



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:33 am BST

PDB ID : 3RMC
Title : Crystal Structure of a replicative DNA polymerase bound to DNA containing
Thymine Glycol
Authors : Aller, P.; Duclos, S.; Wallace, S.S.; Doublié, S.
Deposited on : 2011-04-20
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

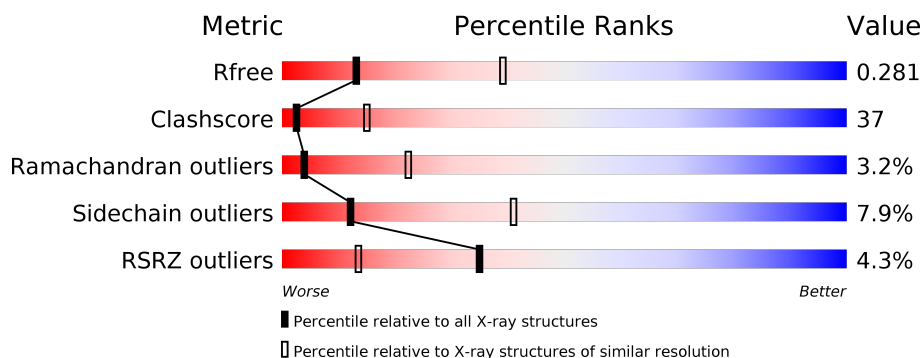
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 | A | 906 | <div> <div>3%</div> <div>45%</div> <div>47%</div> <div>7%</div> </div> |
| 1 | B | 906 | <div> <div>7%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div> |
| 1 | C | 906 | <div> <div>%</div> <div>50%</div> <div>45%</div> <div>5%</div> </div> |
| 1 | D | 906 | <div> <div>7%</div> <div>36%</div> <div>54%</div> <div>8%</div> </div> |
| 2 | E | 18 | <div> <div>33%</div> <div>67%</div> </div> |
| 2 | G | 18 | <div> <div>11%</div> <div>89%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | I | 18 | |
| 2 | K | 18 | |
| 3 | F | 14 | |
| 3 | H | 14 | |
| 3 | J | 14 | |
| 3 | L | 14 | |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31561 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA polymerase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 902 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7323 | 4704 | 1220 | 1367 | 32 | | | |
| 1 | B | 902 | Total | C | N | O | S | 13 | 0 | 0 |
| | | | 7246 | 4643 | 1202 | 1368 | 33 | | | |
| 1 | C | 901 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7339 | 4712 | 1220 | 1374 | 33 | | | |
| 1 | D | 890 | Total | C | N | O | S | 15 | 0 | 0 |
| | | | 7027 | 4507 | 1155 | 1334 | 31 | | | |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 222 | ALA | ASP | ENGINEERED MUTATION | UNP Q38087 |
| A | 327 | ALA | ASP | ENGINEERED MUTATION | UNP Q38087 |
| A | 904 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| A | 905 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| A | 906 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| B | 222 | ALA | ASP | ENGINEERED MUTATION | UNP Q38087 |
| B | 327 | ALA | ASP | ENGINEERED MUTATION | UNP Q38087 |
| B | 904 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| B | 905 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| B | 906 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| C | 222 | ALA | ASP | ENGINEERED MUTATION | UNP Q38087 |
| C | 327 | ALA | ASP | ENGINEERED MUTATION | UNP Q38087 |
| C | 904 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| C | 905 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| C | 906 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| D | 222 | ALA | ASP | ENGINEERED MUTATION | UNP Q38087 |
| D | 327 | ALA | ASP | ENGINEERED MUTATION | UNP Q38087 |
| D | 904 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| D | 905 | HIS | - | EXPRESSION TAG | UNP Q38087 |
| D | 906 | HIS | - | EXPRESSION TAG | UNP Q38087 |

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2 | E | 18 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 370 | 175 | 71 | 107 | 17 | | | |
| 2 | G | 18 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 370 | 175 | 71 | 107 | 17 | | | |
| 2 | I | 18 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 370 | 175 | 71 | 107 | 17 | | | |
| 2 | K | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 287 | 136 | 59 | 79 | 13 | | | |

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 3 | F | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 282 | 136 | 50 | 83 | 13 | | | |
| 3 | H | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 282 | 136 | 50 | 83 | 13 | | | |
| 3 | J | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 282 | 136 | 50 | 83 | 13 | | | |
| 3 | L | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 262 | 126 | 45 | 79 | 12 | | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | A | 43 | Total | O | 0 | 0 |
| | | | 43 | 43 | | |
| 4 | B | 33 | Total | O | 0 | 0 |
| | | | 33 | 33 | | |
| 4 | C | 32 | Total | O | 0 | 0 |
| | | | 32 | 32 | | |
| 4 | D | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | E | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | G | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 4 | H | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 4 | I | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |

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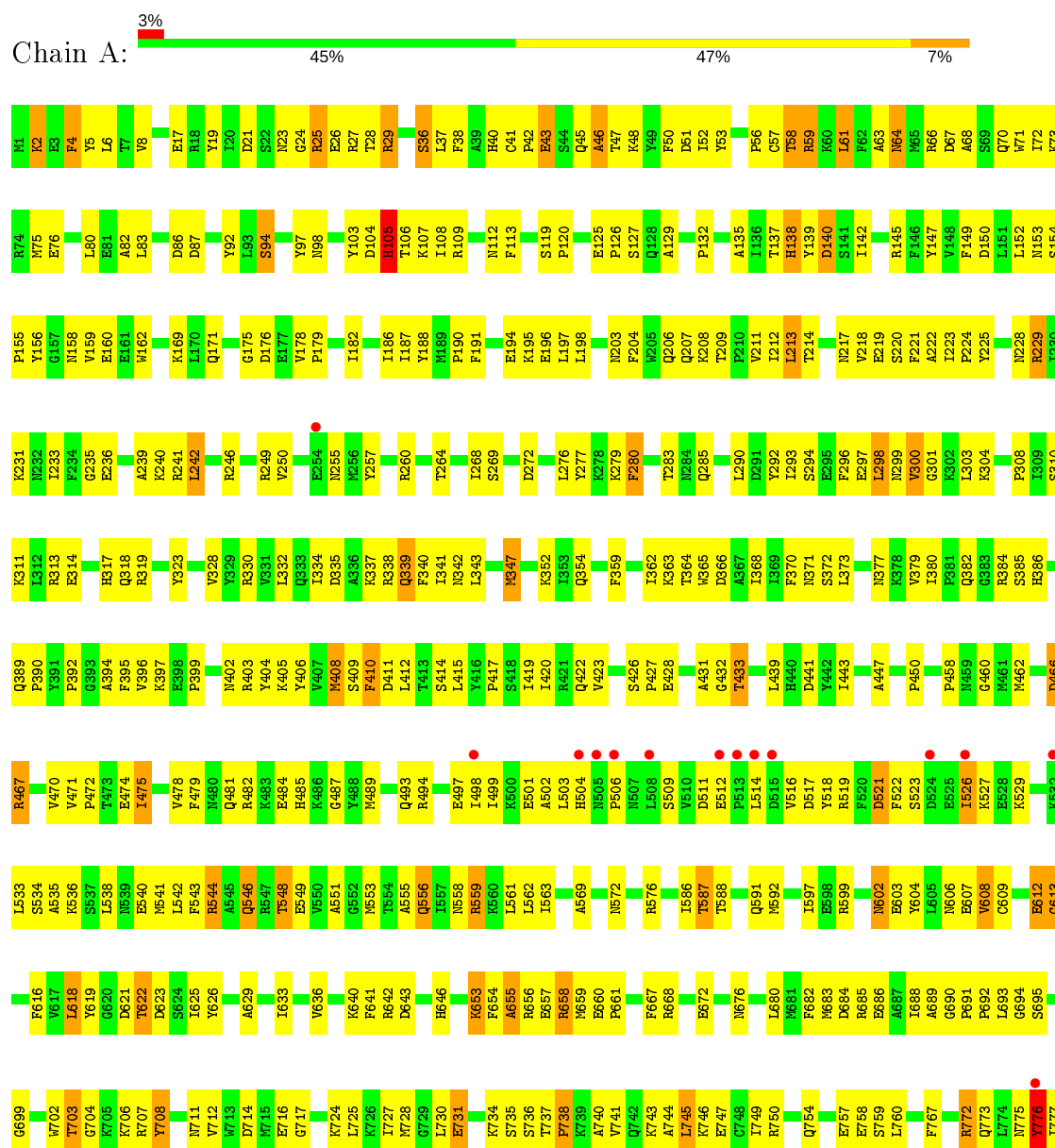
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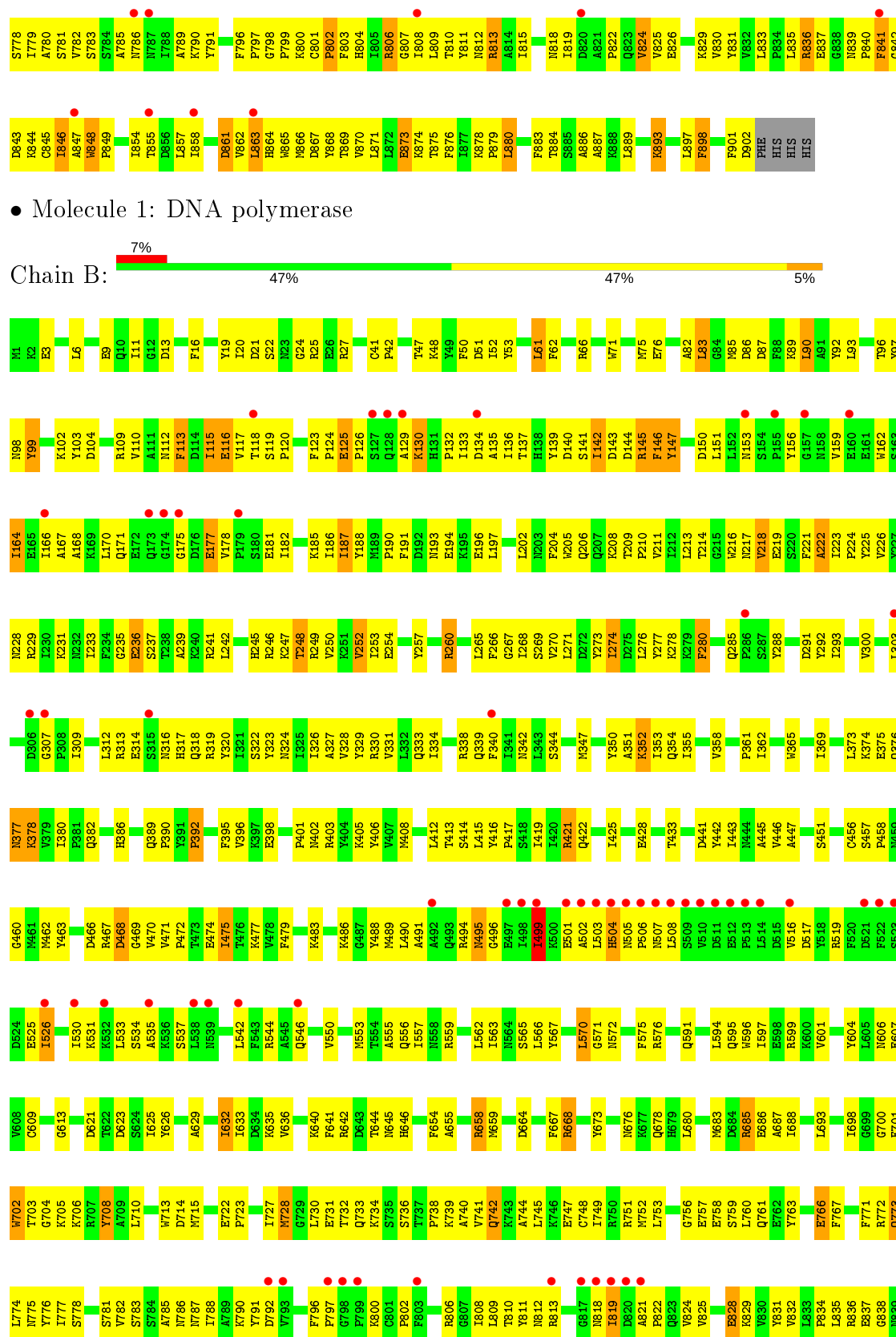
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4 | J | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots

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

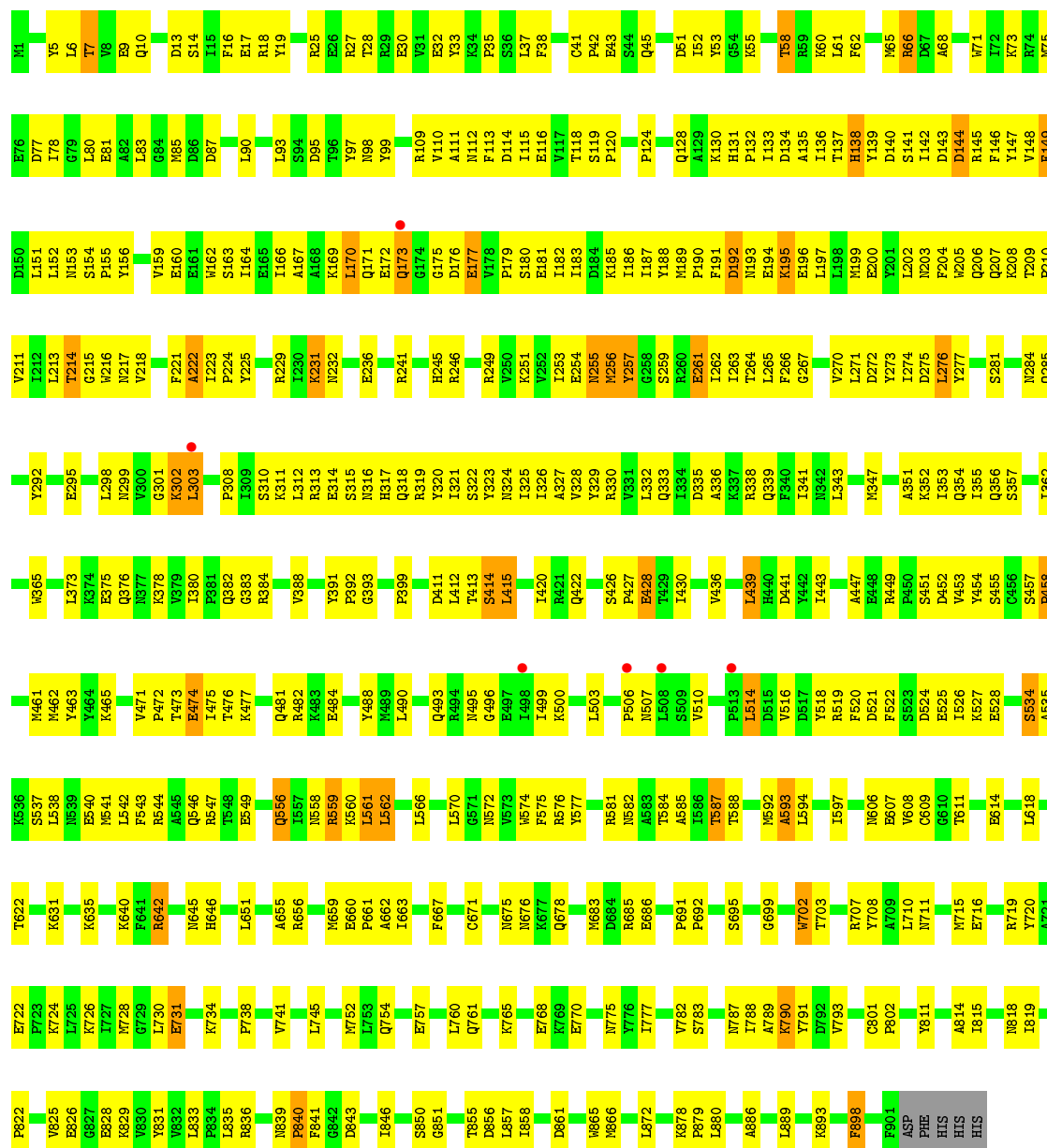
- Molecule 1: DNA polymerase



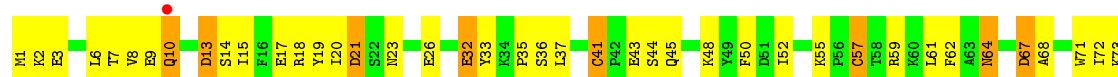


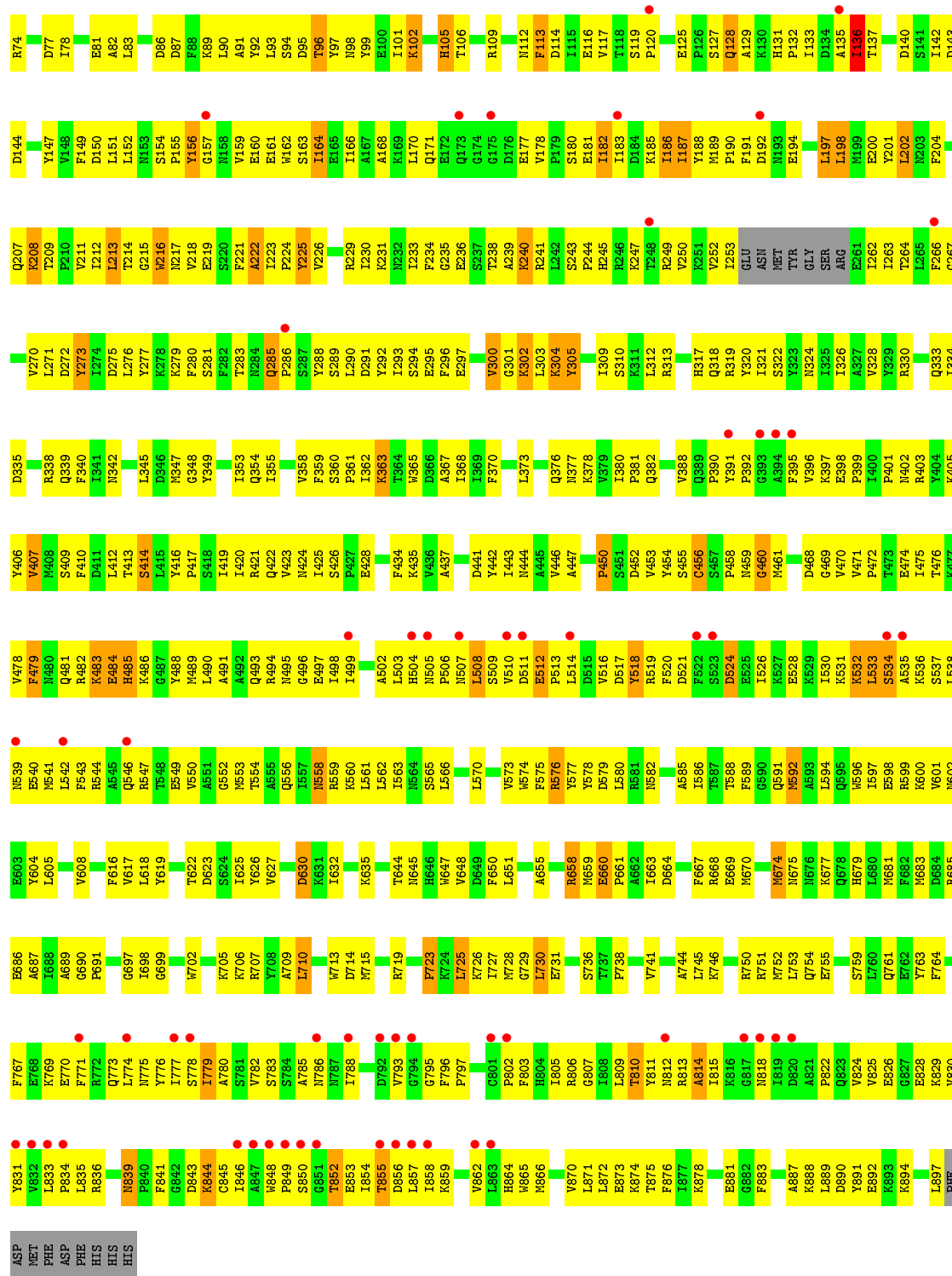


• Molecule 1: DNA polymerase



• Molecule 1: DNA polymerase

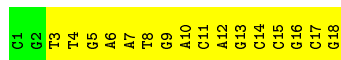






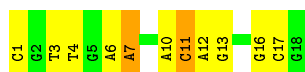
- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C
P*GP*CP*G)-3')

