:280:LEU:HB2 | 2.19 | 0.42 |
| 14:N:174:VAL:O | 14:N:177:ALA:HB3 | 2.20 | 0.42 |
| 13:L:317:MET:O | 13:L:325:LEU:N | 2.52 | 0.42 |
| 11:E:7:ILE:O | 11:E:10:LEU:HB2 | 2.19 | 0.42 |
| 10:M:46:A:H2' | 10:M:48:U:O5' | 2.20 | 0.42 |
| 7:H:2462:U:O2' | 7:H:2463:C:H5' | 2.20 | 0.42 |
| 11:E:62:SER:C | 11:E:64:TYR:H | 2.23 | 0.42 |
| 13:L:682:GLN:HG3 | 13:L:686:LYS:CE | 2.48 | 0.42 |
| 3:C:1499:A:C2 | 3:C:1500:A:C8 | 3.08 | 0.42 |
| 13:L:556:ILE:CG1 | 13:L:601:ILE:HD11 | 2.22 | 0.42 |
| 13:L:627:ARG:O | 13:L:651:GLU:HG3 | 2.20 | 0.42 |
| 11:E:89:ARG:CZ | 11:E:89:ARG:HB2 | 2.47 | 0.42 |
| 7:H:2463:C:C2' | 7:H:2464:C:H5' | 2.49 | 0.42 |
| 13:L:427:ALA:HB1 | 13:L:470:PHE:CG | 2.55 | 0.42 |
| 13:L:611:THR:OG1 | 13:L:642:VAL:HG22 | 2.20 | 0.42 |
| 13:L:535:PRO:HD3 | 13:L:572:TYR:CD1 | 2.55 | 0.42 |
| 11:E:7:ILE:HD13 | 11:E:7:ILE:HA | 1.81 | 0.42 |
| 14:N:223:ILE:C | 14:N:225:ALA:N | 2.70 | 0.42 |
| 10:M:73:G:O2' | 10:M:74:C:C5' | 2.47 | 0.42 |
| 14:N:165:VAL:O | 14:N:187:LEU:O | 2.38 | 0.42 |
| 13:L:324:ARG:O | 13:L:324:ARG:HG3 | 2.20 | 0.42 |
| 13:L:185:ALA:HB3 | 13:L:199:ILE:O | 2.19 | 0.42 |
| 2:B:370:C:O2' | 2:B:371:G:H5' | 2.20 | 0.42 |
| 13:L:600:VAL:HG23 | 13:L:684:GLN:OE1 | 2.16 | 0.42 |
| 8:I:1067:A:O2' | 13:L:634:MET:CG | 2.68 | 0.42 |
| 8:I:1107:G:C8 | 8:I:1108:U:C5 | 3.07 | 0.42 |
| 10:M:75:C:C2 | 10:M:76:A:H5' | 2.55 | 0.42 |
| 8:I:1075:C:C2' | 8:I:1075:C:O2 | 2.68 | 0.42 |
| 8:I:1099:G:C4 | 8:I:1100:C:C5 | 3.08 | 0.42 |
| 8:I:1102:C:C2 | 8:I:1103:A:N7 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:339:C:H2' | 1:A:340:U:C6 | 2.55 | 0.42 |
| 12:K:169:GLY:O | 12:K:170:ALA:HB3 | 2.19 | 0.42 |
| 8:I:1061:U:P | 8:I:1061:U:C3' | 3.03 | 0.41 |
| 8:I:1080:C:C2' | 8:I:1081:U:H5' | 2.49 | 0.41 |
| 14:N:163:PHE:O | 14:N:164:VAL:HG23 | 2.20 | 0.41 |
| 14:N:58:ILE:HD11 | 14:N:185:ILE:HD12 | 2.02 | 0.41 |
| 8:I:1077:A:C8 | 8:I:1078:U:N3 | 2.88 | 0.41 |
| 13:L:9:LEU:HD22 | 13:L:283:PRO:HB2 | 2.02 | 0.41 |
| 12:K:86:ALA:HB1 | 12:K:94:VAL:HG11 | 2.02 | 0.41 |
| 11:E:113:ARG:NH1 | 11:E:120:TYR:CD2 | 2.88 | 0.41 |
| 13:L:302:HIS:O | 13:L:332:SER:HB3 | 2.20 | 0.41 |
| 13:L:321:TYR:O | 13:L:322:VAL:CG1 | 2.63 | 0.41 |
