



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:21 PM GMT

PDB ID : 1T3N
Title : Structure of the catalytic core of DNA polymerase Iota in complex with DNA and dTTP
Authors : Nair, D.T.; Johnson, R.E.; Prakash, S.; Prakash, L.; Aggarwal, A.K.
Deposited on : 2004-04-27
Resolution : 2.30 Å(reported)

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

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

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

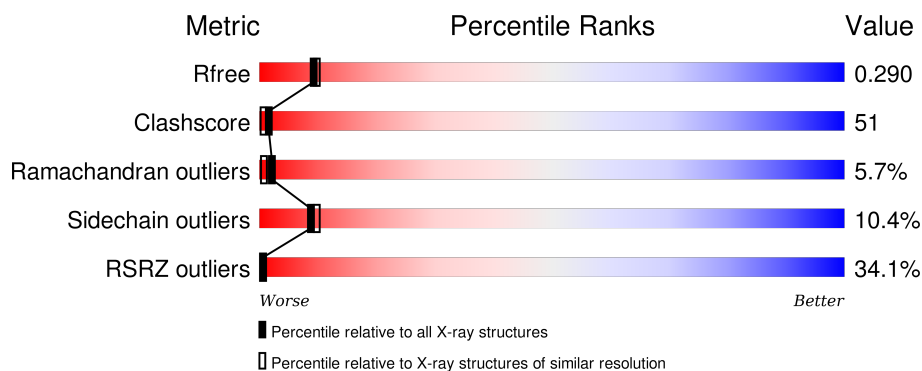
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 3852 (2.30-2.30) |
| Clashscore | 102246 | 4452 (2.30-2.30) |
| Ramachandran outliers | 100387 | 4410 (2.30-2.30) |
| Sidechain outliers | 100360 | 4409 (2.30-2.30) |
| RSRZ outliers | 91569 | 3857 (2.30-2.30) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 1-T | 14 | <div> <div>36%</div> <div>43%</div> <div>57%</div> </div> |
| 1 | 2-T | 14 | <div> <div>36%</div> <div>43%</div> <div>57%</div> </div> |
| 2 | 1-P | 13 | <div> <div>31%</div> <div>38%</div> <div>62%</div> </div> |
| 2 | 2-P | 13 | <div> <div>31%</div> <div>38%</div> <div>62%</div> </div> |
| 3 | 1-A | 388 | <div> <div>34%</div> <div>49%</div> <div>41%</div> <div>8%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | 1-B | 388 | |
| 3 | 2-A | 388 | |
| 3 | 2-B | 388 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | TTP | 1-B | 902 | - | - | - | X |
| 5 | TTP | 2-B | 902 | - | - | - | X |

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13538 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called Template DNA strand.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 1 | 1-T | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 277 | 133 | 47 | 84 | 13 | | | |
| 1 | 2-T | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 277 | 133 | 47 | 84 | 13 | | | |

- Molecule 2 is a DNA chain called Primer DNA strand.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 2 | 1-P | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 270 | 127 | 59 | 72 | 12 | | | |
| 2 | 2-P | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 270 | 127 | 59 | 72 | 12 | | | |

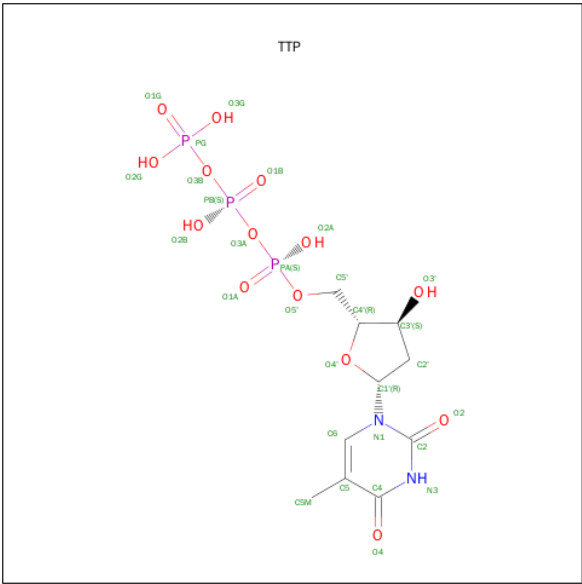
- Molecule 3 is a protein called polymerase (DNA directed) iota.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | 1-A | 388 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2868 | 1801 | 502 | 547 | 18 | | | |
| 3 | 2-A | 388 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2868 | 1801 | 502 | 547 | 18 | | | |
| 3 | 1-B | 388 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2886 | 1812 | 509 | 547 | 18 | | | |
| 3 | 2-B | 388 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2886 | 1812 | 509 | 547 | 18 | | | |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | 1-B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | 2-B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5 | 1-B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 29 | 10 | 2 | 14 | 3 | | |
| 5 | 2-B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 29 | 10 | 2 | 14 | 3 | | |

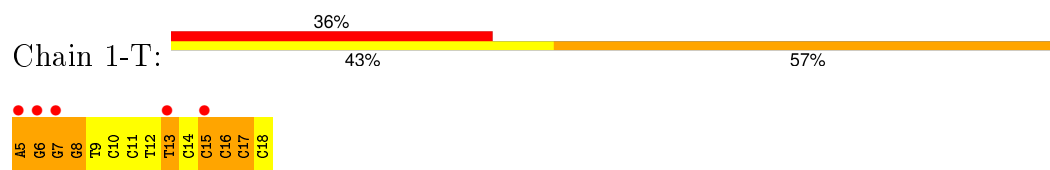
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6 | 1-T | 11 | Total | O | 0 | 0 |
| | | | 11 | 11 | | |
| 6 | 2-T | 209 | Total | O | 0 | 0 |
| | | | 209 | 209 | | |
| 6 | 1-P | 12 | Total | O | 0 | 0 |
| | | | 12 | 12 | | |
| 6 | 2-P | 208 | Total | O | 0 | 0 |
| | | | 208 | 208 | | |
| 6 | 1-A | 207 | Total | O | 0 | 0 |
| | | | 207 | 207 | | |
| 6 | 2-A | 11 | Total | O | 0 | 0 |
| | | | 11 | 11 | | |
| 6 | 1-B | 208 | Total | O | 0 | 0 |
| | | | 208 | 208 | | |
| 6 | 2-B | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |

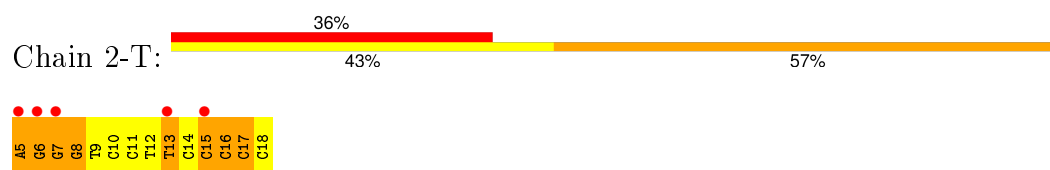
3 Residue-property plots [i](#)

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

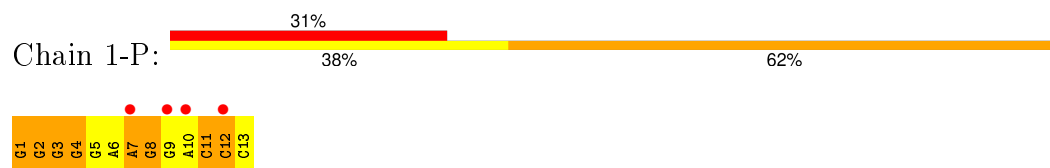
- Molecule 1: Template DNA strand



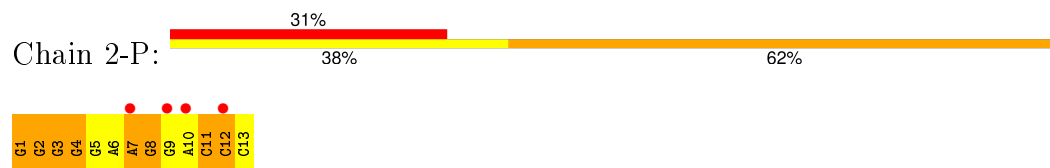
- Molecule 1: Template DNA strand



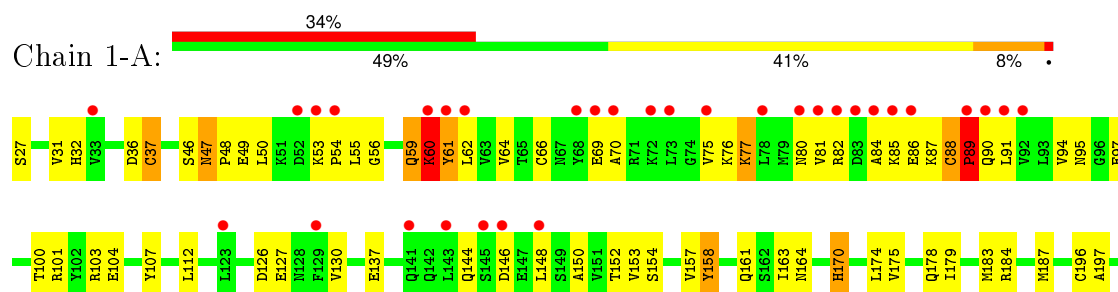
- Molecule 2: Primer DNA strand

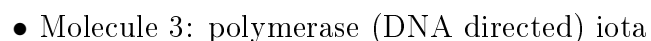
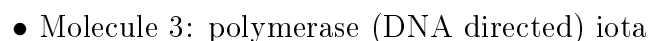


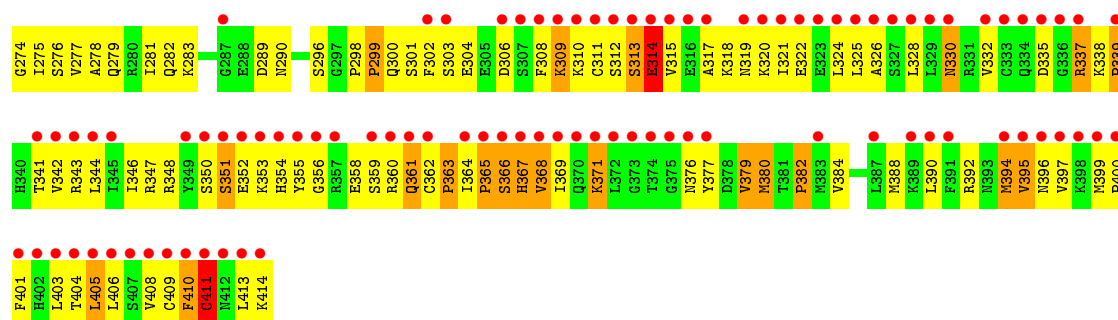
- Molecule 2: Primer DNA strand



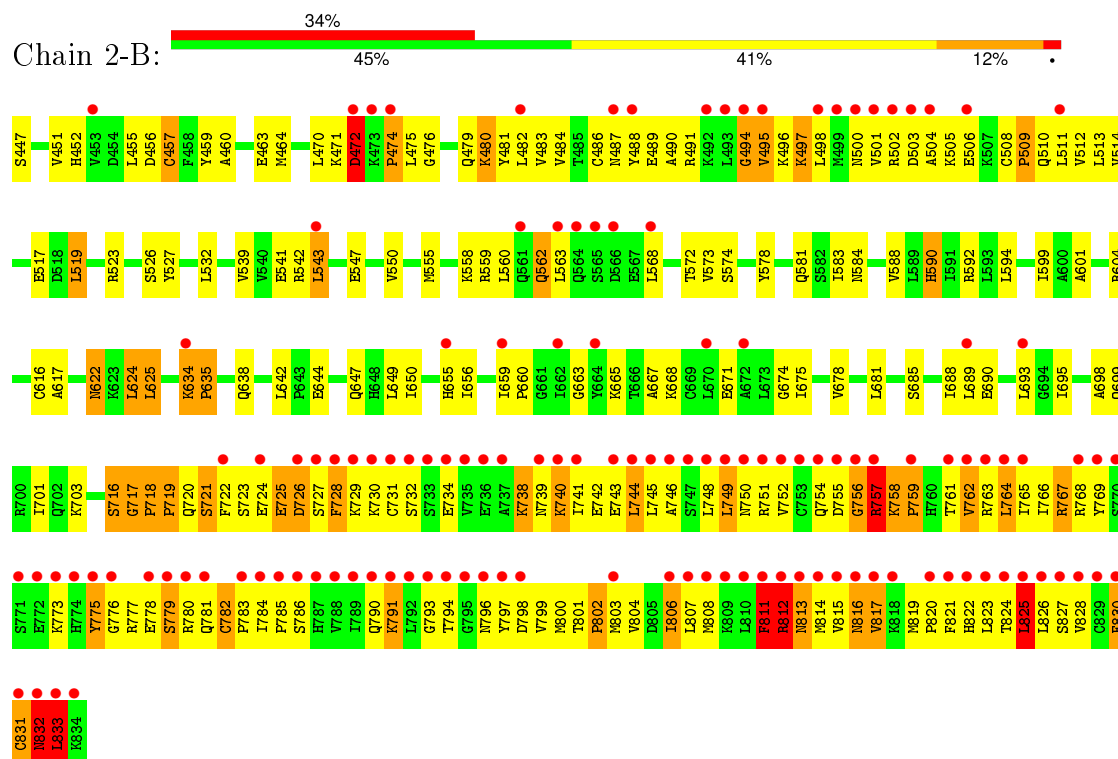
- Molecule 3: polymerase (DNA directed) iota







- Molecule 3: polymerase (DNA directed) iota



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 65 | Depositor |
| Cell constants a, b, c, α , β , γ | 98.83Å 98.83Å 202.75Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 50.00 – 2.30 39.43 – 2.30 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (50.00-2.30) 96.9 (39.43-2.30) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.41 (at 2.29Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.265 , 0.286 0.271 , 0.290 | Depositor DCC |
| R_{free} test set | 4842 reflections (11.20%) | DCC |
| Wilson B-factor (Å ²) | 42.1 | Xtriage |
| Anisotropy | 0.408 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.24 , 73.3 | EDS |
| Estimated twinning fraction | 0.478 for h,-h-k,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Outliers | 1 of 49675 reflections (0.002%) | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 13538 | wwPDB-VP |
| Average B, all atoms (Å ²) | 57.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, MG, TTP

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | 1-T | 0.77 | 0/308 | 1.22 | 3/472 (0.6%) |
| 1 | 2-T | 0.76 | 0/308 | 1.22 | 3/472 (0.6%) |
| 2 | 1-P | 1.20 | 2/285 (0.7%) | 1.55 | 7/440 (1.6%) |
| 2 | 2-P | 1.20 | 2/285 (0.7%) | 1.54 | 7/440 (1.6%) |
| 3 | 1-A | 0.51 | 1/2908 (0.0%) | 0.85 | 8/3946 (0.2%) |
| 3 | 1-B | 0.63 | 2/2928 (0.1%) | 0.99 | 20/3975 (0.5%) |
| 3 | 2-A | 0.50 | 1/2908 (0.0%) | 0.85 | 8/3946 (0.2%) |
| 3 | 2-B | 0.63 | 3/2928 (0.1%) | 0.99 | 21/3975 (0.5%) |
| All | All | 0.62 | 11/12858 (0.1%) | 0.98 | 77/17666 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 1-T | 1 | 6 |
| 1 | 2-T | 1 | 6 |
| 2 | 1-P | 0 | 3 |
| 2 | 2-P | 0 | 3 |
| 3 | 1-B | 0 | 1 |
| 3 | 2-B | 0 | 1 |
| All | All | 2 | 20 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | 1-P | 12 | DC | C3'-O3' | -12.37 | 1.27 | 1.44 |
| 2 | 2-P | 12 | DC | C3'-O3' | -12.34 | 1.27 | 1.44 |
| 3 | 1-B | 832 | ASN | N-CA | 7.35 | 1.61 | 1.46 |
| 3 | 2-B | 832 | ASN | N-CA | 7.33 | 1.61 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | 2-A | 60 | LYS | CB-CG | -6.49 | 1.35 | 1.52 |
| 3 | 1-A | 60 | LYS | CB-CG | -6.46 | 1.35 | 1.52 |
| 3 | 2-B | 816 | ASN | C-O | -6.18 | 1.11 | 1.23 |
| 3 | 1-B | 816 | ASN | C-O | -6.18 | 1.11 | 1.23 |
| 3 | 2-B | 721 | SER | N-CA | 5.81 | 1.57 | 1.46 |
| 2 | 1-P | 11 | DC | O3'-P | -5.58 | 1.54 | 1.61 |
| 2 | 2-P | 11 | DC | O3'-P | -5.41 | 1.54 | 1.61 |

All (77) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 3 | 1-A | 60 | LYS | CB-CG-CD | -12.63 | 78.75 | 111.60 |
| 3 | 2-A | 60 | LYS | CB-CG-CD | -12.63 | 78.77 | 111.60 |
| 3 | 2-B | 757 | ARG | CB-CG-CD | 10.15 | 138.00 | 111.60 |
| 3 | 1-B | 757 | ARG | CB-CG-CD | 10.15 | 138.00 | 111.60 |
| 3 | 1-B | 831 | CYS | N-CA-C | 9.52 | 136.71 | 111.00 |
| 3 | 2-B | 831 | CYS | N-CA-C | 9.51 | 136.67 | 111.00 |
| 3 | 1-B | 831 | CYS | C-N-CA | 8.07 | 141.88 | 121.70 |
| 3 | 2-B | 831 | CYS | C-N-CA | 8.07 | 141.88 | 121.70 |
| 3 | 1-B | 819 | MET | C-N-CD | -8.05 | 102.88 | 120.60 |
| 3 | 2-B | 819 | MET | C-N-CD | -8.04 | 102.91 | 120.60 |
| 3 | 1-B | 811 | PHE | C-N-CA | 7.78 | 141.16 | 121.70 |
| 3 | 1-B | 757 | ARG | CA-CB-CG | 7.77 | 130.49 | 113.40 |
| 3 | 2-B | 811 | PHE | C-N-CA | 7.75 | 141.06 | 121.70 |
| 3 | 2-B | 757 | ARG | CA-CB-CG | 7.74 | 130.43 | 113.40 |
| 3 | 1-B | 756 | GLY | CA-C-N | -7.67 | 100.33 | 117.20 |
| 3 | 2-B | 756 | GLY | CA-C-N | -7.65 | 100.37 | 117.20 |
| 3 | 1-A | 394 | MET | C-N-CA | 7.35 | 140.08 | 121.70 |
| 3 | 2-A | 394 | MET | C-N-CA | 7.35 | 140.08 | 121.70 |
| 3 | 2-B | 811 | PHE | CB-CG-CD2 | 7.01 | 125.71 | 120.80 |
| 2 | 1-P | 11 | DC | O3'-P-O5' | -6.99 | 90.72 | 104.00 |
| 3 | 1-B | 816 | ASN | C-N-CA | -6.96 | 104.29 | 121.70 |
| 3 | 1-B | 811 | PHE | CB-CG-CD2 | 6.95 | 125.66 | 120.80 |
| 3 | 2-B | 816 | ASN | C-N-CA | -6.95 | 104.34 | 121.70 |
| 3 | 1-A | 394 | MET | CA-C-N | -6.90 | 102.02 | 117.20 |
| 3 | 2-B | 811 | PHE | CA-C-N | -6.89 | 102.04 | 117.20 |
| 3 | 2-A | 394 | MET | CA-C-N | -6.89 | 102.04 | 117.20 |
| 3 | 2-A | 411 | CYS | C-N-CA | 6.87 | 138.88 | 121.70 |
| 3 | 1-A | 411 | CYS | C-N-CA | 6.87 | 138.88 | 121.70 |
| 3 | 1-B | 817 | VAL | N-CA-C | 6.86 | 129.53 | 111.00 |
| 3 | 1-B | 811 | PHE | CA-C-N | -6.86 | 102.10 | 117.20 |
| 3 | 2-B | 817 | VAL | N-CA-C | 6.84 | 129.47 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 2-B | 756 | GLY | C-N-CA | 6.77 | 138.63 | 121.70 |
| 3 | 2-A | 60 | LYS | CA-CB-CG | 6.76 | 128.28 | 113.40 |
| 3 | 1-A | 60 | LYS | CA-CB-CG | 6.76 | 128.26 | 113.40 |
| 3 | 1-B | 756 | GLY | C-N-CA | 6.75 | 138.57 | 121.70 |
| 3 | 1-A | 59 | GLN | CA-C-N | -6.61 | 102.66 | 117.20 |
| 2 | 2-P | 3 | DG | C5'-C4'-C3' | -6.61 | 102.20 | 114.10 |
| 3 | 2-A | 59 | GLN | CA-C-N | -6.61 | 102.67 | 117.20 |
| 2 | 1-P | 3 | DG | C5'-C4'-C3' | -6.60 | 102.22 | 114.10 |
| 3 | 2-B | 764 | LEU | N-CA-C | -6.43 | 93.64 | 111.00 |
| 3 | 1-B | 764 | LEU | N-CA-C | -6.40 | 93.73 | 111.00 |
| 1 | 1-T | 15 | DC | C2'-C3'-O3' | 6.39 | 133.69 | 112.60 |
| 1 | 2-T | 15 | DC | C2'-C3'-O3' | 6.37 | 133.62 | 112.60 |
| 2 | 2-P | 11 | DC | C4'-C3'-O3' | 6.27 | 125.37 | 109.70 |
| 2 | 1-P | 11 | DC | C4'-C3'-O3' | 6.25 | 125.33 | 109.70 |
| 3 | 1-A | 394 | MET | O-C-N | 6.03 | 132.35 | 122.70 |
| 2 | 2-P | 11 | DC | O3'-P-O5' | -6.03 | 92.55 | 104.00 |
| 3 | 2-A | 394 | MET | O-C-N | 6.01 | 132.32 | 122.70 |
| 2 | 2-P | 12 | DC | O4'-C4'-C3' | -5.98 | 102.11 | 104.50 |
| 2 | 1-P | 12 | DC | O4'-C4'-C3' | -5.87 | 102.15 | 104.50 |
| 3 | 1-B | 833 | LEU | CA-CB-CG | 5.83 | 128.70 | 115.30 |
| 3 | 2-B | 833 | LEU | CA-CB-CG | 5.83 | 128.70 | 115.30 |
| 2 | 1-P | 12 | DC | N1-C1'-C2' | 5.80 | 123.62 | 112.60 |
| 3 | 2-B | 832 | ASN | C-N-CA | 5.79 | 136.17 | 121.70 |
| 2 | 2-P | 12 | DC | N1-C1'-C2' | 5.78 | 123.58 | 112.60 |
| 3 | 1-B | 832 | ASN | C-N-CA | 5.72 | 136.01 | 121.70 |
| 1 | 1-T | 13 | DT | C4'-C3'-O3' | 5.56 | 123.60 | 109.70 |
| 1 | 2-T | 13 | DT | C4'-C3'-O3' | 5.53 | 123.52 | 109.70 |
| 3 | 1-B | 758 | LYS | N-CA-C | 5.51 | 125.89 | 111.00 |
| 3 | 2-B | 758 | LYS | N-CA-C | 5.51 | 125.87 | 111.00 |
| 3 | 1-B | 832 | ASN | CA-C-N | -5.45 | 105.20 | 117.20 |
| 3 | 2-B | 831 | CYS | O-C-N | 5.43 | 131.39 | 122.70 |
| 3 | 2-B | 832 | ASN | CA-C-N | -5.43 | 105.26 | 117.20 |
| 3 | 1-B | 831 | CYS | O-C-N | 5.41 | 131.36 | 122.70 |
| 3 | 2-B | 634 | LYS | N-CA-C | 5.38 | 125.53 | 111.00 |
| 3 | 1-B | 634 | LYS | N-CA-C | 5.37 | 125.50 | 111.00 |
| 1 | 2-T | 13 | DT | C4'-C3'-C2' | 5.31 | 107.88 | 103.10 |
| 2 | 2-P | 4 | DG | C5'-C4'-C3' | -5.27 | 104.61 | 114.10 |
| 2 | 1-P | 4 | DG | C5'-C4'-C3' | -5.25 | 104.65 | 114.10 |
| 1 | 1-T | 13 | DT | C4'-C3'-C2' | 5.23 | 107.81 | 103.10 |
| 3 | 1-B | 756 | GLY | O-C-N | 5.21 | 131.04 | 122.70 |
| 3 | 2-B | 756 | GLY | O-C-N | 5.21 | 131.03 | 122.70 |
| 3 | 1-A | 214 | LYS | N-CA-C | 5.18 | 124.99 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 2-A | 214 | LYS | N-CA-C | 5.15 | 124.91 | 111.00 |
| 2 | 2-P | 7 | DA | C4'-C3'-O3' | 5.12 | 122.53 | 112.30 |
| 2 | 1-P | 7 | DA | C4'-C3'-O3' | 5.06 | 122.42 | 112.30 |
| 3 | 2-B | 757 | ARG | N-CA-CB | 5.05 | 119.68 | 110.60 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | 1-T | 13 | DT | C3' |
| 1 | 2-T | 13 | DT | C3' |

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | 1-B | 816 | ASN | Mainchain |
| 2 | 1-P | 1 | DG | Sidechain |
| 2 | 1-P | 2 | DG | Sidechain |
| 2 | 1-P | 8 | DG | Sidechain |
| 1 | 1-T | 16 | DC | Sidechain |
| 1 | 1-T | 17 | DC | Sidechain |
| 1 | 1-T | 5 | DA | Sidechain |
| 1 | 1-T | 6 | DG | Sidechain |
| 1 | 1-T | 7 | DG | Sidechain |
| 1 | 1-T | 8 | DG | Sidechain |
| 3 | 2-B | 816 | ASN | Mainchain |
| 2 | 2-P | 1 | DG | Sidechain |
| 2 | 2-P | 2 | DG | Sidechain |
| 2 | 2-P | 8 | DG | Sidechain |
| 1 | 2-T | 16 | DC | Sidechain |
| 1 | 2-T | 17 | DC | Sidechain |
| 1 | 2-T | 5 | DA | Sidechain |
| 1 | 2-T | 6 | DG | Sidechain |
| 1 | 2-T | 7 | DG | Sidechain |
| 1 | 2-T | 8 | DG | Sidechain |

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1-T | 277 | 0 | 159 | 59 | 0 |
| 1 | 2-T | 277 | 0 | 159 | 55 | 0 |
| 2 | 1-P | 270 | 0 | 145 | 46 | 0 |
| 2 | 2-P | 270 | 0 | 145 | 39 | 0 |
| 3 | 1-A | 2868 | 0 | 2764 | 247 | 0 |
| 3 | 1-B | 2886 | 0 | 2789 | 306 | 0 |
| 3 | 2-A | 2868 | 0 | 2764 | 252 | 0 |
| 3 | 2-B | 2886 | 0 | 2789 | 306 | 0 |
| 4 | 1-B | 1 | 0 | 0 | 0 | 0 |
| 4 | 2-B | 1 | 0 | 0 | 0 | 0 |
| 5 | 1-B | 29 | 0 | 10 | 2 | 0 |
| 5 | 2-B | 29 | 0 | 10 | 4 | 0 |
| 6 | 1-A | 207 | 0 | 0 | 18 | 0 |
| 6 | 1-B | 208 | 0 | 0 | 20 | 0 |
| 6 | 1-P | 12 | 0 | 0 | 0 | 0 |
| 6 | 1-T | 11 | 0 | 0 | 1 | 0 |
| 6 | 2-A | 11 | 0 | 0 | 0 | 0 |
| 6 | 2-B | 10 | 0 | 0 | 1 | 0 |
| 6 | 2-P | 208 | 0 | 0 | 18 | 0 |
| 6 | 2-T | 209 | 0 | 0 | 29 | 0 |
| All | All | 13538 | 0 | 11734 | 1236 | 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 51.