Chain G: 11% 89%



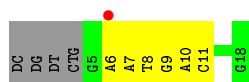
- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C
P*GP*CP*G)-3')

Chain I: 39% 50% 11%



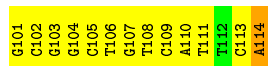
- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C
P*GP*CP*G)-3')

Chain K: 6% 44% 33% 22%



- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain F: 7% 86% 7%



- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain H: 21% 79%



- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain J: 50% 50%



- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')



| | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|----|
| G101 | C102 | G103 | G104 | C105 | T106 | G107 | T108 | C109 | A110 | T111 | T112 | C113 | DA |
|------|------|------|------|------|------|------|------|------|------|------|------|------|----|

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 133.99Å 123.77Å 163.64Å 90.00° 95.57° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.00 49.30 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 90.5 (50.00-3.00) 96.5 (49.30-3.00) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.01 (at 3.01Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.222 , 0.282 0.219 , 0.281 | Depositor DCC |
| R_{free} test set | 19675 reflections (9.40%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 68.4 | Xtriage |
| Anisotropy | 0.120 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 69.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 31561 | wwPDB-VP |
| Average B, all atoms (Å ²) | 92.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CTG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.46 | 0/7503 | 0.68 | 0/10148 |
| 1 | B | 0.42 | 0/7421 | 0.62 | 0/10054 |
| 1 | C | 0.46 | 0/7519 | 0.66 | 0/10166 |
| 1 | D | 0.34 | 0/7198 | 0.59 | 1/9779 (0.0%) |
| 2 | E | 0.40 | 0/390 | 0.71 | 0/598 |
| 2 | G | 0.39 | 0/390 | 0.69 | 0/598 |
| 2 | I | 0.60 | 0/390 | 0.77 | 0/598 |
| 2 | K | 0.31 | 0/323 | 0.67 | 0/497 |
| 3 | F | 0.33 | 0/315 | 0.77 | 0/484 |
| 3 | H | 0.30 | 0/315 | 0.70 | 0/484 |
| 3 | J | 0.62 | 0/315 | 0.89 | 0/484 |
| 3 | L | 0.28 | 0/292 | 0.64 | 0/449 |
| All | All | 0.42 | 0/32371 | 0.65 | 1/44339 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 2 | I | 0 | 2 |
| 3 | F | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1 | D | 533 | LEU | CA-CB-CG | 5.08 | 126.97 | 115.30 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 92 | TYR | Sidechain |
| 3 | F | 114 | DA | Sidechain |
| 2 | I | 11 | DC | Sidechain |
| 2 | I | 7 | DA | 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 | A | 7323 | 0 | 7185 | 536 | 0 |
| 1 | B | 7246 | 0 | 7027 | 512 | 0 |
| 1 | C | 7339 | 0 | 7210 | 456 | 0 |
| 1 | D | 7027 | 0 | 6703 | 622 | 0 |
| 2 | E | 370 | 0 | 205 | 19 | 0 |
| 2 | G | 370 | 0 | 205 | 34 | 0 |
| 2 | I | 370 | 0 | 205 | 14 | 0 |
| 2 | K | 287 | 0 | 157 | 11 | 0 |
| 3 | F | 282 | 0 | 158 | 27 | 0 |
| 3 | H | 282 | 0 | 158 | 19 | 0 |
| 3 | J | 282 | 0 | 158 | 21 | 0 |
| 3 | L | 262 | 0 | 149 | 18 | 0 |
| 4 | A | 43 | 0 | 0 | 3 | 0 |
| 4 | B | 33 | 0 | 0 | 2 | 0 |
| 4 | C | 32 | 0 | 0 | 3 | 0 |
| 4 | D | 2 | 0 | 0 | 0 | 0 |
| 4 | E | 1 | 0 | 0 | 0 | 0 |
| 4 | G | 3 | 0 | 0 | 0 | 0 |
| 4 | H | 3 | 0 | 0 | 1 | 0 |
| 4 | I | 3 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| All | All | 31561 | 0 | 29520 | 2248 | 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 37.