| 8:I:1072:C:OP2 | 8:I:1073:A:OP1 | 2.39 | 0.41 |
| 8:I:1086:A:C3' | 8:I:1087:G:C5' | 2.95 | 0.41 |
| 14:N:109:SER:O | 14:N:111:ARG:N | 2.54 | 0.41 |
| 14:N:191:ASP:OD1 | 14:N:191:ASP:O | 2.39 | 0.41 |
| 10:M:50:G:C5 | 10:M:65:G:C2 | 3.09 | 0.41 |
| 10:M:66:U:C4 | 10:M:67:C:N4 | 2.88 | 0.41 |
| 14:N:80:ILE:HD13 | 14:N:208:ILE:HG23 | 2.02 | 0.41 |
| 3:C:1422:G:C2 | 3:C:1423:G:C5 | 3.08 | 0.41 |
| 14:N:102:LEU:HD12 | 14:N:102:LEU:H | 1.81 | 0.41 |
| 13:L:88:VAL:HG12 | 13:L:121:VAL:HG12 | 2.01 | 0.41 |
| 10:M:74:C:H2' | 10:M:75:C:O4' | 2.20 | 0.41 |
| 14:N:163:PHE:CD2 | 14:N:186:ALA:HA | 2.55 | 0.41 |
| 14:N:17:PHE:CD1 | 14:N:44:LEU:HD21 | 2.55 | 0.41 |
| 10:M:24:G:C4 | 10:M:25:U:C6 | 3.08 | 0.41 |
| 13:L:203:GLU:HA | 13:L:206:LEU:HB2 | 2.01 | 0.41 |
| 12:K:92:ASP:CG | 12:K:93:TYR:N | 2.73 | 0.41 |
| 8:I:1083:U:H2' | 8:I:1083:U:O2 | 2.19 | 0.41 |
| 8:I:1094:U:H3 | 8:I:1096:A:H5" | 1.85 | 0.41 |
| 10:M:4:G:H2' | 10:M:5:U:O5' | 2.21 | 0.41 |
| 14:N:136:VAL:O | 14:N:140:HIS:HB2 | 2.21 | 0.41 |
| 13:L:20:HIS:CE1 | 13:L:21:ILE:HG22 | 2.54 | 0.41 |
| 13:L:95:GLU:OE1 | 13:L:402:ILE:HA | 2.19 | 0.41 |
| 6:G:1885:A:H8 | 6:G:1885:A:H5' | 1.86 | 0.41 |
| 13:L:416:LYS:HG2 | 13:L:474:ALA:HA | 2.01 | 0.41 |
| 14:N:9:GLU:HB2 | 14:N:10:LEU:H | 1.73 | 0.41 |
| 14:N:168:THR:HG23 | 14:N:192:SER:OG | 2.19 | 0.41 |
| 6:G:1862:G:O2' | 6:G:1863:G:H5' | 2.19 | 0.41 |
| 12:K:79:LYS:O | 12:K:96:GLY:HA3 | 2.20 | 0.41 |
| 13:L:108:PHE:HE2 | 13:L:134:ALA:HB1 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1087:G:O3' | 8:I:1089:G:H5' | 2.21 | 0.41 |
| 8:I:1087:G:C2' | 8:I:1103:A:H2 | 2.31 | 0.41 |
| 13:L:13:ARG:HD3 | 13:L:276:VAL:O | 2.21 | 0.41 |
| 9:J:2097:C:O2' | 9:J:2098:U:H5' | 2.20 | 0.41 |
| 13:L:459:LEU:O | 13:L:463:VAL:HG23 | 2.20 | 0.41 |
| 5:F:2655:G:N3 | 5:F:2655:G:H2' | 2.35 | 0.41 |
| 13:L:484:ARG:O | 13:L:647:VAL:HG23 | 2.06 | 0.41 |
| 8:I:1061:U:O2' | 8:I:1070:A:N3 | 2.45 | 0.41 |
| 8:I:1081:U:O4 | 8:I:1086:A:C4 | 2.74 | 0.41 |
| 8:I:1085:A:O2' | 8:I:1086:A:O5' | 2.39 | 0.41 |
| 13:L:87:HIS:HB3 | 13:L:90:PHE:HE1 | 1.86 | 0.41 |
| 14:N:143:GLU:O | 14:N:147:LYS:HB2 | 2.20 | 0.41 |
| 11:E:48:PRO:C | 11:E:49:ASN:HD22 | 2.24 | 0.41 |