All (1236) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 3:B:729:LYS:O | 3:B:730:LYS:HG2 | 1.26 | 1.34 |
| 3:B:729:LYS:O | 3:B:730:LYS:HG2 | 1.26 | 1.33 |
| 3:B:763:ARG:O | 3:B:828:VAL:HG13 | 1.33 | 1.28 |
| 3:B:763:ARG:O | 3:B:828:VAL:HG13 | 1.33 | 1.27 |
| 3:A:60:LYS:O | 3:A:61:TYR:HD1 | 1.22 | 1.21 |
| 3:B:807:LEU:O | 3:B:811:PHE:CD1 | 1.95 | 1.20 |
| 2:P:8:DG:H3' | 3:B:776:GLY:O | 1.42 | 1.19 |
| 2:P:8:DG:H3' | 3:B:776:GLY:O | 1.41 | 1.19 |
| 3:A:409:CYS:SG | 3:A:411:CYS:HB2 | 1.82 | 1.18 |
| 3:A:60:LYS:O | 3:A:61:TYR:HD1 | 1.22 | 1.18 |
| 3:B:807:LEU:O | 3:B:811:PHE:CD1 | 1.95 | 1.18 |
| 3:A:409:CYS:SG | 3:A:411:CYS:HB2 | 1.82 | 1.18 |
| 3:B:780:ARG:NH2 | 3:B:812:ARG:O | 1.77 | 1.17 |
| 3:B:807:LEU:O | 3:B:811:PHE:HD1 | 1.26 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:60:LYS:O | 3:A:61:TYR:CD1 | 1.98 | 1.17 |
| 3:A:60:LYS:O | 3:A:61:TYR:CD1 | 1.98 | 1.17 |
| 3:B:780:ARG:NH2 | 3:B:812:ARG:O | 1.77 | 1.17 |
| 1:T:6:DG:H2'' | 1:T:7:DG:H5' | 1.19 | 1.15 |
| 3:A:366:SER:O | 3:A:367:HIS:CG | 2.00 | 1.15 |
| 2:P:8:DG:C3' | 3:B:776:GLY:O | 1.94 | 1.14 |
| 2:P:8:DG:C3' | 3:B:776:GLY:O | 1.96 | 1.13 |
| 3:A:366:SER:O | 3:A:367:HIS:CG | 2.00 | 1.13 |
| 1:T:6:DG:H2'' | 1:T:7:DG:H5' | 1.19 | 1.09 |
| 1:T:11:DC:H2'' | 1:T:12:DT:H5'' | 1.25 | 1.09 |
| 3:B:825:LEU:H | 3:B:825:LEU:HD23 | 1.18 | 1.08 |
| 3:B:778:GLU:O | 3:B:779:SER:HB3 | 1.51 | 1.08 |
| 3:B:825:LEU:H | 3:B:825:LEU:HD23 | 1.18 | 1.08 |
| 3:A:342:VAL:HG13 | 3:A:364:ILE:HD11 | 1.14 | 1.08 |
| 3:A:342:VAL:HG13 | 3:A:364:ILE:HD11 | 1.14 | 1.08 |
| 1:T:11:DC:H2'' | 1:T:12:DT:H5'' | 1.25 | 1.07 |
| 3:A:380:MET:O | 3:A:384:VAL:HG23 | 1.55 | 1.07 |
| 3:B:807:LEU:O | 3:B:811:PHE:HD1 | 1.26 | 1.06 |
| 1:T:11:DC:C2' | 1:T:12:DT:H5'' | 1.87 | 1.05 |
| 3:A:380:MET:O | 3:A:384:VAL:HG23 | 1.55 | 1.05 |
| 1:T:11:DC:C2' | 1:T:12:DT:H5'' | 1.87 | 1.05 |
| 6:T:185:HOH:O | 3:A:158:TYR:O | 1.72 | 1.05 |
| 3:B:501:VAL:HG12 | 3:B:502:ARG:H | 1.19 | 1.04 |
| 3:B:791:LYS:HB3 | 3:B:794:THR:CG2 | 1.87 | 1.04 |
| 3:B:791:LYS:HB3 | 3:B:794:THR:CG2 | 1.87 | 1.04 |
| 1:T:17:DC:OP1 | 3:A:246:THR:OG1 | 1.75 | 1.04 |
| 3:A:392:ARG:O | 3:A:395:VAL:CB | 2.06 | 1.04 |
| 3:B:791:LYS:HB3 | 3:B:794:THR:HG21 | 1.39 | 1.03 |
| 3:B:763:ARG:O | 3:B:828:VAL:CG1 | 2.06 | 1.03 |
| 3:B:763:ARG:O | 3:B:828:VAL:CG1 | 2.06 | 1.03 |
| 3:A:342:VAL:HG13 | 3:A:364:ILE:CD1 | 1.89 | 1.03 |
| 3:A:342:VAL:HG13 | 3:A:364:ILE:CD1 | 1.89 | 1.02 |
| 3:B:501:VAL:HG12 | 3:B:502:ARG:H | 1.19 | 1.02 |
| 3:B:729:LYS:O | 3:B:730:LYS:CG | 2.08 | 1.02 |
| 3:A:392:ARG:O | 3:A:395:VAL:CB | 2.06 | 1.02 |
| 3:B:778:GLU:O | 3:B:779:SER:HB3 | 1.51 | 1.02 |
| 1:T:17:DC:OP1 | 3:A:246:THR:OG1 | 1.75 | 1.01 |
| 3:A:365:PRO:HB2 | 3:A:369:ILE:HD13 | 1.42 | 1.01 |
| 3:B:729:LYS:O | 3:B:730:LYS:CG | 2.08 | 1.01 |
| 6:T:182:HOH:O | 3:A:103:ARG:HD2 | 1.59 | 1.01 |
| 6:P:198:HOH:O | 3:B:486:CYS:SG | 2.18 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:791:LYS:HB3 | 3:B:794:THR:HG21 | 1.39 | 1.01 |
| 3:B:723:SER:HB2 | 3:B:828:VAL:O | 1.61 | 1.01 |
| 2:P:1:DG:H2'' | 2:P:2:DG:H5'' | 1.42 | 1.00 |
| 3:A:365:PRO:HB2 | 3:A:369:ILE:HD13 | 1.42 | 1.00 |
| 3:A:328:LEU:O | 3:A:332:VAL:HG23 | 1.60 | 1.00 |
| 3:A:328:LEU:O | 3:A:332:VAL:HG23 | 1.61 | 0.99 |
| 3:B:723:SER:HB2 | 3:B:828:VAL:O | 1.61 | 0.99 |
| 3:A:366:SER:O | 3:A:367:HIS:ND1 | 1.95 | 0.99 |
| 3:B:752:VAL:O | 3:B:755:ASP:O | 1.81 | 0.99 |
| 1:T:14:DC:H2'' | 1:T:15:DC:H5' | 1.42 | 0.99 |
| 3:B:752:VAL:O | 3:B:755:ASP:O | 1.81 | 0.99 |
| 3:A:107:TYR:OH | 3:A:299:PRO:HG3 | 1.63 | 0.99 |
| 3:A:107:TYR:OH | 3:A:299:PRO:HG3 | 1.64 | 0.98 |
| 3:A:366:SER:O | 3:A:367:HIS:ND1 | 1.95 | 0.98 |
| 2:P:1:DG:H2'' | 2:P:2:DG:H5'' | 1.42 | 0.97 |
| 1:T:14:DC:H2'' | 1:T:15:DC:H5' | 1.42 | 0.97 |
| 2:P:8:DG:OP2 | 3:B:779:SER:OG | 1.82 | 0.96 |
| 2:P:8:DG:OP2 | 3:B:779:SER:OG | 1.83 | 0.96 |
| 3:A:404:THR:HG22 | 3:A:405:LEU:H | 1.29 | 0.96 |
| 2:P:8:DG:O5' | 3:B:777:ARG:HA | 1.66 | 0.95 |
| 3:A:308:PHE:CB | 3:A:405:LEU:HD22 | 1.97 | 0.95 |
| 3:A:404:THR:HG22 | 3:A:405:LEU:H | 1.29 | 0.94 |
| 3:A:308:PHE:CB | 3:A:405:LEU:HD22 | 1.97 | 0.94 |
| 6:T:211:HOH:O | 3:A:290:ASN:HB2 | 1.66 | 0.94 |
| 2:P:8:DG:O5' | 3:B:777:ARG:HA | 1.64 | 0.93 |
| 3:B:826:LEU:O | 3:B:826:LEU:HD12 | 1.69 | 0.93 |
| 3:B:734:GLU:OE2 | 3:B:821:PHE:HA | 1.68 | 0.93 |
| 1:T:12:DT:OP1 | 3:A:363:PRO:CD | 2.15 | 0.93 |
| 3:B:826:LEU:HD12 | 3:B:826:LEU:O | 1.68 | 0.93 |
| 3:A:366:SER:O | 3:A:367:HIS:CE1 | 2.22 | 0.92 |
| 3:A:103:ARG:HD2 | 6:A:581:HOH:O | 1.68 | 0.92 |
| 3:B:759:PRO:HD3 | 3:B:833:LEU:CD1 | 1.99 | 0.92 |
| 3:B:734:GLU:OE2 | 3:B:821:PHE:HA | 1.68 | 0.92 |
| 3:A:366:SER:O | 3:A:367:HIS:CE1 | 2.22 | 0.92 |
| 6:T:123:HOH:O | 3:A:289:ASP:OD1 | 1.87 | 0.92 |
| 3:B:759:PRO:HD3 | 3:B:833:LEU:CD1 | 1.99 | 0.92 |
| 6:T:231:HOH:O | 3:A:27:SER:N | 2.02 | 0.91 |
| 3:B:542:ARG:HG3 | 3:B:716:SER:OG | 1.70 | 0.91 |
| 3:B:542:ARG:HG3 | 3:B:716:SER:OG | 1.70 | 0.91 |
| 3:A:317:ALA:HA | 3:A:320:LYS:HG3 | 1.52 | 0.91 |
| 3:B:791:LYS:O | 3:B:794:THR:HG22 | 1.72 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:6:DG:H2'' | 1:T:7:DG:C5' | 2.01 | 0.90 |
| 1:T:12:DT:OP1 | 3:A:363:PRO:HD2 | 1.71 | 0.90 |
| 1:T:6:DG:H2'' | 1:T:7:DG:C5' | 2.00 | 0.90 |
| 3:A:317:ALA:HA | 3:A:320:LYS:HG3 | 1.51 | 0.90 |
| 3:B:762:VAL:HG21 | 3:B:803:MET:CE | 2.01 | 0.90 |
| 3:B:724:GLU:O | 3:B:744:LEU:HD12 | 1.72 | 0.90 |
| 3:B:791:LYS:O | 3:B:794:THR:HG22 | 1.72 | 0.89 |
| 3:A:346:ILE:O | 3:A:358:GLU:CB | 2.21 | 0.89 |
| 3:B:822:HIS:O | 3:B:823:LEU:HG | 1.72 | 0.89 |
| 3:B:762:VAL:HG21 | 3:B:803:MET:CE | 2.01 | 0.89 |
| 3:A:392:ARG:O | 3:A:395:VAL:CA | 2.21 | 0.89 |
| 3:B:822:HIS:O | 3:B:823:LEU:HG | 1.72 | 0.89 |
| 6:P:226:HOH:O | 3:B:717:GLY:HA3 | 1.71 | 0.89 |
| 2:P:6:DA:H2' | 2:P:7:DA:C8 | 2.08 | 0.89 |
| 3:A:346:ILE:O | 3:A:358:GLU:CB | 2.21 | 0.89 |
| 3:B:724:GLU:O | 3:B:744:LEU:HD12 | 1.72 | 0.89 |
| 3:A:366:SER:O | 3:A:367:HIS:CD2 | 2.26 | 0.88 |
| 3:A:348:ARG:HA | 3:A:403:LEU:CB | 2.04 | 0.88 |
| 3:A:348:ARG:HA | 3:A:403:LEU:CB | 2.04 | 0.88 |
| 3:A:366:SER:O | 3:A:367:HIS:CD2 | 2.26 | 0.88 |
| 6:T:122:HOH:O | 3:A:231:HIS:ND1 | 2.05 | 0.88 |
| 3:A:392:ARG:O | 3:A:395:VAL:CA | 2.21 | 0.88 |
| 2:P:6:DA:H2' | 2:P:7:DA:C8 | 2.08 | 0.88 |
| 3:B:486:CYS:SG | 6:B:1098:HOH:O | 2.29 | 0.88 |
| 3:A:371:LYS:H | 3:A:371:LYS:HD3 | 1.39 | 0.87 |
| 3:A:290:ASN:HB2 | 6:A:610:HOH:O | 1.73 | 0.86 |
| 3:B:763:ARG:C | 3:B:764:LEU:HD12 | 1.95 | 0.86 |
| 3:B:763:ARG:C | 3:B:764:LEU:HD12 | 1.95 | 0.86 |
| 3:A:360:ARG:HB3 | 3:A:390:LEU:HD22 | 1.58 | 0.86 |
| 6:T:270:HOH:O | 3:A:94:VAL:HG13 | 1.74 | 0.86 |
| 3:A:347:ARG:CB | 3:A:356:GLY:O | 2.23 | 0.86 |
| 3:A:347:ARG:CB | 3:A:356:GLY:O | 2.23 | 0.86 |
| 3:A:164:ASN:H | 3:A:170:HIS:HD2 | 1.20 | 0.85 |
| 3:A:164:ASN:H | 3:A:170:HIS:HD2 | 1.20 | 0.85 |
| 3:A:343:ARG:O | 3:A:344:LEU:HD12 | 1.77 | 0.85 |
| 3:A:371:LYS:H | 3:A:371:LYS:HD3 | 1.39 | 0.85 |
| 3:A:343:ARG:O | 3:A:344:LEU:HD12 | 1.76 | 0.85 |
| 1:T:6:DG:C2' | 1:T:7:DG:H5' | 2.05 | 0.85 |
| 3:B:756:GLY:O | 3:B:757:ARG:HD3 | 1.77 | 0.84 |
| 3:B:471:LYS:HD3 | 3:B:472:ASP:H | 1.43 | 0.84 |
| 3:B:756:GLY:O | 3:B:757:ARG:HD3 | 1.78 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:759:PRO:HD3 | 3:B:833:LEU:HD11 | 1.57 | 0.84 |
| 3:B:762:VAL:HG21 | 3:B:803:MET:HE1 | 1.58 | 0.84 |
| 3:B:471:LYS:HD3 | 3:B:472:ASP:H | 1.43 | 0.84 |
| 3:B:724:GLU:HG2 | 3:B:748:LEU:HD23 | 1.60 | 0.84 |
| 3:B:475:LEU:O | 3:B:486:CYS:HB2 | 1.78 | 0.84 |
| 3:B:762:VAL:HG21 | 3:B:803:MET:HE1 | 1.59 | 0.84 |
| 3:A:313:SER:O | 3:A:315:VAL:HG12 | 1.78 | 0.83 |
| 3:A:313:SER:O | 3:A:315:VAL:N | 2.11 | 0.83 |
| 3:B:759:PRO:HD3 | 3:B:833:LEU:HD11 | 1.57 | 0.83 |
| 3:A:313:SER:O | 3:A:315:VAL:N | 2.11 | 0.83 |
| 3:B:763:ARG:O | 3:B:764:LEU:HD12 | 1.78 | 0.83 |
| 3:A:313:SER:O | 3:A:315:VAL:HG12 | 1.78 | 0.83 |
| 3:A:360:ARG:HB3 | 3:A:390:LEU:HD22 | 1.58 | 0.83 |
| 3:B:763:ARG:O | 3:B:764:LEU:HD12 | 1.78 | 0.83 |
| 1:T:6:DG:C2' | 1:T:7:DG:H5' | 2.05 | 0.83 |
| 3:B:475:LEU:O | 3:B:486:CYS:HB2 | 1.78 | 0.83 |
| 1:T:12:DT:OP1 | 3:A:363:PRO:CD | 2.26 | 0.82 |
| 3:B:584:ASN:H | 3:B:590:HIS:HD2 | 1.23 | 0.82 |
| 1:T:12:DT:H2'' | 1:T:13:DT:C6 | 2.13 | 0.82 |
| 3:A:365:PRO:O | 3:A:369:ILE:HB | 1.79 | 0.82 |
| 6:P:220:HOH:O | 3:B:674:GLY:C | 2.17 | 0.82 |
| 3:A:365:PRO:O | 3:A:369:ILE:HB | 1.80 | 0.82 |
| 3:B:584:ASN:H | 3:B:590:HIS:HD2 | 1.24 | 0.82 |
| 1:T:12:DT:H2'' | 1:T:13:DT:C6 | 2.13 | 0.82 |
| 3:B:724:GLU:HG2 | 3:B:748:LEU:HD23 | 1.60 | 0.82 |
| 3:B:755:ASP:OD2 | 3:B:756:GLY:O | 1.97 | 0.82 |
| 3:B:755:ASP:OD2 | 3:B:756:GLY:O | 1.97 | 0.81 |
| 6:P:206:HOH:O | 3:B:523:ARG:HD3 | 1.80 | 0.81 |
| 3:A:314:GLU:CD | 3:A:401:PHE:CB | 2.50 | 0.81 |
| 3:B:721:SER:HB3 | 3:B:831:CYS:HB2 | 1.62 | 0.81 |
| 3:A:367:HIS:CD2 | 3:A:368:VAL:HG22 | 2.16 | 0.81 |
| 3:A:367:HIS:CD2 | 3:A:368:VAL:HG22 | 2.16 | 0.80 |
| 3:A:314:GLU:CD | 3:A:401:PHE:CB | 2.50 | 0.80 |
| 3:B:690:GLU:HG3 | 3:B:695:ILE:HA | 1.64 | 0.80 |
| 1:T:15:DC:H2'' | 1:T:16:DC:H5'' | 1.62 | 0.80 |
| 3:B:721:SER:HB3 | 3:B:831:CYS:HB2 | 1.63 | 0.80 |
| 3:B:690:GLU:HG3 | 3:B:695:ILE:HA | 1.64 | 0.80 |
| 3:B:763:ARG:HB3 | 3:B:781:GLN:HG2 | 1.63 | 0.80 |
| 3:A:306:ASP:O | 3:A:405:LEU:HB3 | 1.81 | 0.80 |
| 3:A:409:CYS:SG | 3:A:411:CYS:CB | 2.69 | 0.80 |
| 3:B:812:ARG:HH11 | 3:B:812:ARG:HG3 | 1.48 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:158:TYR:O | 6:A:584:HOH:O | 2.00 | 0.79 |
| 3:A:409:CYS:SG | 3:A:411:CYS:CB | 2.69 | 0.79 |
| 3:B:685:SER:HB3 | 3:B:688:ILE:HG22 | 1.63 | 0.79 |
| 3:B:802:PRO:O | 3:B:806:ILE:HG23 | 1.82 | 0.79 |
| 1:T:15:DC:H2'' | 1:T:16:DC:H5'' | 1.62 | 0.79 |
| 3:B:802:PRO:O | 3:B:806:ILE:HG23 | 1.82 | 0.79 |
| 3:B:685:SER:HB3 | 3:B:688:ILE:HG22 | 1.63 | 0.79 |
| 3:B:812:ARG:HH11 | 3:B:812:ARG:HG3 | 1.48 | 0.79 |
| 3:B:822:HIS:O | 3:B:823:LEU:CG | 2.30 | 0.79 |
| 3:A:306:ASP:O | 3:A:405:LEU:HB3 | 1.81 | 0.79 |
| 3:A:371:LYS:HD3 | 3:A:371:LYS:N | 1.98 | 0.79 |
| 3:A:94:VAL:HG13 | 6:A:668:HOH:O | 1.84 | 0.78 |
| 3:B:734:GLU:OE2 | 3:B:821:PHE:CA | 2.32 | 0.78 |
| 3:B:763:ARG:HB3 | 3:B:781:GLN:HG2 | 1.63 | 0.78 |
| 3:A:404:THR:HG22 | 3:A:405:LEU:N | 1.99 | 0.78 |
| 3:B:734:GLU:OE2 | 3:B:821:PHE:CB | 2.31 | 0.78 |
| 3:B:822:HIS:O | 3:B:823:LEU:CG | 2.30 | 0.78 |
| 3:B:800:MET:O | 3:B:804:VAL:HG23 | 1.84 | 0.78 |
| 1:T:7:DG:H5'' | 3:B:519:LEU:HG | 1.65 | 0.78 |
| 1:T:12:DT:H2' | 1:T:13:DT:H72 | 1.65 | 0.78 |
| 3:A:404:THR:HG22 | 3:A:405:LEU:N | 1.99 | 0.78 |
| 3:B:721:SER:HB2 | 3:B:831:CYS:HB3 | 1.66 | 0.78 |
| 3:B:825:LEU:CD2 | 3:B:825:LEU:H | 1.89 | 0.77 |
| 3:B:734:GLU:OE2 | 3:B:821:PHE:CB | 2.31 | 0.77 |
| 3:A:371:LYS:HD3 | 3:A:371:LYS:N | 1.98 | 0.77 |
| 1:T:12:DT:OP1 | 3:A:363:PRO:HD2 | 1.84 | 0.77 |
| 3:B:807:LEU:O | 3:B:811:PHE:CE1 | 2.37 | 0.77 |
| 3:B:800:MET:O | 3:B:804:VAL:HG23 | 1.84 | 0.77 |
| 3:B:734:GLU:OE2 | 3:B:821:PHE:CA | 2.32 | 0.77 |
| 1:T:12:DT:OP1 | 3:A:363:PRO:HD3 | 1.85 | 0.77 |
| 3:A:324:LEU:O | 3:A:328:LEU:HG | 1.85 | 0.76 |
| 3:B:825:LEU:H | 3:B:825:LEU:CD2 | 1.89 | 0.76 |
| 3:B:717:GLY:HA3 | 6:B:1126:HOH:O | 1.84 | 0.76 |
| 3:B:740:LYS:O | 3:B:744:LEU:HD23 | 1.85 | 0.76 |
| 3:B:727:SER:HB2 | 3:B:825:LEU:HB3 | 1.66 | 0.76 |
| 3:B:807:LEU:O | 3:B:811:PHE:CE1 | 2.37 | 0.76 |
| 1:T:11:DC:H2'' | 1:T:12:DT:C5' | 2.13 | 0.76 |
| 1:T:12:DT:H2' | 1:T:13:DT:H72 | 1.65 | 0.76 |
| 3:B:791:LYS:HB3 | 3:B:794:THR:HG22 | 1.68 | 0.76 |
| 3:B:721:SER:HB2 | 3:B:831:CYS:HB3 | 1.66 | 0.76 |
| 3:A:377:TYR:HD1 | 3:A:377:TYR:O | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:501:VAL:HG12 | 3:B:502:ARG:N | 1.98 | 0.76 |
| 3:A:377:TYR:HD1 | 3:A:377:TYR:O | 1.68 | 0.76 |
| 1:T:7:DG:H5" | 3:B:519:LEU:HG | 1.67 | 0.75 |
| 3:A:85:LYS:HA | 3:A:91:LEU:HD23 | 1.67 | 0.75 |
| 3:A:85:LYS:HA | 3:A:91:LEU:HD23 | 1.67 | 0.75 |
| 3:B:790:GLN:O | 3:B:791:LYS:NZ | 2.16 | 0.75 |
| 3:A:324:LEU:O | 3:A:328:LEU:HG | 1.85 | 0.75 |
| 3:B:740:LYS:O | 3:B:744:LEU:HD23 | 1.85 | 0.75 |
| 3:B:725:GLU:HB2 | 3:B:827:SER:HA | 1.69 | 0.75 |
| 3:A:59:GLN:O | 3:A:62:LEU:N | 2.19 | 0.75 |
| 3:B:791:LYS:HE3 | 3:B:791:LYS:HA | 1.69 | 0.75 |
| 3:B:791:LYS:HE3 | 3:B:791:LYS:HA | 1.69 | 0.75 |
| 3:B:825:LEU:N | 3:B:825:LEU:HD23 | 2.01 | 0.75 |
| 3:A:59:GLN:O | 3:A:62:LEU:N | 2.19 | 0.75 |
| 3:A:289:ASP:OD1 | 6:A:523:HOH:O | 2.03 | 0.75 |
| 3:B:727:SER:HB2 | 3:B:825:LEU:HB3 | 1.66 | 0.74 |
| 2:P:8:DG:O5' | 3:B:777:ARG:CA | 2.35 | 0.74 |
| 3:A:314:GLU:OE2 | 3:A:401:PHE:CB | 2.35 | 0.74 |
| 3:B:825:LEU:N | 3:B:825:LEU:HD23 | 2.01 | 0.74 |
| 3:B:724:GLU:HG2 | 3:B:748:LEU:CD2 | 2.18 | 0.74 |
| 3:B:791:LYS:HB3 | 3:B:794:THR:HG22 | 1.68 | 0.74 |
| 1:T:13:DT:H2' | 1:T:14:DC:C6 | 2.23 | 0.74 |
| 3:B:725:GLU:HB2 | 3:B:827:SER:HA | 1.68 | 0.74 |
| 3:A:365:PRO:HB2 | 3:A:369:ILE:CD1 | 2.17 | 0.74 |
| 1:T:11:DC:H2" | 1:T:12:DT:C5' | 2.13 | 0.74 |
| 3:A:395:VAL:O | 3:A:397:VAL:N | 2.21 | 0.74 |
| 3:B:743:GLU:O | 3:B:746:ALA:HB3 | 1.88 | 0.74 |
| 3:B:725:GLU:OE1 | 3:B:827:SER:HB3 | 1.88 | 0.74 |
| 3:A:395:VAL:O | 3:A:397:VAL:N | 2.21 | 0.74 |
| 3:B:778:GLU:O | 3:B:779:SER:CB | 2.32 | 0.73 |
| 3:B:501:VAL:HG12 | 3:B:502:ARG:N | 1.98 | 0.73 |
| 3:A:377:TYR:CD1 | 3:A:377:TYR:O | 2.41 | 0.73 |
| 3:B:592:ARG:HH11 | 3:B:592:ARG:HG2 | 1.51 | 0.73 |
| 1:T:13:DT:H2' | 1:T:14:DC:C6 | 2.23 | 0.73 |
| 3:B:724:GLU:HG2 | 3:B:748:LEU:CD2 | 2.17 | 0.73 |
| 3:B:743:GLU:O | 3:B:746:ALA:HB3 | 1.88 | 0.73 |
| 3:B:725:GLU:OE1 | 3:B:827:SER:HB3 | 1.88 | 0.73 |
| 3:A:314:GLU:OE1 | 3:A:401:PHE:CB | 2.36 | 0.73 |
| 3:A:339:PRO:HG3 | 3:A:413:LEU:CD2 | 2.19 | 0.73 |
| 3:A:342:VAL:CG1 | 3:A:364:ILE:HD11 | 2.08 | 0.73 |
| 3:B:762:VAL:HG11 | 3:B:806:ILE:HD11 | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:592:ARG:HH11 | 3:B:592:ARG:HG2 | 1.51 | 0.73 |
| 3:A:314:GLU:OE2 | 3:A:401:PHE:CB | 2.35 | 0.73 |
| 3:B:767:ARG:HB2 | 3:B:775:TYR:O | 1.88 | 0.73 |
| 3:A:365:PRO:HB2 | 3:A:369:ILE:CD1 | 2.17 | 0.73 |
| 3:A:377:TYR:CD1 | 3:A:377:TYR:O | 2.41 | 0.73 |
| 2:P:2:DG:H2'' | 2:P:3:DG:O5' | 1.89 | 0.72 |
| 3:B:767:ARG:HB2 | 3:B:775:TYR:O | 1.88 | 0.72 |
| 2:P:8:DG:C4' | 3:B:776:GLY:O | 2.36 | 0.72 |
| 3:A:342:VAL:CG1 | 3:A:364:ILE:HD11 | 2.08 | 0.72 |
| 2:P:2:DG:H2'' | 2:P:3:DG:O5' | 1.89 | 0.72 |
| 3:A:314:GLU:OE1 | 3:A:401:PHE:CB | 2.36 | 0.72 |
| 3:B:762:VAL:HB | 3:B:784:ILE:HD11 | 1.71 | 0.72 |
| 2:P:8:DG:O5' | 3:B:777:ARG:CA | 2.38 | 0.72 |
| 3:B:727:SER:CB | 3:B:825:LEU:HB3 | 2.20 | 0.72 |
| 3:B:762:VAL:HG11 | 3:B:806:ILE:HD11 | 1.71 | 0.72 |
| 3:A:337:ARG:HG2 | 3:A:414:LYS:O | 1.89 | 0.72 |
| 3:A:379:VAL:O | 3:A:382:PRO:CD | 2.38 | 0.72 |
| 3:A:379:VAL:O | 3:A:382:PRO:CD | 2.38 | 0.72 |
| 3:B:727:SER:CB | 3:B:825:LEU:HB3 | 2.20 | 0.72 |
| 3:A:337:ARG:HG2 | 3:A:414:LYS:O | 1.89 | 0.72 |
| 3:A:339:PRO:HG3 | 3:A:413:LEU:CD2 | 2.19 | 0.72 |
| 3:B:721:SER:HB3 | 3:B:831:CYS:CB | 2.19 | 0.71 |
| 6:T:172:HOH:O | 3:A:239:ILE:O | 2.09 | 0.71 |
| 3:A:270:GLU:HG3 | 3:A:275:ILE:HA | 1.70 | 0.71 |
| 3:B:724:GLU:N | 3:B:748:LEU:HD21 | 2.05 | 0.71 |
| 3:B:762:VAL:HB | 3:B:784:ILE:HD11 | 1.71 | 0.71 |
| 3:B:801:THR:CB | 3:B:802:PRO:CD | 2.69 | 0.71 |
| 3:A:303:SER:HB2 | 3:A:409:CYS:HA | 1.73 | 0.71 |
| 3:A:88:CYS:O | 3:A:90:GLN:N | 2.24 | 0.71 |
| 6:T:256:HOH:O | 3:A:58:GLN:OE1 | 2.08 | 0.71 |
| 3:B:801:THR:CB | 3:B:802:PRO:CD | 2.69 | 0.71 |
| 3:A:88:CYS:O | 3:A:90:GLN:N | 2.24 | 0.71 |
| 1:T:14:DC:H2' | 1:T:15:DC:C5 | 2.26 | 0.71 |
| 3:B:721:SER:HB3 | 3:B:831:CYS:CB | 2.20 | 0.71 |
| 3:A:270:GLU:HG3 | 3:A:275:ILE:HA | 1.70 | 0.71 |
| 3:B:790:GLN:O | 3:B:791:LYS:NZ | 2.16 | 0.70 |
| 3:B:724:GLU:N | 3:B:748:LEU:HD21 | 2.05 | 0.70 |
| 3:B:573:VAL:HB | 3:B:594:LEU:HD22 | 1.72 | 0.70 |
| 3:B:622:ASN:ND2 | 3:B:625:LEU:H | 1.89 | 0.70 |
| 3:B:721:SER:CB | 3:B:831:CYS:HB3 | 2.21 | 0.70 |
| 3:B:622:ASN:ND2 | 3:B:625:LEU:H | 1.89 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:778:GLU:O | 3:B:779:SER:CB | 2.32 | 0.70 |
| 3:B:674:GLY:C | 6:B:1120:HOH:O | 2.29 | 0.70 |
| 1:T:14:DC:H2' | 1:T:15:DC:C5 | 2.26 | 0.70 |
| 3:A:84:ALA:HA | 3:A:87:LYS:HG2 | 1.74 | 0.70 |
| 3:B:573:VAL:HB | 3:B:594:LEU:HD22 | 1.71 | 0.70 |
| 3:A:303:SER:HB2 | 3:A:409:CYS:HA | 1.72 | 0.70 |
| 3:B:721:SER:CB | 3:B:831:CYS:HB3 | 2.21 | 0.70 |
| 2:P:8:DG:C4' | 3:B:776:GLY:O | 2.38 | 0.70 |