All (2248) 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:202:LEU:HD21 | 1:D:241:ARG:HD3 | 1.26 | 1.14 |
| 1:D:533:LEU:HD13 | 1:D:534:SER:H | 1.05 | 1.12 |
| 1:D:116:GLU:HB2 | 1:D:135:ALA:HB3 | 1.32 | 1.12 |
| 1:C:642:ARG:HE | 1:C:646:HIS:CD2 | 1.67 | 1.12 |
| 3:J:104:DG:H2'' | 3:J:105:DC:H5'' | 1.20 | 1.12 |
| 2:E:6:DA:H2'' | 2:E:7:DA:H5' | 1.31 | 1.11 |
| 2:E:4:CTG:H5' | 2:E:4:CTG:H6 | 1.33 | 1.11 |
| 1:C:231:LYS:HG2 | 1:C:236:GLU:HA | 1.33 | 1.10 |
| 3:F:104:DG:H2'' | 3:F:105:DC:H5'' | 1.09 | 1.07 |
| 3:J:104:DG:C2' | 3:J:105:DC:H5'' | 1.85 | 1.07 |
| 1:B:85:MET:HE2 | 1:B:87:ASP:H | 1.15 | 1.06 |
| 1:B:732:THR:HG23 | 1:B:733:GLN:HE21 | 1.20 | 1.05 |
| 1:C:41:CYS:HB3 | 1:C:58:THR:HG22 | 1.36 | 1.04 |
| 3:F:104:DG:C2' | 3:F:105:DC:H5'' | 1.87 | 1.03 |
| 1:A:502:ALA:HB1 | 1:A:538:LEU:HD22 | 1.42 | 1.02 |
| 1:A:839:ASN:HB2 | 1:A:840:PRO:HD2 | 1.42 | 1.01 |
| 1:D:785:ALA:HB1 | 1:D:788:ILE:HD11 | 1.41 | 1.01 |
| 1:A:642:ARG:H | 1:A:646:HIS:HD2 | 1.07 | 1.01 |
| 1:D:493:GLN:HG3 | 1:D:494:ARG:H | 1.26 | 1.00 |
| 1:D:815:ILE:HG22 | 1:D:858:ILE:HG21 | 1.42 | 1.00 |
| 1:A:362:ILE:HD13 | 2:E:3:DT:H5' | 1.40 | 1.00 |
| 1:D:533:LEU:HD13 | 1:D:534:SER:N | 1.77 | 0.99 |
| 1:A:153:ASN:HD22 | 1:A:158:ASN:HD22 | 1.10 | 0.99 |
| 1:A:703:THR:HG21 | 1:A:707:ARG:HH11 | 1.26 | 0.98 |
| 1:D:214:THR:HG22 | 1:D:215:GLY:H | 1.26 | 0.97 |
| 1:B:164:ILE:H | 1:B:164:ILE:HD13 | 1.25 | 0.97 |
| 1:C:163:SER:HB3 | 1:C:318:GLN:HE22 | 1.29 | 0.96 |
| 1:A:835:LEU:HD11 | 1:A:846:ILE:HG22 | 1.43 | 0.96 |
| 1:A:72:ILE:O | 1:A:76:GLU:HG3 | 1.66 | 0.95 |
| 3:L:110:DA:H2'' | 3:L:111:DT:H5' | 1.46 | 0.94 |
| 1:B:395:PHE:HB2 | 1:B:591:GLN:HE21 | 1.32 | 0.94 |
| 1:C:195:LYS:NZ | 1:C:195:LYS:H | 1.64 | 0.94 |
| 2:E:6:DA:H2'' | 2:E:7:DA:C5' | 1.98 | 0.94 |
| 1:B:499:ILE:H | 1:B:499:ILE:HD13 | 1.32 | 0.94 |
| 1:C:711:ASN:HD21 | 1:C:754:GLN:HE21 | 0.96 | 0.94 |
| 1:A:703:THR:HG21 | 1:A:707:ARG:NH1 | 1.83 | 0.92 |
| 1:D:164:ILE:HD13 | 1:D:164:ILE:H | 1.34 | 0.92 |
| 1:A:836:ARG:NH1 | 1:A:865:TRP:HA | 1.83 | 0.92 |
| 1:B:505:ASN:ND2 | 1:B:507:ASN:HD22 | 1.67 | 0.92 |
| 3:F:104:DG:H2'' | 3:F:105:DC:C5' | 1.97 | 0.92 |
| 1:B:217:ASN:H | 1:B:274:ILE:HG21 | 1.35 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:193:ASN:HD22 | 1:B:196:GLU:HG2 | 1.33 | 0.91 |
| 1:B:83:LEU:H | 1:B:83:LEU:HD12 | 1.35 | 0.91 |
| 1:C:137:THR:HB | 1:C:328:VAL:HG21 | 1.50 | 0.91 |
| 1:D:109:ARG:NH1 | 1:D:142:ILE:HD11 | 1.85 | 0.91 |
| 1:A:502:ALA:O | 1:A:538:LEU:HD13 | 1.71 | 0.90 |
| 1:C:392:PRO:O | 1:C:587:THR:HG21 | 1.70 | 0.90 |
| 1:A:736:SER:HA | 1:A:782:VAL:HB | 1.53 | 0.90 |
| 2:K:6:DA:H2'' | 2:K:7:DA:H5'' | 1.50 | 0.90 |
| 1:B:894:LYS:HB2 | 1:B:894:LYS:NZ | 1.87 | 0.89 |
| 3:F:110:DA:H2'' | 3:F:111:DT:H5' | 1.54 | 0.89 |
| 1:A:897:LEU:HD12 | 1:A:897:LEU:H | 1.38 | 0.89 |
| 1:B:668:ARG:HG3 | 1:B:668:ARG:HH11 | 1.38 | 0.88 |
| 2:E:12:DA:H2'' | 2:E:13:DG:H5' | 1.52 | 0.88 |
| 1:B:219:GLU:HA | 1:B:223:ILE:HD12 | 1.53 | 0.88 |
| 1:A:559:ARG:HG2 | 1:A:559:ARG:HH11 | 1.38 | 0.87 |
| 1:D:541:MET:O | 1:D:544:ARG:HG2 | 1.74 | 0.87 |
| 1:D:132:PRO:HA | 1:D:229:ARG:HE | 1.39 | 0.87 |
| 1:D:198:LEU:HD11 | 1:D:230:ILE:HG12 | 1.54 | 0.87 |
| 1:D:481:GLN:HB3 | 1:D:559:ARG:HE | 1.38 | 0.86 |
| 1:A:708:TYR:CE2 | 1:A:728:MET:HG3 | 2.11 | 0.86 |
| 1:A:791:TYR:HB3 | 1:A:801:CYS:SG | 2.15 | 0.86 |
| 1:A:25:ARG:HB2 | 1:A:25:ARG:HH11 | 1.39 | 0.86 |
| 1:C:660:GLU:HB2 | 1:C:661:PRO:HD3 | 1.57 | 0.86 |
| 1:C:711:ASN:ND2 | 1:C:754:GLN:HE21 | 1.74 | 0.85 |
| 1:D:159:VAL:HG12 | 1:D:160:GLU:H | 1.40 | 0.85 |
| 1:A:176:ASP:HA | 1:A:319:ARG:HH21 | 1.42 | 0.85 |
| 1:B:115:ILE:HG22 | 1:B:136:ILE:HG23 | 1.58 | 0.85 |
| 1:B:745:LEU:O | 1:B:749:ILE:HG13 | 1.77 | 0.85 |
| 1:C:642:ARG:NH1 | 1:C:646:HIS:HB3 | 1.92 | 0.84 |
| 1:D:493:GLN:HG3 | 1:D:494:ARG:N | 1.93 | 0.84 |
| 1:C:855:THR:HG22 | 1:C:857:LEU:H | 1.43 | 0.84 |
| 1:A:127:SER:HA | 1:A:228:ASN:ND2 | 1.92 | 0.84 |
| 1:B:271:LEU:HB3 | 1:B:276:LEU:HD11 | 1.59 | 0.84 |
| 2:E:5:DG:H2'' | 2:E:6:DA:OP2 | 1.78 | 0.83 |
| 1:D:10:GLN:HA | 1:D:15:ILE:HG22 | 1.59 | 0.83 |
| 1:D:814:ALA:HB3 | 1:D:841:PHE:CE1 | 2.13 | 0.83 |
| 2:I:4:CTG:H5'' | 2:I:4:CTG:H6 | 1.61 | 0.83 |
| 1:B:777:ILE:HD11 | 1:B:853:GLU:HG2 | 1.58 | 0.83 |
| 3:L:104:DG:H2'' | 3:L:105:DC:C5' | 2.09 | 0.83 |
| 2:K:6:DA:H2'' | 2:K:7:DA:C5' | 2.07 | 0.83 |
| 1:A:2:LYS:NZ | 1:A:2:LYS:HA | 1.94 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:130:LYS:HE3 | 1:C:131:HIS:HE1 | 1.42 | 0.82 |
| 1:B:508:LEU:HD23 | 1:B:508:LEU:H | 1.44 | 0.82 |
| 1:D:133:ILE:HG12 | 1:D:229:ARG:HD2 | 1.62 | 0.82 |
| 1:D:212:ILE:HD11 | 1:D:345:LEU:HD21 | 1.62 | 0.82 |
| 1:B:347:MET:HE1 | 1:B:562:LEU:HD11 | 1.59 | 0.82 |
| 1:D:503:LEU:HD11 | 1:D:539:ASN:HD22 | 1.42 | 0.82 |
| 1:B:248:THR:HG22 | 1:B:265:LEU:HA | 1.62 | 0.82 |
| 1:A:836:ARG:HH11 | 1:A:865:TRP:HA | 1.44 | 0.81 |
| 1:D:61:LEU:HD23 | 1:D:62:PHE:N | 1.94 | 0.81 |
| 1:C:836:ARG:HH12 | 1:C:865:TRP:HA | 1.44 | 0.81 |
| 3:L:104:DG:H2" | 3:L:105:DC:H5" | 1.62 | 0.81 |
| 1:B:818:ASN:ND2 | 1:B:821:ALA:HB2 | 1.95 | 0.81 |
| 1:D:391:TYR:HB2 | 1:D:392:PRO:HD2 | 1.61 | 0.81 |
| 1:D:223:ILE:HB | 1:D:224:PRO:HD3 | 1.62 | 0.81 |
| 1:C:516:VAL:HG11 | 1:C:526:ILE:HD13 | 1.62 | 0.81 |
| 1:D:164:ILE:HG21 | 1:D:186:ILE:CD1 | 2.11 | 0.81 |
| 1:A:236:GLU:HG2 | 1:A:240:LYS:HE2 | 1.60 | 0.81 |
| 1:C:295:GLU:OE1 | 1:C:301:GLY:HA2 | 1.81 | 0.81 |
| 1:A:642:ARG:H | 1:A:646:HIS:CD2 | 1.97 | 0.80 |
| 1:C:818:ASN:ND2 | 1:C:857:LEU:HD11 | 1.96 | 0.80 |
| 1:D:803:PHE:HB2 | 2:K:11:DC:H4' | 1.62 | 0.80 |
| 1:D:843:ASP:OD1 | 1:D:844:LYS:HD3 | 1.82 | 0.80 |
| 1:A:2:LYS:HZ3 | 1:A:2:LYS:HA | 1.46 | 0.80 |
| 1:A:544:ARG:HH11 | 1:A:544:ARG:HB2 | 1.45 | 0.80 |
| 1:D:149:PHE:HB3 | 1:D:197:LEU:HD21 | 1.63 | 0.80 |
| 1:D:164:ILE:HG21 | 1:D:186:ILE:HD12 | 1.63 | 0.80 |
| 1:D:495:ASN:HD22 | 1:D:521:ASP:HA | 1.43 | 0.80 |
| 1:D:444:ASN:HA | 1:D:599:ARG:NH1 | 1.96 | 0.80 |
| 1:D:597:ILE:O | 1:D:601:VAL:HG23 | 1.81 | 0.80 |
| 1:A:303:LEU:HD12 | 1:A:323:TYR:HA | 1.64 | 0.80 |
| 1:D:140:ASP:HB3 | 1:D:143:ASP:HB3 | 1.62 | 0.80 |
| 1:B:658:ARG:HG2 | 1:D:897:LEU:HD21 | 1.63 | 0.80 |
| 1:D:793:VAL:HG22 | 1:D:796:PHE:O | 1.82 | 0.80 |
| 1:B:808:ILE:HG22 | 1:B:812:ASN:HD21 | 1.45 | 0.80 |
| 1:A:422:GLN:NE2 | 1:A:680:LEU:H | 1.79 | 0.79 |
| 1:B:27:ARG:HG3 | 1:B:27:ARG:HH11 | 1.47 | 0.79 |
| 1:D:533:LEU:CD1 | 1:D:534:SER:H | 1.93 | 0.79 |
| 1:B:797:PRO:HG3 | 1:B:806:ARG:NH1 | 1.97 | 0.79 |
| 1:D:214:THR:HG22 | 1:D:215:GLY:N | 1.96 | 0.79 |
| 1:D:398:GLU:HA | 1:D:705:LYS:HE3 | 1.63 | 0.79 |
| 1:A:362:ILE:HG12 | 1:A:572:ASN:ND2 | 1.97 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:499:ILE:N | 1:B:499:ILE:HD13 | 1.96 | 0.79 |
| 1:D:109:ARG:HB2 | 1:D:211:VAL:HG23 | 1.63 | 0.79 |
| 1:D:818:ASN:OD1 | 1:D:855:THR:HG21 | 1.82 | 0.79 |
| 1:A:25:ARG:NH1 | 1:A:25:ARG:HB2 | 1.98 | 0.79 |
| 1:B:162:TRP:HA | 1:B:318:GLN:HE22 | 1.46 | 0.79 |
| 1:C:791:TYR:CD2 | 1:C:801:CYS:HA | 2.17 | 0.79 |
| 1:C:686:GLU:HG3 | 1:C:715:MET:CE | 2.13 | 0.79 |
| 1:B:117:VAL:HG22 | 1:B:133:ILE:HA | 1.64 | 0.78 |
| 1:B:863:LEU:HD12 | 1:B:866:MET:HE3 | 1.66 | 0.78 |
| 1:B:800:LYS:HD3 | 3:H:108:DT:H4' | 1.62 | 0.78 |
| 1:D:426:SER:HB2 | 1:D:472:PRO:HD3 | 1.63 | 0.78 |
| 1:B:231:LYS:HG3 | 1:B:236:GLU:HA | 1.65 | 0.78 |
| 1:C:195:LYS:H | 1:C:195:LYS:HZ3 | 1.31 | 0.78 |
| 1:B:534:SER:OG | 1:B:537:SER:HB2 | 1.82 | 0.78 |
| 1:C:73:LYS:NZ | 1:C:73:LYS:HB3 | 1.97 | 0.78 |
| 1:C:642:ARG:HD3 | 1:C:642:ARG:N | 1.99 | 0.78 |
| 1:A:43:GLU:CD | 1:A:43:GLU:H | 1.87 | 0.78 |
| 1:C:116:GLU:HB2 | 1:C:135:ALA:HB3 | 1.65 | 0.78 |
| 3:F:106:DT:H1' | 3:F:107:DG:H5' | 1.66 | 0.78 |
| 1:A:127:SER:HA | 1:A:228:ASN:HD22 | 1.48 | 0.77 |
| 1:B:223:ILE:HB | 1:B:224:PRO:HD3 | 1.65 | 0.77 |
| 1:B:505:ASN:HD22 | 1:B:507:ASN:HD22 | 1.32 | 0.77 |
| 1:C:642:ARG:NE | 1:C:646:HIS:CD2 | 2.51 | 0.77 |
| 1:D:132:PRO:HA | 1:D:229:ARG:NE | 1.99 | 0.77 |
| 3:J:104:DG:H2'' | 3:J:105:DC:C5' | 2.10 | 0.77 |
| 1:A:246:ARG:HH11 | 1:A:246:ARG:HG2 | 1.48 | 0.77 |
| 1:D:150:ASP:HB3 | 1:D:188:TYR:HE1 | 1.48 | 0.77 |
| 1:D:598:GLU:CG | 1:D:617:VAL:HG21 | 2.14 | 0.77 |
| 1:B:151:LEU:HA | 1:B:191:PHE:O | 1.84 | 0.77 |
| 1:B:322:SER:O | 1:B:326:ILE:HG12 | 1.85 | 0.77 |
| 1:D:494:ARG:O | 1:D:497:GLU:HG2 | 1.85 | 0.77 |
| 2:E:4:CTG:H2' | 2:E:4:CTG:O6 | 1.84 | 0.77 |
| 2:K:6:DA:C2' | 2:K:7:DA:H5'' | 2.15 | 0.77 |
| 1:D:182:ILE:HD13 | 1:D:182:ILE:O | 1.86 | 0.77 |
| 1:B:218:VAL:O | 1:B:223:ILE:HG13 | 1.84 | 0.76 |
| 1:B:751:ARG:HH11 | 1:B:759:SER:HB3 | 1.49 | 0.76 |
| 1:B:222:ALA:O | 1:B:226:VAL:HG23 | 1.83 | 0.76 |
| 1:D:597:ILE:HD11 | 1:D:663:ILE:HG23 | 1.67 | 0.76 |
| 1:D:849:PRO:HG2 | 1:D:852:THR:OG1 | 1.85 | 0.76 |
| 2:I:6:DA:H2'' | 2:I:7:DA:H5' | 1.67 | 0.76 |
| 1:C:373:LEU:HB3 | 1:C:378:LYS:HB2 | 1.66 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:546:GLN:HE21 | 1:A:546:GLN:C | 1.88 | 0.76 |
| 1:B:369:ILE:HG22 | 1:B:373:LEU:HD12 | 1.68 | 0.76 |
| 1:B:818:ASN:HD22 | 1:B:821:ALA:HB2 | 1.47 | 0.76 |
| 1:A:25:ARG:CB | 1:A:25:ARG:HH11 | 1.99 | 0.76 |
| 1:C:62:PHE:CE2 | 1:C:68:ALA:HA | 2.21 | 0.76 |
| 1:C:836:ARG:NH1 | 1:C:865:TRP:HA | 2.01 | 0.76 |
| 1:D:305:TYR:OH | 1:D:312:LEU:HB2 | 1.85 | 0.76 |
| 1:D:815:ILE:HG21 | 1:D:858:ILE:HD13 | 1.68 | 0.76 |
| 3:J:105:DC:H2' | 3:J:106:DT:H71 | 1.68 | 0.75 |
| 1:C:482:ARG:HH12 | 1:C:556:GLN:HE21 | 1.32 | 0.75 |
| 1:D:218:VAL:HA | 1:D:222:ALA:HB3 | 1.67 | 0.75 |
| 2:I:4:CTG:C6 | 2:I:4:CTG:H5'' | 2.16 | 0.75 |
| 1:D:407:VAL:HG13 | 1:D:689:ALA:HB3 | 1.68 | 0.75 |
| 1:C:85:MET:HA | 1:C:380:ILE:HD11 | 1.69 | 0.75 |
| 3:L:110:DA:H2'' | 3:L:111:DT:C5' | 2.16 | 0.75 |
| 1:A:428:GLU:OE2 | 1:A:428:GLU:N | 2.20 | 0.75 |
| 1:A:139:TYR:CE2 | 1:A:332:LEU:HD21 | 2.21 | 0.75 |
| 1:A:384:ARG:HD3 | 1:A:385:SER:N | 2.02 | 0.74 |
| 1:B:166:ILE:H | 1:B:166:ILE:HD12 | 1.51 | 0.74 |
| 1:B:854:ILE:HD11 | 1:B:858:ILE:HG13 | 1.68 | 0.74 |
| 1:C:195:LYS:HZ3 | 1:C:195:LYS:N | 1.84 | 0.74 |
| 1:D:738:PRO:HB3 | 1:D:780:ALA:O | 1.87 | 0.74 |
| 1:D:512:GLU:CB | 1:D:513:PRO:HA | 2.17 | 0.74 |
| 1:A:153:ASN:HD22 | 1:A:158:ASN:ND2 | 1.83 | 0.74 |
| 1:A:847:ALA:O | 1:A:848:TRP:HB3 | 1.86 | 0.74 |
| 1:C:216:TRP:O | 1:C:217:ASN:HB2 | 1.87 | 0.74 |
| 1:D:856:ASP:HA | 1:D:859:LYS:HB2 | 1.68 | 0.74 |
| 1:D:835:LEU:HD12 | 1:D:835:LEU:O | 1.87 | 0.74 |
| 1:B:775:ASN:HD21 | 1:B:777:ILE:HB | 1.53 | 0.74 |
| 1:D:202:LEU:CD2 | 1:D:241:ARG:HD3 | 2.11 | 0.74 |
| 1:A:404:TYR:CD1 | 1:A:618:LEU:HD13 | 2.23 | 0.74 |
| 1:D:82:ALA:N | 1:D:382:GLN:HE21 | 1.86 | 0.74 |
| 1:A:653:LYS:HD3 | 1:A:657:GLU:CD | 2.07 | 0.74 |
| 1:C:231:LYS:HG2 | 1:C:236:GLU:CA | 2.16 | 0.74 |
| 1:D:97:TYR:HB3 | 1:D:101:ILE:HD11 | 1.67 | 0.74 |
| 1:A:171:GLN:HE22 | 1:A:319:ARG:HH12 | 1.35 | 0.73 |
| 1:A:636:VAL:O | 1:A:640:LYS:HD2 | 1.88 | 0.73 |
| 1:C:81:GLU:HG2 | 1:C:83:LEU:HD22 | 1.67 | 0.73 |
| 1:D:117:VAL:HG13 | 1:D:132:PRO:O | 1.88 | 0.73 |
| 1:A:818:ASN:HD22 | 1:A:857:LEU:HD11 | 1.54 | 0.73 |
| 2:E:8:DT:H2' | 2:E:9:DG:C8 | 2.23 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:10:DA:H2'' | 2:K:11:DC:H5' | 1.70 | 0.73 |