| 11:E:32:PHE:HD1 | 11:E:86:ARG:HA | 1.85 | 0.41 |
| 14:N:80:ILE:O | 14:N:83:MET:HB2 | 2.20 | 0.41 |
| 14:N:97:TRP:CZ2 | 14:N:102:LEU:HD13 | 2.49 | 0.41 |
| 12:K:76:ALA:HB3 | 12:K:94:VAL:HG11 | 1.99 | 0.41 |
| 9:J:2097:C:H2' | 9:J:2098:U:O4' | 2.20 | 0.41 |
| 14:N:142:LEU:CD2 | 14:N:146:GLN:NE2 | 2.83 | 0.41 |
| 3:C:1419:G:C2 | 3:C:1420:C:C2 | 3.08 | 0.41 |
| 13:L:442:THR:HG23 | 13:L:447:GLY:O | 2.20 | 0.41 |
| 8:I:1063:G:C6 | 8:I:1064:C:N4 | 2.89 | 0.41 |
| 8:I:1066:U:C2 | 8:I:1069:A:P | 3.13 | 0.41 |
| 10:M:69:C:C4 | 10:M:70:G:N7 | 2.88 | 0.41 |
| 14:N:75:LYS:HG2 | 14:N:78:GLN:HE21 | 1.83 | 0.41 |
| 13:L:88:VAL:CG1 | 13:L:121:VAL:HG12 | 2.51 | 0.41 |
| 12:K:42:GLU:HG2 | 12:K:176:GLY:O | 2.21 | 0.41 |
| 13:L:486:THR:O | 13:L:600:VAL:CA | 2.67 | 0.41 |
| 8:I:1071:G:N2 | 8:I:1089:G:H2' | 2.36 | 0.41 |
| 8:I:1056:G:H21 | 8:I:1104:C:H42 | 1.69 | 0.41 |
| 8:I:1095:A:C6 | 13:L:614:GLU:OE1 | 2.62 | 0.41 |
| 10:M:14:A:N6 | 10:M:46:A:H2 | 2.19 | 0.41 |
| 13:L:85:PRO:HG2 | 13:L:94:VAL:HG22 | 2.02 | 0.41 |
| 14:N:69:LEU:HD12 | 14:N:92:TYR:HA | 2.03 | 0.41 |
| 10:M:25:U:C4 | 10:M:26:A:C5 | 3.09 | 0.41 |
| 13:L:579:GLU:O | 13:L:583:LYS:HB2 | 2.21 | 0.41 |
| 14:N:203:GLY:O | 14:N:204:ASN:C | 2.59 | 0.41 |
| 14:N:142:LEU:CD2 | 14:N:146:GLN:HE21 | 2.34 | 0.41 |
| 13:L:116:PRO:HB3 | 13:L:666:ARG:HG2 | 2.02 | 0.41 |
| 9:J:2172:U:H2' | 9:J:2174:C:O4' | 2.21 | 0.41 |
| 13:L:327:PHE:CE1 | 13:L:376:ALA:HB2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:L:561:VAL:HG13 | 13:L:602:LEU:HD12 | 1.98 | 0.41 |
| 13:L:648:PRO:HG2 | 13:L:651:GLU:HG3 | 2.03 | 0.41 |
| 8:I:1095:A:H5" | 13:L:618:GLY:H | 1.84 | 0.41 |
| 8:I:1097:U:C2 | 8:I:1098:A:C8 | 3.09 | 0.41 |
| 12:K:51:PRO:HB3 | 12:K:204:ALA:HB2 | 2.02 | 0.41 |
| 3:C:1495:U:C2 | 3:C:1496:C:C5 | 3.08 | 0.41 |
| 13:L:583:LYS:C | 13:L:583:LYS:HE2 | 2.42 | 0.41 |
| 13:L:344:THR:HG21 | 13:L:396:ARG:HA | 2.03 | 0.41 |
| 13:L:409:ILE:HA | 13:L:480:GLN:O | 2.20 | 0.40 |
| 13:L:627:ARG:HB3 | 13:L:651:GLU:HB3 | 2.02 | 0.40 |
| 8:I:1097:U:O2 | 8:I:1098:A:O4' | 2.38 | 0.40 |
| 8:I:1105:U:O2' | 8:I:1106:G:P | 2.79 | 0.40 |
| 12:K:46:LYS:NZ | 12:K:172:HIS:CB | 2.84 | 0.40 |