| 3:A:47:ASN:ND2 | 3:A:49:GLU:HG2 | 2.07 | 0.70 |
| 1:T:12:DT:OP1 | 3:A:363:PRO:HD3 | 1.91 | 0.70 |
| 3:B:762:VAL:HG21 | 3:B:803:MET:HE3 | 1.73 | 0.70 |
| 3:A:84:ALA:HA | 3:A:87:LYS:HG2 | 1.74 | 0.70 |
| 1:T:11:DC:C3' | 1:T:12:DT:H5'' | 2.22 | 0.70 |
| 1:T:12:DT:O2 | 6:B:1005:HOH:O | 2.07 | 0.70 |
| 3:B:584:ASN:H | 3:B:590:HIS:CD2 | 2.09 | 0.70 |
| 1:T:14:DC:H2' | 1:T:15:DC:C6 | 2.27 | 0.70 |
| 3:A:366:SER:C | 3:A:367:HIS:CG | 2.63 | 0.69 |
| 3:B:734:GLU:HG3 | 3:B:821:PHE:CB | 2.22 | 0.69 |
| 3:B:721:SER:HA | 3:B:833:LEU:HD23 | 1.73 | 0.69 |
| 3:A:409:CYS:HG | 3:A:411:CYS:HB2 | 1.57 | 0.69 |
| 1:T:14:DC:H2' | 1:T:15:DC:C6 | 2.27 | 0.69 |
| 3:B:734:GLU:HG3 | 3:B:821:PHE:CB | 2.22 | 0.69 |
| 3:B:526:SER:OG | 3:B:542:ARG:NH2 | 2.26 | 0.69 |
| 3:A:47:ASN:ND2 | 3:A:49:GLU:HG2 | 2.07 | 0.69 |
| 3:B:812:ARG:HH11 | 3:B:812:ARG:CG | 2.06 | 0.69 |
| 1:T:18:DC:OP1 | 6:T:172:HOH:O | 2.11 | 0.69 |
| 3:B:768:ARG:HH21 | 3:B:812:ARG:NH2 | 1.91 | 0.69 |
| 3:A:366:SER:C | 3:A:367:HIS:CG | 2.63 | 0.69 |
| 3:B:584:ASN:H | 3:B:590:HIS:CD2 | 2.09 | 0.69 |
| 3:A:371:LYS:HE2 | 3:A:376:ASN:HB2 | 1.75 | 0.69 |
| 1:T:11:DC:C3' | 1:T:12:DT:H5'' | 2.22 | 0.69 |
| 2:P:11:DC:H2'' | 2:P:12:DC:O4' | 1.92 | 0.69 |
| 3:B:768:ARG:HH21 | 3:B:812:ARG:NH2 | 1.91 | 0.69 |
| 1:T:5:DA:H4' | 3:B:480:LYS:HB2 | 1.75 | 0.68 |
| 3:B:812:ARG:HH11 | 3:B:812:ARG:CG | 2.06 | 0.68 |
| 3:B:526:SER:OG | 3:B:542:ARG:NH2 | 2.25 | 0.68 |
| 3:B:721:SER:HA | 3:B:833:LEU:HD23 | 1.74 | 0.68 |
| 3:A:164:ASN:H | 3:A:170:HIS:CD2 | 2.09 | 0.68 |
| 3:A:371:LYS:HE2 | 3:A:376:ASN:HB2 | 1.75 | 0.68 |
| 3:A:27:SER:N | 6:A:630:HOH:O | 2.27 | 0.68 |
| 3:B:523:ARG:HD3 | 6:B:1106:HOH:O | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:729:LYS:HA | 3:B:825:LEU:CD2 | 2.23 | 0.68 |
| 3:B:763:ARG:HA | 3:B:780:ARG:O | 1.94 | 0.68 |
| 3:B:729:LYS:HA | 3:B:825:LEU:CD2 | 2.23 | 0.67 |
| 3:A:164:ASN:H | 3:A:170:HIS:CD2 | 2.08 | 0.67 |
| 3:B:457:CYS:HA | 5:B:902:TTP:O1B | 1.94 | 0.67 |
| 3:A:107:TYR:OH | 3:A:299:PRO:CG | 2.40 | 0.67 |
| 3:A:320:LYS:HB2 | 3:A:406:LEU:CD1 | 2.25 | 0.67 |
| 3:A:343:ARG:C | 3:A:344:LEU:HD12 | 2.15 | 0.67 |
| 3:B:762:VAL:HG21 | 3:B:803:MET:HE3 | 1.74 | 0.67 |
| 3:A:306:ASP:OD1 | 3:A:405:LEU:HD23 | 1.95 | 0.67 |
| 3:B:745:LEU:HD21 | 3:B:828:VAL:HG11 | 1.76 | 0.67 |
| 3:A:95:ASN:HD21 | 3:A:97:GLU:HB2 | 1.59 | 0.67 |
| 1:T:5:DA:H2'' | 1:T:6:DG:O5' | 1.95 | 0.67 |
| 3:A:320:LYS:HB2 | 3:A:406:LEU:CD1 | 2.25 | 0.67 |
| 3:A:343:ARG:C | 3:A:344:LEU:HD12 | 2.15 | 0.67 |
| 6:T:230:HOH:O | 3:A:296:SER:O | 2.12 | 0.66 |
| 3:A:306:ASP:OD1 | 3:A:405:LEU:HD23 | 1.95 | 0.66 |
| 3:B:763:ARG:HA | 3:B:780:ARG:O | 1.94 | 0.66 |
| 6:P:253:HOH:O | 3:B:504:ALA:HB2 | 1.95 | 0.66 |
| 3:A:341:THR:HG23 | 3:A:362:CYS:O | 1.95 | 0.66 |
| 1:T:5:DA:H2'' | 1:T:6:DG:O5' | 1.95 | 0.66 |
| 6:P:220:HOH:O | 3:B:675:ILE:N | 2.29 | 0.66 |
| 3:B:745:LEU:HD21 | 3:B:828:VAL:HG11 | 1.76 | 0.66 |
| 3:A:341:THR:HG23 | 3:A:362:CYS:O | 1.95 | 0.66 |
| 1:T:7:DG:H4' | 3:B:519:LEU:HD12 | 1.78 | 0.66 |
| 3:A:95:ASN:HD21 | 3:A:97:GLU:HB2 | 1.59 | 0.66 |
| 3:A:112:LEU:C | 3:A:112:LEU:HD23 | 2.15 | 0.66 |
| 3:B:451:VAL:CG1 | 3:B:550:VAL:HB | 2.26 | 0.66 |
| 6:T:117:HOH:O | 3:A:210:SER:OG | 2.13 | 0.66 |
| 3:B:685:SER:HB3 | 3:B:688:ILE:CG2 | 2.25 | 0.66 |
| 3:A:112:LEU:C | 3:A:112:LEU:HD23 | 2.15 | 0.66 |
| 3:B:568:LEU:HD23 | 3:B:568:LEU:O | 1.96 | 0.66 |
| 6:T:159:HOH:O | 3:A:137:GLU:HG3 | 1.94 | 0.66 |
| 1:T:10:DC:H2'' | 1:T:11:DC:O5' | 1.96 | 0.66 |
| 3:B:685:SER:HB3 | 3:B:688:ILE:CG2 | 2.24 | 0.66 |
| 3:A:59:GLN:O | 3:A:61:TYR:N | 2.23 | 0.65 |
| 1:T:10:DC:H2'' | 1:T:11:DC:O5' | 1.96 | 0.65 |
| 3:B:568:LEU:O | 3:B:568:LEU:HD23 | 1.97 | 0.65 |
| 3:B:762:VAL:CG2 | 3:B:803:MET:HE1 | 2.27 | 0.65 |
| 3:B:451:VAL:CG1 | 3:B:550:VAL:HB | 2.27 | 0.65 |
| 2:P:11:DC:H2'' | 2:P:12:DC:O4' | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:107:TYR:OH | 3:A:299:PRO:CG | 2.41 | 0.65 |
| 3:A:392:ARG:O | 3:A:395:VAL:HA | 1.95 | 0.65 |
| 3:B:622:ASN:HD21 | 3:B:625:LEU:H | 1.44 | 0.65 |
| 3:A:392:ARG:O | 3:A:395:VAL:HA | 1.95 | 0.65 |
| 3:B:808:MET:HA | 3:B:811:PHE:HB2 | 1.79 | 0.65 |
| 3:A:299:PRO:HD3 | 6:A:502:HOH:O | 1.97 | 0.65 |
| 2:P:4:DG:H2'' | 2:P:5:DG:H8 | 1.62 | 0.65 |
| 3:A:409:CYS:HG | 3:A:411:CYS:HB2 | 1.61 | 0.65 |
| 3:B:740:LYS:HZ2 | 3:B:741:ILE:HG13 | 1.62 | 0.64 |
| 1:T:5:DA:H4' | 3:B:480:LYS:HB2 | 1.77 | 0.64 |
| 2:P:4:DG:H2'' | 2:P:5:DG:H8 | 1.62 | 0.64 |
| 3:B:622:ASN:HD21 | 3:B:625:LEU:H | 1.45 | 0.64 |
| 3:A:88:CYS:SG | 3:A:91:LEU:HB2 | 2.37 | 0.64 |
| 6:T:102:HOH:O | 3:A:299:PRO:HD3 | 1.96 | 0.64 |
| 3:B:808:MET:HA | 3:B:811:PHE:HB2 | 1.79 | 0.64 |
| 3:A:88:CYS:SG | 3:A:91:LEU:HB2 | 2.38 | 0.64 |
| 3:B:762:VAL:CG2 | 3:B:803:MET:HE1 | 2.28 | 0.64 |
| 3:B:721:SER:CB | 3:B:831:CYS:CB | 2.76 | 0.64 |
| 3:A:59:GLN:CD | 3:A:64:VAL:HG11 | 2.18 | 0.63 |
| 3:A:59:GLN:O | 3:A:61:TYR:N | 2.23 | 0.63 |
| 3:B:721:SER:CB | 3:B:831:CYS:CB | 2.76 | 0.63 |
| 3:B:767:ARG:CB | 3:B:775:TYR:O | 2.45 | 0.63 |
| 1:T:14:DC:C2' | 1:T:15:DC:C6 | 2.81 | 0.63 |
| 3:B:622:ASN:HD22 | 3:B:622:ASN:C | 2.02 | 0.63 |
| 3:A:319:ASN:HA | 3:A:322:GLU:OE1 | 1.99 | 0.63 |
| 1:T:7:DG:H4' | 3:B:519:LEU:HD12 | 1.81 | 0.63 |
| 3:B:765:ILE:N | 3:B:827:SER:O | 2.22 | 0.63 |
| 3:A:347:ARG:HA | 3:A:356:GLY:O | 1.99 | 0.63 |
| 3:B:767:ARG:CB | 3:B:775:TYR:O | 2.45 | 0.63 |
| 1:T:14:DC:C2' | 1:T:15:DC:C6 | 2.81 | 0.63 |
| 3:A:309:LYS:O | 3:A:310:LYS:HE3 | 1.99 | 0.63 |
| 3:A:371:LYS:HE2 | 3:A:376:ASN:O | 1.99 | 0.62 |
| 3:A:371:LYS:HE2 | 3:A:376:ASN:O | 1.99 | 0.62 |
| 3:B:527:TYR:OH | 3:B:719:PRO:HG3 | 1.99 | 0.62 |
| 3:B:729:LYS:O | 3:B:730:LYS:CB | 2.48 | 0.62 |
| 3:A:59:GLN:CD | 3:A:64:VAL:HG11 | 2.18 | 0.62 |
| 3:A:319:ASN:HA | 3:A:322:GLU:OE1 | 1.99 | 0.62 |
| 3:A:309:LYS:O | 3:A:310:LYS:HE3 | 1.99 | 0.62 |
| 3:B:717:GLY:O | 3:B:718:PRO:O | 2.18 | 0.62 |
| 3:A:347:ARG:HA | 3:A:356:GLY:O | 1.99 | 0.62 |
| 3:A:318:LYS:O | 3:A:322:GLU:HG3 | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:622:ASN:C | 3:B:622:ASN:HD22 | 2.02 | 0.62 |
| 3:A:379:VAL:O | 3:A:382:PRO:N | 2.32 | 0.62 |
| 3:A:163:ILE:HG21 | 3:A:174:LEU:HD11 | 1.82 | 0.62 |
| 3:B:729:LYS:O | 3:B:730:LYS:CB | 2.48 | 0.62 |
| 3:A:55:LEU:HD12 | 3:A:56:GLY:H | 1.64 | 0.62 |
| 3:B:723:SER:C | 3:B:748:LEU:HD21 | 2.20 | 0.62 |
| 3:B:717:GLY:O | 3:B:718:PRO:O | 2.18 | 0.62 |
| 3:A:318:LYS:O | 3:A:322:GLU:HG3 | 2.00 | 0.62 |
| 3:A:343:ARG:O | 3:A:344:LEU:CD1 | 2.48 | 0.61 |
| 3:B:765:ILE:N | 3:B:827:SER:O | 2.22 | 0.61 |
| 3:A:163:ILE:HG21 | 3:A:174:LEU:HD11 | 1.82 | 0.61 |
| 3:A:379:VAL:O | 3:A:382:PRO:HD2 | 2.00 | 0.61 |
| 3:A:55:LEU:HD12 | 3:A:56:GLY:H | 1.64 | 0.61 |
| 3:A:371:LYS:NZ | 3:A:376:ASN:HB2 | 2.15 | 0.61 |
| 3:B:740:LYS:NZ | 3:B:741:ILE:HG13 | 2.15 | 0.61 |
| 2:P:4:DG:H2" | 2:P:5:DG:C8 | 2.35 | 0.61 |
| 3:B:495:VAL:HG12 | 3:B:497:LYS:HE2 | 1.82 | 0.61 |
| 3:B:527:TYR:OH | 3:B:719:PRO:HG3 | 1.99 | 0.61 |
| 3:A:379:VAL:O | 3:A:382:PRO:N | 2.33 | 0.61 |
| 3:A:347:ARG:CA | 3:A:356:GLY:O | 2.48 | 0.61 |
| 3:A:347:ARG:CA | 3:A:356:GLY:O | 2.48 | 0.61 |
| 3:B:464:MET:HE2 | 3:B:471:LYS:HA | 1.82 | 0.61 |
| 3:A:379:VAL:O | 3:A:382:PRO:HD2 | 2.00 | 0.61 |
| 3:B:740:LYS:NZ | 3:B:741:ILE:HG13 | 2.15 | 0.61 |
| 3:B:555:MET:CE | 3:B:599:ILE:HD12 | 2.31 | 0.61 |
| 3:B:504:ALA:HB2 | 6:B:1152:HOH:O | 2.01 | 0.61 |
| 3:A:107:TYR:HH | 3:A:299:PRO:HG3 | 1.63 | 0.61 |
| 3:B:718:PRO:HG3 | 6:B:1123:HOH:O | 2.00 | 0.61 |
| 3:A:371:LYS:NZ | 3:A:376:ASN:HB2 | 2.15 | 0.61 |
| 3:A:371:LYS:CE | 3:A:376:ASN:HB2 | 2.29 | 0.61 |
| 3:A:384:VAL:O | 3:A:388:MET:HG2 | 2.01 | 0.61 |
| 3:B:532:LEU:HD23 | 3:B:532:LEU:C | 2.22 | 0.60 |
| 3:B:532:LEU:HD23 | 3:B:532:LEU:C | 2.22 | 0.60 |
| 3:A:59:GLN:C | 3:A:61:TYR:H | 2.04 | 0.60 |
| 3:A:322:GLU:O | 3:A:326:ALA:HB2 | 2.02 | 0.60 |
| 3:A:371:LYS:CE | 3:A:376:ASN:HB2 | 2.30 | 0.60 |
| 3:B:723:SER:C | 3:B:748:LEU:HD21 | 2.20 | 0.60 |
| 6:T:128:HOH:O | 3:A:158:TYR:OH | 2.15 | 0.60 |
| 3:B:740:LYS:HZ2 | 3:B:741:ILE:HG13 | 1.66 | 0.60 |
| 2:P:4:DG:H2" | 2:P:5:DG:C8 | 2.35 | 0.60 |
| 3:A:343:ARG:O | 3:A:344:LEU:CD1 | 2.48 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:457:CYS:HA | 5:B:902:TTP:O1B | 2.01 | 0.60 |
| 3:B:764:LEU:O | 3:B:779:SER:HA | 2.02 | 0.60 |
| 3:B:475:LEU:HD12 | 3:B:476:GLY:H | 1.67 | 0.60 |
| 3:A:384:VAL:O | 3:A:388:MET:HG2 | 2.01 | 0.60 |
| 3:B:555:MET:CE | 3:B:599:ILE:HD12 | 2.31 | 0.60 |
| 1:T:15:DC:H2'' | 1:T:16:DC:C5' | 2.32 | 0.60 |
| 3:B:690:GLU:HA | 3:B:698:ALA:CB | 2.32 | 0.60 |
| 3:B:495:VAL:HG12 | 3:B:497:LYS:HE2 | 1.82 | 0.60 |
| 3:A:161:GLN:NE2 | 3:A:225:SER:OG | 2.35 | 0.60 |
| 3:B:764:LEU:O | 3:B:779:SER:HA | 2.02 | 0.60 |
| 3:B:689:LEU:HD11 | 3:B:701:ILE:HD11 | 1.83 | 0.60 |
| 3:B:689:LEU:HD11 | 3:B:701:ILE:HD11 | 1.84 | 0.59 |
| 3:B:475:LEU:HD12 | 3:B:476:GLY:H | 1.67 | 0.59 |
| 3:A:322:GLU:O | 3:A:326:ALA:HB2 | 2.02 | 0.59 |
| 3:A:59:GLN:C | 3:A:61:TYR:H | 2.04 | 0.59 |
| 3:B:479:GLN:O | 3:B:482:LEU:N | 2.33 | 0.59 |
| 2:P:12:DC:H5'' | 2:P:13:DOC:OP2 | 2.02 | 0.59 |
| 1:T:15:DC:H2'' | 1:T:16:DC:C5' | 2.32 | 0.59 |
| 1:T:8:DG:H2' | 1:T:9:DT:H72 | 1.84 | 0.59 |
| 3:B:722:PHE:O | 3:B:830:PHE:HB2 | 2.03 | 0.59 |
| 3:B:690:GLU:HA | 3:B:698:ALA:CB | 2.31 | 0.59 |
| 3:B:479:GLN:O | 3:B:482:LEU:N | 2.33 | 0.59 |
| 1:T:12:DT:H2' | 1:T:13:DT:C7 | 2.32 | 0.59 |
| 3:A:309:LYS:O | 3:A:310:LYS:HB2 | 2.03 | 0.59 |
| 3:A:314:GLU:CA | 3:A:314:GLU:OE1 | 2.51 | 0.59 |
| 2:P:6:DA:H5' | 3:B:781:GLN:HB2 | 1.85 | 0.59 |
| 3:B:659:ILE:HD11 | 3:B:678:VAL:HG22 | 1.85 | 0.59 |
| 1:T:13:DT:C2' | 1:T:14:DC:C6 | 2.85 | 0.59 |
| 3:A:161:GLN:NE2 | 3:A:225:SER:OG | 2.36 | 0.59 |
| 3:B:767:ARG:CG | 3:B:775:TYR:O | 2.51 | 0.58 |
| 3:A:311:CYS:O | 3:A:312:SER:HB3 | 2.03 | 0.58 |
| 3:A:215:PRO:O | 3:A:217:GLN:HG3 | 2.03 | 0.58 |
| 1:T:12:DT:H2' | 1:T:13:DT:C7 | 2.32 | 0.58 |
| 3:B:659:ILE:HD11 | 3:B:678:VAL:HG22 | 1.86 | 0.58 |
| 3:B:497:LYS:H | 3:B:497:LYS:HD2 | 1.68 | 0.58 |
| 3:A:314:GLU:CA | 3:A:314:GLU:OE1 | 2.51 | 0.58 |
| 3:A:50:LEU:HD23 | 3:A:53:LYS:HD3 | 1.85 | 0.58 |
| 3:A:215:PRO:O | 3:A:217:GLN:HG3 | 2.04 | 0.58 |
| 1:T:13:DT:C2' | 1:T:14:DC:C6 | 2.85 | 0.58 |
| 3:B:767:ARG:CG | 3:B:775:TYR:O | 2.51 | 0.58 |
| 3:A:317:ALA:HA | 3:A:320:LYS:CG | 2.31 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:50:LEU:HA | 3:A:53:LYS:HD3 | 1.85 | 0.58 |
| 3:A:50:LEU:HD23 | 3:A:53:LYS:HD3 | 1.85 | 0.58 |
| 1:T:8:DG:H2' | 1:T:9:DT:H72 | 1.84 | 0.58 |
| 3:B:464:MET:HE2 | 3:B:471:LYS:HA | 1.86 | 0.58 |
| 3:A:59:GLN:NE2 | 3:A:64:VAL:HG11 | 2.19 | 0.58 |
| 3:A:54:PRO:O | 3:A:91:LEU:HD12 | 2.04 | 0.58 |
| 3:A:311:CYS:O | 3:A:312:SER:HB3 | 2.03 | 0.58 |
| 3:B:801:THR:CB | 3:B:802:PRO:HD3 | 2.33 | 0.58 |
| 3:A:54:PRO:O | 3:A:91:LEU:HD12 | 2.04 | 0.58 |
| 3:B:675:ILE:N | 6:B:1120:HOH:O | 2.37 | 0.58 |
| 1:T:5:DA:C2' | 1:T:6:DG:O5' | 2.51 | 0.57 |
| 2:P:6:DA:H5' | 3:B:781:GLN:HB2 | 1.86 | 0.57 |
| 3:B:801:THR:CB | 3:B:802:PRO:HD3 | 2.33 | 0.57 |
| 3:B:739:ASN:O | 3:B:742:GLU:HG3 | 2.05 | 0.57 |
| 3:A:50:LEU:HA | 3:A:53:LYS:HD3 | 1.84 | 0.57 |
| 2:P:7:DA:H5'' | 6:B:1149:HOH:O | 2.04 | 0.57 |
| 3:A:59:GLN:NE2 | 3:A:64:VAL:HG11 | 2.19 | 0.57 |
| 3:A:309:LYS:O | 3:A:310:LYS:HB2 | 2.03 | 0.57 |
| 3:B:560:LEU:HD12 | 3:B:592:ARG:NH1 | 2.19 | 0.57 |
| 3:B:739:ASN:O | 3:B:742:GLU:HG3 | 2.05 | 0.57 |
| 3:B:497:LYS:HD2 | 3:B:497:LYS:H | 1.68 | 0.57 |
| 1:T:5:DA:C2' | 1:T:6:DG:O5' | 2.51 | 0.57 |
| 3:B:722:PHE:O | 3:B:830:PHE:HB2 | 2.03 | 0.57 |
| 3:A:314:GLU:N | 3:A:314:GLU:OE1 | 2.37 | 0.57 |
| 3:A:314:GLU:OE1 | 3:A:314:GLU:N | 2.37 | 0.57 |
| 1:T:14:DC:H2'' | 1:T:15:DC:C5' | 2.28 | 0.57 |
| 3:A:306:ASP:HB2 | 3:A:324:LEU:HD21 | 1.86 | 0.57 |
| 3:A:367:HIS:HD2 | 3:A:368:VAL:HG22 | 1.70 | 0.57 |
| 3:B:560:LEU:HD12 | 3:B:592:ARG:NH1 | 2.19 | 0.57 |
| 3:B:592:ARG:HG2 | 3:B:592:ARG:NH1 | 2.20 | 0.57 |
| 3:A:36:ASP:O | 3:A:37:CYS:C | 2.43 | 0.57 |
| 3:B:742:GLU:O | 3:B:746:ALA:HB2 | 2.05 | 0.56 |
| 3:B:456:ASP:O | 3:B:457:CYS:C | 2.43 | 0.56 |
| 3:A:317:ALA:O | 3:A:321:ILE:HD13 | 2.05 | 0.56 |
| 3:A:366:SER:O | 3:A:367:HIS:NE2 | 2.38 | 0.56 |
| 3:B:456:ASP:O | 3:B:457:CYS:C | 2.43 | 0.56 |
| 3:A:306:ASP:HB2 | 3:A:324:LEU:HD21 | 1.86 | 0.56 |
| 3:A:380:MET:O | 3:A:384:VAL:CG2 | 2.44 | 0.56 |
| 3:A:317:ALA:O | 3:A:321:ILE:HD13 | 2.05 | 0.56 |
| 3:B:497:LYS:NZ | 3:B:497:LYS:HB3 | 2.20 | 0.56 |
| 3:A:36:ASP:O | 3:A:37:CYS:C | 2.43 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:279:GLN:O | 3:A:283:LYS:HG3 | 2.06 | 0.56 |
| 3:B:464:MET:CE | 3:B:487:ASN:HD22 | 2.19 | 0.56 |
| 3:B:497:LYS:HB3 | 3:B:497:LYS:NZ | 2.20 | 0.56 |
| 2:P:11:DC:OP1 | 3:B:665:LYS:CB | 2.54 | 0.56 |
| 3:B:740:LYS:HD3 | 3:B:741:ILE:N | 2.19 | 0.56 |
| 3:A:366:SER:O | 3:A:367:HIS:NE2 | 2.38 | 0.56 |
| 1:T:7:DG:H2'' | 1:T:8:DG:OP2 | 2.05 | 0.56 |
| 3:B:592:ARG:NH1 | 3:B:592:ARG:HG2 | 2.20 | 0.56 |
| 3:A:204:LEU:CD1 | 3:A:240:PRO:HD2 | 2.35 | 0.56 |
| 3:B:782:CYS:SG | 3:B:806:ILE:HD12 | 2.46 | 0.56 |
| 2:P:6:DA:H2'' | 2:P:7:DA:O4' | 2.05 | 0.56 |
| 3:B:742:GLU:O | 3:B:746:ALA:HB2 | 2.05 | 0.56 |
| 3:A:279:GLN:O | 3:A:283:LYS:HG3 | 2.05 | 0.56 |
| 2:P:8:DG:C5' | 3:B:777:ARG:HA | 2.36 | 0.56 |
| 1:T:7:DG:H5'' | 3:B:519:LEU:CG | 2.36 | 0.56 |
| 3:B:740:LYS:HD3 | 3:B:741:ILE:N | 2.20 | 0.56 |
| 3:B:782:CYS:SG | 3:B:806:ILE:HD12 | 2.46 | 0.56 |
| 3:A:261:LEU:HD23 | 3:A:261:LEU:O | 2.07 | 0.55 |
| 3:B:699:GLN:O | 3:B:703:LYS:HG2 | 2.07 | 0.55 |
| 3:A:204:LEU:CD1 | 3:A:240:PRO:HD2 | 2.36 | 0.55 |
| 6:T:269:HOH:O | 3:A:94:VAL:HA | 2.06 | 0.55 |
| 3:A:47:ASN:HD21 | 3:A:49:GLU:HG2 | 1.72 | 0.55 |
| 1:T:14:DC:H2'' | 1:T:15:DC:C5' | 2.28 | 0.55 |
| 3:A:157:VAL:HG11 | 3:A:161:GLN:O | 2.07 | 0.55 |
| 2:P:11:DC:OP1 | 3:B:665:LYS:CB | 2.55 | 0.55 |
| 6:T:269:HOH:O | 3:A:95:ASN:N | 2.23 | 0.55 |
| 3:A:339:PRO:HD3 | 3:A:413:LEU:HD22 | 1.89 | 0.55 |
| 3:A:54:PRO:CA | 3:A:70:ALA:HB2 | 2.37 | 0.55 |
| 3:A:339:PRO:HD3 | 3:A:413:LEU:HD22 | 1.89 | 0.55 |
| 3:B:464:MET:CE | 3:B:487:ASN:HD22 | 2.19 | 0.55 |
| 3:A:157:VAL:HG11 | 3:A:161:GLN:O | 2.07 | 0.55 |
| 3:A:137:GLU:HG3 | 6:A:559:HOH:O | 2.07 | 0.55 |
| 1:T:7:DG:H2'' | 1:T:8:DG:OP2 | 2.05 | 0.55 |
| 3:B:583:ILE:HG21 | 3:B:594:LEU:HD11 | 1.89 | 0.55 |
| 3:A:261:LEU:O | 3:A:261:LEU:HD23 | 2.07 | 0.55 |
| 3:B:699:GLN:O | 3:B:703:LYS:HG2 | 2.07 | 0.55 |
| 3:B:716:SER:O | 3:B:716:SER:OG | 2.23 | 0.55 |
| 3:B:738:LYS:CB | 3:B:808:MET:SD | 2.95 | 0.55 |
| 3:B:762:VAL:CG1 | 3:B:806:ILE:HD11 | 2.36 | 0.55 |
| 3:A:231:HIS:ND1 | 6:A:522:HOH:O | 2.33 | 0.55 |
| 3:B:738:LYS:CB | 3:B:808:MET:SD | 2.95 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:491:ARG:HA | 3:B:496:LYS:O | 2.07 | 0.55 |
| 2:P:6:DA:H2'' | 2:P:7:DA:O4' | 2.05 | 0.54 |
| 6:T:210:HOH:O | 3:A:277:VAL:HG21 | 2.07 | 0.54 |
| 3:B:729:LYS:HA | 3:B:825:LEU:HD22 | 1.89 | 0.54 |
| 3:B:779:SER:H | 3:B:811:PHE:HE2 | 1.55 | 0.54 |
| 3:A:308:PHE:O | 3:A:310:LYS:N | 2.37 | 0.54 |
| 3:B:728:PHE:CZ | 3:B:740:LYS:HG3 | 2.42 | 0.54 |
| 3:B:583:ILE:HG21 | 3:B:594:LEU:HD11 | 1.89 | 0.54 |
| 3:B:491:ARG:HA | 3:B:496:LYS:O | 2.07 | 0.54 |
| 3:B:721:SER:HA | 3:B:833:LEU:CD2 | 2.38 | 0.54 |
| 3:B:741:ILE:HA | 3:B:744:LEU:HD21 | 1.89 | 0.54 |
| 3:B:762:VAL:CG1 | 3:B:806:ILE:HD11 | 2.36 | 0.54 |
| 3:B:741:ILE:HA | 3:B:744:LEU:HD21 | 1.89 | 0.54 |
| 1:T:7:DG:OP2 | 3:B:725:GLU:N | 2.33 | 0.54 |
| 2:P:4:DG:OP2 | 3:A:300:GLN:NE2 | 2.40 | 0.54 |
| 3:B:745:LEU:O | 3:B:749:LEU:HD22 | 2.08 | 0.54 |
| 3:A:341:THR:O | 3:A:411:CYS:O | 2.25 | 0.54 |
| 3:B:728:PHE:HZ | 3:B:740:LYS:HG3 | 1.73 | 0.54 |
| 3:A:367:HIS:HD2 | 3:A:368:VAL:HG22 | 1.69 | 0.54 |
| 3:A:47:ASN:HD21 | 3:A:49:GLU:HG2 | 1.72 | 0.54 |
| 2:P:8:DG:C5' | 3:B:777:ARG:HA | 2.38 | 0.54 |
| 3:A:343:ARG:HG3 | 3:A:361:GLN:HB2 | 1.90 | 0.54 |
| 3:A:341:THR:O | 3:A:411:CYS:O | 2.25 | 0.54 |
| 3:A:163:ILE:HD13 | 3:A:174:LEU:HD11 | 1.90 | 0.54 |
| 3:A:247:ALA:O | 3:A:251:GLU:HG3 | 2.08 | 0.54 |
| 3:B:506:GLU:O | 3:B:509:PRO:HD3 | 2.08 | 0.54 |
| 3:B:726:ASP:HB3 | 3:B:744:LEU:HB3 | 1.90 | 0.54 |
| 3:A:388:MET:N | 3:A:388:MET:HE2 | 2.23 | 0.54 |
| 3:B:474:PRO:HG3 | 3:B:489:GLU:O | 2.07 | 0.54 |
| 3:B:506:GLU:O | 3:B:509:PRO:HD3 | 2.08 | 0.54 |
| 3:B:509:PRO:C | 3:B:511:LEU:H | 2.11 | 0.54 |
| 3:B:509:PRO:C | 3:B:511:LEU:H | 2.11 | 0.54 |