| 1:D:229:ARG:NH1 | 1:D:233:ILE:HD11 | 2.04 | 0.73 |
| 1:D:441:ASP:HB3 | 1:D:447:ALA:HB2 | 1.70 | 0.73 |
| 1:B:193:ASN:ND2 | 1:B:196:GLU:HG2 | 2.03 | 0.73 |
| 1:C:642:ARG:HD3 | 1:C:642:ARG:H | 1.50 | 0.73 |
| 1:C:412:LEU:HD13 | 1:C:415:LEU:HD13 | 1.70 | 0.73 |
| 1:B:516:VAL:HG13 | 1:B:544:ARG:HH11 | 1.52 | 0.73 |
| 1:C:308:PRO:HG2 | 1:C:311:LYS:HG2 | 1.70 | 0.73 |
| 1:D:81:GLU:OE2 | 1:D:83:LEU:HD21 | 1.89 | 0.73 |
| 1:C:180:SER:O | 1:C:183:ILE:HG22 | 1.88 | 0.73 |
| 1:A:392:PRO:O | 1:A:587:THR:HG21 | 1.89 | 0.73 |
| 1:B:83:LEU:N | 1:B:83:LEU:HD12 | 2.03 | 0.73 |
| 1:C:163:SER:HB3 | 1:C:318:GLN:NE2 | 2.04 | 0.73 |
| 1:D:597:ILE:HG12 | 1:D:683:MET:HE1 | 1.71 | 0.73 |
| 1:A:501:GLU:HA | 1:A:504:HIS:ND1 | 2.04 | 0.72 |
| 3:H:106:DT:H1' | 3:H:107:DG:H5' | 1.71 | 0.72 |
| 1:A:482:ARG:HH21 | 1:A:556:GLN:HE22 | 1.36 | 0.72 |
| 1:B:27:ARG:HG3 | 1:B:27:ARG:NH1 | 2.02 | 0.72 |
| 1:B:446:VAL:HG22 | 1:B:446:VAL:O | 1.87 | 0.72 |
| 1:C:109:ARG:NH1 | 1:C:208:LYS:HA | 2.03 | 0.72 |
| 1:D:204:PHE:CE1 | 1:D:208:LYS:HG3 | 2.25 | 0.72 |
| 1:D:62:PHE:HB3 | 1:D:67:ASP:OD1 | 1.89 | 0.72 |
| 1:A:862:VAL:O | 1:A:864:HIS:N | 2.23 | 0.72 |
| 1:D:140:ASP:OD1 | 1:D:142:ILE:HG12 | 1.89 | 0.72 |
| 1:A:808:ILE:O | 1:A:811:TYR:HB3 | 1.90 | 0.72 |
| 1:B:217:ASN:OD1 | 1:B:274:ILE:HD13 | 1.90 | 0.72 |
| 1:A:41:CYS:HB2 | 1:A:42:PRO:HD2 | 1.70 | 0.72 |
| 1:D:222:ALA:O | 1:D:226:VAL:HG23 | 1.89 | 0.72 |
| 1:D:398:GLU:CA | 1:D:705:LYS:HE3 | 2.19 | 0.72 |
| 1:D:326:ILE:O | 1:D:330:ARG:HG2 | 1.90 | 0.72 |
| 1:B:749:ILE:HG22 | 1:B:753:LEU:HD12 | 1.70 | 0.71 |
| 1:D:802:PRO:HD2 | 1:D:805:ILE:HD12 | 1.72 | 0.71 |
| 1:B:621:ASP:OD1 | 3:H:114:DA:H5' | 1.90 | 0.71 |
| 3:J:104:DG:C3' | 3:J:105:DC:H5'' | 2.19 | 0.71 |
| 1:A:153:ASN:ND2 | 1:A:158:ASN:HD22 | 1.85 | 0.71 |
| 1:B:781:SER:HB2 | 1:B:832:VAL:HB | 1.72 | 0.71 |
| 1:D:495:ASN:ND2 | 1:D:521:ASP:HA | 2.05 | 0.71 |
| 2:G:14:DC:H2'' | 2:G:15:DC:H5'' | 1.73 | 0.71 |
| 1:B:347:MET:CE | 1:B:562:LEU:HD11 | 2.21 | 0.71 |
| 1:A:40:HIS:HD2 | 1:A:57:CYS:SG | 2.14 | 0.71 |
| 1:A:818:ASN:ND2 | 1:A:857:LEU:HD11 | 2.05 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:706:LYS:HE3 | 3:F:113:DC:O2 | 1.91 | 0.71 |
| 1:C:109:ARG:HH12 | 1:C:208:LYS:CD | 2.04 | 0.71 |
| 1:C:322:SER:O | 1:C:326:ILE:HG13 | 1.90 | 0.71 |
| 1:C:656:ARG:HA | 1:C:660:GLU:HG3 | 1.73 | 0.71 |
| 1:D:434:PHE:CE1 | 1:D:460:GLY:HA2 | 2.26 | 0.71 |
| 1:C:130:LYS:HG3 | 1:C:131:HIS:ND1 | 2.05 | 0.71 |
| 1:C:41:CYS:HB3 | 1:C:58:THR:CG2 | 2.18 | 0.71 |
| 2:I:10:DA:H2'' | 2:I:11:DC:H5' | 1.72 | 0.71 |
| 1:B:517:ASP:OD1 | 1:B:519:ARG:HB2 | 1.91 | 0.70 |
| 1:C:272:ASP:OD1 | 1:C:274:ILE:HG22 | 1.90 | 0.70 |
| 1:C:176:ASP:OD2 | 1:C:319:ARG:HD3 | 1.89 | 0.70 |
| 1:D:846:ILE:HD11 | 1:D:862:VAL:HG11 | 1.71 | 0.70 |
| 1:C:835:LEU:HD11 | 1:C:846:ILE:HB | 1.72 | 0.70 |
| 1:D:322:SER:O | 1:D:326:ILE:HG12 | 1.90 | 0.70 |
| 1:D:535:ALA:HB1 | 1:D:539:ASN:ND2 | 2.05 | 0.70 |
| 1:D:109:ARG:NH2 | 1:D:208:LYS:HB3 | 2.06 | 0.70 |
| 1:C:183:ILE:HD12 | 1:C:186:ILE:HD12 | 1.72 | 0.70 |
| 1:D:109:ARG:HH11 | 1:D:142:ILE:HD11 | 1.55 | 0.70 |
| 1:A:707:ARG:NH2 | 1:A:731:GLU:OE1 | 2.25 | 0.70 |
| 1:B:732:THR:CG2 | 1:B:733:GLN:HE21 | 2.02 | 0.70 |
| 1:D:41:CYS:HB3 | 1:D:57:CYS:HA | 1.72 | 0.70 |
| 1:B:312:LEU:O | 1:B:312:LEU:HD13 | 1.92 | 0.70 |
| 1:B:811:TYR:OH | 1:B:822:PRO:HG2 | 1.91 | 0.70 |
| 1:C:711:ASN:HD21 | 1:C:754:GLN:NE2 | 1.81 | 0.70 |
| 1:A:536:LYS:HD3 | 1:A:536:LYS:O | 1.92 | 0.70 |
| 1:B:408:MET:CE | 1:B:685:ARG:HD3 | 2.22 | 0.70 |
| 1:C:587:THR:HG22 | 1:C:588:THR:N | 2.05 | 0.70 |
| 1:A:514:LEU:HD12 | 1:A:526:ILE:HG23 | 1.73 | 0.70 |
| 1:A:642:ARG:NH1 | 1:A:642:ARG:HB2 | 2.07 | 0.70 |
| 1:C:13:ASP:OD2 | 1:C:66:ARG:HB2 | 1.91 | 0.70 |
| 1:B:785:ALA:HB1 | 1:B:788:ILE:HD11 | 1.74 | 0.69 |
| 1:D:597:ILE:HG21 | 1:D:683:MET:HE1 | 1.74 | 0.69 |
| 1:A:362:ILE:CD1 | 1:A:572:ASN:HD22 | 2.05 | 0.69 |
| 1:A:384:ARG:HD3 | 1:A:385:SER:H | 1.56 | 0.69 |
| 1:B:164:ILE:HD13 | 1:B:164:ILE:N | 2.05 | 0.69 |
| 1:B:875:THR:O | 1:B:879:PRO:HG3 | 1.92 | 0.69 |
| 1:D:114:ASP:HB3 | 1:D:328:VAL:HG13 | 1.73 | 0.69 |
| 1:D:82:ALA:HB3 | 1:D:382:GLN:HG3 | 1.75 | 0.69 |
| 1:A:685:ARG:NH2 | 1:A:714:ASP:OD2 | 2.25 | 0.69 |
| 1:B:326:ILE:O | 1:B:330:ARG:HG2 | 1.92 | 0.69 |
| 1:C:176:ASP:O | 1:C:177:GLU:HB2 | 1.91 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:12:DA:H2" | 2:E:13:DG:C5' | 2.22 | 0.69 |
| 1:B:204:PHE:HE1 | 1:B:208:LYS:HD2 | 1.57 | 0.69 |
| 1:D:330:ARG:O | 1:D:334:ILE:HG13 | 1.92 | 0.69 |
| 1:A:335:ASP:OD2 | 1:A:341:ILE:HG12 | 1.92 | 0.69 |
| 1:D:204:PHE:O | 1:D:208:LYS:HG2 | 1.92 | 0.69 |
| 1:D:442:TYR:HB3 | 1:D:592:MET:HE3 | 1.75 | 0.69 |
| 1:C:655:ALA:O | 1:C:660:GLU:HG2 | 1.93 | 0.69 |
| 1:D:6:LEU:HB2 | 1:D:18:ARG:O | 1.93 | 0.69 |
| 1:A:606:ASN:HD21 | 1:A:613:GLY:N | 1.91 | 0.69 |
| 1:B:732:THR:HG23 | 1:B:733:GLN:NE2 | 2.03 | 0.69 |
| 1:C:382:GLN:HG2 | 1:C:383:GLY:N | 2.07 | 0.69 |
| 1:D:149:PHE:HB3 | 1:D:197:LEU:CD2 | 2.21 | 0.69 |
| 1:D:234:PHE:HB3 | 1:D:238:THR:HB | 1.74 | 0.69 |
| 2:I:16:DG:H2" | 2:I:17:DC:O5' | 1.92 | 0.69 |
| 1:C:223:ILE:HB | 1:C:224:PRO:HD3 | 1.75 | 0.69 |
| 1:D:201:TYR:O | 1:D:204:PHE:HB3 | 1.92 | 0.69 |
| 1:A:474:GLU:O | 1:A:478:VAL:HG23 | 1.92 | 0.69 |
| 1:C:524:ASP:HA | 1:C:527:LYS:HE2 | 1.75 | 0.68 |
| 1:D:811:TYR:HA | 1:D:841:PHE:CZ | 2.27 | 0.68 |
| 1:C:354:GLN:HB3 | 1:C:356:GLN:OE1 | 1.93 | 0.68 |
| 1:D:214:THR:CG2 | 1:D:215:GLY:H | 2.04 | 0.68 |
| 1:A:606:ASN:HD21 | 1:A:613:GLY:CA | 2.05 | 0.68 |
| 1:D:373:LEU:HD12 | 1:D:380:ILE:HG22 | 1.75 | 0.68 |
| 1:C:482:ARG:NH1 | 1:C:560:LYS:HB2 | 2.08 | 0.68 |
| 1:B:217:ASN:H | 1:B:274:ILE:CG2 | 2.05 | 0.68 |
| 1:C:14:SER:OG | 1:C:30:GLU:HG2 | 1.92 | 0.68 |
| 1:C:449:ARG:HH12 | 1:C:452:ASP:HA | 1.58 | 0.68 |
| 1:D:147:TYR:HA | 1:D:187:ILE:HG23 | 1.76 | 0.68 |
| 1:D:777:ILE:HG22 | 1:D:777:ILE:O | 1.94 | 0.68 |
| 1:D:159:VAL:HG11 | 1:D:317:HIS:CB | 2.24 | 0.68 |
| 1:D:159:VAL:HG11 | 1:D:317:HIS:HB3 | 1.76 | 0.68 |
| 1:B:808:ILE:HD13 | 1:B:824:VAL:HG11 | 1.75 | 0.68 |
| 1:C:791:TYR:CE2 | 1:C:802:PRO:HD3 | 2.28 | 0.68 |
| 1:D:132:PRO:CA | 1:D:229:ARG:HH21 | 2.07 | 0.68 |
| 1:A:308:PRO:HG2 | 1:A:311:LYS:HG2 | 1.74 | 0.67 |
| 1:A:466:ASP:OD2 | 1:A:467:ARG:HD3 | 1.95 | 0.67 |
| 1:A:64:ASN:HD22 | 1:A:64:ASN:C | 1.97 | 0.67 |
| 1:D:658:ARG:HH11 | 1:D:658:ARG:HG3 | 1.57 | 0.67 |
| 1:B:6:LEU:HG | 1:B:19:TYR:HA | 1.76 | 0.67 |
| 1:B:894:LYS:HZ2 | 1:B:894:LYS:HB2 | 1.57 | 0.67 |
| 1:D:159:VAL:HG12 | 1:D:160:GLU:N | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:293:ILE:HD12 | 1:D:294:SER:N | 2.10 | 0.67 |
| 1:A:835:LEU:HD21 | 1:A:846:ILE:CG2 | 2.25 | 0.67 |
| 1:C:145:ARG:HB2 | 1:C:147:TYR:HE1 | 1.60 | 0.67 |
| 1:C:188:TYR:O | 1:C:189:MET:HG3 | 1.94 | 0.67 |
| 1:D:214:THR:CG2 | 1:D:273:TYR:HB2 | 2.24 | 0.67 |
| 1:A:502:ALA:CB | 1:A:538:LEU:HD22 | 2.23 | 0.67 |
| 1:A:660:GLU:HB2 | 1:A:661:PRO:HD3 | 1.77 | 0.67 |
| 1:B:641:PHE:HA | 1:B:646:HIS:HD2 | 1.58 | 0.67 |
| 1:D:775:ASN:HB3 | 1:D:778:SER:OG | 1.95 | 0.67 |
| 1:D:797:PRO:HG2 | 1:D:806:ARG:NH1 | 2.09 | 0.67 |
| 1:A:621:ASP:OD2 | 3:F:114:DA:H5' | 1.95 | 0.67 |
| 1:A:380:ILE:HD12 | 1:A:576:ARG:CZ | 2.25 | 0.67 |
| 1:A:824:VAL:HG13 | 1:A:849:PRO:HG3 | 1.76 | 0.67 |
| 1:B:553:MET:O | 1:B:557:ILE:HG12 | 1.94 | 0.67 |
| 1:C:170:LEU:HD23 | 1:C:177:GLU:HG2 | 1.77 | 0.67 |
| 1:C:28:THR:O | 1:C:28:THR:HG23 | 1.95 | 0.67 |
| 1:D:509:SER:HB2 | 1:D:532:LYS:O | 1.95 | 0.67 |
| 1:A:544:ARG:HB2 | 1:A:544:ARG:NH1 | 2.10 | 0.67 |
| 1:C:221:PHE:O | 1:C:224:PRO:HD2 | 1.94 | 0.67 |
| 1:A:27:ARG:HG3 | 1:A:27:ARG:HH11 | 1.58 | 0.67 |
| 1:B:134:ASP:OD1 | 1:B:151:LEU:HB3 | 1.95 | 0.67 |
| 1:B:483:LYS:O | 1:B:486:LYS:HG2 | 1.95 | 0.67 |
| 1:B:766:GLU:HG3 | 1:B:767:PHE:N | 2.09 | 0.67 |
| 1:B:98:ASN:O | 1:B:99:TYR:HB3 | 1.94 | 0.67 |
| 3:F:101:DG:H2'' | 3:F:102:DC:O5' | 1.95 | 0.67 |
| 2:G:16:DG:H2'' | 2:G:17:DC:H5'' | 1.77 | 0.67 |
| 2:G:4:CTG:H6 | 2:G:4:CTG:H5'' | 1.76 | 0.67 |
| 1:A:347:MET:HB2 | 1:A:558:ASN:OD1 | 1.94 | 0.66 |
| 1:B:319:ARG:HH11 | 1:B:319:ARG:HG2 | 1.60 | 0.66 |
| 1:B:116:GLU:CB | 1:B:135:ALA:HB3 | 2.25 | 0.66 |
| 1:B:894:LYS:HB2 | 1:B:894:LYS:HZ3 | 1.60 | 0.66 |
| 1:B:499:ILE:HG12 | 1:B:542:LEU:HD13 | 1.77 | 0.66 |
| 1:D:505:ASN:N | 1:D:506:PRO:HD3 | 2.10 | 0.66 |
| 1:D:533:LEU:CD1 | 1:D:534:SER:N | 2.55 | 0.66 |
| 1:D:561:LEU:HD23 | 1:D:561:LEU:O | 1.96 | 0.66 |
| 1:B:700:GLY:HA2 | 1:B:753:LEU:HD21 | 1.76 | 0.66 |
| 1:A:642:ARG:HH11 | 1:A:642:ARG:HB2 | 1.60 | 0.66 |
| 1:B:216:TRP:HA | 1:B:274:ILE:HG22 | 1.78 | 0.66 |
| 1:D:481:GLN:CB | 1:D:559:ARG:HE | 2.08 | 0.66 |
| 1:A:83:LEU:HD12 | 1:A:83:LEU:N | 2.10 | 0.66 |
| 1:B:351:ALA:O | 1:B:352:LYS:HB2 | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:102:LYS:HD2 | 1:B:103:TYR:H | 1.60 | 0.66 |
| 1:B:599:ARG:HH11 | 1:B:599:ARG:HG2 | 1.60 | 0.66 |
| 1:B:728:MET:HG3 | 3:H:113:DC:H5' | 1.78 | 0.66 |
| 1:D:281:SER:HB3 | 1:D:283:THR:HG22 | 1.78 | 0.66 |
| 1:C:52:ILE:HB | 1:C:428:GLU:HG2 | 1.77 | 0.66 |
| 1:D:504:HIS:C | 1:D:506:PRO:HD3 | 2.14 | 0.66 |
| 1:B:159:VAL:HG21 | 1:B:317:HIS:CD2 | 2.30 | 0.66 |
| 1:C:193:ASN:HD22 | 1:C:195:LYS:NZ | 1.94 | 0.66 |
| 1:A:730:LEU:HB3 | 1:A:883:PHE:CZ | 2.31 | 0.66 |
| 1:B:253:ILE:HD12 | 1:B:254:GLU:H | 1.59 | 0.66 |
| 1:D:15:ILE:HD11 | 1:D:92:TYR:CD2 | 2.31 | 0.66 |
| 1:D:685:ARG:C | 1:D:685:ARG:HD2 | 2.17 | 0.66 |
| 3:H:110:DA:H2'' | 3:H:111:DT:C5' | 2.26 | 0.66 |
| 1:A:712:VAL:HG22 | 1:A:724:LYS:O | 1.96 | 0.65 |
| 1:B:326:ILE:HG23 | 1:B:330:ARG:CZ | 2.26 | 0.65 |
| 1:B:749:ILE:HG22 | 1:B:753:LEU:CD1 | 2.26 | 0.65 |
| 1:B:186:ILE:HG22 | 1:B:187:ILE:N | 2.11 | 0.65 |
| 1:C:439:LEU:HD12 | 1:C:443:ILE:HD11 | 1.78 | 0.65 |
| 1:C:757:GLU:HB2 | 1:C:889:LEU:HD22 | 1.76 | 0.65 |
| 1:A:403:ARG:HD2 | 1:A:887:ALA:O | 1.96 | 0.65 |
| 1:A:485:HIS:C | 1:A:487:GLY:H | 1.98 | 0.65 |
| 1:C:130:LYS:HE3 | 1:C:131:HIS:CE1 | 2.29 | 0.65 |
| 1:D:517:ASP:OD1 | 1:D:519:ARG:HG2 | 1.96 | 0.65 |
| 3:J:110:DA:H2'' | 3:J:111:DT:C5' | 2.27 | 0.65 |
| 1:D:396:VAL:HB | 2:K:7:DA:OP1 | 1.97 | 0.65 |
| 1:C:78:ILE:CD1 | 1:C:80:LEU:HD23 | 2.25 | 0.65 |
| 1:D:151:LEU:HD11 | 1:D:154:SER:OG | 1.97 | 0.65 |
| 1:D:112:ASN:HB3 | 1:D:214:THR:HB | 1.77 | 0.65 |
| 3:L:104:DG:H2'' | 3:L:105:DC:H5' | 1.79 | 0.65 |
| 1:A:203:ASN:O | 1:A:207:GLN:HG2 | 1.97 | 0.65 |
| 1:A:744:ALA:HB2 | 1:A:767:PHE:CE2 | 2.31 | 0.65 |
| 1:D:216:TRP:CZ2 | 1:D:293:ILE:HG12 | 2.32 | 0.65 |
| 1:D:594:LEU:O | 1:D:597:ILE:HG22 | 1.96 | 0.65 |
| 1:B:421:ARG:HB3 | 1:B:680:LEU:CD1 | 2.26 | 0.65 |
| 1:C:109:ARG:HH12 | 1:C:208:LYS:HD3 | 1.62 | 0.65 |
| 1:C:726:LYS:HG3 | 1:C:728:MET:HE3 | 1.79 | 0.65 |
| 1:D:813:ARG:HG3 | 1:D:814:ALA:H | 1.60 | 0.65 |
| 1:A:71:TRP:CZ3 | 1:A:82:ALA:HB1 | 2.32 | 0.65 |
| 1:D:149:PHE:CE2 | 1:D:201:TYR:HA | 2.32 | 0.65 |
| 1:C:81:GLU:HB2 | 1:C:384:ARG:HH22 | 1.60 | 0.64 |
| 1:C:818:ASN:HB2 | 4:C:921:HOH:O | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:598:GLU:HG2 | 1:D:617:VAL:HG21 | 1.78 | 0.64 |
| 1:A:176:ASP:HA | 1:A:319:ARG:NH2 | 2.13 | 0.64 |
| 1:A:396:VAL:HG22 | 1:A:621:ASP:OD1 | 1.98 | 0.64 |