| 14:N:213:LEU:CD2 | 14:N:214:ILE:HD13 | 2.50 | 0.40 |
| 14:N:39:ILE:HG22 | 14:N:40:HIS:N | 2.34 | 0.40 |
| 12:K:51:PRO:O | 12:K:52:ARG:HB2 | 2.22 | 0.40 |
| 14:N:75:LYS:HA | 14:N:78:GLN:HE21 | 1.86 | 0.40 |
| 5:F:2669:G:C2 | 5:F:2670:A:C8 | 3.08 | 0.40 |
| 13:L:635:GLU:HA | 13:L:636:PRO:HD2 | 1.95 | 0.40 |
| 3:C:1446:U:O3' | 3:C:1447:A:H8 | 2.04 | 0.40 |
| 12:K:124:GLY:O | 12:K:125:SER:CB | 2.68 | 0.40 |
| 9:J:2128:C:C3' | 9:J:2129:C:H5" | 2.50 | 0.40 |
| 6:G:1847:A:N3 | 6:G:1847:A:H2' | 2.36 | 0.40 |
| 14:N:98:LEU:H | 14:N:101:MET:HE3 | 1.85 | 0.40 |
| 11:E:126:LYS:HD2 | 11:E:127:GLU:H | 1.87 | 0.40 |
| 6:G:1860:G:H2' | 6:G:1861:G:C8 | 2.56 | 0.40 |
| 7:H:2478:A:H3' | 7:H:2479:G:H8 | 1.87 | 0.40 |
| 13:L:177:ILE:HD12 | 13:L:271:LEU:HD12 | 2.03 | 0.40 |
| 5:F:2660:A:O2' | 13:L:660:ARG:HB2 | 2.21 | 0.40 |
| 8:I:1085:A:C1' | 8:I:1086:A:O5' | 2.70 | 0.40 |
| 8:I:1097:U:C6 | 8:I:1098:A:C8 | 3.09 | 0.40 |
| 14:N:115:LEU:HD23 | 14:N:153:ARG:NE | 2.35 | 0.40 |
| 14:N:164:VAL:HG13 | 14:N:165:VAL:N | 2.36 | 0.40 |
| 3:C:1469:G:H2' | 3:C:1470:G:C8 | 2.55 | 0.40 |
| 3:C:1452:C:H4' | 3:C:1456:G:O5' | 2.22 | 0.40 |
| 13:L:345:THR:HG21 | 13:L:387:ASP:OD1 | 2.21 | 0.40 |
| 14:N:116:GLU:HA | 14:N:119:GLU:HB2 | 2.02 | 0.40 |
| 14:N:113:HIS:O | 14:N:116:GLU:HG2 | 2.21 | 0.40 |
| 13:L:17:ILE:N | 13:L:17:ILE:CD1 | 2.84 | 0.40 |
| 11:E:30:ALA:HA | 11:E:31:PRO:HD3 | 1.96 | 0.40 |
| 8:I:1069:A:N7 | 8:I:1073:A:C5 | 2.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:1091:G:C2 | 8:I:1101:U:N3 | 2.90 | 0.40 |
| 13:L:92:ILE:CG2 | 13:L:93:GLU:H | 2.35 | 0.40 |
| 12:K:64:LEU:HD22 | 12:K:193:ILE:CB | 2.51 | 0.40 |
| 6:G:1886:C:H2' | 6:G:1887:C:H6 | 1.86 | 0.40 |
| 13:L:301:ILE:HD12 | 13:L:399:LEU:HD11 | 2.02 | 0.40 |
| 5:F:2667:C:C5 | 5:F:2668:G:N7 | 2.90 | 0.40 |
| 6:G:1882:C:H2' | 6:G:1882:C:O2 | 2.20 | 0.40 |
| 8:I:1095:A:O4' | 13:L:617:MET:SD | 2.60 | 0.40 |
| 11:E:46:LYS:HB2 | 11:E:92:ASP:O | 2.21 | 0.40 |
| 14:N:169:LYS:HB3 | 14:N:170:GLU:OE2 | 2.22 | 0.40 |
| 13:L:100:VAL:HG21 | 13:L:314:PHE:CD2 | 2.56 | 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 PDB entries followed by that with respect to all EM entries.