| 3:A:54:PRO:CA | 3:A:70:ALA:HB2 | 2.37 | 0.54 |
| 3:A:163:ILE:HD13 | 3:A:174:LEU:HD11 | 1.90 | 0.54 |
| 3:B:647:GLN:O | 3:B:650:ILE:HG22 | 2.08 | 0.54 |
| 3:B:723:SER:O | 3:B:751:ARG:NH2 | 2.41 | 0.53 |
| 1:T:7:DG:H5'' | 3:B:519:LEU:CG | 2.38 | 0.53 |
| 3:A:126:ASP:OD1 | 3:A:127:GLU:HG3 | 2.08 | 0.53 |
| 3:A:126:ASP:OD1 | 3:A:127:GLU:HG3 | 2.09 | 0.53 |
| 3:A:343:ARG:HG3 | 3:A:361:GLN:HB2 | 1.90 | 0.53 |
| 3:B:729:LYS:HA | 3:B:825:LEU:HD22 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:464:MET:HE1 | 3:B:487:ASN:HD22 | 1.74 | 0.53 |
| 3:A:337:ARG:CG | 3:A:414:LYS:O | 2.56 | 0.53 |
| 3:B:491:ARG:CZ | 3:B:498:LEU:HD11 | 2.39 | 0.53 |
| 6:P:231:HOH:O | 3:B:558:LYS:NZ | 2.41 | 0.53 |
| 3:B:604:ARG:HE | 3:B:638:GLN:HE21 | 1.55 | 0.53 |
| 3:A:88:CYS:N | 3:A:89:PRO:CD | 2.71 | 0.53 |
| 3:A:84:ALA:HA | 3:A:87:LYS:NZ | 2.24 | 0.53 |
| 3:B:558:LYS:NZ | 6:B:1131:HOH:O | 2.41 | 0.53 |
| 1:T:14:DC:C2' | 1:T:15:DC:H5' | 2.28 | 0.53 |
| 3:A:350:SER:O | 3:A:351:SER:O | 2.26 | 0.53 |
| 3:B:728:PHE:HZ | 3:B:740:LYS:HG3 | 1.72 | 0.53 |
| 2:P:7:DA:C5' | 6:B:1149:HOH:O | 2.57 | 0.53 |
| 3:B:474:PRO:HG3 | 3:B:489:GLU:O | 2.07 | 0.53 |
| 3:B:728:PHE:CZ | 3:B:740:LYS:HG3 | 2.43 | 0.53 |
| 6:T:227:HOH:O | 3:A:290:ASN:ND2 | 2.29 | 0.53 |
| 3:A:84:ALA:HA | 3:A:87:LYS:NZ | 2.23 | 0.53 |
| 3:B:745:LEU:O | 3:B:749:LEU:HD22 | 2.08 | 0.53 |
| 3:A:247:ALA:O | 3:A:251:GLU:HG3 | 2.08 | 0.53 |
| 3:B:495:VAL:HG12 | 3:B:495:VAL:O | 2.09 | 0.53 |
| 3:B:723:SER:O | 3:B:751:ARG:NH2 | 2.41 | 0.53 |
| 3:B:604:ARG:HE | 3:B:638:GLN:HE21 | 1.54 | 0.53 |
| 3:B:766:ILE:CB | 3:B:778:GLU:CB | 2.86 | 0.53 |
| 3:A:317:ALA:HA | 3:A:320:LYS:CG | 2.30 | 0.53 |
| 3:A:360:ARG:NH1 | 3:A:394:MET:SD | 2.82 | 0.53 |
| 3:B:471:LYS:CD | 3:B:472:ASP:H | 2.19 | 0.53 |
| 3:A:314:GLU:OE1 | 3:A:314:GLU:HA | 2.09 | 0.53 |
| 3:B:647:GLN:O | 3:B:650:ILE:HG22 | 2.09 | 0.53 |
| 3:A:337:ARG:CG | 3:A:414:LYS:O | 2.56 | 0.53 |
| 3:A:161:GLN:OE1 | 3:A:224:GLU:HB2 | 2.09 | 0.53 |
| 3:A:350:SER:O | 3:A:351:SER:O | 2.26 | 0.53 |
| 3:B:539:VAL:CG2 | 6:B:1077:HOH:O | 2.57 | 0.53 |
| 6:P:182:HOH:O | 3:B:720:GLN:NE2 | 2.42 | 0.53 |
| 3:B:495:VAL:HG12 | 3:B:495:VAL:O | 2.09 | 0.53 |
| 3:A:31:VAL:HG12 | 3:A:130:VAL:HB | 1.91 | 0.53 |
| 3:B:716:SER:OG | 3:B:716:SER:O | 2.23 | 0.53 |
| 3:B:766:ILE:CB | 3:B:778:GLU:CB | 2.86 | 0.53 |
| 3:A:161:GLN:OE1 | 3:A:224:GLU:HB2 | 2.09 | 0.52 |
| 3:A:360:ARG:NH1 | 3:A:394:MET:SD | 2.82 | 0.52 |
| 3:B:616:CYS:SG | 3:B:634:LYS:O | 2.67 | 0.52 |
| 3:A:88:CYS:N | 3:A:89:PRO:CD | 2.71 | 0.52 |
| 3:B:726:ASP:HB3 | 3:B:744:LEU:HB3 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:328:LEU:O | 3:A:332:VAL:CG2 | 2.47 | 0.52 |
| 2:P:2:DG:H2' | 6:A:597:HOH:O | 2.10 | 0.52 |
| 3:B:797:TYR:CD1 | 3:B:797:TYR:O | 2.62 | 0.52 |
| 3:A:371:LYS:HZ1 | 3:A:376:ASN:HB2 | 1.74 | 0.52 |
| 3:A:31:VAL:HG12 | 3:A:130:VAL:HB | 1.90 | 0.52 |
| 3:A:314:GLU:HA | 3:A:314:GLU:OE1 | 2.09 | 0.52 |
| 3:B:616:CYS:SG | 3:B:634:LYS:O | 2.67 | 0.52 |
| 6:T:126:HOH:O | 3:A:134:GLU:HG3 | 2.08 | 0.52 |
| 1:T:14:DC:C2' | 1:T:15:DC:H5' | 2.28 | 0.52 |
| 3:A:321:ILE:O | 3:A:325:LEU:HB2 | 2.09 | 0.52 |
| 3:B:471:LYS:CD | 3:B:472:ASP:H | 2.19 | 0.52 |
| 3:B:491:ARG:CZ | 3:B:498:LEU:HD11 | 2.39 | 0.52 |
| 3:B:488:TYR:C | 3:B:490:ALA:H | 2.12 | 0.52 |
| 3:B:562:GLN:N | 3:B:562:GLN:HE21 | 2.07 | 0.52 |
| 3:A:320:LYS:HB2 | 3:A:406:LEU:HD12 | 1.92 | 0.52 |
| 3:B:471:LYS:HD3 | 3:B:472:ASP:N | 2.20 | 0.52 |
| 3:A:196:CYS:SG | 3:A:214:LYS:O | 2.67 | 0.52 |
| 3:B:681:LEU:HD12 | 3:B:681:LEU:O | 2.10 | 0.52 |
| 3:A:320:LYS:HB2 | 3:A:406:LEU:HD12 | 1.92 | 0.52 |
| 3:A:88:CYS:O | 3:A:91:LEU:N | 2.41 | 0.52 |
| 3:B:491:ARG:NH2 | 3:B:498:LEU:HD11 | 2.25 | 0.52 |
| 3:B:555:MET:HE1 | 3:B:599:ILE:HD12 | 1.92 | 0.52 |
| 3:B:488:TYR:C | 3:B:490:ALA:H | 2.12 | 0.52 |
| 2:P:8:DG:O3' | 3:B:776:GLY:O | 2.27 | 0.52 |
| 3:B:779:SER:H | 3:B:811:PHE:HE2 | 1.55 | 0.52 |
| 1:T:5:DA:O5' | 1:T:5:DA:N3 | 2.39 | 0.52 |
| 3:A:196:CYS:SG | 3:A:214:LYS:O | 2.67 | 0.52 |
| 2:P:4:DG:OP2 | 3:A:300:GLN:NE2 | 2.43 | 0.52 |
| 3:B:721:SER:HA | 3:B:833:LEU:CD2 | 2.38 | 0.52 |
| 3:A:313:SER:O | 3:A:315:VAL:CG1 | 2.56 | 0.52 |
| 3:B:741:ILE:HD12 | 3:B:808:MET:SD | 2.50 | 0.51 |
| 3:B:797:TYR:CD1 | 3:B:797:TYR:O | 2.62 | 0.51 |
| 2:P:8:DG:OP1 | 3:B:777:ARG:C | 2.49 | 0.51 |
| 3:A:332:VAL:HG21 | 3:A:410:PHE:CE1 | 2.45 | 0.51 |
| 3:A:332:VAL:HG21 | 3:A:410:PHE:CE1 | 2.45 | 0.51 |
| 3:B:681:LEU:HD12 | 3:B:681:LEU:O | 2.10 | 0.51 |
| 3:B:741:ILE:HD12 | 3:B:808:MET:SD | 2.50 | 0.51 |
| 3:B:738:LYS:CB | 3:B:808:MET:CE | 2.88 | 0.51 |
| 3:A:31:VAL:CG1 | 3:A:130:VAL:HB | 2.39 | 0.51 |
| 3:A:330:ASN:O | 3:A:330:ASN:ND2 | 2.44 | 0.51 |
| 6:T:248:HOH:O | 3:A:169:LEU:HD12 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:741:ILE:HA | 3:B:744:LEU:CD2 | 2.40 | 0.51 |
| 3:A:103:ARG:HD3 | 6:A:603:HOH:O | 2.10 | 0.51 |
| 3:A:94:VAL:HA | 6:A:667:HOH:O | 2.10 | 0.51 |
| 3:A:330:ASN:ND2 | 3:A:330:ASN:O | 2.44 | 0.51 |
| 3:B:451:VAL:HG12 | 3:B:550:VAL:HB | 1.92 | 0.51 |
| 3:B:624:LEU:HD21 | 3:B:660:PRO:HD2 | 1.93 | 0.51 |
| 3:B:741:ILE:HA | 3:B:744:LEU:CD2 | 2.40 | 0.51 |
| 3:A:321:ILE:O | 3:A:325:LEU:HB2 | 2.09 | 0.51 |
| 3:B:624:LEU:HD21 | 3:B:660:PRO:HD2 | 1.93 | 0.51 |
| 2:P:5:DG:C2' | 2:P:6:DA:O5' | 2.59 | 0.51 |
| 3:B:451:VAL:HG12 | 3:B:550:VAL:HB | 1.92 | 0.51 |
| 3:B:532:LEU:HD23 | 3:B:532:LEU:O | 2.10 | 0.51 |
| 3:B:511:LEU:HD23 | 3:B:512:VAL:O | 2.11 | 0.51 |
| 3:B:501:VAL:C | 3:B:503:ASP:N | 2.63 | 0.51 |
| 3:A:270:GLU:HA | 3:A:278:ALA:CB | 2.41 | 0.51 |
| 3:B:532:LEU:HD23 | 3:B:532:LEU:O | 2.10 | 0.51 |
| 3:B:562:GLN:HE21 | 3:B:562:GLN:N | 2.08 | 0.51 |
| 3:B:745:LEU:HD21 | 3:B:828:VAL:CG1 | 2.41 | 0.51 |
| 3:B:573:VAL:HG12 | 6:B:1037:HOH:O | 2.11 | 0.51 |
| 3:A:31:VAL:CG1 | 3:A:130:VAL:HB | 2.40 | 0.51 |
| 3:B:740:LYS:HD3 | 3:B:741:ILE:HG13 | 1.92 | 0.51 |
| 3:B:738:LYS:CB | 3:B:808:MET:CE | 2.88 | 0.51 |
| 3:B:797:TYR:HD1 | 3:B:797:TYR:O | 1.93 | 0.51 |
| 3:A:236:ILE:HD12 | 3:A:237:LYS:N | 2.26 | 0.51 |
| 3:B:497:LYS:O | 3:B:500:ASN:ND2 | 2.44 | 0.51 |
| 3:B:539:VAL:HG23 | 6:B:1077:HOH:O | 2.11 | 0.51 |
| 6:T:101:HOH:O | 3:A:161:GLN:NE2 | 2.43 | 0.50 |
| 3:A:127:GLU:OE1 | 3:A:207:LYS:NZ | 2.41 | 0.50 |
| 3:A:308:PHE:O | 3:A:310:LYS:N | 2.37 | 0.50 |
| 3:A:388:MET:N | 3:A:388:MET:HE2 | 2.26 | 0.50 |
| 2:P:5:DG:C2' | 2:P:6:DA:O5' | 2.59 | 0.50 |
| 1:T:14:DC:H6 | 1:T:14:DC:H5'' | 1.77 | 0.50 |
| 3:A:88:CYS:O | 3:A:91:LEU:N | 2.41 | 0.50 |
| 2:P:8:DG:OP1 | 3:B:777:ARG:C | 2.50 | 0.50 |
| 3:B:497:LYS:O | 3:B:500:ASN:ND2 | 2.43 | 0.50 |
| 3:B:740:LYS:HD3 | 3:B:741:ILE:HG13 | 1.92 | 0.50 |
| 3:B:491:ARG:NH2 | 3:B:498:LEU:HD11 | 2.25 | 0.50 |
| 3:B:797:TYR:HD1 | 3:B:797:TYR:O | 1.93 | 0.50 |
| 3:B:764:LEU:HD13 | 3:B:807:LEU:HA | 1.94 | 0.50 |
| 3:A:328:LEU:O | 3:A:332:VAL:CG2 | 2.47 | 0.50 |
| 3:B:498:LEU:HD12 | 3:B:498:LEU:N | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:332:VAL:HG21 | 3:A:410:PHE:CD1 | 2.46 | 0.50 |
| 3:A:317:ALA:CA | 3:A:320:LYS:HG3 | 2.33 | 0.50 |
| 3:B:812:ARG:CG | 3:B:812:ARG:NH1 | 2.74 | 0.50 |
| 3:B:511:LEU:HD23 | 3:B:512:VAL:O | 2.11 | 0.50 |
| 3:A:320:LYS:HB2 | 3:A:406:LEU:HD11 | 1.93 | 0.50 |
| 3:B:471:LYS:HD3 | 3:B:472:ASP:N | 2.20 | 0.50 |
| 1:T:14:DC:H2'' | 1:T:15:DC:C6 | 2.47 | 0.50 |
| 3:A:270:GLU:HA | 3:A:278:ALA:CB | 2.41 | 0.50 |
| 3:B:498:LEU:N | 3:B:498:LEU:HD12 | 2.26 | 0.50 |
| 3:A:82:ARG:HA | 3:A:85:LYS:HB2 | 1.94 | 0.50 |
| 3:A:235:HIS:ND1 | 3:A:237:LYS:HG2 | 2.27 | 0.50 |
| 1:T:14:DC:H5'' | 1:T:14:DC:H6 | 1.77 | 0.49 |
| 1:T:5:DA:O5' | 1:T:5:DA:N3 | 2.39 | 0.49 |
| 3:A:239:ILE:HD11 | 3:A:258:VAL:HG22 | 1.94 | 0.49 |
| 3:B:761:THR:HG22 | 3:B:762:VAL:N | 2.27 | 0.49 |
| 1:T:8:DG:H2'' | 1:T:9:DT:C6 | 2.47 | 0.49 |
| 3:B:826:LEU:HD12 | 3:B:826:LEU:C | 2.31 | 0.49 |
| 3:B:767:ARG:NH1 | 3:B:824:THR:HB | 2.27 | 0.49 |
| 3:B:501:VAL:CG1 | 3:B:502:ARG:H | 2.04 | 0.49 |
| 3:B:501:VAL:C | 3:B:503:ASP:N | 2.64 | 0.49 |
| 3:A:236:ILE:HD12 | 3:A:237:LYS:N | 2.27 | 0.49 |
| 3:A:239:ILE:HD11 | 3:A:258:VAL:HG22 | 1.95 | 0.49 |
| 2:P:5:DG:H2' | 2:P:6:DA:H8 | 1.78 | 0.49 |
| 2:P:8:DG:H2'' | 2:P:9:DG:H8 | 1.77 | 0.49 |
| 3:A:332:VAL:HG21 | 3:A:410:PHE:CD1 | 2.46 | 0.49 |
| 3:A:371:LYS:HZ1 | 3:A:376:ASN:HB2 | 1.76 | 0.49 |
| 3:A:82:ARG:HA | 3:A:85:LYS:HB2 | 1.94 | 0.49 |
| 3:A:235:HIS:ND1 | 3:A:237:LYS:HG2 | 2.28 | 0.49 |
| 3:A:88:CYS:O | 3:A:88:CYS:SG | 2.71 | 0.49 |
| 2:P:5:DG:H2' | 2:P:6:DA:H8 | 1.77 | 0.49 |
| 1:T:8:DG:H2'' | 1:T:9:DT:C6 | 2.47 | 0.49 |
| 3:B:491:ARG:HH22 | 5:B:902:TTP:PG | 2.36 | 0.49 |
| 3:B:764:LEU:HD13 | 3:B:807:LEU:HA | 1.94 | 0.49 |
| 3:B:767:ARG:NH1 | 3:B:824:THR:HB | 2.27 | 0.49 |
| 3:A:50:LEU:O | 3:A:53:LYS:HG2 | 2.13 | 0.49 |
| 3:A:88:CYS:O | 3:A:88:CYS:SG | 2.71 | 0.49 |
| 2:P:12:DC:H2'' | 3:B:543:LEU:HD21 | 1.94 | 0.49 |
| 3:B:601:ALA:HA | 3:B:638:GLN:HE22 | 1.77 | 0.49 |
| 1:T:14:DC:H2'' | 1:T:15:DC:C6 | 2.47 | 0.49 |
| 3:B:601:ALA:HA | 3:B:638:GLN:HE22 | 1.77 | 0.49 |
| 3:A:404:THR:CG2 | 3:A:405:LEU:N | 2.73 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:501:VAL:CG1 | 3:B:502:ARG:H | 2.04 | 0.49 |
| 3:B:808:MET:O | 3:B:811:PHE:HB2 | 2.13 | 0.49 |
| 3:B:808:MET:O | 3:B:811:PHE:HB2 | 2.13 | 0.49 |
| 3:A:84:ALA:HA | 3:A:87:LYS:HZ3 | 1.78 | 0.48 |
| 2:P:11:DC:C2' | 2:P:12:DC:O5' | 2.61 | 0.48 |
| 1:T:5:DA:O3' | 3:B:480:LYS:HG2 | 2.13 | 0.48 |
| 3:A:100:THR:O | 3:A:104:GLU:HG3 | 2.13 | 0.48 |
| 3:B:761:THR:HG22 | 3:B:762:VAL:N | 2.27 | 0.48 |
| 3:A:50:LEU:O | 3:A:53:LYS:HG2 | 2.13 | 0.48 |
| 3:A:410:PHE:HD2 | 3:A:410:PHE:HA | 1.60 | 0.48 |
| 2:P:8:DG:H2'' | 2:P:9:DG:H8 | 1.77 | 0.48 |
| 3:B:826:LEU:HD12 | 3:B:826:LEU:C | 2.31 | 0.48 |
| 3:A:55:LEU:HD12 | 3:A:56:GLY:N | 2.27 | 0.48 |
| 3:A:343:ARG:HB3 | 3:A:409:CYS:HB3 | 1.96 | 0.48 |
| 3:A:343:ARG:HB3 | 3:A:409:CYS:HB3 | 1.96 | 0.48 |
| 3:A:320:LYS:HB2 | 3:A:406:LEU:HD11 | 1.93 | 0.48 |
| 1:T:5:DA:H8 | 3:B:479:GLN:OE1 | 1.97 | 0.48 |
| 3:A:380:MET:O | 3:A:384:VAL:CG2 | 2.44 | 0.48 |
| 3:B:799:VAL:O | 3:B:803:MET:HG2 | 2.14 | 0.48 |
| 2:P:7:DA:H5' | 3:B:779:SER:O | 2.14 | 0.48 |
| 3:A:303:SER:OG | 3:A:408:VAL:O | 2.24 | 0.48 |
| 3:B:763:ARG:O | 3:B:764:LEU:CD1 | 2.57 | 0.48 |
| 3:B:779:SER:N | 3:B:811:PHE:CE2 | 2.82 | 0.48 |
| 3:A:318:LYS:HE2 | 3:A:322:GLU:OE2 | 2.14 | 0.48 |
| 3:A:150:ALA:O | 3:A:152:THR:HG23 | 2.14 | 0.48 |
| 6:P:177:HOH:O | 3:B:539:VAL:HG23 | 2.14 | 0.48 |
| 3:A:46:SER:O | 3:A:48:PRO:HD3 | 2.13 | 0.48 |
| 3:A:369:ILE:HG13 | 3:A:379:VAL:HG21 | 1.96 | 0.48 |
| 3:B:734:GLU:CG | 3:B:821:PHE:CB | 2.91 | 0.48 |
| 3:A:161:GLN:NE2 | 6:A:501:HOH:O | 2.46 | 0.48 |
| 6:P:137:HOH:O | 3:B:573:VAL:HG12 | 2.14 | 0.48 |
| 3:B:634:LYS:O | 3:B:635:PRO:O | 2.32 | 0.48 |
| 3:B:763:ARG:O | 3:B:764:LEU:CD1 | 2.57 | 0.48 |
| 3:A:318:LYS:HE2 | 3:A:322:GLU:OE2 | 2.14 | 0.48 |
| 3:A:46:SER:O | 3:A:48:PRO:HD3 | 2.13 | 0.48 |
| 2:P:8:DG:O3' | 3:B:776:GLY:O | 2.30 | 0.47 |
| 2:P:13:DOC:H5' | 3:B:547:GLU:OE2 | 2.14 | 0.47 |
| 3:A:100:THR:O | 3:A:104:GLU:HG3 | 2.14 | 0.47 |
| 3:B:689:LEU:HD11 | 3:B:693:LEU:HD12 | 1.95 | 0.47 |
| 3:B:779:SER:N | 3:B:811:PHE:CE2 | 2.82 | 0.47 |
| 3:B:799:VAL:O | 3:B:803:MET:HG2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:55:LEU:HD12 | 3:A:56:GLY:N | 2.27 | 0.47 |
| 3:A:365:PRO:CB | 3:A:369:ILE:HD13 | 2.30 | 0.47 |
| 3:B:734:GLU:CG | 3:B:821:PHE:CB | 2.91 | 0.47 |
| 3:B:456:ASP:OD1 | 3:B:635:PRO:O | 2.32 | 0.47 |
| 3:A:161:GLN:NE2 | 3:A:222:LEU:HB2 | 2.30 | 0.47 |
| 3:B:801:THR:CB | 3:B:802:PRO:HD2 | 2.45 | 0.47 |
| 1:T:6:DG:OP1 | 3:B:517:GLU:HG2 | 2.14 | 0.47 |
| 3:A:150:ALA:O | 3:A:152:THR:HG23 | 2.14 | 0.47 |
| 6:T:200:HOH:O | 3:A:343:ARG:NH2 | 2.43 | 0.47 |
| 6:T:198:HOH:O | 2:P:2:DG:H2' | 2.13 | 0.47 |
| 2:P:12:DC:H5'' | 2:P:13:DOC:OP2 | 2.15 | 0.47 |
| 3:A:304:GLU:HB2 | 3:A:328:LEU:HD21 | 1.97 | 0.47 |
| 3:B:734:GLU:CD | 3:B:821:PHE:CB | 2.82 | 0.47 |
| 3:B:634:LYS:O | 3:B:635:PRO:O | 2.32 | 0.47 |
| 3:B:495:VAL:O | 3:B:497:LYS:HD2 | 2.15 | 0.47 |
| 3:B:767:ARG:HH11 | 3:B:824:THR:HB | 1.79 | 0.47 |
| 2:P:5:DG:H2'' | 2:P:6:DA:O4' | 2.15 | 0.47 |
| 1:T:5:DA:O3' | 3:B:480:LYS:HG2 | 2.15 | 0.47 |
| 3:B:759:PRO:HG2 | 3:B:830:PHE:CD1 | 2.50 | 0.47 |
| 3:A:161:GLN:NE2 | 3:A:222:LEU:HB2 | 2.30 | 0.47 |
| 3:B:779:SER:N | 3:B:811:PHE:CZ | 2.82 | 0.47 |
| 3:B:798:ASP:O | 3:B:802:PRO:HD2 | 2.15 | 0.47 |
| 3:B:745:LEU:HD21 | 3:B:828:VAL:CG1 | 2.41 | 0.47 |
| 3:B:502:ARG:HD3 | 3:B:505:LYS:CB | 2.44 | 0.47 |
| 3:A:369:ILE:HG13 | 3:A:379:VAL:HG21 | 1.96 | 0.47 |
| 3:B:734:GLU:CD | 3:B:821:PHE:CB | 2.82 | 0.47 |
| 3:A:184:ARG:HA | 3:A:187:MET:CE | 2.45 | 0.47 |
| 3:B:502:ARG:HD3 | 3:B:505:LYS:CB | 2.45 | 0.47 |
| 3:A:81:VAL:O | 3:A:85:LYS:HB2 | 2.15 | 0.47 |
| 2:P:11:DC:C2' | 2:P:12:DC:O5' | 2.61 | 0.47 |
| 3:B:456:ASP:OD1 | 3:B:635:PRO:O | 2.32 | 0.47 |
| 3:B:539:VAL:N | 6:B:1067:HOH:O | 2.30 | 0.47 |
| 3:B:624:LEU:CD2 | 3:B:660:PRO:HD2 | 2.45 | 0.47 |
| 3:A:184:ARG:HA | 3:A:187:MET:CE | 2.45 | 0.47 |
| 3:B:813:ASN:O | 3:B:814:MET:C | 2.52 | 0.47 |
| 3:A:81:VAL:O | 3:A:85:LYS:HB2 | 2.15 | 0.47 |
| 3:B:779:SER:N | 3:B:811:PHE:CZ | 2.82 | 0.47 |
| 3:B:798:ASP:O | 3:B:802:PRO:HD2 | 2.15 | 0.47 |
| 3:B:767:ARG:HH11 | 3:B:824:THR:HB | 1.79 | 0.47 |
| 3:B:791:LYS:CB | 3:B:794:THR:HG21 | 2.26 | 0.47 |
| 1:T:6:DG:OP1 | 1:T:6:DG:H4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:794:THR:HG23 | 3:B:796:ASN:ND2 | 2.30 | 0.47 |
| 3:B:624:LEU:CD2 | 3:B:660:PRO:HD2 | 2.45 | 0.47 |
| 6:T:129:HOH:O | 3:A:114:GLU:OE1 | 2.20 | 0.47 |
| 1:T:8:DG:H2' | 1:T:9:DT:C7 | 2.45 | 0.47 |
| 3:B:759:PRO:HG2 | 3:B:830:PHE:CD1 | 2.50 | 0.47 |
| 1:T:8:DG:H2' | 1:T:9:DT:C7 | 2.45 | 0.47 |
| 6:P:297:HOH:O | 3:B:572:THR:HG21 | 2.15 | 0.47 |
| 3:B:497:LYS:HZ2 | 3:B:497:LYS:HB3 | 1.79 | 0.47 |
| 3:A:388:MET:HA | 3:A:388:MET:CE | 2.45 | 0.46 |
| 3:B:689:LEU:HD11 | 3:B:693:LEU:HD12 | 1.96 | 0.46 |
| 2:P:5:DG:H2'' | 2:P:6:DA:O4' | 2.15 | 0.46 |
| 1:T:6:DG:H4' | 1:T:6:DG:OP1 | 2.15 | 0.46 |
| 3:A:379:VAL:N | 6:A:593:HOH:O | 2.48 | 0.46 |
| 3:A:54:PRO:HB3 | 3:A:70:ALA:HB2 | 1.97 | 0.46 |
| 3:B:588:VAL:O | 3:B:592:ARG:HG3 | 2.15 | 0.46 |
| 1:T:12:DT:C2' | 1:T:13:DT:C6 | 2.93 | 0.46 |
| 3:A:61:TYR:O | 3:A:62:LEU:HD23 | 2.14 | 0.46 |
| 3:B:495:VAL:O | 3:B:497:LYS:HD2 | 2.15 | 0.46 |
| 3:A:54:PRO:HB3 | 3:A:70:ALA:HB2 | 1.97 | 0.46 |
| 3:B:665:LYS:O | 3:B:668:LYS:HB2 | 2.16 | 0.46 |
| 3:B:782:CYS:SG | 3:B:782:CYS:O | 2.73 | 0.46 |
| 3:B:740:LYS:NZ | 3:B:741:ILE:CG1 | 2.78 | 0.46 |
| 3:A:304:GLU:HB2 | 3:A:328:LEU:HD21 | 1.97 | 0.46 |
| 3:B:588:VAL:O | 3:B:592:ARG:HG3 | 2.15 | 0.46 |
| 6:T:248:HOH:O | 3:A:169:LEU:CD1 | 2.64 | 0.46 |
| 3:A:317:ALA:CA | 3:A:320:LYS:HG3 | 2.33 | 0.46 |
| 3:B:464:MET:HE1 | 3:B:487:ASN:HD22 | 1.80 | 0.46 |
| 3:B:665:LYS:O | 3:B:668:LYS:HB2 | 2.16 | 0.46 |
| 3:A:296:SER:O | 6:A:629:HOH:O | 2.20 | 0.46 |
| 3:A:302:PHE:O | 3:A:328:LEU:HD22 | 2.16 | 0.46 |
| 3:B:762:VAL:O | 3:B:781:GLN:HG2 | 2.15 | 0.46 |
| 1:T:12:DT:C2' | 1:T:13:DT:C6 | 2.93 | 0.46 |
| 3:A:410:PHE:O | 3:A:411:CYS:O | 2.33 | 0.46 |
| 1:T:5:DA:H8 | 3:B:479:GLN:OE1 | 1.99 | 0.46 |
| 6:T:101:HOH:O | 3:A:222:LEU:HB2 | 2.14 | 0.46 |
| 3:A:50:LEU:HA | 3:A:53:LYS:CD | 2.46 | 0.46 |
| 3:B:791:LYS:CB | 3:B:794:THR:HG21 | 2.27 | 0.46 |
| 2:P:9:DG:P | 3:B:776:GLY:H | 2.38 | 0.46 |
| 3:A:302:PHE:O | 3:A:328:LEU:HD22 | 2.16 | 0.46 |
| 3:B:555:MET:HE2 | 3:B:599:ILE:HD12 | 1.98 | 0.46 |
| 1:T:12:DT:H2'' | 1:T:13:DT:H6 | 1.76 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:313:SER:O | 3:A:315:VAL:CG1 | 2.56 | 0.46 |
| 3:B:459:TYR:CZ | 5:B:902:TTP:H1' | 2.51 | 0.46 |
| 6:P:257:HOH:O | 3:B:447:SER:HB2 | 2.16 | 0.46 |
| 3:B:782:CYS:O | 3:B:782:CYS:SG | 2.73 | 0.46 |
| 3:A:301:SER:O | 3:A:302:PHE:HD2 | 1.98 | 0.46 |
| 3:B:460:ALA:O | 3:B:464:MET:HG3 | 2.16 | 0.46 |
| 3:A:127:GLU:OE1 | 3:A:207:LYS:NZ | 2.41 | 0.46 |
| 3:A:301:SER:O | 3:A:302:PHE:HD2 | 1.98 | 0.46 |
| 3:A:339:PRO:HG2 | 3:A:410:PHE:CD1 | 2.51 | 0.46 |
| 3:B:501:VAL:C | 3:B:503:ASP:H | 2.19 | 0.46 |
| 3:A:54:PRO:HG3 | 3:A:69:GLU:HG3 | 1.98 | 0.46 |
| 3:A:339:PRO:HG2 | 3:A:410:PHE:CD1 | 2.51 | 0.46 |
| 3:B:740:LYS:NZ | 3:B:741:ILE:CG1 | 2.78 | 0.46 |
| 3:A:410:PHE:O | 3:A:411:CYS:O | 2.33 | 0.46 |
| 3:A:153:VAL:HG22 | 3:A:154:SER:N | 2.31 | 0.46 |