| 1:B:777:ILE:CD1 | 1:B:853:GLU:HG2 | 2.27 | 0.64 |
| 1:D:604:TYR:O | 1:D:608:VAL:HG23 | 1.97 | 0.64 |
| 1:B:116:GLU:HB2 | 1:B:135:ALA:HB3 | 1.77 | 0.64 |
| 1:C:114:ASP:HB3 | 1:C:328:VAL:HG22 | 1.77 | 0.64 |
| 3:F:102:DC:H2" | 3:F:103:DG:OP2 | 1.96 | 0.64 |
| 2:G:11:DC:H2" | 2:G:12:DA:H5' | 1.78 | 0.64 |
| 1:B:668:ARG:NH1 | 1:B:668:ARG:HG3 | 2.07 | 0.64 |
| 1:C:147:TYR:HB3 | 1:C:149:PHE:HE1 | 1.62 | 0.64 |
| 1:D:761:GLN:HG2 | 1:D:891:TYR:C | 2.18 | 0.64 |
| 1:D:783:SER:HA | 3:L:111:DT:OP1 | 1.97 | 0.64 |
| 1:C:153:ASN:HB2 | 1:C:192:ASP:O | 1.98 | 0.64 |
| 1:B:501:GLU:HG3 | 1:B:501:GLU:O | 1.96 | 0.64 |
| 1:C:159:VAL:HG21 | 1:C:317:HIS:CD2 | 2.33 | 0.64 |
| 1:A:540:GLU:O | 1:A:544:ARG:HD3 | 1.98 | 0.64 |
| 1:B:636:VAL:O | 1:B:640:LYS:HG3 | 1.97 | 0.64 |
| 1:C:271:LEU:HB3 | 1:C:276:LEU:CD2 | 2.28 | 0.64 |
| 1:D:164:ILE:H | 1:D:164:ILE:CD1 | 2.11 | 0.64 |
| 1:D:355:ILE:O | 1:D:358:VAL:HG23 | 1.96 | 0.64 |
| 1:A:621:ASP:O | 3:F:114:DA:H4' | 1.97 | 0.64 |
| 1:D:78:ILE:O | 1:D:78:ILE:HG22 | 1.98 | 0.64 |
| 1:A:470:VAL:O | 1:A:474:GLU:HG2 | 1.98 | 0.64 |
| 1:B:338:ARG:O | 1:B:339:GLN:HB2 | 1.96 | 0.64 |
| 1:D:163:SER:HB2 | 1:D:166:ILE:CD1 | 2.28 | 0.64 |
| 2:G:14:DC:C2' | 2:G:15:DC:H5" | 2.28 | 0.64 |
| 1:B:362:ILE:HD11 | 1:B:572:ASN:HB3 | 1.80 | 0.64 |
| 1:C:302:LYS:HE3 | 1:C:302:LYS:HA | 1.78 | 0.64 |
| 1:A:555:ALA:HB1 | 1:A:559:ARG:HH12 | 1.62 | 0.63 |
| 1:B:164:ILE:H | 1:B:164:ILE:CD1 | 2.00 | 0.63 |
| 1:B:641:PHE:HA | 1:B:646:HIS:CD2 | 2.33 | 0.63 |
| 1:B:76:GLU:HG2 | 1:B:382:GLN:HE22 | 1.63 | 0.63 |
| 1:C:120:PRO:HD2 | 1:C:131:HIS:HE2 | 1.64 | 0.63 |
| 1:C:330:ARG:O | 1:C:333:GLN:HB2 | 1.97 | 0.63 |
| 1:C:465:LYS:NZ | 1:C:675:ASN:HD21 | 1.96 | 0.63 |
| 1:A:43:GLU:CD | 1:A:43:GLU:N | 2.52 | 0.63 |
| 1:D:116:GLU:HB3 | 1:D:320:TYR:OH | 1.98 | 0.63 |
| 1:D:767:PHE:O | 1:D:771:PHE:HB2 | 1.97 | 0.63 |
| 1:A:439:LEU:O | 1:A:443:ILE:HG13 | 1.98 | 0.63 |
| 1:C:187:ILE:HG22 | 1:C:187:ILE:O | 1.97 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:270:VAL:O | 1:C:271:LEU:HD23 | 1.99 | 0.63 |
| 1:C:524:ASP:HA | 1:C:527:LYS:CE | 2.28 | 0.63 |
| 2:E:4:CTG:H5' | 2:E:4:CTG:C6 | 2.22 | 0.63 |
| 1:B:119:SER:HB2 | 1:B:124:PRO:HG3 | 1.80 | 0.63 |
| 1:B:401:PRO:O | 1:B:402:ASN:HB2 | 1.98 | 0.63 |
| 1:C:642:ARG:CD | 1:C:642:ARG:H | 2.11 | 0.63 |
| 1:D:125:GLU:HG3 | 1:D:127:SER:H | 1.62 | 0.63 |
| 1:D:171:GLN:OE1 | 1:D:303:LEU:HD11 | 1.98 | 0.63 |
| 1:A:708:TYR:CZ | 1:A:728:MET:HG3 | 2.33 | 0.63 |
| 1:B:20:ILE:CG2 | 1:B:24:GLY:HA2 | 2.29 | 0.63 |
| 1:B:334:ILE:O | 1:B:338:ARG:HG2 | 1.99 | 0.63 |
| 1:C:382:GLN:HG2 | 1:C:383:GLY:H | 1.61 | 0.63 |
| 1:A:223:ILE:HB | 1:A:224:PRO:HD3 | 1.79 | 0.63 |
| 1:C:204:PHE:CE1 | 1:C:208:LYS:HG3 | 2.33 | 0.63 |
| 1:D:189:MET:HB3 | 1:D:191:PHE:CZ | 2.34 | 0.63 |
| 1:D:21:ASP:HB2 | 1:D:23:ASN:OD1 | 1.98 | 0.63 |
| 1:B:117:VAL:HG21 | 1:B:225:TYR:CE2 | 2.34 | 0.63 |
| 1:C:422:GLN:HG3 | 1:C:678:GLN:O | 1.99 | 0.63 |
| 1:C:791:TYR:CD2 | 1:C:802:PRO:HD3 | 2.34 | 0.63 |
| 1:D:864:HIS:C | 1:D:866:MET:H | 2.01 | 0.63 |
| 1:A:559:ARG:HH11 | 1:A:559:ARG:CG | 2.10 | 0.63 |
| 1:A:276:LEU:HD21 | 1:A:341:ILE:HD13 | 1.79 | 0.63 |
| 1:A:836:ARG:HG3 | 1:A:867:ASP:HA | 1.80 | 0.63 |
| 1:B:406:TYR:CD2 | 1:B:633:ILE:HG13 | 2.34 | 0.63 |
| 1:D:183:ILE:O | 1:D:186:ILE:HG12 | 1.99 | 0.63 |
| 1:C:6:LEU:HD13 | 1:C:211:VAL:HG21 | 1.81 | 0.62 |
| 1:D:219:GLU:OE1 | 1:D:262:ILE:HD13 | 1.99 | 0.62 |
| 1:D:444:ASN:HA | 1:D:599:ARG:HH11 | 1.62 | 0.62 |
| 1:D:605:LEU:HD22 | 1:D:632:ILE:HD11 | 1.80 | 0.62 |
| 2:K:8:DT:H2'' | 2:K:9:DG:C8 | 2.34 | 0.62 |
| 1:A:239:ALA:O | 1:A:242:LEU:HB2 | 1.99 | 0.62 |
| 1:B:740:ALA:HB2 | 1:B:778:SER:HB2 | 1.81 | 0.62 |
| 2:G:6:DA:H2'' | 2:G:7:DA:C5' | 2.28 | 0.62 |
| 1:A:338:ARG:HB3 | 1:A:340:PHE:CE1 | 2.33 | 0.62 |
| 1:B:470:VAL:O | 1:B:474:GLU:HB2 | 1.99 | 0.62 |
| 1:D:170:LEU:HD22 | 1:D:177:GLU:HG2 | 1.79 | 0.62 |
| 1:D:751:ARG:NH1 | 1:D:763:TYR:HB2 | 2.15 | 0.62 |
| 3:J:110:DA:H2'' | 3:J:111:DT:H5' | 1.80 | 0.62 |
| 1:B:273:TYR:OH | 1:B:340:PHE:HB2 | 2.00 | 0.62 |
| 1:C:787:ASN:HD22 | 1:C:790:LYS:HD2 | 1.64 | 0.62 |
| 1:D:713:TRP:CZ3 | 1:D:723:PRO:HD3 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:167:ALA:O | 1:C:176:ASP:HB2 | 2.00 | 0.62 |
| 1:D:7:THR:HG21 | 1:D:267:GLY:O | 2.00 | 0.62 |
| 1:B:837:GLU:HG2 | 1:B:838:GLY:N | 2.14 | 0.62 |
| 1:C:195:LYS:NZ | 1:C:195:LYS:N | 2.39 | 0.62 |
| 1:A:129:ALA:HA | 1:A:225:TYR:CE1 | 2.34 | 0.62 |
| 1:A:467:ARG:HG3 | 1:A:467:ARG:HH11 | 1.64 | 0.62 |
| 1:A:362:ILE:HD11 | 1:A:569:ALA:HA | 1.81 | 0.62 |
| 1:A:810:THR:HG22 | 1:A:841:PHE:HB3 | 1.82 | 0.62 |
| 1:C:540:GLU:O | 1:C:544:ARG:HG3 | 2.00 | 0.62 |
| 1:D:738:PRO:HG2 | 1:D:741:VAL:HB | 1.81 | 0.62 |
| 1:A:499:ILE:HB | 1:A:542:LEU:HD13 | 1.80 | 0.62 |
| 1:C:154:SER:C | 1:C:156:TYR:H | 2.01 | 0.62 |
| 1:D:247:LYS:O | 1:D:266:PHE:HB2 | 1.99 | 0.62 |
| 1:D:294:SER:HB3 | 1:D:300:VAL:HG21 | 1.80 | 0.62 |
| 1:B:468:ASP:N | 1:B:468:ASP:OD2 | 2.33 | 0.62 |
| 1:C:839:ASN:OD1 | 1:C:841:PHE:HB2 | 1.99 | 0.62 |
| 1:D:90:LEU:HD12 | 1:D:363:LYS:HE3 | 1.81 | 0.62 |
| 1:A:204:PHE:CE1 | 1:A:208:LYS:HD2 | 2.35 | 0.62 |
| 1:B:171:GLN:NE2 | 1:B:303:LEU:HD13 | 2.15 | 0.62 |
| 1:C:365:TRP:CE2 | 1:C:566:LEU:HD13 | 2.34 | 0.62 |
| 1:D:725:LEU:H | 1:D:725:LEU:HD13 | 1.65 | 0.62 |
| 1:A:218:VAL:HG23 | 1:A:222:ALA:HB3 | 1.81 | 0.61 |
| 1:B:499:ILE:CG1 | 1:B:542:LEU:HD13 | 2.30 | 0.61 |
| 1:D:313:ARG:HG3 | 1:D:317:HIS:HD2 | 1.65 | 0.61 |
| 1:D:707:ARG:HA | 1:D:729:GLY:HA3 | 1.82 | 0.61 |
| 1:D:750:ARG:HH11 | 1:D:754:GLN:NE2 | 1.97 | 0.61 |
| 1:D:736:SER:HA | 1:D:782:VAL:HB | 1.82 | 0.61 |
| 2:I:4:CTG:C5' | 2:I:4:CTG:H6 | 2.29 | 0.61 |
| 1:B:129:ALA:HB1 | 1:B:229:ARG:HG2 | 1.82 | 0.61 |
| 1:B:319:ARG:O | 1:B:323:TYR:HB2 | 2.00 | 0.61 |
| 1:A:362:ILE:HD13 | 2:E:3:DT:C5' | 2.24 | 0.61 |
| 1:A:656:ARG:HA | 1:A:660:GLU:HG3 | 1.83 | 0.61 |
| 1:B:82:ALA:O | 1:B:382:GLN:HB2 | 2.00 | 0.61 |
| 1:C:97:TYR:O | 1:C:352:LYS:HE2 | 2.00 | 0.61 |
| 1:D:576:ARG:HB2 | 1:D:576:ARG:NH1 | 2.16 | 0.61 |
| 1:D:811:TYR:CB | 1:D:846:ILE:HB | 2.30 | 0.61 |
| 1:A:745:LEU:HD13 | 1:A:876:PHE:HD1 | 1.65 | 0.61 |
| 1:B:233:ILE:N | 1:B:233:ILE:HD12 | 2.15 | 0.61 |
| 1:C:455:SER:OG | 1:C:676:ASN:HA | 1.99 | 0.61 |
| 1:D:818:ASN:OD1 | 1:D:857:LEU:HD12 | 2.01 | 0.61 |
| 3:F:110:DA:H2" | 3:F:111:DT:C5' | 2.28 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:280:PHE:N | 1:A:280:PHE:CD1 | 2.66 | 0.61 |
| 1:B:797:PRO:HG3 | 1:B:806:ARG:HH12 | 1.65 | 0.61 |
| 1:C:514:LEU:HD21 | 1:C:526:ILE:HG23 | 1.82 | 0.61 |
| 1:C:775:ASN:OD1 | 1:C:777:ILE:N | 2.30 | 0.61 |
| 1:D:198:LEU:HD13 | 1:D:198:LEU:O | 2.00 | 0.61 |
| 1:D:441:ASP:O | 1:D:446:VAL:HG12 | 2.00 | 0.61 |
| 1:D:725:LEU:N | 1:D:725:LEU:HD13 | 2.15 | 0.61 |
| 2:G:4:CTG:H6 | 2:G:4:CTG:C5' | 2.31 | 0.61 |
| 1:B:685:ARG:HG2 | 1:B:685:ARG:HH11 | 1.66 | 0.61 |
| 1:D:575:PHE:HE2 | 1:D:577:TYR:HB2 | 1.65 | 0.61 |
| 1:A:154:SER:HB2 | 1:A:155:PRO:HD2 | 1.82 | 0.61 |
| 1:A:410:PHE:CD1 | 1:A:410:PHE:N | 2.68 | 0.61 |
| 1:A:840:PRO:C | 1:A:842:GLY:H | 2.04 | 0.61 |
| 1:A:303:LEU:HD12 | 1:A:323:TYR:CA | 2.31 | 0.61 |
| 1:C:135:ALA:O | 1:C:136:ILE:HG13 | 2.01 | 0.61 |
| 1:D:533:LEU:HD12 | 1:D:536:LYS:H | 1.66 | 0.61 |
| 1:D:779:ILE:CG1 | 1:D:871:LEU:HD21 | 2.31 | 0.61 |
| 1:A:276:LEU:CD2 | 1:A:341:ILE:HD13 | 2.30 | 0.61 |
| 1:A:153:ASN:ND2 | 1:A:158:ASN:HB3 | 2.16 | 0.61 |
| 1:A:132:PRO:HB3 | 1:A:194:GLU:OE2 | 2.01 | 0.61 |
| 1:A:408:MET:CE | 1:A:655:ALA:HB2 | 2.31 | 0.61 |
| 1:B:621:ASP:HB3 | 3:H:114:DA:H5'' | 1.83 | 0.61 |
| 1:C:195:LYS:HZ3 | 1:C:195:LYS:HB2 | 1.64 | 0.61 |
| 1:C:542:LEU:O | 1:C:546:GLN:HG3 | 2.01 | 0.61 |
| 1:C:720:TYR:CE1 | 1:C:724:LYS:HD2 | 2.36 | 0.61 |
| 1:C:78:ILE:HD11 | 1:C:80:LEU:HD23 | 1.82 | 0.61 |
| 1:D:156:TYR:N | 1:D:156:TYR:CD2 | 2.65 | 0.61 |
| 1:D:833:LEU:HB2 | 1:D:848:TRP:HH2 | 1.65 | 0.61 |
| 1:D:508:LEU:HD13 | 1:D:509:SER:N | 2.15 | 0.60 |
| 1:D:403:ARG:HH22 | 1:D:889:LEU:HD21 | 1.64 | 0.60 |
| 1:B:504:HIS:O | 1:B:506:PRO:HD3 | 2.01 | 0.60 |
| 1:C:642:ARG:HE | 1:C:646:HIS:HD2 | 1.39 | 0.60 |
| 1:C:642:ARG:HH11 | 1:C:646:HIS:HB3 | 1.65 | 0.60 |
| 1:A:836:ARG:HG3 | 1:A:867:ASP:CA | 2.31 | 0.60 |
| 1:B:365:TRP:CD2 | 1:B:566:LEU:HD13 | 2.36 | 0.60 |
| 1:D:471:VAL:HB | 1:D:472:PRO:HD3 | 1.82 | 0.60 |
| 3:H:110:DA:H2'' | 3:H:111:DT:H5' | 1.83 | 0.60 |
| 2:G:10:DA:H2'' | 2:G:11:DC:C5' | 2.31 | 0.60 |
| 2:G:16:DG:H2'' | 2:G:17:DC:C5' | 2.32 | 0.60 |
| 1:A:38:PHE:CD2 | 1:A:59:ARG:HA | 2.36 | 0.60 |
| 1:A:685:ARG:NH1 | 1:A:688:ILE:HG13 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:772:ARG:HD2 | 1:A:868:TYR:CD2 | 2.36 | 0.60 |
| 1:C:203:ASN:O | 1:C:207:GLN:HG2 | 2.01 | 0.60 |
| 1:D:216:TRP:HB2 | 1:D:290:LEU:HD12 | 1.83 | 0.60 |
| 1:D:833:LEU:HB2 | 1:D:848:TRP:CH2 | 2.36 | 0.60 |
| 3:F:104:DG:C3' | 3:F:105:DC:H5'' | 2.31 | 0.60 |
| 1:B:629:ALA:HA | 1:B:632:ILE:HG12 | 1.82 | 0.60 |
| 1:D:191:PHE:HD1 | 1:D:197:LEU:HD23 | 1.65 | 0.60 |
| 1:D:191:PHE:CD1 | 1:D:197:LEU:HD23 | 2.35 | 0.60 |
| 1:A:725:LEU:HD11 | 1:A:750:ARG:HB2 | 1.82 | 0.60 |
| 1:B:126:PRO:HG3 | 1:B:221:PHE:HD1 | 1.66 | 0.60 |
| 1:B:421:ARG:HG2 | 1:B:421:ARG:HH11 | 1.67 | 0.60 |
| 1:C:151:LEU:HD21 | 1:C:154:SER:HB3 | 1.83 | 0.60 |
| 1:D:416:TYR:HB2 | 1:D:417:PRO:HD3 | 1.83 | 0.60 |
| 1:D:469:GLY:C | 1:D:472:PRO:HD2 | 2.22 | 0.60 |
| 1:D:519:ARG:HH11 | 1:D:519:ARG:HG3 | 1.67 | 0.60 |
| 1:A:783:SER:HA | 3:F:111:DT:OP1 | 2.01 | 0.60 |
| 2:K:10:DA:H2'' | 2:K:11:DC:C5' | 2.31 | 0.60 |
| 1:B:288:TYR:CD1 | 1:B:293:ILE:HD11 | 2.37 | 0.60 |
| 1:C:152:LEU:HD11 | 1:C:190:PRO:HB2 | 1.84 | 0.60 |
| 1:C:327:ALA:O | 1:C:330:ARG:HB2 | 2.01 | 0.60 |
| 1:C:73:LYS:HB3 | 1:C:73:LYS:HZ3 | 1.67 | 0.60 |
| 1:C:822:PRO:HD2 | 1:C:855:THR:OG1 | 2.01 | 0.60 |
| 1:A:137:THR:HB | 1:A:328:VAL:HG21 | 1.83 | 0.59 |
| 1:A:194:GLU:OE1 | 1:A:229:ARG:NH1 | 2.34 | 0.59 |
| 1:A:813:ARG:HB2 | 1:A:813:ARG:HH11 | 1.67 | 0.59 |
| 1:D:231:LYS:O | 1:D:235:GLY:HA2 | 2.02 | 0.59 |
| 1:A:855:THR:HG22 | 1:A:857:LEU:HG | 1.83 | 0.59 |
| 1:A:862:VAL:C | 1:A:864:HIS:H | 2.04 | 0.59 |
| 1:B:505:ASN:ND2 | 1:B:507:ASN:ND2 | 2.46 | 0.59 |
| 1:D:194:GLU:O | 1:D:198:LEU:HB2 | 2.02 | 0.59 |
| 1:A:482:ARG:HE | 1:A:556:GLN:NE2 | 2.00 | 0.59 |
| 1:B:102:LYS:HD2 | 1:B:103:TYR:N | 2.18 | 0.59 |
| 1:B:706:LYS:HD2 | 3:H:113:DC:H1' | 1.84 | 0.59 |
| 1:B:777:ILE:HD11 | 1:B:853:GLU:CG | 2.31 | 0.59 |
| 1:C:302:LYS:HD3 | 1:C:303:LEU:N | 2.17 | 0.59 |
| 1:D:159:VAL:HG11 | 1:D:317:HIS:CG | 2.37 | 0.59 |
| 1:D:835:LEU:CD2 | 1:D:846:ILE:HG23 | 2.33 | 0.59 |
| 1:A:132:PRO:HA | 1:A:229:ARG:NH1 | 2.17 | 0.59 |
| 1:A:514:LEU:HD13 | 1:A:529:LYS:HZ3 | 1.68 | 0.59 |
| 1:D:503:LEU:O | 1:D:503:LEU:HD23 | 2.03 | 0.59 |
| 1:D:136:ILE:HG23 | 1:D:149:PHE:HB2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:68:ALA:O | 1:D:71:TRP:HB3 | 2.02 | 0.59 |
| 2:I:10:DA:H2" | 2:I:11:DC:C5' | 2.32 | 0.59 |
| 1:A:839:ASN:HB2 | 1:A:840:PRO:CD | 2.22 | 0.59 |
| 1:B:642:ARG:H | 1:B:646:HIS:HD2 | 1.50 | 0.59 |
| 1:D:171:GLN:HE22 | 1:D:303:LEU:CD1 | 2.15 | 0.59 |
| 1:A:279:LYS:HD3 | 1:A:359:PHE:HD1 | 1.68 | 0.59 |