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 |
|---|---|---|---|---|---|---|
| 11 | E | 123/135 (91%) | 83 (68%) | 24 (20%) | 16 (13%) | 0 7 |
| 12 | K | 183/229 (80%) | 90 (49%) | 50 (27%) | 43 (24%) | 0 2 |
| 13 | L | 645/691 (93%) | 583 (90%) | 55 (8%) | 7 (1%) | 17 63 |
| 14 | N | 233/256 (91%) | 150 (64%) | 51 (22%) | 32 (14%) | 0 6 |
| All | All | 1184/1311 (90%) | 906 (76%) | 180 (15%) | 98 (8%) | 2 18 |

All (98) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | E | 28 | LYS |
| 11 | E | 47 | LYS |
| 11 | E | 91 | LYS |
| 11 | E | 92 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | K | 19 | VAL |
| 12 | K | 35 | ALA |
| 12 | K | 46 | LYS |
| 12 | K | 57 | ASN |
| 12 | K | 63 | SER |
| 12 | K | 160 | ARG |
| 12 | K | 161 | ILE |
| 12 | K | 166 | ASP |
| 12 | K | 172 | HIS |
| 12 | K | 173 | ALA |
| 12 | K | 174 | PRO |
| 12 | K | 179 | SER |
| 12 | K | 182 | PRO |
| 12 | K | 191 | ALA |
| 12 | K | 192 | PHE |
| 12 | K | 201 | PRO |
| 12 | K | 205 | LYS |
| 12 | K | 209 | LEU |
| 12 | K | 213 | TYR |
| 12 | K | 216 | THR |
| 12 | K | 220 | PRO |
| 13 | L | 322 | VAL |
| 14 | N | 15 | VAL |
| 14 | N | 52 | GLU |
| 14 | N | 77 | ALA |
| 14 | N | 84 | GLU |
| 14 | N | 154 | LEU |
| 14 | N | 165 | VAL |
| 14 | N | 195 | ASP |
| 14 | N | 226 | ARG |
| 11 | E | 12 | ARG |
| 11 | E | 29 | GLY |
| 11 | E | 72 | GLY |
| 12 | K | 62 | VAL |
| 12 | K | 125 | SER |
| 12 | K | 133 | PRO |
| 12 | K | 148 | ASN |
| 12 | K | 211 | SER |
| 12 | K | 214 | VAL |
| 13 | L | 10 | LYS |
| 14 | N | 8 | LYS |
| 14 | N | 9 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | N | 32 | ILE |
| 14 | N | 78 | GLN |
| 14 | N | 88 | ALA |
| 14 | N | 110 | GLN |
| 14 | N | 194 | PRO |
| 14 | N | 204 | ASN |
| 14 | N | 217 | ARG |
| 14 | N | 238 | LEU |
| 11 | E | 45 | PRO |
| 11 | E | 62 | SER |
| 11 | E | 96 | VAL |
| 11 | E | 115 | LYS |
| 12 | K | 49 | ILE |
| 12 | K | 140 | PRO |
| 12 | K | 198 | ALA |
| 12 | K | 204 | ALA |
| 12 | K | 210 | ARG |
| 12 | K | 217 | THR |
| 13 | L | 403 | GLU |
| 13 | L | 444 | PRO |
| 14 | N | 28 | PHE |
| 14 | N | 53 | ARG |
| 14 | N | 79 | ASP |
| 14 | N | 83 | MET |
| 14 | N | 101 | MET |
| 14 | N | 150 | SER |
| 14 | N | 237 | ALA |
| 11 | E | 51 | ALA |
| 11 | E | 79 | GLU |
| 12 | K | 55 | ASP |
| 12 | K | 64 | LEU |
| 12 | K | 77 | ILE |
| 12 | K | 183 | GLU |
| 12 | K | 202 | GLU |
| 14 | N | 18 | GLY |
| 14 | N | 20 | GLU |
| 14 | N | 97 | TRP |
| 14 | N | 130 | ARG |
| 14 | N | 216 | SER |
| 14 | N | 239 | VAL |
| 12 | K | 159 | GLY |
| 13 | L | 69 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | L | 203 | GLU |
| 14 | N | 181 | PHE |
| 11 | E | 18 | VAL |
| 12 | K | 130 | ILE |
| 12 | K | 149 | ILE |
| 12 | K | 175 | VAL |
| 11 | E | 43 | VAL |
| 13 | L | 554 | PRO |
| 11 | E | 48 | PRO |
| 12 | K | 103 | ILE |