| 3:A:61:TYR:O | 3:A:62:LEU:HD23 | 2.14 | 0.46 |
| 3:A:146:ASP:C | 3:A:148:LEU:H | 2.20 | 0.46 |
| 3:B:762:VAL:O | 3:B:781:GLN:HG2 | 2.15 | 0.45 |
| 3:B:813:ASN:O | 3:B:814:MET:C | 2.52 | 0.45 |
| 3:B:794:THR:HG23 | 3:B:796:ASN:ND2 | 2.30 | 0.45 |
| 3:A:86:GLU:O | 3:A:89:PRO:HD3 | 2.16 | 0.45 |
| 2:P:12:DC:H2" | 3:B:543:LEU:HD21 | 1.98 | 0.45 |
| 3:B:725:GLU:HB2 | 3:B:827:SER:CA | 2.43 | 0.45 |
| 3:B:592:ARG:NH1 | 3:B:592:ARG:CG | 2.80 | 0.45 |
| 3:A:354:HIS:O | 3:A:355:TYR:C | 2.55 | 0.45 |
| 6:P:177:HOH:O | 3:B:539:VAL:CG2 | 2.64 | 0.45 |
| 3:B:501:VAL:C | 3:B:503:ASP:H | 2.19 | 0.45 |
| 3:A:392:ARG:O | 3:A:395:VAL:N | 2.50 | 0.45 |
| 3:A:54:PRO:HG3 | 3:A:69:GLU:HG3 | 1.97 | 0.45 |
| 3:B:728:PHE:HB2 | 3:B:731:CYS:HB2 | 1.99 | 0.45 |
| 3:A:365:PRO:CB | 3:A:369:ILE:HD13 | 2.30 | 0.45 |
| 3:B:460:ALA:O | 3:B:464:MET:HG3 | 2.16 | 0.45 |
| 3:B:592:ARG:CG | 3:B:592:ARG:NH1 | 2.80 | 0.45 |
| 3:A:50:LEU:HA | 3:A:53:LYS:CG | 2.47 | 0.45 |
| 1:T:6:DG:OP1 | 3:B:517:GLU:HG2 | 2.17 | 0.45 |
| 3:A:86:GLU:O | 3:A:89:PRO:HD3 | 2.16 | 0.45 |
| 3:A:265:SER:OG | 3:A:268:ILE:HB | 2.17 | 0.45 |
| 3:A:388:MET:CE | 3:A:388:MET:HA | 2.45 | 0.45 |
| 3:B:822:HIS:O | 3:B:823:LEU:CB | 2.64 | 0.45 |
| 3:A:341:THR:CG2 | 3:A:362:CYS:O | 2.64 | 0.45 |
| 3:A:388:MET:N | 3:A:388:MET:CE | 2.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:1:DG:H2'' | 2:P:2:DG:C5' | 2.31 | 0.45 |
| 3:A:354:HIS:O | 3:A:355:TYR:C | 2.55 | 0.45 |
| 3:B:667:ALA:O | 3:B:671:GLU:HG3 | 2.17 | 0.45 |
| 3:A:60:LYS:O | 3:A:61:TYR:CG | 2.63 | 0.45 |
| 3:A:388:MET:CE | 3:A:388:MET:N | 2.80 | 0.45 |
| 3:B:667:ALA:O | 3:B:671:GLU:HG3 | 2.17 | 0.45 |
| 3:B:720:GLN:NE2 | 6:B:1082:HOH:O | 2.46 | 0.45 |
| 3:A:410:PHE:O | 3:A:411:CYS:C | 2.55 | 0.45 |
| 1:T:8:DG:C8 | 1:T:9:DT:H72 | 2.52 | 0.45 |
| 3:B:822:HIS:O | 3:B:823:LEU:CB | 2.64 | 0.45 |
| 6:P:230:HOH:O | 3:B:539:VAL:HG11 | 2.17 | 0.45 |
| 3:A:184:ARG:HA | 3:A:187:MET:HE3 | 1.99 | 0.45 |
| 1:T:10:DC:C2' | 1:T:11:DC:O5' | 2.62 | 0.45 |
| 3:A:175:VAL:O | 3:A:178:GLN:HB2 | 2.17 | 0.45 |
| 2:P:5:DG:H2'' | 2:P:6:DA:O5' | 2.17 | 0.45 |
| 1:T:8:DG:C8 | 1:T:9:DT:H72 | 2.52 | 0.45 |
| 3:A:265:SER:OG | 3:A:268:ILE:HB | 2.17 | 0.45 |
| 3:B:479:GLN:O | 3:B:480:LYS:C | 2.56 | 0.44 |
| 6:P:249:HOH:O | 3:B:781:GLN:HG3 | 2.16 | 0.44 |
| 2:P:5:DG:H2'' | 2:P:6:DA:O5' | 2.17 | 0.44 |
| 1:T:10:DC:C2' | 1:T:11:DC:O5' | 2.62 | 0.44 |
| 3:B:512:VAL:HG12 | 3:B:513:LEU:N | 2.32 | 0.44 |
| 3:B:512:VAL:HG12 | 3:B:513:LEU:N | 2.32 | 0.44 |
| 3:B:728:PHE:HB2 | 3:B:731:CYS:HB2 | 1.98 | 0.44 |
| 3:A:208:LEU:HD21 | 3:A:240:PRO:HD3 | 2.00 | 0.44 |
| 3:B:479:GLN:O | 3:B:480:LYS:C | 2.56 | 0.44 |
| 1:T:5:DA:C8 | 3:B:479:GLN:OE1 | 2.71 | 0.44 |
| 3:A:55:LEU:O | 3:A:66:CYS:HB2 | 2.17 | 0.44 |
| 3:A:175:VAL:O | 3:A:178:GLN:HB2 | 2.17 | 0.44 |
| 3:A:335:ASP:OD1 | 3:A:337:ARG:HB2 | 2.18 | 0.44 |
| 3:A:75:VAL:HG12 | 3:A:75:VAL:O | 2.17 | 0.44 |
| 3:A:335:ASP:OD1 | 3:A:337:ARG:HB2 | 2.18 | 0.44 |
| 3:B:725:GLU:HB2 | 3:B:827:SER:CA | 2.43 | 0.44 |
| 3:A:75:VAL:O | 3:A:75:VAL:HG12 | 2.17 | 0.44 |
| 3:A:153:VAL:HG22 | 3:A:154:SER:N | 2.32 | 0.44 |
| 3:A:60:LYS:O | 3:A:61:TYR:CG | 2.63 | 0.44 |
| 3:A:410:PHE:O | 3:A:411:CYS:C | 2.55 | 0.44 |
| 3:A:347:ARG:CB | 3:A:356:GLY:HA3 | 2.48 | 0.44 |
| 3:B:559:ARG:CZ | 3:B:599:ILE:CD1 | 2.96 | 0.44 |
| 3:B:750:ASN:O | 3:B:754:GLN:HB2 | 2.18 | 0.44 |
| 3:B:801:THR:CB | 3:B:802:PRO:HD2 | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:392:ARG:O | 3:A:395:VAL:N | 2.50 | 0.44 |
| 3:B:750:ASN:O | 3:B:754:GLN:HB2 | 2.18 | 0.44 |
| 3:A:301:SER:O | 3:A:302:PHE:CD2 | 2.71 | 0.44 |
| 3:A:405:LEU:HA | 3:A:405:LEU:HD12 | 1.67 | 0.44 |
| 3:B:685:SER:CB | 3:B:688:ILE:HG22 | 2.42 | 0.44 |
| 6:T:148:HOH:O | 3:A:257:SER:HB2 | 2.18 | 0.44 |
| 3:B:802:PRO:O | 3:B:806:ILE:CG2 | 2.60 | 0.44 |
| 3:A:346:ILE:N | 3:A:358:GLU:O | 2.51 | 0.44 |
| 1:T:17:DC:H2'' | 1:T:18:DC:OP2 | 2.18 | 0.44 |
| 3:A:55:LEU:O | 3:A:66:CYS:HB2 | 2.17 | 0.44 |
| 3:A:146:ASP:C | 3:A:148:LEU:H | 2.20 | 0.44 |
| 3:A:50:LEU:HA | 3:A:53:LYS:CG | 2.47 | 0.44 |
| 3:B:744:LEU:HD11 | 3:B:828:VAL:HG23 | 2.00 | 0.43 |
| 3:B:743:GLU:O | 3:B:746:ALA:CB | 2.63 | 0.43 |
| 1:T:13:DT:H2'' | 1:T:14:DC:O4' | 2.18 | 0.43 |
| 3:B:471:LYS:O | 3:B:472:ASP:OD1 | 2.35 | 0.43 |
| 3:A:54:PRO:HB3 | 3:A:70:ALA:CB | 2.48 | 0.43 |
| 3:B:459:TYR:CZ | 5:B:902:TTP:H1' | 2.53 | 0.43 |
| 3:B:539:VAL:HG11 | 6:B:1130:HOH:O | 2.18 | 0.43 |
| 3:A:270:GLU:HA | 3:A:278:ALA:HB2 | 2.00 | 0.43 |
| 1:T:17:DC:H2'' | 1:T:18:DC:OP2 | 2.18 | 0.43 |
| 3:B:560:LEU:HD23 | 3:B:563:LEU:HD12 | 2.00 | 0.43 |
| 3:A:101:ARG:HH11 | 3:A:101:ARG:HG3 | 1.83 | 0.43 |
| 3:B:764:LEU:HA | 3:B:828:VAL:HA | 2.01 | 0.43 |
| 2:P:8:DG:C5' | 3:B:776:GLY:O | 2.66 | 0.43 |
| 3:B:560:LEU:HD23 | 3:B:563:LEU:HD12 | 2.00 | 0.43 |
| 3:A:208:LEU:HD21 | 3:A:240:PRO:HD3 | 1.99 | 0.43 |
| 3:A:301:SER:O | 3:A:302:PHE:CD2 | 2.71 | 0.43 |
| 2:P:1:DG:H2'' | 2:P:2:DG:C5' | 2.31 | 0.43 |
| 3:B:573:VAL:HG22 | 3:B:574:SER:N | 2.33 | 0.43 |
| 1:T:13:DT:H2'' | 1:T:14:DC:O4' | 2.18 | 0.43 |
| 3:B:559:ARG:CZ | 3:B:599:ILE:CD1 | 2.96 | 0.43 |
| 3:B:822:HIS:O | 3:B:823:LEU:CD2 | 2.66 | 0.43 |
| 3:A:88:CYS:N | 3:A:89:PRO:HD3 | 2.33 | 0.43 |
| 3:B:622:ASN:C | 3:B:622:ASN:ND2 | 2.72 | 0.43 |
| 3:B:759:PRO:CD | 3:B:833:LEU:HD11 | 2.40 | 0.43 |
| 3:A:346:ILE:N | 3:A:358:GLU:O | 2.51 | 0.43 |
| 3:A:347:ARG:CB | 3:A:356:GLY:HA3 | 2.48 | 0.43 |
| 3:B:508:CYS:C | 3:B:510:GLN:H | 2.21 | 0.43 |
| 3:B:716:SER:O | 3:B:717:GLY:O | 2.36 | 0.43 |
| 3:A:335:ASP:C | 3:A:335:ASP:OD1 | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:101:ARG:HH11 | 3:A:101:ARG:HG3 | 1.83 | 0.43 |
| 3:A:371:LYS:HE2 | 3:A:376:ASN:CB | 2.47 | 0.43 |
| 3:A:50:LEU:HA | 3:A:53:LYS:CD | 2.46 | 0.43 |
| 3:A:50:LEU:HA | 3:A:53:LYS:HG2 | 2.01 | 0.43 |
| 3:A:318:LYS:HD3 | 3:A:318:LYS:C | 2.39 | 0.43 |
| 1:T:5:DA:C8 | 3:B:479:GLN:OE1 | 2.72 | 0.43 |
| 3:A:388:MET:CA | 3:A:388:MET:CE | 2.97 | 0.43 |
| 3:B:716:SER:O | 3:B:717:GLY:O | 2.36 | 0.43 |
| 2:P:8:DG:O5' | 3:B:777:ARG:C | 2.56 | 0.43 |
| 3:A:335:ASP:C | 3:A:335:ASP:OD1 | 2.56 | 0.43 |
| 3:B:508:CYS:C | 3:B:510:GLN:H | 2.21 | 0.43 |
| 3:B:572:THR:HG21 | 6:B:1197:HOH:O | 2.18 | 0.43 |
| 3:B:802:PRO:O | 3:B:806:ILE:CG2 | 2.60 | 0.43 |
| 3:B:471:LYS:O | 3:B:472:ASP:OD1 | 2.35 | 0.43 |
| 3:A:54:PRO:HB3 | 3:A:70:ALA:CB | 2.48 | 0.43 |
| 3:A:318:LYS:C | 3:A:318:LYS:HD3 | 2.39 | 0.43 |
| 3:A:46:SER:C | 3:A:48:PRO:HD3 | 2.39 | 0.43 |
| 3:A:255:ILE:HD11 | 3:A:264:PHE:CD1 | 2.53 | 0.43 |
| 2:P:7:DA:H5' | 3:B:779:SER:O | 2.19 | 0.43 |
| 3:B:573:VAL:HG22 | 3:B:574:SER:N | 2.33 | 0.43 |
| 3:B:508:CYS:O | 3:B:510:GLN:N | 2.52 | 0.43 |
| 3:A:255:ILE:HD11 | 3:A:264:PHE:CD1 | 2.53 | 0.43 |
| 3:A:179:ILE:O | 3:A:183:MET:HG3 | 2.19 | 0.43 |
| 1:T:14:DC:OP1 | 3:A:360:ARG:NH2 | 2.52 | 0.43 |
| 3:A:388:MET:CE | 3:A:388:MET:CA | 2.97 | 0.43 |
| 3:A:46:SER:C | 3:A:48:PRO:HD3 | 2.39 | 0.43 |
| 3:B:581:GLN:OE1 | 3:B:642:LEU:HB2 | 2.19 | 0.43 |
| 3:B:764:LEU:HG | 3:B:828:VAL:HG22 | 2.00 | 0.42 |
| 3:B:484:VAL:HG21 | 5:B:902:TTP:O2 | 2.18 | 0.42 |
| 3:B:744:LEU:HD11 | 3:B:828:VAL:HG23 | 2.00 | 0.42 |
| 1:T:12:DT:H2'' | 1:T:13:DT:H6 | 1.75 | 0.42 |
| 3:A:405:LEU:HD12 | 3:A:405:LEU:HA | 1.67 | 0.42 |
| 3:A:320:LYS:CB | 3:A:406:LEU:HD12 | 2.50 | 0.42 |
| 3:B:483:VAL:HG23 | 3:B:501:VAL:HA | 2.01 | 0.42 |
| 3:A:295:LEU:HD22 | 6:A:698:HOH:O | 2.18 | 0.42 |
| 3:A:88:CYS:N | 3:A:89:PRO:HD3 | 2.33 | 0.42 |
| 1:T:7:DG:C4' | 3:B:519:LEU:HD12 | 2.47 | 0.42 |
| 3:A:112:LEU:O | 3:A:112:LEU:HD23 | 2.19 | 0.42 |
| 3:B:712:PRO:HB3 | 6:B:1127:HOH:O | 2.20 | 0.42 |
| 3:B:761:THR:CG2 | 3:B:762:VAL:N | 2.82 | 0.42 |
| 3:A:341:THR:CG2 | 3:A:362:CYS:O | 2.64 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:408:VAL:CG1 | 3:A:409:CYS:N | 2.82 | 0.42 |
| 3:A:320:LYS:CB | 3:A:406:LEU:HD12 | 2.50 | 0.42 |
| 3:A:95:ASN:N | 6:A:667:HOH:O | 2.37 | 0.42 |
| 3:A:270:GLU:HA | 3:A:278:ALA:HB2 | 2.00 | 0.42 |
| 3:A:179:ILE:O | 3:A:183:MET:HG3 | 2.20 | 0.42 |
| 3:B:483:VAL:HG23 | 3:B:501:VAL:HA | 2.01 | 0.42 |
| 3:A:54:PRO:CB | 3:A:70:ALA:HB2 | 2.49 | 0.42 |
| 3:B:560:LEU:HD12 | 3:B:592:ARG:HH12 | 1.83 | 0.42 |
| 1:T:18:DC:OP1 | 6:T:103:HOH:O | 2.22 | 0.42 |
| 3:B:767:ARG:HD3 | 3:B:769:TYR:CB | 2.50 | 0.42 |
| 3:B:824:THR:HG22 | 3:B:825:LEU:HG | 2.02 | 0.42 |
| 2:P:9:DG:P | 3:B:776:GLY:H | 2.43 | 0.42 |
| 3:A:75:VAL:O | 3:A:77:LYS:N | 2.52 | 0.42 |
| 6:P:223:HOH:O | 3:B:718:PRO:HG3 | 2.20 | 0.42 |
| 3:B:584:ASN:N | 3:B:590:HIS:HD2 | 2.04 | 0.42 |
| 3:B:761:THR:CG2 | 3:B:762:VAL:N | 2.82 | 0.42 |
| 3:B:685:SER:CB | 3:B:688:ILE:HG22 | 2.43 | 0.42 |
| 3:B:560:LEU:HD12 | 3:B:592:ARG:HH12 | 1.83 | 0.42 |
| 3:B:508:CYS:O | 3:B:510:GLN:N | 2.52 | 0.42 |
| 3:A:75:VAL:O | 3:A:77:LYS:N | 2.52 | 0.42 |
| 3:B:581:GLN:NE2 | 3:B:644:GLU:HB2 | 2.35 | 0.42 |
| 1:T:12:DT:P | 3:A:363:PRO:HD3 | 2.58 | 0.42 |
| 3:B:764:LEU:HG | 3:B:828:VAL:HG22 | 2.00 | 0.42 |
| 3:B:743:GLU:O | 3:B:746:ALA:CB | 2.63 | 0.42 |
| 3:B:511:LEU:C | 3:B:511:LEU:HD23 | 2.40 | 0.42 |
| 2:P:8:DG:H2'' | 2:P:9:DG:C8 | 2.54 | 0.42 |
| 2:P:11:DC:H2'' | 2:P:12:DC:O5' | 2.19 | 0.42 |
| 6:T:235:HOH:O | 3:A:108:LYS:NZ | 2.45 | 0.42 |
| 3:A:32:HIS:O | 3:A:197:ALA:HA | 2.20 | 0.42 |
| 3:B:780:ARG:NH2 | 3:B:812:ARG:C | 2.66 | 0.42 |
| 3:A:408:VAL:CG1 | 3:A:409:CYS:N | 2.82 | 0.42 |
| 3:B:481:TYR:C | 3:B:501:VAL:HG13 | 2.40 | 0.42 |
| 3:A:369:ILE:HG13 | 3:A:379:VAL:CG2 | 2.50 | 0.42 |
| 3:B:755:ASP:CG | 3:B:756:GLY:O | 2.58 | 0.42 |
| 3:B:722:PHE:CD1 | 3:B:722:PHE:N | 2.88 | 0.42 |
| 3:B:822:HIS:O | 3:B:823:LEU:CD2 | 2.66 | 0.42 |
| 3:B:562:GLN:H | 3:B:562:GLN:HE21 | 1.68 | 0.42 |
| 3:A:214:LYS:HB2 | 3:A:215:PRO:HD3 | 2.02 | 0.42 |
| 3:A:281:ILE:HG22 | 3:A:282:GLN:N | 2.35 | 0.42 |
| 3:A:342:VAL:HG12 | 3:A:410:PHE:CD2 | 2.55 | 0.41 |
| 3:B:685:SER:O | 3:B:688:ILE:HG22 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:50:LEU:HA | 3:A:53:LYS:HG2 | 2.00 | 0.41 |
| 3:B:581:GLN:OE1 | 3:B:642:LEU:HB2 | 2.19 | 0.41 |
| 2:P:8:DG:C5' | 3:B:776:GLY:O | 2.67 | 0.41 |
| 3:B:824:THR:HG22 | 3:B:825:LEU:HG | 2.02 | 0.41 |
| 3:A:369:ILE:HG13 | 3:A:379:VAL:CG2 | 2.50 | 0.41 |
| 3:B:722:PHE:HE1 | 3:B:833:LEU:HG | 1.85 | 0.41 |
| 3:A:321:ILE:O | 3:A:325:LEU:HD13 | 2.20 | 0.41 |
| 3:A:54:PRO:CB | 3:A:70:ALA:HB2 | 2.49 | 0.41 |
| 3:B:767:ARG:HD3 | 3:B:769:TYR:CB | 2.50 | 0.41 |
| 3:B:555:MET:HE1 | 3:B:599:ILE:HD12 | 2.02 | 0.41 |
| 3:B:562:GLN:H | 3:B:562:GLN:HE21 | 1.68 | 0.41 |
| 3:B:581:GLN:NE2 | 3:B:644:GLU:HB2 | 2.35 | 0.41 |
| 3:B:655:HIS:CE1 | 3:B:656:ILE:HG12 | 2.56 | 0.41 |
| 3:B:722:PHE:HE1 | 3:B:833:LEU:HG | 1.85 | 0.41 |
| 3:A:321:ILE:O | 3:A:325:LEU:HD13 | 2.20 | 0.41 |
| 3:B:616:CYS:SG | 3:B:635:PRO:O | 2.79 | 0.41 |
| 3:B:764:LEU:HA | 3:B:828:VAL:HA | 2.01 | 0.41 |
| 3:A:395:VAL:C | 3:A:397:VAL:H | 2.24 | 0.41 |
| 3:B:541:GLU:HA | 3:B:716:SER:HB3 | 2.03 | 0.41 |
| 1:T:10:DC:H2'' | 1:T:11:DC:H6 | 1.85 | 0.41 |
| 3:B:479:GLN:O | 3:B:481:TYR:N | 2.54 | 0.41 |
| 3:B:716:SER:C | 3:B:717:GLY:O | 2.59 | 0.41 |
| 3:A:112:LEU:O | 3:A:112:LEU:HD23 | 2.19 | 0.41 |
| 3:B:655:HIS:CE1 | 3:B:656:ILE:HG12 | 2.55 | 0.41 |
| 2:P:5:DG:H2' | 2:P:6:DA:C8 | 2.56 | 0.41 |
| 2:P:6:DA:C2' | 2:P:7:DA:C8 | 2.93 | 0.41 |
| 3:A:60:LYS:O | 3:A:61:TYR:CB | 2.68 | 0.41 |
| 3:B:685:SER:O | 3:B:688:ILE:HG22 | 2.20 | 0.41 |
| 3:B:452:HIS:O | 3:B:617:ALA:HA | 2.21 | 0.41 |
| 1:T:7:DG:C4' | 3:B:519:LEU:HD12 | 2.49 | 0.41 |
| 3:B:470:LEU:HD13 | 3:B:475:LEU:CD2 | 2.50 | 0.41 |
| 3:B:541:GLU:HA | 3:B:716:SER:HB3 | 2.03 | 0.41 |
| 3:B:532:LEU:CD2 | 3:B:532:LEU:C | 2.89 | 0.41 |
| 3:A:265:SER:HA | 3:A:266:PRO:HD3 | 1.94 | 0.41 |
| 3:A:338:LYS:HA | 3:A:339:PRO:HD2 | 1.94 | 0.41 |
| 1:T:8:DG:H2'' | 1:T:9:DT:H6 | 1.85 | 0.41 |
| 3:B:758:LYS:HA | 3:B:759:PRO:HD2 | 1.89 | 0.41 |
| 3:B:470:LEU:HD13 | 3:B:475:LEU:CD2 | 2.50 | 0.41 |
| 3:B:616:CYS:SG | 3:B:635:PRO:O | 2.78 | 0.41 |
| 3:B:559:ARG:CZ | 3:B:599:ILE:HD13 | 2.51 | 0.41 |
| 1:T:5:DA:H1' | 3:B:479:GLN:HB3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:483:VAL:HB | 3:B:500:ASN:O | 2.21 | 0.41 |
| 3:B:475:LEU:HD12 | 3:B:476:GLY:N | 2.34 | 0.41 |
| 3:B:759:PRO:CD | 3:B:833:LEU:CD1 | 2.84 | 0.41 |
| 2:P:8:DG:H4' | 3:B:777:ARG:HA | 2.03 | 0.41 |
| 3:B:744:LEU:HG | 3:B:745:LEU:N | 2.36 | 0.41 |
| 2:P:8:DG:O5' | 3:B:777:ARG:C | 2.59 | 0.41 |
| 1:T:8:DG:H2'' | 1:T:9:DT:H6 | 1.85 | 0.41 |
| 2:P:10:DA:H2'' | 2:P:11:DC:H5'' | 2.03 | 0.41 |
| 3:A:214:LYS:HB2 | 3:A:215:PRO:HD3 | 2.02 | 0.41 |
| 1:T:14:DC:OP1 | 3:A:359:SER:O | 2.38 | 0.41 |
| 2:P:8:DG:H2'' | 2:P:9:DG:C8 | 2.54 | 0.41 |
| 3:B:479:GLN:O | 3:B:481:TYR:N | 2.54 | 0.41 |
| 3:A:60:LYS:O | 3:A:61:TYR:CB | 2.68 | 0.41 |
| 3:A:60:LYS:C | 3:A:61:TYR:CD1 | 2.85 | 0.41 |
| 3:A:395:VAL:C | 3:A:397:VAL:H | 2.24 | 0.41 |
| 3:B:758:LYS:HA | 3:B:759:PRO:HD2 | 1.89 | 0.41 |
| 3:A:371:LYS:HE2 | 3:A:376:ASN:CB | 2.48 | 0.41 |
| 3:A:274:GLY:O | 3:A:278:ALA:HB2 | 2.21 | 0.41 |
| 3:B:573:VAL:CB | 3:B:594:LEU:HD22 | 2.47 | 0.41 |
| 6:P:253:HOH:O | 3:B:504:ALA:CB | 2.60 | 0.41 |
| 3:B:511:LEU:HD23 | 3:B:511:LEU:C | 2.40 | 0.41 |
| 3:A:230:ILE:HD12 | 3:A:230:ILE:HA | 1.97 | 0.41 |
| 1:T:10:DC:H2'' | 1:T:11:DC:H6 | 1.85 | 0.41 |
| 3:B:744:LEU:HG | 3:B:745:LEU:N | 2.36 | 0.41 |
| 3:A:302:PHE:HZ | 3:A:335:ASP:OD2 | 2.04 | 0.41 |
| 3:B:722:PHE:CD1 | 3:B:722:PHE:N | 2.88 | 0.41 |
| 3:B:716:SER:C | 3:B:717:GLY:O | 2.59 | 0.41 |
| 3:A:274:GLY:O | 3:A:278:ALA:HB2 | 2.21 | 0.41 |
| 3:A:84:ALA:CA | 3:A:87:LYS:HG2 | 2.47 | 0.41 |
| 2:P:10:DA:H2'' | 2:P:11:DC:H5'' | 2.03 | 0.41 |
| 3:B:559:ARG:CZ | 3:B:599:ILE:HD13 | 2.51 | 0.41 |
| 3:B:509:PRO:C | 3:B:511:LEU:N | 2.74 | 0.41 |
| 3:B:604:ARG:HH21 | 3:B:638:GLN:HE21 | 1.69 | 0.41 |
| 1:T:5:DA:C5' | 1:T:5:DA:N3 | 2.84 | 0.41 |
| 3:A:84:ALA:CA | 3:A:87:LYS:HG2 | 2.47 | 0.41 |
| 3:A:351:SER:O | 3:A:353:LYS:N | 2.54 | 0.41 |
| 3:B:562:GLN:NE2 | 3:B:562:GLN:N | 2.69 | 0.41 |
| 3:B:781:GLN:HG3 | 6:B:1149:HOH:O | 2.20 | 0.41 |
| 3:B:799:VAL:HG12 | 3:B:799:VAL:O | 2.21 | 0.41 |
| 2:P:9:DG:OP2 | 3:B:776:GLY:N | 2.54 | 0.41 |
| 2:P:1:DG:O5' | 3:A:304:GLU:HA | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:584:ASN:N | 3:B:590:HIS:HD2 | 2.04 | 0.41 |
| 3:A:32:HIS:O | 3:A:197:ALA:HA | 2.20 | 0.41 |
| 3:B:604:ARG:HH21 | 3:B:638:GLN:HE21 | 1.69 | 0.40 |
| 3:A:342:VAL:HG12 | 3:A:410:PHE:CD2 | 2.55 | 0.40 |
| 1:T:5:DA:N3 | 1:T:5:DA:C5' | 2.84 | 0.40 |
| 3:A:227:GLN:O | 3:A:230:ILE:HG22 | 2.21 | 0.40 |
| 3:B:546:ASP:HA | 6:B:1046:HOH:O | 2.19 | 0.40 |
| 3:B:497:LYS:HZ2 | 3:B:497:LYS:HB3 | 1.84 | 0.40 |
| 3:B:494:GLY:C | 3:B:496:LYS:N | 2.73 | 0.40 |
| 3:B:452:HIS:O | 3:B:617:ALA:HA | 2.21 | 0.40 |
| 3:B:812:ARG:HD3 | 3:B:812:ARG:HA | 1.94 | 0.40 |
| 3:B:481:TYR:C | 3:B:501:VAL:HG13 | 2.41 | 0.40 |
| 3:B:604:ARG:HE | 3:B:638:GLN:NE2 | 2.19 | 0.40 |
| 3:B:748:LEU:O | 3:B:751:ARG:N | 2.53 | 0.40 |
| 3:A:338:LYS:HA | 3:A:339:PRO:HD2 | 1.94 | 0.40 |
| 3:A:281:ILE:HG22 | 3:A:282:GLN:N | 2.35 | 0.40 |
| 2:P:9:DG:P | 3:B:775:TYR:CB | 3.09 | 0.40 |
| 3:B:501:VAL:O | 3:B:503:ASP:N | 2.54 | 0.40 |
| 3:A:53:LYS:HA | 3:A:54:PRO:HD3 | 1.97 | 0.40 |
| 2:P:12:DC:OP2 | 3:B:663:GLY:HA2 | 2.21 | 0.40 |
| 3:A:351:SER:O | 3:A:353:LYS:N | 2.54 | 0.40 |
| 3:A:230:ILE:HD12 | 3:A:230:ILE:HA | 1.98 | 0.40 |
| 3:A:303:SER:CB | 3:A:409:CYS:HA | 2.48 | 0.40 |
| 3:B:501:VAL:O | 3:B:503:ASP:N | 2.55 | 0.40 |
| 3:B:463:GLU:HG3 | 3:B:514:VAL:HG21 | 2.04 | 0.40 |
| 2:P:8:DG:OP1 | 3:B:777:ARG:O | 2.38 | 0.40 |
| 2:P:8:DG:OP1 | 3:B:778:GLU:CA | 2.69 | 0.40 |
| 3:A:303:SER:CB | 3:A:409:CYS:HA | 2.49 | 0.40 |
| 3:B:764:LEU:O | 3:B:779:SER:CB | 2.69 | 0.40 |
| 2:P:7:DA:H5'' | 6:P:249:HOH:O | 2.22 | 0.40 |
| 2:P:12:DC:OP2 | 3:B:663:GLY:HA2 | 2.21 | 0.40 |
| 3:B:475:LEU:HD12 | 3:B:476:GLY:N | 2.34 | 0.40 |
| 3:A:277:VAL:HG21 | 6:A:609:HOH:O | 2.22 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|---|
| 3 | 1-A | 386/388 (100%) | 338 (88%) | 27 (7%) | 21 (5%) | 2 | 1 |
| 3 | 1-B | 386/388 (100%) | 319 (83%) | 44 (11%) | 23 (6%) | 2 | 1 |
| 3 | 2-A | 386/388 (100%) | 337 (87%) | 28 (7%) | 21 (5%) | 2 | 1 |
| 3 | 2-B | 386/388 (100%) | 319 (83%) | 44 (11%) | 23 (6%) | 2 | 1 |
| All | All | 1544/1552 (100%) | 1313 (85%) | 143 (9%) | 88 (6%) | 2 | 1 |