| 1:A:807:GLY:HA2 | 1:A:845:CYS:O | 2.03 | 0.59 |
| 1:D:305:TYR:OH | 1:D:309:ILE:HA | 2.03 | 0.59 |
| 1:D:542:LEU:HD11 | 1:D:546:GLN:HE21 | 1.67 | 0.59 |
| 1:D:286:PRO:HB3 | 1:D:782:VAL:HG11 | 1.83 | 0.59 |
| 1:A:290:LEU:O | 1:A:294:SER:HB2 | 2.03 | 0.59 |
| 1:A:811:TYR:CZ | 1:A:815:ILE:HD13 | 2.38 | 0.59 |
| 1:D:598:GLU:HG3 | 1:D:617:VAL:HG21 | 1.83 | 0.59 |
| 1:D:777:ILE:HG23 | 1:D:831:TYR:CE1 | 2.37 | 0.59 |
| 1:C:170:LEU:HA | 1:C:177:GLU:HG2 | 1.85 | 0.59 |
| 1:C:277:TYR:O | 1:C:281:SER:HB3 | 2.03 | 0.59 |
| 1:C:471:VAL:HB | 1:C:472:PRO:HD3 | 1.84 | 0.59 |
| 1:D:132:PRO:HA | 1:D:229:ARG:NH2 | 2.18 | 0.59 |
| 1:D:335:ASP:O | 1:D:339:GLN:N | 2.32 | 0.59 |
| 1:A:298:LEU:HD12 | 1:A:298:LEU:N | 2.17 | 0.58 |
| 1:B:471:VAL:HG11 | 1:B:570:LEU:HD11 | 1.85 | 0.58 |
| 1:D:77:ASP:O | 1:D:78:ILE:HD13 | 2.03 | 0.58 |
| 1:A:40:HIS:CD2 | 1:A:57:CYS:SG | 2.95 | 0.58 |
| 1:B:505:ASN:HD22 | 1:B:507:ASN:ND2 | 2.01 | 0.58 |
| 1:C:274:ILE:HG23 | 1:C:275:ASP:N | 2.17 | 0.58 |
| 1:D:770:GLU:O | 1:D:774:LEU:HG | 2.03 | 0.58 |
| 1:A:745:LEU:HD13 | 1:A:876:PHE:CD1 | 2.38 | 0.58 |
| 1:D:285:GLN:HE21 | 1:D:285:GLN:H | 1.52 | 0.58 |
| 1:D:594:LEU:HD11 | 1:D:625:ILE:HG22 | 1.86 | 0.58 |
| 1:D:777:ILE:HG23 | 1:D:831:TYR:HE1 | 1.68 | 0.58 |
| 1:D:779:ILE:HG13 | 1:D:871:LEU:HD21 | 1.84 | 0.58 |
| 1:B:425:ILE:HG23 | 1:B:463:TYR:CE2 | 2.39 | 0.58 |
| 1:C:42:PRO:HG2 | 1:C:45:GLN:HG3 | 1.84 | 0.58 |
| 1:D:381:PRO:O | 1:D:576:ARG:HD2 | 2.03 | 0.58 |
| 1:D:412:LEU:HD12 | 1:D:623:ASP:HA | 1.85 | 0.58 |
| 1:D:848:TRP:CG | 1:D:854:ILE:HB | 2.38 | 0.58 |
| 3:J:111:DT:H2" | 3:J:112:DT:H5" | 1.85 | 0.58 |
| 1:C:162:TRP:HB3 | 1:C:188:TYR:CZ | 2.38 | 0.58 |
| 1:A:120:PRO:HG2 | 1:A:156:TYR:CE1 | 2.39 | 0.58 |
| 1:A:364:THR:O | 1:A:368:ILE:HG13 | 2.03 | 0.58 |
| 1:A:494:ARG:NH2 | 1:A:521:ASP:HB3 | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:743:LYS:O | 1:A:746:LYS:HB3 | 2.04 | 0.58 |
| 1:B:204:PHE:CE1 | 1:B:208:LYS:HD2 | 2.37 | 0.58 |
| 1:B:369:ILE:HG22 | 1:B:373:LEU:CD1 | 2.32 | 0.58 |
| 1:B:664:ASP:OD2 | 1:B:668:ARG:NH1 | 2.36 | 0.58 |
| 1:B:408:MET:HE2 | 1:B:685:ARG:HD3 | 1.86 | 0.58 |
| 1:B:83:LEU:CD1 | 1:B:83:LEU:H | 2.14 | 0.58 |
| 1:D:197:LEU:O | 1:D:197:LEU:HD22 | 2.04 | 0.58 |
| 1:D:397:LYS:O | 1:D:399:PRO:HD3 | 2.02 | 0.58 |
| 1:A:467:ARG:HG3 | 1:A:467:ARG:NH1 | 2.18 | 0.58 |
| 1:B:739:LYS:HE2 | 1:B:742:GLN:HE22 | 1.66 | 0.58 |
| 1:C:788:ILE:HG13 | 1:C:826:GLU:OE1 | 2.04 | 0.58 |
| 1:D:82:ALA:H | 1:D:382:GLN:HE21 | 1.50 | 0.58 |
| 1:D:786:ASN:HB2 | 3:L:110:DA:OP1 | 2.04 | 0.58 |
| 1:A:685:ARG:NH2 | 1:A:717:GLY:H | 2.01 | 0.58 |
| 1:A:779:ILE:O | 1:A:779:ILE:HG13 | 2.03 | 0.58 |
| 1:B:217:ASN:OD1 | 1:B:274:ILE:CD1 | 2.51 | 0.58 |
| 1:C:137:THR:HG21 | 1:C:325:ILE:HA | 1.85 | 0.58 |
| 1:D:9:GLU:HG3 | 1:D:267:GLY:H | 1.69 | 0.58 |
| 1:A:236:GLU:CG | 1:A:240:LYS:HE2 | 2.30 | 0.58 |
| 1:A:139:TYR:CD2 | 1:A:332:LEU:HD21 | 2.38 | 0.58 |
| 1:C:465:LYS:HZ3 | 1:C:675:ASN:HD21 | 1.52 | 0.58 |
| 3:H:102:DC:H2" | 3:H:103:DG:OP2 | 2.04 | 0.58 |
| 1:B:317:HIS:O | 1:B:320:TYR:HB3 | 2.04 | 0.58 |
| 1:C:831:TYR:CD2 | 1:C:850:SER:HA | 2.38 | 0.57 |
| 1:A:42:PRO:HG2 | 1:A:45:GLN:HB2 | 1.86 | 0.57 |
| 1:A:523:SER:O | 1:A:527:LYS:HB3 | 2.04 | 0.57 |
| 1:B:16:PHE:HB3 | 1:B:245:HIS:CE1 | 2.40 | 0.57 |
| 1:D:132:PRO:HA | 1:D:229:ARG:HH21 | 1.68 | 0.57 |
| 1:D:305:TYR:CE2 | 1:D:312:LEU:HD13 | 2.39 | 0.57 |
| 1:A:708:TYR:CE2 | 1:A:728:MET:CG | 2.85 | 0.57 |
| 1:B:117:VAL:CG2 | 1:B:133:ILE:HG12 | 2.34 | 0.57 |
| 1:B:855:THR:HG21 | 1:B:857:LEU:HD12 | 1.86 | 0.57 |
| 1:D:229:ARG:HH11 | 1:D:233:ILE:HD11 | 1.68 | 0.57 |
| 2:I:4:CTG:O6 | 2:I:4:CTG:H5" | 2.03 | 0.57 |
| 1:A:27:ARG:HG3 | 1:A:27:ARG:NH1 | 2.16 | 0.57 |
| 1:A:405:LYS:O | 1:A:690:GLY:HA2 | 2.04 | 0.57 |
| 1:C:111:ALA:CB | 1:C:210:PRO:HB3 | 2.34 | 0.57 |
| 1:C:193:ASN:HD22 | 1:C:195:LYS:HZ1 | 1.51 | 0.57 |
| 1:D:313:ARG:HG3 | 1:D:317:HIS:CD2 | 2.40 | 0.57 |
| 1:B:771:PHE:CE2 | 1:B:872:LEU:HB2 | 2.39 | 0.57 |
| 1:C:183:ILE:HD12 | 1:C:186:ILE:CD1 | 2.33 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:726:LYS:CG | 1:C:728:MET:HE3 | 2.33 | 0.57 |
| 1:D:150:ASP:HB3 | 1:D:188:TYR:CE1 | 2.36 | 0.57 |
| 1:D:15:ILE:HG13 | 1:D:15:ILE:O | 2.04 | 0.57 |
| 1:D:347:MET:HG2 | 1:D:358:VAL:HG13 | 1.87 | 0.57 |
| 1:D:518:TYR:CD1 | 1:D:518:TYR:N | 2.73 | 0.57 |
| 1:D:810:THR:HG22 | 1:D:846:ILE:HG22 | 1.85 | 0.57 |
| 1:A:109:ARG:NH1 | 1:A:140:ASP:OD2 | 2.37 | 0.57 |
| 1:A:839:ASN:CB | 1:A:840:PRO:HD2 | 2.22 | 0.57 |
| 1:B:273:TYR:HA | 1:B:276:LEU:HB2 | 1.87 | 0.57 |
| 1:C:191:PHE:CD2 | 1:C:197:LEU:HA | 2.40 | 0.57 |
| 1:C:231:LYS:O | 1:C:231:LYS:HD2 | 2.05 | 0.57 |
| 1:D:290:LEU:O | 1:D:290:LEU:HD23 | 2.04 | 0.57 |
| 1:D:503:LEU:HG | 1:D:535:ALA:HB2 | 1.85 | 0.57 |
| 1:A:602:ASN:ND2 | 1:A:616:PHE:HB2 | 2.20 | 0.57 |
| 1:B:210:PRO:HG2 | 1:B:213:LEU:HD13 | 1.86 | 0.57 |
| 1:B:835:LEU:HD21 | 1:B:862:VAL:HG13 | 1.85 | 0.57 |
| 1:C:465:LYS:NZ | 1:C:675:ASN:ND2 | 2.53 | 0.57 |
| 1:D:214:THR:O | 1:D:218:VAL:HG21 | 2.04 | 0.57 |
| 1:D:295:GLU:OE1 | 1:D:302:LYS:HG3 | 2.05 | 0.57 |
| 1:D:365:TRP:CE2 | 1:D:566:LEU:HD13 | 2.40 | 0.57 |
| 1:B:221:PHE:C | 1:B:224:PRO:HD2 | 2.25 | 0.57 |
| 1:B:342:ASN:HB2 | 4:B:923:HOH:O | 2.05 | 0.57 |
| 1:B:642:ARG:H | 1:B:646:HIS:CD2 | 2.23 | 0.57 |
| 1:C:811:TYR:HA | 1:C:846:ILE:HD11 | 1.86 | 0.57 |
| 1:D:249:ARG:O | 1:D:264:THR:HG22 | 2.05 | 0.57 |
| 1:D:285:GLN:NE2 | 1:D:285:GLN:H | 2.02 | 0.57 |
| 1:A:395:PHE:HA | 4:A:942:HOH:O | 2.03 | 0.57 |
| 1:C:124:PRO:HB2 | 1:C:225:TYR:HE2 | 1.68 | 0.57 |
| 1:D:214:THR:HG21 | 1:D:273:TYR:HD2 | 1.69 | 0.57 |
| 1:D:405:LYS:O | 1:D:690:GLY:HA2 | 2.05 | 0.57 |
| 1:D:534:SER:O | 1:D:538:LEU:HD13 | 2.05 | 0.57 |
| 1:A:129:ALA:HA | 1:A:225:TYR:CZ | 2.39 | 0.57 |
| 1:A:37:LEU:HD11 | 1:A:72:ILE:HD11 | 1.86 | 0.57 |
| 1:A:654:PHE:HE1 | 1:A:659:MET:HG3 | 1.69 | 0.57 |
| 1:A:66:ARG:O | 1:A:70:GLN:HB2 | 2.04 | 0.57 |
| 1:A:862:VAL:O | 1:A:865:TRP:N | 2.36 | 0.57 |
| 3:F:109:DC:H1' | 3:F:110:DA:H5'' | 1.87 | 0.57 |
| 3:L:101:DG:H2'' | 3:L:102:DC:C6 | 2.40 | 0.57 |
| 1:A:824:VAL:HG11 | 1:A:830:VAL:HG12 | 1.87 | 0.56 |
| 1:B:117:VAL:HG13 | 1:B:132:PRO:O | 2.05 | 0.56 |
| 1:B:347:MET:CE | 1:B:350:TYR:HD2 | 2.18 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:858:ILE:O | 1:B:862:VAL:HG23 | 2.04 | 0.56 |
| 1:D:101:ILE:HG22 | 1:D:102:LYS:N | 2.20 | 0.56 |
| 1:D:270:VAL:O | 1:D:271:LEU:HD23 | 2.05 | 0.56 |
| 1:B:505:ASN:HB3 | 1:B:535:ALA:CB | 2.35 | 0.56 |
| 1:D:229:ARG:HH11 | 1:D:229:ARG:HG2 | 1.69 | 0.56 |
| 1:D:546:GLN:HA | 1:D:549:GLU:HB3 | 1.87 | 0.56 |
| 1:A:411:ASP:OD1 | 1:A:686:GLU:HG3 | 2.06 | 0.56 |
| 1:A:514:LEU:CD2 | 1:A:529:LYS:HE2 | 2.36 | 0.56 |
| 1:B:376:GLN:NE2 | 1:B:378:LYS:NZ | 2.52 | 0.56 |
| 1:B:752:MET:HG2 | 1:B:760:LEU:HD22 | 1.85 | 0.56 |
| 1:C:149:PHE:O | 1:C:197:LEU:HD11 | 2.05 | 0.56 |
| 1:D:305:TYR:HE2 | 1:D:312:LEU:HD13 | 1.70 | 0.56 |
| 1:D:376:GLN:HB2 | 1:D:378:LYS:HG2 | 1.85 | 0.56 |
| 2:G:15:DC:H6 | 2:G:15:DC:H5' | 1.70 | 0.56 |
| 1:A:654:PHE:CE1 | 1:A:659:MET:HG3 | 2.41 | 0.56 |
| 1:A:876:PHE:O | 1:A:879:PRO:HG2 | 2.04 | 0.56 |
| 1:D:575:PHE:CE2 | 1:D:577:TYR:HB2 | 2.39 | 0.56 |
| 3:J:110:DA:H1' | 3:J:111:DT:H5'' | 1.87 | 0.56 |
| 1:B:159:VAL:HG11 | 1:B:313:ARG:O | 2.05 | 0.56 |
| 1:C:451:SER:OG | 1:C:453:VAL:HG22 | 2.05 | 0.56 |
| 1:C:686:GLU:HG3 | 1:C:715:MET:HE1 | 1.86 | 0.56 |
| 1:D:202:LEU:HD21 | 1:D:241:ARG:CD | 2.18 | 0.56 |
| 1:D:810:THR:CG2 | 1:D:846:ILE:HG22 | 2.36 | 0.56 |
| 1:D:89:LYS:O | 1:D:93:LEU:HD13 | 2.05 | 0.56 |
| 3:F:110:DA:H1' | 3:F:111:DT:H5'' | 1.87 | 0.56 |
| 1:B:821:ALA:HB1 | 1:B:822:PRO:HD2 | 1.87 | 0.56 |
| 1:C:139:TYR:CE2 | 1:C:332:LEU:HD21 | 2.41 | 0.56 |
| 1:C:731:GLU:HA | 1:C:734:LYS:HG3 | 1.88 | 0.56 |
| 1:D:878:LYS:O | 1:D:881:GLU:HB2 | 2.06 | 0.56 |
| 2:G:6:DA:H2'' | 2:G:7:DA:H5' | 1.87 | 0.56 |
| 1:A:481:GLN:O | 1:A:484:GLU:HB3 | 2.05 | 0.56 |
| 1:A:509:SER:H | 1:A:534:SER:HB3 | 1.71 | 0.56 |
| 1:A:509:SER:N | 1:A:534:SER:HB3 | 2.19 | 0.56 |
| 1:B:166:ILE:N | 1:B:166:ILE:HD12 | 2.18 | 0.56 |
| 1:B:25:ARG:HH11 | 1:B:25:ARG:HG2 | 1.70 | 0.56 |
| 1:B:738:PRO:HB2 | 1:B:741:VAL:HB | 1.88 | 0.56 |
| 1:B:863:LEU:HA | 1:B:866:MET:HE3 | 1.87 | 0.56 |
| 1:C:316:ASN:OD1 | 1:C:318:GLN:HB3 | 2.06 | 0.56 |
| 1:C:461:MET:SD | 1:C:581:ARG:HD2 | 2.45 | 0.56 |
| 1:C:9:GLU:OE2 | 1:C:266:PHE:HA | 2.05 | 0.56 |
| 1:D:213:LEU:HD22 | 1:D:218:VAL:HG11 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:264:THR:HG23 | 1:D:264:THR:O | 2.06 | 0.56 |
| 1:D:552:GLY:O | 1:D:556:GLN:HB3 | 2.06 | 0.56 |
| 1:A:399:PRO:HG2 | 1:A:704:GLY:HA2 | 1.87 | 0.56 |
| 1:B:644:THR:HG23 | 1:B:645:ASN:N | 2.21 | 0.56 |
| 1:B:85:MET:HE2 | 1:B:87:ASP:N | 2.01 | 0.56 |
| 1:C:189:MET:O | 1:C:191:PHE:CE1 | 2.59 | 0.56 |
| 1:C:475:ILE:HG23 | 1:C:476:THR:N | 2.20 | 0.56 |
| 1:C:506:PRO:HB3 | 1:C:535:ALA:HB2 | 1.87 | 0.56 |
| 1:C:380:ILE:HD12 | 1:C:576:ARG:CZ | 2.35 | 0.56 |
| 1:D:365:TRP:HA | 1:D:368:ILE:HD12 | 1.87 | 0.56 |
| 3:J:105:DC:H2' | 3:J:106:DT:C7 | 2.35 | 0.56 |
| 1:A:246:ARG:NH1 | 1:A:246:ARG:HG2 | 2.20 | 0.56 |
| 1:A:408:MET:HE1 | 1:A:655:ALA:HB2 | 1.88 | 0.56 |
| 1:A:4:PHE:CD1 | 1:A:4:PHE:N | 2.74 | 0.56 |
| 1:D:442:TYR:HB3 | 1:D:592:MET:CE | 2.34 | 0.56 |
| 1:D:830:VAL:HA | 1:D:850:SER:HB3 | 1.88 | 0.56 |
| 1:A:653:LYS:HD3 | 1:A:657:GLU:OE1 | 2.06 | 0.56 |
| 1:C:642:ARG:HE | 1:C:646:HIS:CG | 2.19 | 0.56 |
| 1:C:720:TYR:CZ | 1:C:724:LYS:HD2 | 2.40 | 0.56 |
| 1:D:132:PRO:HA | 1:D:229:ARG:CZ | 2.35 | 0.56 |
| 1:D:154:SER:HB2 | 1:D:313:ARG:NH1 | 2.20 | 0.56 |
| 1:D:453:VAL:HG23 | 1:D:454:TYR:CD1 | 2.40 | 0.56 |
| 1:D:419:ILE:HD13 | 1:D:589:PHE:HD1 | 1.69 | 0.56 |
| 1:D:777:ILE:O | 1:D:777:ILE:CG2 | 2.53 | 0.56 |
| 3:J:105:DC:H5' | 3:J:105:DC:H6 | 1.71 | 0.56 |
| 1:A:4:PHE:O | 1:A:19:TYR:HB2 | 2.05 | 0.56 |
| 1:B:270:VAL:C | 1:B:271:LEU:HD12 | 2.26 | 0.56 |
| 1:C:154:SER:O | 1:C:156:TYR:N | 2.39 | 0.56 |
| 1:D:151:LEU:HD13 | 1:D:151:LEU:C | 2.27 | 0.56 |
| 1:A:501:GLU:HA | 1:A:504:HIS:CE1 | 2.41 | 0.55 |
| 1:A:880:LEU:O | 1:A:883:PHE:HB2 | 2.05 | 0.55 |
| 1:D:402:ASN:CG | 1:D:403:ARG:H | 2.09 | 0.55 |
| 1:D:455:SER:HA | 1:D:675:ASN:O | 2.06 | 0.55 |
| 1:D:554:THR:O | 1:D:558:ASN:HB2 | 2.06 | 0.55 |
| 3:J:105:DC:H6 | 3:J:105:DC:C5' | 2.19 | 0.55 |
| 1:A:19:TYR:HE1 | 1:A:29:ARG:HG2 | 1.71 | 0.55 |
| 1:A:686:GLU:O | 1:A:716:GLU:N | 2.33 | 0.55 |
| 1:C:214:THR:HG21 | 1:C:341:ILE:HD11 | 1.88 | 0.55 |
| 1:D:131:HIS:O | 1:D:229:ARG:NE | 2.39 | 0.55 |
| 1:D:48:LYS:O | 1:D:377:ASN:HB3 | 2.06 | 0.55 |
| 1:A:279:LYS:HZ2 | 2:E:3:DT:H71 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:489:MET:SD | 1:A:553:MET:HG2 | 2.46 | 0.55 |
| 1:B:516:VAL:CG1 | 1:B:544:ARG:HH11 | 2.18 | 0.55 |
| 1:C:453:VAL:HG23 | 1:C:454:TYR:CG | 2.42 | 0.55 |
| 1:D:109:ARG:HH21 | 1:D:208:LYS:CB | 2.19 | 0.55 |
| 1:D:516:VAL:HG12 | 1:D:517:ASP:N | 2.21 | 0.55 |
| 1:D:513:PRO:HA | 1:D:541:MET:CE | 2.36 | 0.55 |
| 1:A:113:PHE:CE1 | 1:A:218:VAL:HG21 | 2.42 | 0.55 |
| 1:A:211:VAL:HG12 | 1:A:212:ILE:HG12 | 1.89 | 0.55 |
| 1:A:362:ILE:HD11 | 1:A:572:ASN:HD22 | 1.70 | 0.55 |
| 1:B:113:PHE:HB2 | 1:B:137:THR:O | 2.07 | 0.55 |