### 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 PDB entries followed by that with respect to all EM entries.

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 |
|---|---|---|---|---|---|
| 11 | E | 104/111 (94%) | 95 (91%) | 9 (9%) | 13 45 |
| 12 | K | 61/181 (34%) | 54 (88%) | 7 (12%) | 7 32 |
| 13 | L | 553/582 (95%) | 510 (92%) | 43 (8%) | 16 51 |
| 14 | N | 202/220 (92%) | 182 (90%) | 20 (10%) | 10 39 |
| All | All | 920/1094 (84%) | 841 (91%) | 79 (9%) | 18 47 |

All (79) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | E | 20 | LYS |
| 11 | E | 41 | ARG |
| 11 | E | 53 | ARG |
| 11 | E | 62 | SER |
| 11 | E | 83 | VAL |
| 11 | E | 84 | LEU |
| 11 | E | 89 | ARG |
| 11 | E | 102 | ARG |
| 11 | E | 120 | TYR |
| 12 | K | 20 | TYR |
| 12 | K | 36 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | K | 41 | VAL |
| 12 | K | 58 | VAL |
| 12 | K | 64 | LEU |
| 12 | K | 77 | ILE |
| 12 | K | 101 | GLN |
| 13 | L | 33 | LEU |
| 13 | L | 69 | VAL |
| 13 | L | 100 | VAL |
| 13 | L | 162 | VAL |
| 13 | L | 166 | LEU |
| 13 | L | 167 | PRO |
| 13 | L | 170 | ARG |
| 13 | L | 171 | GLU |
| 13 | L | 181 | LEU |
| 13 | L | 190 | ASN |
| 13 | L | 196 | ILE |
| 13 | L | 203 | GLU |
| 13 | L | 232 | LEU |
| 13 | L | 238 | THR |
| 13 | L | 253 | LEU |
| 13 | L | 260 | LEU |
| 13 | L | 273 | LEU |
| 13 | L | 280 | LEU |
| 13 | L | 284 | LEU |
| 13 | L | 315 | LYS |
| 13 | L | 321 | TYR |
| 13 | L | 326 | THR |
| 13 | L | 328 | ILE |
| 13 | L | 336 | THR |
| 13 | L | 352 | VAL |
| 13 | L | 369 | LEU |
| 13 | L | 373 | ASP |
| 13 | L | 377 | VAL |
| 13 | L | 385 | THR |
| 13 | L | 389 | LEU |
| 13 | L | 403 | GLU |
| 13 | L | 416 | LYS |
| 13 | L | 420 | ASP |
| 13 | L | 461 | ILE |
| 13 | L | 473 | ASP |
| 13 | L | 536 | LYS |
| 13 | L | 614 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | L | 616 | TYR |
| 13 | L | 619 | ASP |
| 13 | L | 634 | MET |
| 13 | L | 647 | VAL |
| 13 | L | 659 | LEU |
| 13 | L | 660 | ARG |
| 14 | N | 10 | LEU |
| 14 | N | 15 | VAL |
| 14 | N | 16 | HIS |
| 14 | N | 17 | PHE |
| 14 | N | 22 | LYS |
| 14 | N | 24 | TRP |
| 14 | N | 36 | ARG |
| 14 | N | 44 | LEU |
| 14 | N | 59 | GLU |
| 14 | N | 79 | ASP |
| 14 | N | 102 | LEU |
| 14 | N | 130 | ARG |
| 14 | N | 137 | ARG |
| 14 | N | 145 | LEU |
| 14 | N | 178 | ARG |
| 14 | N | 187 | LEU |
| 14 | N | 196 | LEU |
| 14 | N | 204 | ASN |
| 14 | N | 215 | LEU |
| 14 | N | 221 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | E | 9 | GLN |
| 11 | E | 49 | ASN |
| 11 | E | 75 | HIS |
| 13 | L | 20 | HIS |
| 13 | L | 124 | GLN |
| 13 | L | 137 | ASN |
| 13 | L | 154 | GLN |
| 13 | L | 165 | GLN |
| 13 | L | 208 | GLN |
| 13 | L | 226 | ASN |
| 13 | L | 458 | HIS |
| 13 | L | 475 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | L | 480 | GLN |
| 13 | L | 500 | GLN |
| 13 | L | 506 | GLN |
| 13 | L | 543 | GLN |
| 13 | L | 551 | GLN |
| 13 | L | 625 | ASN |
| 13 | L | 641 | GLN |
| 13 | L | 677 | GLN |
| 14 | N | 37 | ASN |
| 14 | N | 40 | HIS |
| 14 | N | 78 | GLN |
| 14 | N | 146 | GLN |
| 14 | N | 204 | ASN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A | 11/12 (91%) | 1 (9%) | 0 |