All (88) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1-A | 60 | LYS |
| 3 | 1-A | 61 | TYR |
| 3 | 1-A | 76 | LYS |
| 3 | 1-A | 80 | ASN |
| 3 | 1-A | 89 | PRO |
| 3 | 1-A | 309 | LYS |
| 3 | 1-A | 314 | GLU |
| 3 | 1-A | 351 | SER |
| 3 | 1-A | 352 | GLU |
| 3 | 1-A | 395 | VAL |
| 3 | 1-A | 396 | ASN |
| 3 | 1-A | 399 | MET |
| 3 | 1-A | 400 | PRO |
| 3 | 1-A | 411 | CYS |
| 3 | 1-B | 480 | LYS |
| 3 | 1-B | 635 | PRO |
| 3 | 1-B | 773 | LYS |
| 3 | 1-B | 779 | SER |
| 3 | 1-B | 812 | ARG |
| 3 | 1-B | 815 | VAL |
| 3 | 1-B | 825 | LEU |
| 3 | 1-B | 832 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1-B | 833 | LEU |
| 3 | 2-A | 60 | LYS |
| 3 | 2-A | 61 | TYR |
| 3 | 2-A | 76 | LYS |
| 3 | 2-A | 80 | ASN |
| 3 | 2-A | 89 | PRO |
| 3 | 2-A | 309 | LYS |
| 3 | 2-A | 314 | GLU |
| 3 | 2-A | 351 | SER |
| 3 | 2-A | 352 | GLU |
| 3 | 2-A | 395 | VAL |
| 3 | 2-A | 396 | ASN |
| 3 | 2-A | 399 | MET |
| 3 | 2-A | 400 | PRO |
| 3 | 2-A | 411 | CYS |
| 3 | 2-B | 480 | LYS |
| 3 | 2-B | 635 | PRO |
| 3 | 2-B | 773 | LYS |
| 3 | 2-B | 779 | SER |
| 3 | 2-B | 812 | ARG |
| 3 | 2-B | 815 | VAL |
| 3 | 2-B | 825 | LEU |
| 3 | 2-B | 832 | ASN |
| 3 | 2-B | 833 | LEU |
| 3 | 1-A | 77 | LYS |
| 3 | 1-A | 380 | MET |
| 3 | 1-B | 717 | GLY |
| 3 | 1-B | 718 | PRO |
| 3 | 1-B | 738 | LYS |
| 3 | 2-A | 77 | LYS |
| 3 | 2-A | 380 | MET |
| 3 | 2-B | 717 | GLY |
| 3 | 2-B | 718 | PRO |
| 3 | 2-B | 738 | LYS |
| 3 | 1-A | 37 | CYS |
| 3 | 1-A | 158 | TYR |
| 3 | 1-B | 457 | CYS |
| 3 | 1-B | 472 | ASP |
| 3 | 1-B | 474 | PRO |
| 3 | 1-B | 817 | VAL |
| 3 | 2-A | 37 | CYS |
| 3 | 2-B | 457 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 2-B | 472 | ASP |
| 3 | 2-B | 474 | PRO |
| 3 | 2-B | 817 | VAL |
| 3 | 1-A | 88 | CYS |
| 3 | 1-A | 367 | HIS |
| 3 | 1-A | 405 | LEU |
| 3 | 1-B | 578 | TYR |
| 3 | 1-B | 775 | TYR |
| 3 | 1-B | 793 | GLY |
| 3 | 2-A | 88 | CYS |
| 3 | 2-A | 158 | TYR |
| 3 | 2-A | 367 | HIS |
| 3 | 2-A | 405 | LEU |
| 3 | 2-B | 578 | TYR |
| 3 | 2-B | 775 | TYR |
| 3 | 2-B | 793 | GLY |
| 3 | 2-B | 757 | ARG |
| 3 | 1-B | 757 | ARG |
| 3 | 1-B | 494 | GLY |
| 3 | 1-B | 509 | PRO |
| 3 | 2-B | 494 | GLY |
| 3 | 2-B | 509 | PRO |
| 3 | 1-B | 495 | VAL |
| 3 | 2-B | 495 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 3 | 1-A | 299/353 (85%) | 274 (92%) | 25 (8%) | 14 | 16 |
| 3 | 1-B | 304/353 (86%) | 266 (88%) | 38 (12%) | 6 | 6 |
| 3 | 2-A | 299/353 (85%) | 274 (92%) | 25 (8%) | 14 | 16 |
| 3 | 2-B | 304/353 (86%) | 266 (88%) | 38 (12%) | 6 | 6 |
| All | All | 1206/1412 (85%) | 1080 (90%) | 126 (10%) | 9 | 10 |