| 1:B:668:ARG:HH11 | 1:B:668:ARG:CG | 2.14 | 0.55 |
| 1:C:499:ILE:CG2 | 1:C:542:LEU:HB2 | 2.37 | 0.55 |
| 1:D:412:LEU:HD21 | 1:D:683:MET:HE3 | 1.87 | 0.55 |
| 1:A:347:MET:HE3 | 1:A:347:MET:HA | 1.87 | 0.55 |
| 1:A:597:ILE:HG12 | 1:A:667:PHE:CE2 | 2.41 | 0.55 |
| 1:A:781:SER:O | 1:A:831:TYR:HA | 2.06 | 0.55 |
| 1:B:145:ARG:HG3 | 1:B:185:LYS:O | 2.07 | 0.55 |
| 1:B:129:ALA:HB1 | 1:B:229:ARG:CD | 2.36 | 0.55 |
| 1:B:796:PHE:CD1 | 1:B:813:ARG:NH1 | 2.74 | 0.55 |
| 1:C:37:LEU:C | 1:C:38:PHE:CD1 | 2.80 | 0.55 |
| 1:C:528:GLU:HA | 1:C:528:GLU:OE2 | 2.07 | 0.55 |
| 1:C:791:TYR:HD2 | 1:C:801:CYS:HA | 1.68 | 0.55 |
| 1:D:741:VAL:HG12 | 1:D:745:LEU:HG | 1.88 | 0.55 |
| 1:D:824:VAL:HG23 | 1:D:830:VAL:HG11 | 1.87 | 0.55 |
| 1:A:604:TYR:O | 1:A:608:VAL:HG22 | 2.07 | 0.55 |
| 1:B:115:ILE:HD13 | 1:B:115:ILE:H | 1.71 | 0.55 |
| 2:G:10:DA:H2" | 2:G:11:DC:H5" | 1.89 | 0.55 |
| 1:A:414:SER:O | 1:A:417:PRO:HD2 | 2.07 | 0.55 |
| 1:B:147:TYR:CD1 | 1:B:147:TYR:N | 2.75 | 0.55 |
| 1:B:3:GLU:HG2 | 1:B:21:ASP:HA | 1.89 | 0.55 |
| 1:B:20:ILE:HG22 | 1:B:24:GLY:HA2 | 1.87 | 0.55 |
| 1:B:772:ARG:NH2 | 1:B:868:TYR:HB2 | 2.21 | 0.55 |
| 1:C:10:GLN:HG3 | 1:C:65:MET:HE1 | 1.87 | 0.55 |
| 1:C:251:LYS:HB3 | 1:C:262:ILE:HG13 | 1.87 | 0.55 |
| 1:A:213:LEU:CD1 | 1:A:223:ILE:HD11 | 2.36 | 0.55 |
| 1:A:420:ILE:HG12 | 1:A:586:ILE:HD11 | 1.87 | 0.55 |
| 1:A:846:ILE:HD12 | 1:A:847:ALA:O | 2.07 | 0.55 |
| 1:B:792:ASP:HA | 1:B:809:LEU:HD21 | 1.87 | 0.55 |
| 1:B:878:LYS:O | 1:B:878:LYS:HD3 | 2.06 | 0.55 |
| 1:C:202:LEU:HD23 | 1:C:241:ARG:HH21 | 1.72 | 0.55 |
| 1:D:159:VAL:HG21 | 1:D:317:HIS:CD2 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:52:ILE:CG2 | 1:D:381:PRO:HD3 | 2.37 | 0.55 |
| 1:D:814:ALA:HB3 | 1:D:841:PHE:CD1 | 2.41 | 0.55 |
| 2:E:16:DG:N2 | 3:F:103:DG:N2 | 2.54 | 0.55 |
| 1:B:347:MET:HE3 | 1:B:350:TYR:HD2 | 1.72 | 0.55 |
| 1:C:41:CYS:CB | 1:C:58:THR:HG22 | 2.25 | 0.55 |
| 1:C:81:GLU:HG2 | 1:C:83:LEU:CD2 | 2.36 | 0.55 |
| 1:D:395:PHE:HB3 | 1:D:594:LEU:HD23 | 1.89 | 0.55 |
| 2:G:15:DC:H2'' | 2:G:16:DG:O5' | 2.06 | 0.55 |
| 1:A:782:VAL:HG12 | 1:A:783:SER:N | 2.22 | 0.55 |
| 1:A:782:VAL:HG22 | 1:A:831:TYR:HD1 | 1.71 | 0.55 |
| 1:B:182:ILE:O | 1:B:186:ILE:HG13 | 2.07 | 0.55 |
| 1:A:517:ASP:OD1 | 1:A:519:ARG:HB2 | 2.06 | 0.54 |
| 1:B:145:ARG:HB3 | 1:B:147:TYR:CE1 | 2.41 | 0.54 |
| 1:B:504:HIS:C | 1:B:506:PRO:HD3 | 2.28 | 0.54 |
| 1:C:111:ALA:HB3 | 1:C:210:PRO:HB3 | 1.89 | 0.54 |
| 1:C:195:LYS:CB | 1:C:195:LYS:HZ3 | 2.21 | 0.54 |
| 1:C:392:PRO:HG2 | 1:C:584:THR:HG23 | 1.89 | 0.54 |
| 2:I:12:DA:H2'' | 2:I:13:DG:H5' | 1.89 | 0.54 |
| 1:A:702:TRP:CD1 | 1:A:708:TYR:HB3 | 2.42 | 0.54 |
| 1:D:216:TRP:CH2 | 1:D:293:ILE:HG12 | 2.41 | 0.54 |
| 1:D:512:GLU:CB | 1:D:513:PRO:CA | 2.85 | 0.54 |
| 1:D:530:ILE:O | 1:D:532:LYS:N | 2.40 | 0.54 |
| 3:F:107:DG:H2'' | 3:F:108:DT:OP2 | 2.06 | 0.54 |
| 1:A:4:PHE:CE2 | 1:A:103:TYR:HB2 | 2.42 | 0.54 |
| 1:B:116:GLU:N | 1:B:135:ALA:O | 2.39 | 0.54 |
| 1:B:898:PHE:HD1 | 1:B:898:PHE:H | 1.55 | 0.54 |
| 1:D:450:PRO:HB2 | 1:D:456:CYS:SG | 2.48 | 0.54 |
| 1:D:514:LEU:HD11 | 1:D:532:LYS:CB | 2.37 | 0.54 |
| 1:B:621:ASP:HB3 | 3:H:114:DA:C5' | 2.36 | 0.54 |
| 1:A:41:CYS:HB3 | 1:A:58:THR:HG22 | 1.89 | 0.54 |
| 1:B:27:ARG:HH11 | 1:B:27:ARG:CG | 2.17 | 0.54 |
| 1:C:147:TYR:HB3 | 1:C:149:PHE:CE1 | 2.42 | 0.54 |
| 1:D:482:ARG:C | 1:D:484:GLU:H | 2.11 | 0.54 |
| 1:A:798:GLY:N | 1:A:801:CYS:SG | 2.80 | 0.54 |
| 1:B:421:ARG:HG2 | 1:B:421:ARG:NH1 | 2.23 | 0.54 |
| 1:C:143:ASP:O | 1:C:144:ASP:HB3 | 2.07 | 0.54 |
| 1:C:738:PRO:HG2 | 1:C:741:VAL:CG2 | 2.37 | 0.54 |
| 1:D:514:LEU:HD12 | 1:D:514:LEU:N | 2.22 | 0.54 |
| 1:D:750:ARG:NH1 | 1:D:754:GLN:NE2 | 2.55 | 0.54 |
| 1:A:279:LYS:HE3 | 1:A:280:PHE:CE1 | 2.42 | 0.54 |
| 1:A:395:PHE:HB2 | 1:A:591:GLN:OE1 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:708:TYR:C | 1:A:708:TYR:CD2 | 2.81 | 0.54 |
| 1:A:835:LEU:HD21 | 1:A:846:ILE:HG21 | 1.88 | 0.54 |
| 1:B:395:PHE:HB2 | 1:B:591:GLN:NE2 | 2.11 | 0.54 |
| 1:B:836:ARG:NH2 | 1:B:864:HIS:O | 2.41 | 0.54 |
| 1:C:375:GLU:HA | 1:C:375:GLU:OE2 | 2.08 | 0.54 |
| 1:D:848:TRP:HB2 | 1:D:849:PRO:HD2 | 1.88 | 0.54 |
| 2:G:12:DA:H2'' | 2:G:13:DG:O5' | 2.08 | 0.54 |
| 1:A:373:LEU:HD11 | 1:A:470:VAL:HG11 | 1.90 | 0.54 |
| 1:A:362:ILE:CD1 | 1:A:569:ALA:HA | 2.37 | 0.54 |
| 1:A:782:VAL:HG22 | 1:A:831:TYR:CD1 | 2.43 | 0.54 |
| 1:B:361:PRO:HB3 | 1:B:565:SER:HB2 | 1.89 | 0.54 |
| 1:C:412:LEU:HG | 1:C:683:MET:CE | 2.38 | 0.54 |
| 1:C:477:LYS:HG2 | 1:C:481:GLN:NE2 | 2.23 | 0.54 |
| 1:C:685:ARG:HD2 | 1:C:685:ARG:C | 2.28 | 0.54 |
| 1:D:13:ASP:HB3 | 1:D:64:ASN:HB2 | 1.88 | 0.54 |
| 1:D:600:LYS:HE3 | 1:D:669:GLU:OE2 | 2.08 | 0.54 |
| 1:A:835:LEU:HD11 | 1:A:846:ILE:CG2 | 2.29 | 0.54 |
| 1:B:609:CYS:HA | 1:B:635:LYS:HE3 | 1.90 | 0.54 |
| 1:C:215:GLY:HA3 | 1:C:218:VAL:CG2 | 2.37 | 0.54 |
| 1:D:312:LEU:HG | 1:D:320:TYR:HB2 | 1.90 | 0.54 |
| 1:A:408:MET:HG2 | 1:A:688:ILE:HG12 | 1.90 | 0.54 |
| 1:B:353:ILE:HG13 | 1:B:354:GLN:O | 2.07 | 0.54 |
| 1:C:135:ALA:O | 1:C:136:ILE:CG1 | 2.56 | 0.54 |
| 1:C:836:ARG:HH11 | 1:C:836:ARG:HG3 | 1.73 | 0.54 |
| 1:D:856:ASP:HA | 1:D:859:LYS:CB | 2.38 | 0.54 |
| 1:A:897:LEU:CD1 | 1:A:897:LEU:H | 2.16 | 0.54 |
| 1:B:118:THR:OG1 | 1:B:313:ARG:HD2 | 2.07 | 0.54 |
| 1:B:629:ALA:CA | 1:B:632:ILE:HG12 | 2.38 | 0.54 |
| 1:C:181:GLU:CD | 1:C:181:GLU:H | 2.11 | 0.54 |
| 1:C:373:LEU:HD22 | 1:C:378:LYS:HD2 | 1.88 | 0.54 |
| 1:C:453:VAL:HG23 | 1:C:454:TYR:N | 2.23 | 0.54 |
| 1:D:286:PRO:O | 1:D:829:LYS:HD3 | 2.08 | 0.54 |
| 1:D:488:TYR:HD1 | 1:D:519:ARG:HH21 | 1.56 | 0.54 |
| 1:B:112:ASN:O | 1:B:113:PHE:HB3 | 2.08 | 0.53 |
| 1:B:120:PRO:HG2 | 1:B:156:TYR:CE2 | 2.43 | 0.53 |
| 1:C:154:SER:C | 1:C:156:TYR:N | 2.61 | 0.53 |
| 1:C:686:GLU:HG3 | 1:C:715:MET:HE3 | 1.88 | 0.53 |
| 1:D:140:ASP:CB | 1:D:143:ASP:HB3 | 2.35 | 0.53 |
| 1:D:368:ILE:CD1 | 1:D:562:LEU:HD11 | 2.39 | 0.53 |
| 1:D:697:GLY:HA3 | 1:D:753:LEU:O | 2.07 | 0.53 |
| 1:A:108:ILE:HG23 | 1:A:211:VAL:HG11 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:668:ARG:O | 1:A:672:GLU:HG3 | 2.09 | 0.53 |
| 1:B:273:TYR:O | 1:B:277:TYR:N | 2.39 | 0.53 |
| 1:C:215:GLY:HA3 | 1:C:218:VAL:HG21 | 1.90 | 0.53 |
| 1:C:825:VAL:HB | 1:C:828:GLU:CD | 2.28 | 0.53 |
| 1:D:156:TYR:N | 1:D:156:TYR:HD2 | 2.05 | 0.53 |
| 1:D:285:GLN:NE2 | 1:D:285:GLN:N | 2.56 | 0.53 |
| 1:D:300:VAL:HG12 | 1:D:301:GLY:N | 2.23 | 0.53 |
| 1:D:807:GLY:HA2 | 1:D:845:CYS:O | 2.07 | 0.53 |
| 1:B:177:GLU:HG2 | 1:B:303:LEU:HD11 | 1.90 | 0.53 |
| 1:C:109:ARG:HG2 | 1:C:210:PRO:HA | 1.91 | 0.53 |
| 1:D:20:ILE:HD13 | 1:D:26:GLU:HA | 1.90 | 0.53 |
| 1:D:883:PHE:CD2 | 1:D:883:PHE:N | 2.76 | 0.53 |
| 3:H:106:DT:H2'' | 3:H:107:DG:O5' | 2.07 | 0.53 |
| 3:L:101:DG:H2'' | 3:L:102:DC:C5 | 2.42 | 0.53 |
| 1:B:216:TRP:CH2 | 1:B:293:ILE:HG21 | 2.43 | 0.53 |
| 1:B:516:VAL:HG22 | 1:B:517:ASP:N | 2.22 | 0.53 |
| 1:B:831:TYR:CE2 | 1:B:850:SER:HA | 2.43 | 0.53 |
| 1:C:71:TRP:O | 1:C:75:MET:HG2 | 2.07 | 0.53 |
| 2:G:14:DC:H2'' | 2:G:15:DC:C5' | 2.38 | 0.53 |
| 1:B:147:TYR:H | 1:B:147:TYR:HD1 | 1.56 | 0.53 |
| 1:C:113:PHE:CE1 | 1:C:213:LEU:HD11 | 2.44 | 0.53 |
| 1:C:163:SER:OG | 1:C:166:ILE:HG13 | 2.09 | 0.53 |
| 1:C:362:ILE:HD12 | 1:C:575:PHE:HB2 | 1.89 | 0.53 |
| 1:C:35:PRO:HD3 | 1:C:65:MET:HG2 | 1.91 | 0.53 |
| 2:G:3:DT:H2'' | 2:G:4:CTG:OP2 | 2.08 | 0.53 |
| 1:A:279:LYS:NZ | 2:E:3:DT:H71 | 2.24 | 0.53 |
| 1:A:313:ARG:O | 1:A:317:HIS:HB2 | 2.09 | 0.53 |
| 1:A:347:MET:HA | 1:A:347:MET:CE | 2.38 | 0.53 |
| 1:A:776:TYR:CZ | 1:A:777:ILE:HG13 | 2.43 | 0.53 |
| 1:C:163:SER:CB | 1:C:166:ILE:HD12 | 2.39 | 0.53 |
| 1:D:271:LEU:HB3 | 1:D:276:LEU:HD11 | 1.91 | 0.53 |
| 1:D:617:VAL:O | 1:D:617:VAL:HG23 | 2.09 | 0.53 |
| 1:D:825:VAL:HB | 1:D:828:GLU:CG | 2.38 | 0.53 |
| 1:D:839:ASN:HD22 | 1:D:839:ASN:N | 2.04 | 0.53 |
| 1:A:509:SER:H | 1:A:534:SER:CB | 2.22 | 0.53 |
| 1:A:693:LEU:HD12 | 1:A:694:GLY:N | 2.23 | 0.53 |
| 1:B:456:CYS:SG | 1:B:462:MET:HG2 | 2.49 | 0.53 |
| 1:B:428:GLU:OE1 | 1:B:470:VAL:HG23 | 2.08 | 0.53 |
| 1:B:597:ILE:HD13 | 1:B:667:PHE:CZ | 2.44 | 0.53 |
| 1:B:825:VAL:HB | 1:B:828:GLU:HG3 | 1.91 | 0.53 |
| 1:D:305:TYR:HE1 | 1:D:309:ILE:HG22 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:815:ILE:CG2 | 1:D:858:ILE:HG21 | 2.26 | 0.53 |
| 1:D:864:HIS:O | 1:D:866:MET:N | 2.36 | 0.53 |
| 2:G:8:DT:C2' | 2:G:9:DG:C8 | 2.92 | 0.53 |
| 1:A:48:LYS:HE3 | 1:A:377:ASN:OD1 | 2.09 | 0.53 |
| 1:B:811:TYR:HH | 1:B:822:PRO:HG2 | 1.71 | 0.53 |
| 1:D:668:ARG:HG3 | 1:D:679:HIS:CE1 | 2.43 | 0.53 |
| 1:A:153:ASN:HD22 | 1:A:158:ASN:HB3 | 1.73 | 0.53 |
| 1:A:840:PRO:O | 1:A:842:GLY:N | 2.41 | 0.53 |
| 1:D:485:HIS:HB3 | 1:D:556:GLN:CB | 2.39 | 0.53 |
| 1:D:8:VAL:HG11 | 1:D:93:LEU:HD11 | 1.91 | 0.53 |
| 1:A:152:LEU:HD11 | 1:A:190:PRO:HB2 | 1.90 | 0.53 |
| 1:A:362:ILE:HG12 | 1:A:572:ASN:HD22 | 1.74 | 0.53 |
| 1:A:706:LYS:CE | 3:F:113:DC:O2 | 2.56 | 0.53 |
| 1:C:686:GLU:OE1 | 1:C:716:GLU:HG3 | 2.09 | 0.53 |
| 1:D:147:TYR:CE2 | 1:D:187:ILE:HD13 | 2.44 | 0.53 |
| 1:D:546:GLN:O | 1:D:550:VAL:HG23 | 2.09 | 0.53 |
| 1:D:738:PRO:HB2 | 1:D:778:SER:O | 2.08 | 0.53 |
| 1:A:485:HIS:C | 1:A:487:GLY:N | 2.59 | 0.52 |
| 1:A:612:GLU:HG2 | 1:A:612:GLU:O | 2.09 | 0.52 |
| 1:A:622:THR:HG22 | 1:A:623:ASP:N | 2.24 | 0.52 |
| 1:A:789:ALA:O | 1:A:791:TYR:N | 2.42 | 0.52 |
| 1:B:186:ILE:O | 1:B:187:ILE:HG13 | 2.09 | 0.52 |
| 1:C:195:LYS:HZ2 | 1:C:195:LYS:H | 1.50 | 0.52 |
| 1:C:645:ASN:OD1 | 1:C:719:ARG:NH1 | 2.40 | 0.52 |
| 1:D:416:TYR:HD2 | 1:D:586:ILE:CG2 | 2.22 | 0.52 |
| 1:A:516:VAL:HG21 | 1:A:522:PHE:CE2 | 2.44 | 0.52 |
| 1:A:625:ILE:HG13 | 1:A:625:ILE:O | 2.08 | 0.52 |
| 1:A:422:GLN:HE21 | 1:A:680:LEU:H | 1.54 | 0.52 |
| 1:B:159:VAL:HG22 | 1:B:313:ARG:HH22 | 1.75 | 0.52 |
| 1:B:747:GLU:HG2 | 1:B:763:TYR:CZ | 2.44 | 0.52 |
| 1:C:119:SER:HA | 1:C:131:HIS:CD2 | 2.43 | 0.52 |
| 1:C:204:PHE:HE1 | 1:C:208:LYS:HG3 | 1.74 | 0.52 |
| 1:C:855:THR:HG22 | 1:C:857:LEU:N | 2.19 | 0.52 |
| 1:D:114:ASP:CB | 1:D:328:VAL:HG13 | 2.39 | 0.52 |
| 1:A:855:THR:CG2 | 1:A:857:LEU:HG | 2.39 | 0.52 |
| 1:B:117:VAL:HG22 | 1:B:132:PRO:O | 2.10 | 0.52 |
| 1:B:162:TRP:HA | 1:B:318:GLN:NE2 | 2.20 | 0.52 |
| 1:B:11:ILE:HD12 | 1:B:16:PHE:CD1 | 2.44 | 0.52 |
| 1:B:218:VAL:HG12 | 1:B:223:ILE:HD11 | 1.91 | 0.52 |
| 1:B:810:THR:HG23 | 1:B:813:ARG:HH21 | 1.74 | 0.52 |
| 1:B:887:ALA:HB1 | 1:B:889:LEU:HD12 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:493:GLN:HG3 | 1:C:549:GLU:OE2 | 2.10 | 0.52 |
| 1:D:543:PHE:O | 1:D:547:ARG:HB3 | 2.10 | 0.52 |
| 1:A:471:VAL:HB | 1:A:472:PRO:CD | 2.38 | 0.52 |
| 1:A:727:ILE:HD13 | 1:A:749:ILE:HD12 | 1.90 | 0.52 |
| 1:A:804:HIS:HE2 | 3:F:110:DA:P | 2.32 | 0.52 |
| 1:B:229:ARG:O | 1:B:233:ILE:HD13 | 2.09 | 0.52 |
| 1:B:206:GLN:HE22 | 1:B:246:ARG:HH22 | 1.58 | 0.52 |
| 1:B:599:ARG:HG2 | 1:B:599:ARG:NH1 | 2.22 | 0.52 |
| 1:C:231:LYS:C | 1:C:231:LYS:HE2 | 2.29 | 0.52 |
| 1:C:412:LEU:HD13 | 1:C:415:LEU:CD1 | 2.39 | 0.52 |
| 1:D:403:ARG:NH2 | 1:D:889:LEU:HD21 | 2.24 | 0.52 |
| 1:A:824:VAL:CG1 | 1:A:849:PRO:HG3 | 2.39 | 0.52 |
| 1:B:499:ILE:H | 1:B:499:ILE:CD1 | 2.04 | 0.52 |