| 10 | M | 73/74 (98%) | 26 (35%) | 2 (2%) |
| 2 | B | 8/28 (28%) | 0 | 0 |
| 3 | C | 95/96 (98%) | 11 (11%) | 2 (2%) |
| 4 | D | 11/303 (3%) | 0 | 0 |
| 5 | F | 28/29 (96%) | 7 (25%) | 1 (3%) |
| 6 | G | 53/54 (98%) | 12 (22%) | 1 (1%) |
| 7 | H | 41/42 (97%) | 8 (19%) | 1 (2%) |
| 8 | I | 57/58 (98%) | 34 (59%) | 5 (8%) |
| 9 | J | 72/102 (70%) | 29 (40%) | 2 (2%) |
| All | All | 449/798 (56%) | 128 (28%) | 14 (3%) |

All (128) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 345 | C |
| 3 | C | 1419 | G |
| 3 | C | 1442 | G |
| 3 | C | 1442(A) | G |
| 3 | C | 1442(B) | A |
| 3 | C | 1443 | G |
| 3 | C | 1447 | A |
| 3 | C | 1452 | C |
| 3 | C | 1487 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 1492 | A |
| 3 | C | 1498 | U |
| 3 | C | 1499 | A |
| 5 | F | 2654 | A |
| 5 | F | 2655 | G |
| 5 | F | 2660 | A |
| 5 | F | 2661 | G |
| 5 | F | 2662 | A |
| 5 | F | 2663 | G |
| 5 | F | 2673 | G |
| 6 | G | 1847 | A |
| 6 | G | 1858 | G |
| 6 | G | 1865 | G |
| 6 | G | 1866 | C |
| 6 | G | 1877 | A |
| 6 | G | 1878 | G |
| 6 | G | 1880 | C |
| 6 | G | 1882 | C |
| 6 | G | 1885 | A |
| 6 | G | 1886 | C |
| 6 | G | 1888 | G |
| 6 | G | 1900 | A |
| 7 | H | 2465 | C |
| 7 | H | 2469 | A |
| 7 | H | 2470 | G |
| 7 | H | 2476 | A |
| 7 | H | 2477 | C |
| 7 | H | 2478 | A |
| 7 | H | 2482 | G |
| 7 | H | 2484 | G |
| 8 | I | 1056 | G |
| 8 | I | 1059 | G |
| 8 | I | 1060 | U |
| 8 | I | 1061 | U |
| 8 | I | 1062 | G |
| 8 | I | 1063 | G |
| 8 | I | 1066 | U |
| 8 | I | 1067 | A |
| 8 | I | 1068 | G |
| 8 | I | 1069 | A |
| 8 | I | 1070 | A |
| 8 | I | 1071 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | I | 1072 | C |
| 8 | I | 1073 | A |
| 8 | I | 1074 | G |
| 8 | I | 1077 | A |
| 8 | I | 1083 | U |
| 8 | I | 1084 | A |
| 8 | I | 1086 | A |
| 8 | I | 1087 | G |
| 8 | I | 1088 | A |
| 8 | I | 1089 | G |
| 8 | I | 1090 | U |
| 8 | I | 1091 | G |
| 8 | I | 1093 | G |
| 8 | I | 1096 | A |
| 8 | I | 1097 | U |
| 8 | I | 1098 | A |
| 8 | I | 1099 | G |
| 8 | I | 1101 | U |
| 8 | I | 1103 | A |
| 8 | I | 1104 | C |
| 8 | I | 1105 | U |
| 8 | I | 1106 | G |
| 9 | J | 2099 | U |
| 9 | J | 2103 | C |
| 9 | J | 2104 | G |
| 9 | J | 2110 | G |
| 9 | J | 2111 | C |
| 9 | J | 2112 | G |
| 9 | J | 2116 | G |
| 9 | J | 2118 | U |
| 9 | J | 2119 | A |
| 9 | J | 2120 | G |
| 9 | J | 2122 | U |
| 9 | J | 2127 | G |
| 9 | J | 2128 | C |
| 9 | J | 2129 | C |
| 9 | J | 2130 | U |
| 9 | J | 2159 | G |
| 9 | J | 2161 | C |
| 9 | J | 2162 | G |
| 9 | J | 2164 | C |
| 9 | J | 2165 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | J | 2170 | A |
| 9 | J | 2171 | A |
| 9 | J | 2172 | U |
| 9 | J | 2176 | A |
| 9 | J | 2187 | G |
| 9 | J | 2190 | G |
| 9 | J | 2191 | G |
| 9 | J | 2192 | G |
| 9 | J | 2193 | G |
| 10 | M | 2 | C |
| 10 | M | 5 | U |
| 10 | M | 6 | G |
| 10 | M | 8 | 4SU |
| 10 | M | 9 | A |
| 10 | M | 18 | G |
| 10 | M | 20 | H2U |
| 10 | M | 21 | H2U |
| 10 | M | 22 | A |
| 10 | M | 30 | G |
| 10 | M | 32 | U |
| 10 | M | 34 | U |
| 10 | M | 41 | C |
| 10 | M | 44 | C |
| 10 | M | 45 | U |
| 10 | M | 46 | A |
| 10 | M | 48 | U |
| 10 | M | 49 | 5MC |