All (126) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1-A | 47 | ASN |
| 3 | 1-A | 60 | LYS |
| 3 | 1-A | 89 | PRO |
| 3 | 1-A | 144 | GLN |
| 3 | 1-A | 170 | HIS |
| 3 | 1-A | 229 | LEU |
| 3 | 1-A | 246 | THR |
| 3 | 1-A | 276 | SER |
| 3 | 1-A | 298 | PRO |
| 3 | 1-A | 299 | PRO |
| 3 | 1-A | 313 | SER |
| 3 | 1-A | 314 | GLU |
| 3 | 1-A | 330 | ASN |
| 3 | 1-A | 337 | ARG |
| 3 | 1-A | 339 | PRO |
| 3 | 1-A | 359 | SER |
| 3 | 1-A | 361 | GLN |
| 3 | 1-A | 363 | PRO |
| 3 | 1-A | 365 | PRO |
| 3 | 1-A | 366 | SER |
| 3 | 1-A | 368 | VAL |
| 3 | 1-A | 371 | LYS |
| 3 | 1-A | 379 | VAL |
| 3 | 1-A | 382 | PRO |
| 3 | 1-A | 410 | PHE |
| 3 | 1-B | 455 | LEU |
| 3 | 1-B | 472 | ASP |
| 3 | 1-B | 497 | LYS |
| 3 | 1-B | 519 | LEU |
| 3 | 1-B | 543 | LEU |
| 3 | 1-B | 562 | GLN |
| 3 | 1-B | 590 | HIS |
| 3 | 1-B | 622 | ASN |
| 3 | 1-B | 624 | LEU |
| 3 | 1-B | 625 | LEU |
| 3 | 1-B | 649 | LEU |
| 3 | 1-B | 716 | SER |
| 3 | 1-B | 719 | PRO |
| 3 | 1-B | 725 | GLU |
| 3 | 1-B | 726 | ASP |
| 3 | 1-B | 728 | PHE |
| 3 | 1-B | 732 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1-B | 740 | LYS |
| 3 | 1-B | 744 | LEU |
| 3 | 1-B | 749 | LEU |
| 3 | 1-B | 757 | ARG |
| 3 | 1-B | 759 | PRO |
| 3 | 1-B | 762 | VAL |
| 3 | 1-B | 767 | ARG |
| 3 | 1-B | 782 | CYS |
| 3 | 1-B | 783 | PRO |
| 3 | 1-B | 785 | PRO |
| 3 | 1-B | 786 | SER |
| 3 | 1-B | 791 | LYS |
| 3 | 1-B | 802 | PRO |
| 3 | 1-B | 806 | ILE |
| 3 | 1-B | 811 | PHE |
| 3 | 1-B | 812 | ARG |
| 3 | 1-B | 813 | ASN |
| 3 | 1-B | 820 | PRO |
| 3 | 1-B | 825 | LEU |
| 3 | 1-B | 830 | PHE |
| 3 | 1-B | 832 | ASN |
| 3 | 2-A | 47 | ASN |
| 3 | 2-A | 60 | LYS |
| 3 | 2-A | 89 | PRO |
| 3 | 2-A | 144 | GLN |
| 3 | 2-A | 170 | HIS |
| 3 | 2-A | 229 | LEU |
| 3 | 2-A | 246 | THR |
| 3 | 2-A | 276 | SER |
| 3 | 2-A | 298 | PRO |
| 3 | 2-A | 299 | PRO |
| 3 | 2-A | 313 | SER |
| 3 | 2-A | 314 | GLU |
| 3 | 2-A | 330 | ASN |
| 3 | 2-A | 337 | ARG |
| 3 | 2-A | 339 | PRO |
| 3 | 2-A | 359 | SER |
| 3 | 2-A | 361 | GLN |
| 3 | 2-A | 363 | PRO |
| 3 | 2-A | 365 | PRO |
| 3 | 2-A | 366 | SER |
| 3 | 2-A | 368 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 2-A | 371 | LYS |
| 3 | 2-A | 379 | VAL |
| 3 | 2-A | 382 | PRO |
| 3 | 2-A | 410 | PHE |
| 3 | 2-B | 455 | LEU |
| 3 | 2-B | 472 | ASP |
| 3 | 2-B | 497 | LYS |
| 3 | 2-B | 519 | LEU |
| 3 | 2-B | 543 | LEU |
| 3 | 2-B | 562 | GLN |
| 3 | 2-B | 590 | HIS |
| 3 | 2-B | 622 | ASN |
| 3 | 2-B | 624 | LEU |
| 3 | 2-B | 625 | LEU |
| 3 | 2-B | 649 | LEU |
| 3 | 2-B | 716 | SER |
| 3 | 2-B | 719 | PRO |
| 3 | 2-B | 725 | GLU |
| 3 | 2-B | 726 | ASP |
| 3 | 2-B | 728 | PHE |
| 3 | 2-B | 732 | SER |
| 3 | 2-B | 740 | LYS |
| 3 | 2-B | 744 | LEU |
| 3 | 2-B | 749 | LEU |
| 3 | 2-B | 757 | ARG |
| 3 | 2-B | 759 | PRO |
| 3 | 2-B | 762 | VAL |
| 3 | 2-B | 767 | ARG |
| 3 | 2-B | 782 | CYS |
| 3 | 2-B | 783 | PRO |
| 3 | 2-B | 785 | PRO |
| 3 | 2-B | 786 | SER |
| 3 | 2-B | 791 | LYS |
| 3 | 2-B | 802 | PRO |
| 3 | 2-B | 806 | ILE |
| 3 | 2-B | 811 | PHE |
| 3 | 2-B | 812 | ARG |
| 3 | 2-B | 813 | ASN |
| 3 | 2-B | 820 | PRO |
| 3 | 2-B | 825 | LEU |
| 3 | 2-B | 830 | PHE |
| 3 | 2-B | 832 | ASN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1-A | 47 | ASN |
| 3 | 1-A | 59 | GLN |
| 3 | 1-A | 95 | ASN |
| 3 | 1-A | 161 | GLN |
| 3 | 1-A | 170 | HIS |
| 3 | 1-A | 227 | GLN |
| 3 | 1-A | 256 | ASN |
| 3 | 1-A | 262 | GLN |
| 3 | 1-A | 367 | HIS |
| 3 | 1-B | 478 | GLN |
| 3 | 1-B | 487 | ASN |
| 3 | 1-B | 562 | GLN |
| 3 | 1-B | 590 | HIS |
| 3 | 1-B | 622 | ASN |
| 3 | 1-B | 638 | GLN |
| 3 | 1-B | 682 | GLN |
| 3 | 1-B | 699 | GLN |
| 3 | 1-B | 760 | HIS |
| 3 | 1-B | 813 | ASN |
| 3 | 2-A | 47 | ASN |
| 3 | 2-A | 59 | GLN |
| 3 | 2-A | 95 | ASN |
| 3 | 2-A | 161 | GLN |
| 3 | 2-A | 170 | HIS |
| 3 | 2-A | 227 | GLN |
| 3 | 2-A | 256 | ASN |
| 3 | 2-A | 262 | GLN |
| 3 | 2-A | 330 | ASN |
| 3 | 2-A | 367 | HIS |
| 3 | 2-B | 478 | GLN |
| 3 | 2-B | 487 | ASN |
| 3 | 2-B | 562 | GLN |
| 3 | 2-B | 590 | HIS |
| 3 | 2-B | 622 | ASN |
| 3 | 2-B | 638 | GLN |
| 3 | 2-B | 682 | GLN |
| 3 | 2-B | 699 | GLN |
| 3 | 2-B | 760 | HIS |
| 3 | 2-B | 813 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$ |
| 2 | DOC | 1-P | 13 | 1,2 | 11,19,20 | 1.31 | 1 (9%) | 14,26,29 | 1.41 | 2 (14%) |
| 2 | DOC | 2-P | 13 | 1,2 | 11,19,20 | 1.31 | 1 (9%) | 14,26,29 | 1.41 | 2 (14%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2 | DOC | 1-P | 13 | 1,2 | - | 0/3/18/19 | 0/2/2/2 |
| 2 | DOC | 2-P | 13 | 1,2 | - | 0/3/18/19 | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 1-P | 13 | DOC | C6-N1 | 3.39 | 1.40 | 1.35 |
| 2 | 2-P | 13 | DOC | C6-N1 | 3.41 | 1.40 | 1.35 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 2 | 2-P | 13 | DOC | O4'-C1'-N1 | 2.42 | 111.91 | 107.72 |
| 2 | 1-P | 13 | DOC | O4'-C1'-N1 | 2.43 | 111.92 | 107.72 |
| 2 | 1-P | 13 | DOC | C2-N3-C4 | 3.69 | 120.82 | 115.61 |
| 2 | 2-P | 13 | DOC | C2-N3-C4 | 3.70 | 120.83 | 115.61 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | 1-P | 13 | DOC | 1 | 0 |
| 2 | 2-P | 13 | DOC | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 5 | TTP | 1-B | 902 | 4 | 21,30,30 | 6.19 | 8 (38%) | 31,47,47 | 2.15 | 8 (25%) |
| 5 | TTP | 2-B | 902 | 4 | 21,30,30 | 6.19 | 7 (33%) | 31,47,47 | 2.15 | 8 (25%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 5 | TTP | 1-B | 902 | 4 | - | 0/18/34/34 | 0/2/2/2 |
| 5 | TTP | 2-B | 902 | 4 | - | 0/18/34/34 | 0/2/2/2 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 5 | 2-B | 902 | TTP | C5M-C5 | -26.76 | 0.98 | 1.51 |
| 5 | 1-B | 902 | TTP | C5M-C5 | -26.69 | 0.98 | 1.51 |
| 5 | 1-B | 902 | TTP | PA-O1A | -4.74 | 1.33 | 1.51 |
| 5 | 2-B | 902 | TTP | PA-O1A | -4.64 | 1.34 | 1.51 |
| 5 | 1-B | 902 | TTP | PA-O5' | -4.13 | 1.40 | 1.59 |
| 5 | 2-B | 902 | TTP | PA-O5' | -4.02 | 1.40 | 1.59 |
| 5 | 1-B | 902 | TTP | PG-O1G | 2.06 | 1.57 | 1.51 |
| 5 | 2-B | 902 | TTP | C6-N1 | 2.23 | 1.38 | 1.35 |
| 5 | 1-B | 902 | TTP | C6-N1 | 2.34 | 1.38 | 1.35 |
| 5 | 2-B | 902 | TTP | C4-N3 | 2.42 | 1.37 | 1.33 |
| 5 | 1-B | 902 | TTP | C4-N3 | 2.50 | 1.37 | 1.33 |
| 5 | 2-B | 902 | TTP | O4-C4 | 3.61 | 1.33 | 1.24 |
| 5 | 1-B | 902 | TTP | O4-C4 | 3.69 | 1.33 | 1.24 |
| 5 | 2-B | 902 | TTP | O5'-C5' | 4.14 | 1.61 | 1.44 |
| 5 | 1-B | 902 | TTP | O5'-C5' | 4.23 | 1.62 | 1.44 |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5 | 1-B | 902 | TTP | C2'-C1'-N1 | -4.63 | 102.89 | 114.16 |
| 5 | 1-B | 902 | TTP | C5-C4-N3 | -4.33 | 120.31 | 125.14 |
| 5 | 2-B | 902 | TTP | C2'-C1'-N1 | -4.32 | 103.66 | 114.16 |
| 5 | 2-B | 902 | TTP | C5-C4-N3 | -4.01 | 120.67 | 125.14 |
| 5 | 2-B | 902 | TTP | PB-O3A-PA | -3.91 | 121.75 | 132.73 |
| 5 | 1-B | 902 | TTP | PB-O3A-PA | -3.82 | 122.00 | 132.73 |
| 5 | 2-B | 902 | TTP | PB-O3B-PG | -2.16 | 125.44 | 132.67 |
| 5 | 1-B | 902 | TTP | PB-O3B-PG | -2.05 | 125.79 | 132.67 |
| 5 | 1-B | 902 | TTP | O2A-PA-O1A | -2.04 | 101.47 | 112.53 |
| 5 | 2-B | 902 | TTP | O2A-PA-O1A | -2.03 | 101.54 | 112.53 |
| 5 | 1-B | 902 | TTP | O5'-C5'-C4' | 2.41 | 118.01 | 109.12 |
| 5 | 2-B | 902 | TTP | O5'-C5'-C4' | 2.42 | 118.05 | 109.12 |
| 5 | 1-B | 902 | TTP | O2A-PA-O5' | 2.89 | 123.06 | 108.46 |
| 5 | 2-B | 902 | TTP | O2A-PA-O5' | 2.89 | 123.06 | 108.46 |
| 5 | 1-B | 902 | TTP | C4-N3-C2 | 5.87 | 120.32 | 115.25 |
| 5 | 2-B | 902 | TTP | C4-N3-C2 | 6.18 | 120.59 | 115.25 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | 1-B | 902 | TTP | 2 | 0 |
| 5 | 2-B | 902 | TTP | 4 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------------|
| 1 | 1-T | 14/14 (100%) | 2.01 | 5 (35%) 0 0 | 42, 50, 59, 66 | 14 (100%) |
| 1 | 2-T | 14/14 (100%) | 2.01 | 5 (35%) 0 0 | 42, 50, 59, 66 | 14 (100%) |
| 2 | 1-P | 12/13 (92%) | 1.71 | 4 (33%) 0 0 | 47, 59, 70, 73 | 12 (100%) |
| 2 | 2-P | 12/13 (92%) | 1.71 | 4 (33%) 0 0 | 47, 59, 70, 73 | 12 (100%) |
| 3 | 1-A | 388/388 (100%) | 2.44 | 130 (33%) 0 0 | 20, 51, 100, 100 | 388 (100%) |
| 3 | 1-B | 388/388 (100%) | 2.28 | 132 (34%) 0 0 | 23, 51, 100, 100 | 388 (100%) |
| 3 | 2-A | 388/388 (100%) | 2.44 | 130 (33%) 0 0 | 20, 51, 100, 100 | 388 (100%) |
| 3 | 2-B | 388/388 (100%) | 2.28 | 132 (34%) 0 0 | 23, 51, 100, 100 | 388 (100%) |
| All | All | 1604/1606 (99%) | 2.34 | 542 (33%) 0 0 | 20, 51, 100, 100 | 1604 (100%) |

All (542) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | 1-A | 401 | PHE | 27.9 |
| 3 | 2-A | 401 | PHE | 27.9 |
| 3 | 1-A | 400 | PRO | 27.9 |
| 3 | 2-A | 400 | PRO | 27.9 |
| 3 | 1-B | 731 | CYS | 21.8 |
| 3 | 2-B | 731 | CYS | 21.8 |
| 3 | 1-A | 354 | HIS | 20.0 |
| 3 | 2-A | 354 | HIS | 20.0 |
| 3 | 1-A | 407 | SER | 19.0 |
| 3 | 2-A | 407 | SER | 19.0 |
| 3 | 1-A | 397 | VAL | 16.8 |
| 3 | 2-A | 397 | VAL | 16.8 |
| 3 | 1-A | 399 | MET | 15.7 |
| 3 | 2-A | 399 | MET | 15.7 |
| 3 | 1-B | 816 | ASN | 15.6 |
| 3 | 2-B | 816 | ASN | 15.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | 1-B | 817 | VAL | 15.3 |
| 3 | 2-B | 817 | VAL | 15.3 |
| 3 | 1-B | 774 | HIS | 13.8 |
| 3 | 2-B | 774 | HIS | 13.8 |
| 3 | 1-A | 356 | GLY | 12.5 |
| 3 | 2-A | 356 | GLY | 12.5 |
| 3 | 1-B | 765 | ILE | 12.5 |
| 3 | 2-B | 765 | ILE | 12.5 |
| 3 | 1-B | 797 | TYR | 11.6 |
| 3 | 2-B | 797 | TYR | 11.6 |
| 3 | 1-B | 815 | VAL | 11.6 |
| 3 | 2-B | 815 | VAL | 11.6 |
| 3 | 1-A | 353 | LYS | 11.5 |
| 3 | 2-A | 353 | LYS | 11.5 |
| 3 | 1-A | 310 | LYS | 11.4 |
| 3 | 2-A | 310 | LYS | 11.4 |
| 3 | 1-B | 818 | LYS | 11.4 |
| 3 | 2-B | 818 | LYS | 11.4 |
| 3 | 1-A | 369 | ILE | 11.3 |
| 3 | 2-A | 369 | ILE | 11.3 |
| 3 | 1-A | 355 | TYR | 11.1 |
| 3 | 2-A | 355 | TYR | 11.1 |
| 3 | 1-A | 352 | GLU | 11.0 |
| 3 | 2-A | 352 | GLU | 11.0 |
| 3 | 1-A | 308 | PHE | 10.8 |
| 3 | 2-A | 308 | PHE | 10.8 |
| 3 | 1-A | 311 | CYS | 10.6 |
| 3 | 2-A | 311 | CYS | 10.6 |
| 3 | 1-B | 732 | SER | 10.4 |
| 3 | 2-B | 732 | SER | 10.4 |
| 3 | 1-B | 795 | GLY | 10.4 |
| 3 | 2-B | 795 | GLY | 10.4 |
| 3 | 1-B | 764 | LEU | 10.1 |
| 3 | 2-B | 764 | LEU | 10.1 |
| 3 | 1-B | 789 | ILE | 9.9 |
| 3 | 2-B | 789 | ILE | 9.9 |
| 3 | 1-A | 372 | LEU | 9.5 |
| 3 | 2-A | 372 | LEU | 9.5 |
| 3 | 1-B | 729 | LYS | 9.5 |
| 3 | 2-B | 729 | LYS | 9.5 |
| 3 | 1-A | 366 | SER | 9.5 |
| 3 | 2-A | 366 | SER | 9.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | 1-B | 821 | PHE | 9.3 |
| 3 | 2-B | 821 | PHE | 9.3 |
| 3 | 1-B | 756 | GLY | 9.2 |
| 3 | 2-B | 756 | GLY | 9.2 |
| 3 | 1-A | 395 | VAL | 9.0 |
| 3 | 2-A | 395 | VAL | 9.0 |
| 3 | 1-B | 740 | LYS | 8.9 |
| 3 | 2-B | 740 | LYS | 8.9 |
| 3 | 1-B | 813 | ASN | 8.9 |
| 3 | 2-B | 813 | ASN | 8.9 |
| 3 | 1-B | 495 | VAL | 8.7 |
| 3 | 2-B | 495 | VAL | 8.7 |
| 3 | 1-B | 827 | SER | 8.6 |
| 3 | 2-B | 827 | SER | 8.6 |
| 3 | 1-B | 790 | GLN | 8.5 |
| 3 | 2-B | 790 | GLN | 8.5 |
| 3 | 1-A | 377 | TYR | 8.4 |
| 3 | 2-A | 377 | TYR | 8.4 |
| 3 | 1-A | 82 | ARG | 8.3 |
| 3 | 2-A | 82 | ARG | 8.3 |
| 3 | 1-A | 367 | HIS | 8.3 |
| 3 | 2-A | 367 | HIS | 8.3 |
| 3 | 1-A | 351 | SER | 8.2 |
| 3 | 2-A | 351 | SER | 8.2 |
| 3 | 1-A | 368 | VAL | 8.0 |
| 3 | 2-A | 368 | VAL | 8.0 |
| 3 | 1-B | 730 | LYS | 7.8 |
| 3 | 2-B | 730 | LYS | 7.8 |
| 3 | 1-A | 333 | CYS | 7.7 |
| 3 | 2-A | 333 | CYS | 7.7 |
| 3 | 1-B | 771 | SER | 7.7 |
| 3 | 2-B | 771 | SER | 7.7 |
| 3 | 1-A | 315 | VAL | 7.7 |
| 3 | 2-A | 315 | VAL | 7.7 |
| 3 | 1-A | 345 | ILE | 7.6 |
| 3 | 2-A | 345 | ILE | 7.6 |
| 3 | 1-B | 788 | VAL | 7.6 |
| 3 | 2-B | 788 | VAL | 7.6 |
| 3 | 1-A | 336 | GLY | 7.6 |
| 3 | 2-A | 336 | GLY | 7.6 |
| 3 | 1-B | 565 | SER | 7.5 |
| 3 | 2-B | 565 | SER | 7.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | 1-B | 825 | LEU | 7.5 |
| 3 | 2-B | 825 | LEU | 7.5 |
| 3 | 1-B | 741 | ILE | 7.3 |
| 3 | 2-B | 741 | ILE | 7.3 |
| 3 | 1-A | 405 | LEU | 7.3 |
| 3 | 2-A | 405 | LEU | 7.3 |
| 3 | 1-B | 784 | ILE | 7.3 |
| 3 | 2-B | 784 | ILE | 7.3 |
| 3 | 1-B | 786 | SER | 7.2 |
| 3 | 2-B | 786 | SER | 7.2 |
| 3 | 1-A | 89 | PRO | 7.2 |
| 3 | 2-A | 89 | PRO | 7.2 |
| 1 | 1-T | 6 | DG | 7.1 |
| 1 | 2-T | 6 | DG | 7.1 |
| 3 | 1-A | 81 | VAL | 7.1 |
| 3 | 2-A | 81 | VAL | 7.1 |
| 3 | 1-A | 326 | ALA | 7.0 |
| 3 | 2-A | 326 | ALA | 7.0 |
| 3 | 1-A | 335 | ASP | 7.0 |
| 3 | 2-A | 335 | ASP | 7.0 |
| 3 | 1-A | 320 | LYS | 7.0 |
| 3 | 2-A | 320 | LYS | 7.0 |
| 3 | 1-A | 344 | LEU | 6.9 |
| 3 | 2-A | 344 | LEU | 6.9 |
| 3 | 1-B | 770 | SER | 6.8 |
| 3 | 2-B | 770 | SER | 6.8 |
| 3 | 1-A | 371 | LYS | 6.7 |
| 3 | 2-A | 371 | LYS | 6.7 |
| 3 | 1-A | 370 | GLN | 6.7 |
| 3 | 2-A | 370 | GLN | 6.7 |
| 3 | 1-A | 406 | LEU | 6.7 |
| 3 | 2-A | 406 | LEU | 6.7 |
| 3 | 1-A | 309 | LYS | 6.7 |
| 3 | 2-A | 309 | LYS | 6.7 |
| 3 | 1-A | 61 | TYR | 6.6 |
| 3 | 2-A | 61 | TYR | 6.6 |
| 3 | 1-A | 312 | SER | 6.5 |
| 3 | 2-A | 312 | SER | 6.5 |
| 3 | 1-B | 775 | TYR | 6.5 |
| 3 | 2-B | 775 | TYR | 6.5 |
| 3 | 1-B | 772 | GLU | 6.5 |
| 3 | 2-B | 772 | GLU | 6.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | 1-B | 728 | PHE | 6.5 |
| 3 | 2-B | 728 | PHE | 6.5 |
| 3 | 1-A | 332 | VAL | 6.5 |
| 3 | 1-A | 350 | SER | 6.5 |
| 3 | 2-A | 332 | VAL | 6.5 |
| 3 | 2-A | 350 | SER | 6.5 |
| 3 | 1-B | 506 | GLU | 6.4 |
| 3 | 2-B | 506 | GLU | 6.4 |
| 3 | 1-A | 408 | VAL | 6.4 |
| 3 | 2-A | 408 | VAL | 6.4 |
| 3 | 1-B | 734 | GLU | 6.3 |
| 3 | 2-B | 734 | GLU | 6.3 |
| 3 | 1-B | 755 | ASP | 6.3 |
| 3 | 2-B | 755 | ASP | 6.3 |
| 3 | 1-B | 494 | GLY | 6.3 |
| 3 | 2-B | 494 | GLY | 6.3 |
| 3 | 1-B | 826 | LEU | 6.3 |
| 3 | 2-B | 826 | LEU | 6.3 |
| 3 | 1-A | 349 | TYR | 6.1 |
| 3 | 2-A | 349 | TYR | 6.1 |
| 3 | 1-A | 374 | THR | 6.1 |
| 3 | 2-A | 374 | THR | 6.1 |
| 3 | 1-A | 313 | SER | 6.1 |
| 3 | 2-A | 313 | SER | 6.1 |
| 3 | 1-B | 794 | THR | 6.0 |
| 3 | 2-B | 794 | THR | 6.0 |
| 3 | 1-B | 820 | PRO | 5.9 |
| 3 | 2-B | 820 | PRO | 5.9 |
| 3 | 1-A | 321 | ILE | 5.9 |
| 3 | 2-A | 321 | ILE | 5.9 |
| 3 | 1-A | 375 | GLY | 5.8 |
| 3 | 2-A | 375 | GLY | 5.8 |
| 3 | 1-A | 391 | PHE | 5.8 |
| 3 | 2-A | 391 | PHE | 5.8 |
| 3 | 1-B | 776 | GLY | 5.8 |
| 3 | 2-B | 776 | GLY | 5.8 |
| 3 | 1-A | 214 | LYS | 5.8 |
| 3 | 2-A | 214 | LYS | 5.8 |
| 3 | 1-A | 409 | CYS | 5.8 |
| 3 | 2-A | 409 | CYS | 5.8 |
| 3 | 1-A | 306 | ASP | 5.8 |
| 3 | 2-A | 306 | ASP | 5.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | 1-A | 90 | GLN | 5.7 |
| 3 | 2-A | 90 | GLN | 5.7 |
| 3 | 1-B | 736 | GLU | 5.6 |
| 3 | 2-B | 736 | GLU | 5.6 |
| 3 | 1-B | 796 | ASN | 5.5 |
| 3 | 2-B | 796 | ASN | 5.5 |
| 3 | 1-B | 834 | LYS | 5.5 |
| 3 | 2-B | 834 | LYS | 5.5 |
| 3 | 1-A | 404 | THR | 5.5 |
| 3 | 2-A | 404 | THR | 5.5 |
| 3 | 1-A | 357 | ARG | 5.5 |
| 3 | 2-A | 357 | ARG | 5.5 |
| 3 | 1-A | 390 | LEU | 5.5 |
| 3 | 2-A | 390 | LEU | 5.5 |
| 3 | 1-B | 779 | SER | 5.5 |
| 3 | 2-B | 779 | SER | 5.5 |
| 3 | 1-A | 73 | LEU | 5.4 |
| 3 | 2-A | 73 | LEU | 5.4 |
| 3 | 1-B | 763 | ARG | 5.4 |
| 3 | 2-B | 763 | ARG | 5.4 |
| 3 | 1-B | 664 | TYR | 5.4 |
| 3 | 2-B | 664 | TYR | 5.4 |
| 3 | 1-A | 273 | LEU | 5.3 |
| 3 | 2-A | 273 | LEU | 5.3 |
| 3 | 1-A | 341 | THR | 5.3 |
| 3 | 2-A | 341 | THR | 5.3 |
| 3 | 1-B | 739 | ASN | 5.3 |
| 3 | 2-B | 739 | ASN | 5.3 |
| 3 | 1-A | 342 | VAL | 5.3 |
| 3 | 1-B | 828 | VAL | 5.3 |
| 3 | 2-A | 342 | VAL | 5.3 |
| 3 | 2-B | 828 | VAL | 5.3 |
| 3 | 1-B | 634 | LYS | 5.3 |
| 3 | 2-B | 634 | LYS | 5.3 |
| 3 | 1-A | 396 | ASN | 5.2 |
| 3 | 2-A | 396 | ASN | 5.2 |
| 3 | 1-A | 343 | ARG | 5.2 |
| 3 | 2-A | 343 | ARG | 5.2 |
| 3 | 1-B | 752 | VAL | 5.2 |
| 3 | 2-B | 752 | VAL | 5.2 |
| 3 | 1-B | 753 | CYS | 5.1 |
| 3 | 2-B | 753 | CYS | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | 1-B | 787 | HIS | 5.1 |
| 3 | 2-B | 787 | HIS | 5.1 |
| 3 | 1-A | 362 | CYS | 5.1 |
| 3 | 2-A | 362 | CYS | 5.1 |
| 3 | 1-B | 746 | ALA | 5.0 |
| 3 | 2-B | 746 | ALA | 5.0 |
| 3 | 1-A | 325 | LEU | 5.0 |
| 3 | 2-A | 325 | LEU | 5.0 |
| 3 | 1-A | 244 | TYR | 4.9 |
| 3 | 2-A | 244 | TYR | 4.9 |
| 3 | 1-B | 773 | LYS | 4.9 |
| 3 | 2-B | 773 | LYS | 4.9 |
| 3 | 1-B | 726 | ASP | 4.9 |
| 3 | 2-B | 726 | ASP | 4.9 |
| 3 | 1-A | 319 | ASN | 4.8 |
| 3 | 2-A | 319 | ASN | 4.8 |
| 3 | 1-A | 322 | GLU | 4.7 |
| 3 | 2-A | 322 | GLU | 4.7 |
| 3 | 1-B | 791 | LYS | 4.7 |
| 3 | 2-B | 791 | LYS | 4.7 |
| 3 | 1-A | 83 | ASP | 4.7 |
| 3 | 2-A | 83 | ASP | 4.7 |
| 3 | 1-A | 403 | LEU | 4.7 |
| 3 | 2-A | 403 | LEU | 4.7 |
| 3 | 1-A | 62 | LEU | 4.7 |
| 3 | 2-A | 62 | LEU | 4.7 |
| 3 | 1-B | 811 | PHE | 4.7 |
| 3 | 2-B | 811 | PHE | 4.7 |
| 3 | 1-A | 317 | ALA | 4.6 |
| 3 | 2-A | 317 | ALA | 4.6 |
| 3 | 1-B | 831 | CYS | 4.6 |
| 3 | 2-B | 831 | CYS | 4.6 |
| 3 | 1-A | 339 | PRO | 4.6 |
| 3 | 2-A | 339 | PRO | 4.6 |
| 3 | 1-B | 737 | ALA | 4.6 |
| 3 | 2-B | 737 | ALA | 4.6 |
| 3 | 1-B | 749 | LEU | 4.6 |
| 3 | 2-B | 749 | LEU | 4.6 |
| 3 | 1-B | 792 | LEU | 4.5 |
| 3 | 2-B | 792 | LEU | 4.5 |
| 3 | 1-B | 780 | ARG | 4.5 |
| 3 | 2-B | 780 | ARG | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | 1-B | 735 | VAL | 4.4 |
| 3 | 2-B | 735 | VAL | 4.4 |
| 3 | 1-A | 316 | GLU | 4.4 |
| 3 | 2-A | 316 | GLU | 4.4 |
| 3 | 1-A | 398 | LYS | 4.4 |
| 3 | 2-A | 398 | LYS | 4.4 |
| 3 | 1-A | 414 | LYS | 4.3 |
| 3 | 2-A | 414 | LYS | 4.3 |
| 3 | 1-B | 810 | LEU | 4.3 |
| 3 | 2-B | 810 | LEU | 4.3 |
| 3 | 1-B | 747 | SER | 4.2 |
| 3 | 2-B | 747 | SER | 4.2 |
| 3 | 1-A | 373 | GLY | 4.2 |
| 3 | 2-A | 373 | GLY | 4.2 |
| 3 | 1-A | 360 | ARG | 4.2 |
| 3 | 2-A | 360 | ARG | 4.2 |
| 3 | 1-A | 383 | MET | 4.2 |
| 3 | 2-A | 383 | MET | 4.2 |
| 3 | 1-B | 807 | LEU | 4.2 |
| 3 | 2-B | 807 | LEU | 4.2 |
| 3 | 1-A | 307 | SER | 4.2 |
| 3 | 2-A | 307 | SER | 4.2 |
| 3 | 1-A | 327 | SER | 4.1 |
| 3 | 2-A | 327 | SER | 4.1 |
| 3 | 1-B | 762 | VAL | 4.1 |
| 3 | 2-B | 762 | VAL | 4.1 |
| 3 | 1-A | 389 | LYS | 4.1 |
| 3 | 2-A | 389 | LYS | 4.1 |
| 3 | 1-A | 411 | CYS | 4.0 |
| 3 | 2-A | 411 | CYS | 4.0 |
| 3 | 1-B | 504 | ALA | 4.0 |
| 3 | 2-B | 504 | ALA | 4.0 |
| 3 | 1-B | 832 | ASN | 4.0 |
| 3 | 2-B | 832 | ASN | 4.0 |
| 3 | 1-B | 498 | LEU | 4.0 |
| 3 | 2-B | 498 | LEU | 4.0 |
| 3 | 1-B | 693 | LEU | 3.9 |
| 3 | 2-B | 693 | LEU | 3.9 |
| 3 | 1-B | 806 | ILE | 3.9 |
| 3 | 2-B | 806 | ILE | 3.9 |
| 3 | 1-B | 822 | HIS | 3.9 |
| 3 | 2-B | 822 | HIS | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | 1-A | 402 | HIS | 3.9 |
| 3 | 2-A | 402 | HIS | 3.9 |
| 3 | 1-A | 329 | LEU | 3.9 |
| 3 | 1-B | 803 | MET | 3.9 |
| 3 | 2-A | 329 | LEU | 3.9 |
| 3 | 2-B | 803 | MET | 3.9 |
| 3 | 1-B | 823 | LEU | 3.8 |
| 3 | 2-B | 823 | LEU | 3.8 |
| 3 | 1-A | 145 | SER | 3.8 |
| 3 | 1-B | 733 | SER | 3.8 |
| 3 | 2-A | 145 | SER | 3.8 |
| 3 | 2-B | 733 | SER | 3.8 |
| 3 | 1-B | 493 | LEU | 3.8 |
| 3 | 2-B | 493 | LEU | 3.8 |
| 3 | 1-B | 778 | GLU | 3.8 |
| 3 | 1-B | 809 | LYS | 3.8 |
| 3 | 2-B | 778 | GLU | 3.8 |
| 3 | 2-B | 809 | LYS | 3.8 |
| 3 | 1-A | 387 | LEU | 3.7 |
| 3 | 2-A | 387 | LEU | 3.7 |
| 3 | 1-A | 365 | PRO | 3.7 |
| 3 | 2-A | 365 | PRO | 3.7 |
| 3 | 1-B | 743 | GLU | 3.7 |
| 3 | 2-B | 743 | GLU | 3.7 |
| 3 | 1-B | 566 | ASP | 3.7 |
| 3 | 1-B | 814 | MET | 3.7 |
| 3 | 2-B | 566 | ASP | 3.7 |
| 3 | 2-B | 814 | MET | 3.7 |
| 1 | 1-T | 5 | DA | 3.7 |
| 1 | 2-T | 5 | DA | 3.7 |
| 3 | 1-B | 499 | MET | 3.7 |
| 3 | 2-B | 499 | MET | 3.7 |
| 3 | 1-B | 754 | GLN | 3.7 |
| 3 | 2-B | 754 | GLN | 3.7 |
| 3 | 1-A | 376 | ASN | 3.7 |
| 3 | 2-A | 376 | ASN | 3.7 |
| 3 | 1-A | 146 | ASP | 3.7 |
| 3 | 2-A | 146 | ASP | 3.7 |
| 3 | 1-B | 769 | TYR | 3.6 |
| 3 | 2-B | 769 | TYR | 3.6 |
| 3 | 1-B | 472 | ASP | 3.5 |
| 3 | 2-B | 472 | ASP | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | 1-A | 91 | LEU | 3.5 |
| 3 | 1-B | 745 | LEU | 3.5 |
| 3 | 2-A | 91 | LEU | 3.5 |
| 3 | 2-B | 745 | LEU | 3.5 |
| 3 | 1-B | 824 | THR | 3.5 |
| 3 | 2-B | 824 | THR | 3.5 |
| 3 | 1-A | 359 | SER | 3.4 |
| 3 | 2-A | 359 | SER | 3.4 |
| 3 | 1-B | 750 | ASN | 3.4 |
| 3 | 2-B | 750 | ASN | 3.4 |
| 3 | 1-B | 744 | LEU | 3.4 |
| 3 | 1-B | 761 | THR | 3.4 |
| 3 | 2-B | 744 | LEU | 3.4 |
| 3 | 2-B | 761 | THR | 3.4 |
| 3 | 1-A | 72 | LYS | 3.4 |
| 3 | 2-A | 72 | LYS | 3.4 |
| 3 | 1-B | 689 | LEU | 3.4 |
| 3 | 2-B | 689 | LEU | 3.4 |
| 2 | 1-P | 9 | DG | 3.4 |
| 2 | 2-P | 9 | DG | 3.4 |
| 3 | 1-A | 328 | LEU | 3.3 |
| 3 | 2-A | 328 | LEU | 3.3 |
| 3 | 1-A | 334 | GLN | 3.3 |
| 3 | 2-A | 334 | GLN | 3.3 |
| 3 | 1-B | 768 | ARG | 3.3 |
| 3 | 2-B | 768 | ARG | 3.3 |
| 3 | 1-B | 500 | ASN | 3.3 |
| 3 | 2-B | 500 | ASN | 3.3 |
| 3 | 1-B | 785 | PRO | 3.2 |
| 3 | 2-B | 785 | PRO | 3.2 |
| 3 | 1-B | 568 | LEU | 3.2 |
| 3 | 2-B | 568 | LEU | 3.2 |
| 3 | 1-A | 68 | TYR | 3.1 |
| 3 | 2-A | 68 | TYR | 3.1 |
| 3 | 1-B | 492 | LYS | 3.1 |
| 3 | 2-B | 492 | LYS | 3.1 |
| 3 | 1-B | 798 | ASP | 3.1 |
| 3 | 2-B | 798 | ASP | 3.1 |
| 3 | 1-A | 364 | ILE | 3.1 |
| 3 | 2-A | 364 | ILE | 3.1 |
| 3 | 1-B | 748 | LEU | 3.1 |
| 3 | 2-B | 748 | LEU | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | 1-A | 314 | GLU | 3.1 |
| 3 | 2-A | 314 | GLU | 3.1 |
| 2 | 1-P | 7 | DA | 3.1 |
| 2 | 2-P | 7 | DA | 3.1 |
| 3 | 1-B | 482 | LEU | 3.0 |
| 3 | 2-B | 482 | LEU | 3.0 |
| 3 | 1-A | 75 | VAL | 3.0 |
| 3 | 1-A | 92 | VAL | 3.0 |
| 3 | 2-A | 75 | VAL | 3.0 |
| 3 | 2-A | 92 | VAL | 3.0 |
| 3 | 1-B | 722 | PHE | 3.0 |
| 3 | 2-B | 722 | PHE | 3.0 |
| 3 | 1-B | 759 | PRO | 2.9 |
| 3 | 2-B | 759 | PRO | 2.9 |
| 3 | 1-B | 812 | ARG | 2.9 |
| 3 | 2-B | 812 | ARG | 2.9 |
| 3 | 1-B | 474 | PRO | 2.9 |
| 3 | 2-B | 474 | PRO | 2.9 |
| 3 | 1-A | 52 | ASP | 2.8 |
| 3 | 1-A | 324 | LEU | 2.8 |
| 3 | 1-B | 543 | LEU | 2.8 |
| 3 | 2-A | 52 | ASP | 2.8 |
| 3 | 2-A | 324 | LEU | 2.8 |
| 3 | 2-B | 543 | LEU | 2.8 |
| 3 | 1-A | 337 | ARG | 2.8 |
| 3 | 2-A | 337 | ARG | 2.8 |
| 3 | 1-A | 141 | GLN | 2.8 |
| 3 | 2-A | 141 | GLN | 2.8 |
| 3 | 1-B | 503 | ASP | 2.8 |
| 3 | 2-B | 503 | ASP | 2.8 |
| 3 | 1-B | 829 | CYS | 2.8 |
| 3 | 2-B | 829 | CYS | 2.8 |
| 3 | 1-A | 53 | LYS | 2.8 |
| 3 | 2-A | 53 | LYS | 2.8 |
| 3 | 1-A | 60 | LYS | 2.7 |
| 3 | 2-A | 60 | LYS | 2.7 |
| 3 | 1-B | 561 | GLN | 2.7 |
| 3 | 2-B | 561 | GLN | 2.7 |
| 3 | 1-B | 502 | ARG | 2.7 |
| 3 | 2-B | 502 | ARG | 2.7 |
| 3 | 1-A | 330 | ASN | 2.7 |
| 3 | 2-A | 330 | ASN | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | 1-A | 54 | PRO | 2.7 |
| 3 | 2-A | 54 | PRO | 2.7 |
| 3 | 1-B | 511 | LEU | 2.7 |
| 3 | 2-B | 511 | LEU | 2.7 |
| 3 | 1-A | 143 | LEU | 2.7 |
| 3 | 2-A | 143 | LEU | 2.7 |
| 3 | 1-A | 269 | LEU | 2.6 |
| 3 | 2-A | 269 | LEU | 2.6 |
| 3 | 1-A | 84 | ALA | 2.6 |
| 3 | 2-A | 84 | ALA | 2.6 |
| 3 | 1-A | 80 | ASN | 2.6 |
| 3 | 2-A | 80 | ASN | 2.6 |
| 3 | 1-B | 501 | VAL | 2.6 |
| 3 | 2-B | 501 | VAL | 2.6 |
| 3 | 1-A | 361 | GLN | 2.6 |
| 3 | 2-A | 361 | GLN | 2.6 |
| 3 | 1-A | 394 | MET | 2.6 |
| 3 | 1-B | 672 | ALA | 2.6 |
| 3 | 1-B | 808 | MET | 2.6 |
| 3 | 2-A | 394 | MET | 2.6 |
| 3 | 2-B | 672 | ALA | 2.6 |
| 3 | 2-B | 808 | MET | 2.6 |
| 3 | 1-B | 781 | GLN | 2.6 |
| 3 | 2-B | 781 | GLN | 2.6 |
| 3 | 1-B | 727 | SER | 2.6 |
| 3 | 2-B | 727 | SER | 2.6 |
| 3 | 1-A | 85 | LYS | 2.6 |
| 3 | 2-A | 85 | LYS | 2.6 |
| 3 | 1-A | 33 | VAL | 2.6 |
| 3 | 2-A | 33 | VAL | 2.6 |
| 3 | 1-A | 123 | LEU | 2.5 |
| 3 | 2-A | 123 | LEU | 2.5 |
| 3 | 1-A | 69 | GLU | 2.5 |
| 3 | 2-A | 69 | GLU | 2.5 |
| 3 | 1-A | 265 | SER | 2.4 |
| 3 | 2-A | 265 | SER | 2.4 |
| 3 | 1-A | 412 | ASN | 2.4 |
| 3 | 2-A | 412 | ASN | 2.4 |
| 3 | 1-B | 488 | TYR | 2.4 |
| 3 | 2-B | 488 | TYR | 2.4 |
| 3 | 1-A | 70 | ALA | 2.4 |
| 3 | 2-A | 70 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | 1-A | 86 | GLU | 2.4 |
| 3 | 2-A | 86 | GLU | 2.4 |
| 1 | 1-T | 15 | DC | 2.4 |
| 1 | 2-T | 15 | DC | 2.4 |
| 3 | 1-B | 473 | LYS | 2.4 |
| 3 | 2-B | 473 | LYS | 2.4 |
| 3 | 1-B | 453 | VAL | 2.4 |
| 3 | 2-B | 453 | VAL | 2.4 |
| 3 | 1-B | 655 | HIS | 2.3 |
| 3 | 2-B | 655 | HIS | 2.3 |
| 1 | 1-T | 7 | DG | 2.3 |
| 1 | 2-T | 7 | DG | 2.3 |
| 3 | 1-A | 78 | LEU | 2.3 |
| 3 | 1-A | 148 | LEU | 2.3 |
| 3 | 2-A | 78 | LEU | 2.3 |
| 3 | 2-A | 148 | LEU | 2.3 |
| 3 | 1-A | 410 | PHE | 2.3 |
| 3 | 2-A | 410 | PHE | 2.3 |
| 3 | 1-B | 830 | PHE | 2.3 |
| 3 | 2-B | 830 | PHE | 2.3 |
| 3 | 1-A | 413 | LEU | 2.3 |
| 3 | 2-A | 413 | LEU | 2.3 |
| 3 | 1-B | 564 | GLN | 2.2 |
| 3 | 1-B | 783 | PRO | 2.2 |
| 3 | 2-B | 564 | GLN | 2.2 |
| 3 | 2-B | 783 | PRO | 2.2 |
| 3 | 1-B | 659 | ILE | 2.2 |
| 3 | 2-B | 659 | ILE | 2.2 |
| 3 | 1-A | 302 | PHE | 2.2 |
| 3 | 2-A | 302 | PHE | 2.2 |
| 3 | 1-A | 323 | GLU | 2.2 |
| 3 | 1-B | 662 | ILE | 2.2 |
| 3 | 2-A | 323 | GLU | 2.2 |
| 3 | 2-B | 662 | ILE | 2.2 |
| 3 | 1-A | 287 | GLY | 2.2 |
| 3 | 2-A | 287 | GLY | 2.2 |
| 3 | 1-B | 670 | LEU | 2.2 |
| 3 | 2-B | 670 | LEU | 2.2 |
| 3 | 1-B | 793 | GLY | 2.1 |
| 3 | 2-B | 793 | GLY | 2.1 |
| 3 | 1-B | 757 | ARG | 2.1 |
| 3 | 2-B | 757 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | 1-A | 303 | SER | 2.1 |
| 3 | 2-A | 303 | SER | 2.1 |
| 3 | 1-A | 242 | ILE | 2.1 |
| 3 | 2-A | 242 | ILE | 2.1 |
| 3 | 1-B | 563 | LEU | 2.1 |
| 3 | 2-B | 563 | LEU | 2.1 |
| 3 | 1-B | 751 | ARG | 2.1 |
| 3 | 2-B | 751 | ARG | 2.1 |
| 2 | 1-P | 10 | DA | 2.0 |
| 2 | 2-P | 10 | DA | 2.0 |
| 3 | 1-B | 487 | ASN | 2.0 |
| 3 | 2-B | 487 | ASN | 2.0 |
| 1 | 1-T | 13 | DT | 2.0 |
| 1 | 2-T | 13 | DT | 2.0 |
| 3 | 1-A | 129 | PHE | 2.0 |
| 3 | 2-A | 129 | PHE | 2.0 |
| 3 | 1-B | 724 | GLU | 2.0 |
| 3 | 2-B | 724 | GLU | 2.0 |
| 2 | 1-P | 12 | DC | 2.0 |
| 2 | 2-P | 12 | DC | 2.0 |
| 3 | 1-B | 833 | LEU | 2.0 |
| 3 | 2-B | 833 | LEU | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 2 | DOC | 1-P | 13 | 18/19 | 0.91 | 0.45 | - | 25,30,37,37 | 18 |
| 2 | DOC | 2-P | 13 | 18/19 | 0.91 | 0.45 | - | 25,31,34,36 | 18 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 5 | TTP | 1-B | 902 | 29/29 | 0.87 | 0.41 | 1.37 | 28,31,37,38 | 29 |
| 5 | TTP | 2-B | 902 | 29/29 | 0.87 | 0.41 | 1.37 | 27,33,36,38 | 29 |
| 4 | MG | 1-B | 901 | 1/1 | 0.85 | 0.16 | - | 35,35,35,35 | 1 |
| 4 | MG | 2-B | 901 | 1/1 | 0.85 | 0.16 | - | 35,35,35,35 | 1 |

6.5 Other polymers [i](#)

There are no such residues in this entry.