| 10 | M | 50 | G |
| 10 | M | 55 | PSU |
| 10 | M | 62 | C |
| 10 | M | 64 | C |
| 10 | M | 70 | G |
| 10 | M | 72 | A |
| 10 | M | 73 | G |
| 10 | M | 76 | A |

All (14) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 1442 | G |
| 3 | C | 1498 | U |
| 5 | F | 2662 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | G | 1885 | A |
| 7 | H | 2481 | G |
| 8 | I | 1069 | A |
| 8 | I | 1083 | U |
| 8 | I | 1085 | A |
| 8 | I | 1097 | U |
| 8 | I | 1100 | C |
| 9 | J | 2126 | A |
| 9 | J | 2191 | G |
| 10 | M | 1 | U |
| 10 | M | 33 | U |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 10 | H2U | M | 20 | 10 | 17,21,22 | 0.51 | 0 | 23,30,33 | 0.77 | 1 (4%) |
| 10 | H2U | M | 21 | 10 | 17,21,22 | 0.61 | 0 | 23,30,33 | 0.88 | 1 (4%) |
| 10 | 5MC | M | 49 | 10 | 14,22,23 | 1.17 | 2 (14%) | 17,32,35 | 1.36 | 5 (29%) |
| 10 | 5MU | M | 54 | 10 | 13,22,23 | 0.80 | 0 | 16,32,35 | 3.29 | 4 (25%) |
| 10 | PSU | M | 55 | 10 | 15,21,22 | 1.66 | 4 (26%) | 16,30,33 | 3.67 | 3 (18%) |
| 10 | 4SU | M | 8 | 10 | 12,21,22 | 1.66 | 2 (16%) | 15,30,33 | 2.32 | 1 (6%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 10 | H2U | M | 20 | 10 | - | 0/7/38/39 | 0/2/2/2 |
| 10 | H2U | M | 21 | 10 | - | 0/7/38/39 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 10 | 5MC | M | 49 | 10 | - | 0/3/25/26 | 0/2/2/2 |
| 10 | 5MU | M | 54 | 10 | - | 0/3/25/26 | 0/2/2/2 |
| 10 | PSU | M | 55 | 10 | - | 0/7/25/26 | 0/2/2/2 |
| 10 | 4SU | M | 8 | 10 | - | 0/3/25/26 | 0/2/2/2 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | M | 55 | PSU | C6-C5 | -3.03 | 1.34 | 1.38 |
| 10 | M | 49 | 5MC | C6-C5 | -2.83 | 1.32 | 1.40 |
| 10 | M | 55 | PSU | C5-C1' | -2.25 | 1.50 | 1.52 |
| 10 | M | 55 | PSU | C2'-C1' | -2.10 | 1.51 | 1.53 |
| 10 | M | 8 | 4SU | C6-C5 | -2.10 | 1.33 | 1.38 |
| 10 | M | 49 | 5MC | C5-C4 | 2.00 | 1.44 | 1.41 |
| 10 | M | 55 | PSU | C4-N3 | 3.91 | 1.40 | 1.33 |
| 10 | M | 8 | 4SU | C5-C4 | 4.92 | 1.44 | 1.38 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | M | 8 | 4SU | C5-C4-N3 | -8.75 | 114.28 | 123.56 |
| 10 | M | 54 | 5MU | C5-C4-N3 | -7.86 | 118.75 | 125.35 |
| 10 | M | 55 | PSU | C5-C1'-C2' | -2.74 | 110.78 | 115.44 |
| 10 | M | 21 | H2U | N3-C2-N1 | -2.46 | 114.36 | 116.64 |
| 10 | M | 20 | H2U | N3-C2-N1 | -2.38 | 114.44 | 116.64 |
| 10 | M | 49 | 5MC | CM5-C5-C4 | -2.29 | 119.04 | 121.47 |
| 10 | M | 54 | 5MU | C2'-C1'-N1 | -2.14 | 107.72 | 113.46 |
| 10 | M | 49 | 5MC | C2'-C1'-N1 | -2.06 | 107.93 | 113.46 |
| 10 | M | 54 | 5MU | O2'-C2'-C3' | -2.00 | 105.38 | 111.86 |
| 10 | M | 49 | 5MC | CM5-C5-C6 | 2.17 | 123.02 | 118.63 |
| 10 | M | 49 | 5MC | O4'-C1'-N1 | 2.19 | 112.27 | 108.10 |
| 10 | M | 49 | 5MC | N4-C4-N3 | 2.37 | 120.39 | 116.92 |
| 10 | M | 55 | PSU | O4'-C1'-C2' | 3.22 | 108.17 | 104.69 |
| 10 | M | 54 | 5MU | C4-N3-C2 | 9.74 | 123.28 | 115.16 |
| 10 | M | 55 | PSU | C4-N3-C2 | 13.74 | 126.62 | 115.16 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 10 | M | 20 | H2U | 2 | 0 |
| 10 | M | 49 | 5MC | 7 | 0 |
| 10 | M | 54 | 5MU | 2 | 0 |
| 10 | M | 55 | PSU | 3 | 0 |
| 10 | M | 8 | 4SU | 8 | 0 |

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.