| 1:D:686:GLU:HB3 | 1:D:715:MET:HE1 | 1.91 | 0.52 |
| 1:A:153:ASN:HB3 | 1:A:158:ASN:HD22 | 1.74 | 0.52 |
| 1:B:166:ILE:H | 1:B:166:ILE:CD1 | 2.19 | 0.52 |
| 1:C:139:TYR:CD1 | 1:C:139:TYR:C | 2.83 | 0.52 |
| 1:C:202:LEU:O | 1:C:205:TRP:HB3 | 2.10 | 0.52 |
| 1:C:353:ILE:HD12 | 1:C:357:SER:HB3 | 1.91 | 0.52 |
| 1:D:170:LEU:CD2 | 1:D:177:GLU:HG2 | 2.40 | 0.52 |
| 1:D:191:PHE:HB2 | 1:D:197:LEU:HB2 | 1.92 | 0.52 |
| 2:K:6:DA:H2'' | 2:K:7:DA:H5' | 1.91 | 0.52 |
| 1:A:68:ALA:O | 1:A:72:ILE:HG13 | 2.09 | 0.52 |
| 1:A:858:ILE:O | 1:A:862:VAL:HG23 | 2.10 | 0.52 |
| 1:B:93:LEU:HD23 | 1:B:352:LYS:O | 2.10 | 0.52 |
| 1:D:136:ILE:HD11 | 1:D:201:TYR:CZ | 2.45 | 0.52 |
| 1:D:725:LEU:HG | 1:D:746:LYS:HZ2 | 1.75 | 0.52 |
| 1:D:874:LYS:HG3 | 1:D:875:THR:HG23 | 1.92 | 0.52 |
| 1:A:301:GLY:O | 1:A:330:ARG:NE | 2.33 | 0.52 |
| 1:B:474:GLU:OE2 | 1:B:477:LYS:HD2 | 2.10 | 0.52 |
| 1:B:594:LEU:HG | 1:B:594:LEU:O | 2.10 | 0.52 |
| 1:B:625:ILE:HG13 | 1:B:625:ILE:O | 2.10 | 0.52 |
| 1:B:818:ASN:O | 1:B:819:ILE:C | 2.48 | 0.52 |
| 1:C:241:ARG:HA | 1:C:246:ARG:HD3 | 1.91 | 0.52 |
| 1:C:534:SER:O | 1:C:538:LEU:HG | 2.09 | 0.52 |
| 1:C:53:TYR:CE1 | 1:C:428:GLU:HA | 2.45 | 0.52 |
| 1:C:793:VAL:HG12 | 1:C:793:VAL:O | 2.10 | 0.52 |
| 1:A:135:ALA:HA | 1:A:149:PHE:O | 2.08 | 0.52 |
| 1:B:422:GLN:HG3 | 1:B:678:GLN:O | 2.10 | 0.52 |
| 1:B:808:ILE:HG22 | 1:B:812:ASN:ND2 | 2.20 | 0.52 |
| 1:C:169:LYS:O | 1:C:175:GLY:HA3 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:214:THR:HB | 1:C:271:LEU:O | 2.10 | 0.52 |
| 1:D:113:PHE:HB2 | 1:D:137:THR:O | 2.10 | 0.52 |
| 1:D:573:VAL:C | 1:D:575:PHE:H | 2.13 | 0.52 |
| 1:D:619:TYR:OH | 1:D:706:LYS:HG3 | 2.10 | 0.52 |
| 1:A:104:ASP:O | 1:A:106:THR:N | 2.43 | 0.52 |
| 1:A:529:LYS:HZ3 | 1:A:529:LYS:HB3 | 1.75 | 0.52 |
| 1:A:806:ARG:HD3 | 1:A:843:ASP:OD2 | 2.09 | 0.52 |
| 1:B:878:LYS:C | 1:B:878:LYS:HD3 | 2.31 | 0.52 |
| 1:D:644:THR:O | 1:D:648:VAL:HG23 | 2.09 | 0.52 |
| 1:A:740:ALA:HB2 | 1:A:778:SER:HB2 | 1.90 | 0.51 |
| 1:B:51:ASP:OD1 | 1:B:53:TYR:N | 2.43 | 0.51 |
| 1:B:702:TRP:CD1 | 1:B:708:TYR:HB3 | 2.44 | 0.51 |
| 1:B:96:THR:HG22 | 1:B:97:TYR:CE2 | 2.45 | 0.51 |
| 1:C:170:LEU:HA | 1:C:177:GLU:CG | 2.40 | 0.51 |
| 1:C:752:MET:HG2 | 1:C:889:LEU:CD1 | 2.40 | 0.51 |
| 1:C:878:LYS:HB3 | 1:C:879:PRO:CD | 2.40 | 0.51 |
| 1:D:813:ARG:O | 1:D:815:ILE:N | 2.38 | 0.51 |
| 3:J:105:DC:H2' | 3:J:106:DT:C6 | 2.44 | 0.51 |
| 1:A:897:LEU:N | 1:A:897:LEU:HD12 | 2.18 | 0.51 |
| 1:A:898:PHE:HD1 | 1:A:898:PHE:H | 1.56 | 0.51 |
| 1:A:901:PHE:O | 1:A:902:ASP:HB2 | 2.09 | 0.51 |
| 1:B:728:MET:HG3 | 3:H:113:DC:C5' | 2.39 | 0.51 |
| 1:C:146:PHE:N | 1:C:146:PHE:CD1 | 2.78 | 0.51 |
| 1:D:180:SER:C | 1:D:182:ILE:H | 2.12 | 0.51 |
| 1:D:293:ILE:C | 1:D:293:ILE:HD12 | 2.30 | 0.51 |
| 1:D:52:ILE:HG23 | 1:D:381:PRO:HD3 | 1.92 | 0.51 |
| 1:D:87:ASP:OD1 | 1:D:89:LYS:HG2 | 2.11 | 0.51 |
| 1:A:829:LYS:O | 1:A:830:VAL:HG13 | 2.10 | 0.51 |
| 1:A:880:LEU:HD22 | 1:A:884:THR:HG23 | 1.92 | 0.51 |
| 1:C:482:ARG:HB2 | 1:C:559:ARG:HB3 | 1.93 | 0.51 |
| 1:C:482:ARG:HH12 | 1:C:556:GLN:NE2 | 2.03 | 0.51 |
| 1:D:17:GLU:HG2 | 1:D:18:ARG:N | 2.24 | 0.51 |
| 1:D:171:GLN:HE22 | 1:D:303:LEU:HD13 | 1.75 | 0.51 |
| 1:A:153:ASN:HB3 | 1:A:158:ASN:ND2 | 2.25 | 0.51 |
| 1:B:116:GLU:HB3 | 1:B:135:ALA:HB3 | 1.93 | 0.51 |
| 1:B:253:ILE:HD12 | 1:B:254:GLU:N | 2.25 | 0.51 |
| 1:C:347:MET:CE | 1:C:562:LEU:HD13 | 2.41 | 0.51 |
| 1:D:263:ILE:N | 1:D:263:ILE:HD12 | 2.26 | 0.51 |
| 1:D:508:LEU:HD23 | 1:D:534:SER:HB2 | 1.92 | 0.51 |
| 2:G:16:DG:C2' | 2:G:17:DC:H5'' | 2.40 | 0.51 |
| 1:A:126:PRO:HA | 1:A:225:TYR:HD1 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:499:ILE:HD13 | 1:A:541:MET:HG2 | 1.92 | 0.51 |
| 1:A:362:ILE:CG1 | 1:A:572:ASN:ND2 | 2.71 | 0.51 |
| 1:A:767:PHE:CD1 | 1:A:767:PHE:O | 2.64 | 0.51 |
| 1:B:525:GLU:O | 1:B:526:ILE:HG23 | 2.11 | 0.51 |
| 1:C:308:PRO:CG | 1:C:311:LYS:HG2 | 2.41 | 0.51 |
| 1:C:592:MET:O | 1:C:593:ALA:C | 2.49 | 0.51 |
| 1:D:178:VAL:HG22 | 1:D:326:ILE:HD11 | 1.92 | 0.51 |
| 1:D:434:PHE:CZ | 1:D:460:GLY:HA2 | 2.46 | 0.51 |
| 1:D:645:ASN:OD1 | 1:D:719:ARG:NH1 | 2.44 | 0.51 |
| 1:D:813:ARG:HG3 | 1:D:814:ALA:N | 2.24 | 0.51 |
| 1:A:685:ARG:NH2 | 1:A:717:GLY:N | 2.59 | 0.51 |
| 1:C:514:LEU:HB3 | 1:C:541:MET:CE | 2.41 | 0.51 |
| 1:C:392:PRO:CG | 1:C:584:THR:HG23 | 2.41 | 0.51 |
| 1:C:411:ASP:HB2 | 1:C:686:GLU:OE2 | 2.11 | 0.51 |
| 1:D:755:GLU:HB3 | 1:D:759:SER:OG | 2.09 | 0.51 |
| 1:A:599:ARG:O | 1:A:603:GLU:HG3 | 2.10 | 0.51 |
| 1:B:142:ILE:HG22 | 1:B:143:ASP:N | 2.24 | 0.51 |
| 1:B:188:TYR:CE2 | 1:B:190:PRO:HB3 | 2.45 | 0.51 |
| 1:B:194:GLU:OE1 | 1:B:229:ARG:NH2 | 2.43 | 0.51 |
| 1:D:409:SER:HB3 | 1:D:626:TYR:CD2 | 2.45 | 0.51 |
| 1:A:506:PRO:HB2 | 1:A:535:ALA:HA | 1.93 | 0.51 |
| 1:A:836:ARG:NH1 | 1:A:864:HIS:O | 2.44 | 0.51 |
| 1:B:186:ILE:CG2 | 1:B:187:ILE:N | 2.74 | 0.51 |
| 1:B:216:TRP:CZ2 | 1:B:293:ILE:HG21 | 2.46 | 0.51 |
| 1:C:298:LEU:O | 1:C:299:ASN:HB2 | 2.10 | 0.51 |
| 1:D:280:PHE:CE1 | 1:D:561:LEU:HD11 | 2.46 | 0.51 |
| 1:D:280:PHE:HB2 | 1:D:340:PHE:CZ | 2.46 | 0.51 |
| 1:D:458:PRO:HG3 | 1:D:674:MET:HE1 | 1.93 | 0.51 |
| 3:L:103:DG:H2" | 3:L:104:DG:OP2 | 2.11 | 0.51 |
| 1:A:255:ASN:ND2 | 1:A:257:TYR:CD2 | 2.79 | 0.51 |
| 1:B:863:LEU:HA | 1:B:866:MET:CE | 2.41 | 0.51 |
| 1:C:152:LEU:HD22 | 1:C:160:GLU:HA | 1.93 | 0.51 |
| 1:D:516:VAL:HG12 | 1:D:517:ASP:H | 1.75 | 0.51 |
| 2:G:8:DT:H2" | 2:G:9:DG:C8 | 2.45 | 0.51 |
| 1:B:376:GLN:NE2 | 1:B:378:LYS:HZ3 | 2.09 | 0.51 |
| 1:B:502:ALA:HB1 | 1:B:535:ALA:HB1 | 1.93 | 0.51 |
| 1:B:898:PHE:HA | 1:B:901:PHE:HD1 | 1.75 | 0.51 |
| 1:C:516:VAL:HG21 | 1:C:522:PHE:CE1 | 2.45 | 0.51 |
| 1:C:858:ILE:O | 1:C:861:ASP:HB2 | 2.10 | 0.51 |
| 1:D:197:LEU:C | 1:D:197:LEU:HD13 | 2.31 | 0.51 |
| 1:D:50:PHE:HA | 1:D:55:LYS:O | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:365:TRP:O | 1:A:366:ASP:C | 2.50 | 0.50 |
| 1:A:588:THR:O | 1:A:591:GLN:HB2 | 2.11 | 0.50 |
| 1:B:834:PRO:HD2 | 1:B:871:LEU:HD13 | 1.92 | 0.50 |
| 1:C:163:SER:HB3 | 1:C:166:ILE:HB | 1.92 | 0.50 |
| 1:D:275:ASP:O | 1:D:279:LYS:HB2 | 2.11 | 0.50 |
| 1:D:458:PRO:C | 1:D:460:GLY:H | 2.15 | 0.50 |
| 1:D:726:LYS:HG3 | 1:D:726:LYS:O | 2.10 | 0.50 |
| 1:A:428:GLU:OE1 | 1:A:470:VAL:HG23 | 2.11 | 0.50 |
| 1:A:514:LEU:HD13 | 1:A:529:LYS:NZ | 2.27 | 0.50 |
| 1:B:445:ALA:HB2 | 1:B:596:TRP:CH2 | 2.46 | 0.50 |
| 1:B:597:ILE:HD12 | 1:B:683:MET:SD | 2.50 | 0.50 |
| 1:C:144:ASP:O | 1:C:185:LYS:HD3 | 2.11 | 0.50 |
| 1:C:109:ARG:HD2 | 1:C:209:THR:O | 2.11 | 0.50 |
| 1:C:38:PHE:HB2 | 1:C:83:LEU:HB2 | 1.92 | 0.50 |
| 1:C:436:VAL:HG13 | 1:C:436:VAL:O | 2.11 | 0.50 |
| 1:C:506:PRO:CB | 1:C:535:ALA:HB2 | 2.41 | 0.50 |
| 1:D:305:TYR:CZ | 1:D:312:LEU:HD22 | 2.47 | 0.50 |
| 1:D:150:ASP:OD1 | 1:D:321:ILE:HG12 | 2.11 | 0.50 |
| 1:A:277:TYR:CE2 | 1:A:293:ILE:HD12 | 2.46 | 0.50 |
| 1:A:509:SER:CA | 1:A:534:SER:HB3 | 2.41 | 0.50 |
| 1:A:642:ARG:HH11 | 1:A:642:ARG:CB | 2.25 | 0.50 |
| 1:A:759:SER:O | 1:A:760:LEU:C | 2.48 | 0.50 |
| 1:B:319:ARG:NH1 | 1:B:319:ARG:HG2 | 2.25 | 0.50 |
| 1:C:120:PRO:HD2 | 1:C:131:HIS:NE2 | 2.26 | 0.50 |
| 1:C:142:ILE:HA | 4:C:915:HOH:O | 2.11 | 0.50 |
| 1:C:475:ILE:HD13 | 1:C:566:LEU:HD22 | 1.92 | 0.50 |
| 1:D:388:VAL:O | 1:D:390:PRO:HD3 | 2.11 | 0.50 |
| 1:A:197:LEU:HD23 | 1:A:198:LEU:N | 2.27 | 0.50 |
| 1:A:689:ALA:HB1 | 1:A:711:ASN:O | 2.11 | 0.50 |
| 1:B:162:TRP:HE1 | 1:B:322:SER:HG | 1.57 | 0.50 |
| 1:B:260:ARG:NH1 | 1:B:260:ARG:HG2 | 2.26 | 0.50 |
| 1:B:415:LEU:O | 1:B:419:ILE:HG13 | 2.10 | 0.50 |
| 1:B:668:ARG:NH1 | 1:B:668:ARG:CG | 2.71 | 0.50 |
| 1:B:708:TYR:CE1 | 1:B:728:MET:HB3 | 2.47 | 0.50 |
| 1:C:273:TYR:HA | 1:C:276:LEU:HB2 | 1.94 | 0.50 |
| 1:C:302:LYS:HD3 | 1:C:303:LEU:H | 1.75 | 0.50 |
| 1:C:326:ILE:O | 1:C:327:ALA:C | 2.49 | 0.50 |
| 1:D:519:ARG:NH1 | 1:D:519:ARG:HG3 | 2.24 | 0.50 |
| 1:A:17:GLU:OE2 | 1:A:29:ARG:NH1 | 2.44 | 0.50 |
| 1:A:362:ILE:CG1 | 1:A:572:ASN:HD22 | 2.24 | 0.50 |
| 1:A:840:PRO:C | 1:A:842:GLY:N | 2.65 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:728:MET:CG | 3:H:113:DC:H5' | 2.39 | 0.50 |
| 1:C:333:GLN:O | 1:C:336:ALA:HB3 | 2.11 | 0.50 |
| 1:D:164:ILE:HD13 | 1:D:164:ILE:N | 2.16 | 0.50 |
| 1:D:300:VAL:CG1 | 1:D:301:GLY:N | 2.74 | 0.50 |
| 1:D:82:ALA:H | 1:D:382:GLN:NE2 | 2.09 | 0.50 |
| 1:D:403:ARG:HH22 | 1:D:889:LEU:CD2 | 2.24 | 0.50 |
| 1:D:576:ARG:HG3 | 1:D:576:ARG:O | 2.11 | 0.50 |
| 1:D:741:VAL:O | 1:D:744:ALA:N | 2.45 | 0.50 |
| 1:D:818:ASN:HA | 1:D:857:LEU:CD1 | 2.42 | 0.50 |
| 1:A:23:ASN:HD22 | 1:A:25:ARG:HH22 | 1.58 | 0.50 |
| 1:A:310:SER:C | 1:A:311:LYS:HD3 | 2.32 | 0.50 |
| 1:B:389:GLN:CD | 1:B:390:PRO:HD2 | 2.32 | 0.50 |
| 1:B:483:LYS:CB | 1:B:483:LYS:NZ | 2.75 | 0.50 |
| 1:C:114:ASP:HB3 | 1:C:328:VAL:CG2 | 2.42 | 0.50 |
| 1:D:550:VAL:HA | 1:D:553:MET:HB3 | 1.94 | 0.50 |
| 1:A:659:MET:O | 1:A:660:GLU:C | 2.50 | 0.50 |
| 1:A:693:LEU:HD12 | 1:A:694:GLY:H | 1.77 | 0.50 |
| 1:B:786:ASN:O | 1:B:787:ASN:HB2 | 2.12 | 0.50 |
| 1:C:109:ARG:HH12 | 1:C:208:LYS:HD2 | 1.73 | 0.50 |
| 1:C:449:ARG:NH1 | 1:C:452:ASP:HA | 2.26 | 0.50 |
| 1:C:642:ARG:CZ | 1:C:646:HIS:HB3 | 2.41 | 0.50 |
| 1:D:825:VAL:HG12 | 1:D:826:GLU:N | 2.26 | 0.50 |
| 1:D:846:ILE:HD11 | 1:D:862:VAL:CG1 | 2.39 | 0.50 |
| 2:G:6:DA:H2" | 2:G:7:DA:H5" | 1.94 | 0.50 |
| 1:A:145:ARG:HB2 | 1:A:147:TYR:HE1 | 1.76 | 0.50 |
| 1:A:219:GLU:HG2 | 1:A:219:GLU:O | 2.12 | 0.50 |
| 1:A:803:PHE:O | 1:A:845:CYS:SG | 2.68 | 0.50 |
| 1:B:488:TYR:C | 1:B:490:LEU:H | 2.16 | 0.50 |
| 1:B:687:ALA:HB2 | 1:B:715:MET:CE | 2.40 | 0.50 |
| 1:B:775:ASN:HB3 | 1:B:778:SER:OG | 2.11 | 0.50 |
| 1:C:16:PHE:HB3 | 1:C:245:HIS:CE1 | 2.47 | 0.50 |
| 1:C:738:PRO:HG2 | 1:C:741:VAL:HG21 | 1.94 | 0.50 |
| 1:D:109:ARG:HD3 | 1:D:209:THR:O | 2.11 | 0.50 |
| 1:D:770:GLU:HG2 | 1:D:770:GLU:O | 2.11 | 0.50 |
| 1:D:839:ASN:ND2 | 1:D:839:ASN:N | 2.59 | 0.50 |
| 3:H:112:DT:H73 | 4:H:47:HOH:O | 2.12 | 0.50 |
| 1:B:52:ILE:HG13 | 1:B:53:TYR:CD1 | 2.47 | 0.50 |
| 1:D:131:HIS:HB3 | 1:D:132:PRO:HD2 | 1.93 | 0.50 |
| 1:D:493:GLN:HB2 | 1:D:549:GLU:OE2 | 2.11 | 0.50 |
| 1:D:502:ALA:HB3 | 1:D:538:LEU:HD21 | 1.94 | 0.50 |
| 1:A:730:LEU:HD22 | 1:A:883:PHE:CE1 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:338:ARG:O | 1:C:339:GLN:HB2 | 2.11 | 0.49 |
| 1:C:660:GLU:HB2 | 1:C:661:PRO:CD | 2.34 | 0.49 |
| 1:D:191:PHE:CB | 1:D:197:LEU:HB2 | 2.42 | 0.49 |
| 1:D:321:ILE:HD12 | 1:D:321:ILE:N | 2.27 | 0.49 |
| 1:A:422:GLN:O | 1:A:676:ASN:HB3 | 2.12 | 0.49 |
| 1:A:555:ALA:HB1 | 1:A:559:ARG:NH1 | 2.27 | 0.49 |
| 1:B:887:ALA:O | 1:B:888:LYS:HB2 | 2.12 | 0.49 |
| 1:C:231:LYS:HE2 | 1:C:232:ASN:N | 2.27 | 0.49 |
| 1:C:461:MET:CE | 1:C:581:ARG:HD2 | 2.42 | 0.49 |
| 1:D:458:PRO:HG3 | 1:D:674:MET:CE | 2.42 | 0.49 |
| 1:D:835:LEU:HD21 | 1:D:846:ILE:HG23 | 1.93 | 0.49 |
| 1:B:129:ALA:HB1 | 1:B:229:ARG:CG | 2.42 | 0.49 |
| 1:B:245:HIS:CD2 | 1:B:267:GLY:HA3 | 2.47 | 0.49 |
| 1:B:247:LYS:HE3 | 1:B:266:PHE:CE2 | 2.47 | 0.49 |
| 1:C:138:HIS:CD2 | 1:C:138:HIS:C | 2.85 | 0.49 |
| 1:D:420:ILE:O | 1:D:424:ASN:N | 2.44 | 0.49 |
| 1:D:412:LEU:HD21 | 1:D:683:MET:CE | 2.42 | 0.49 |
| 1:A:420:ILE:HG12 | 1:A:586:ILE:CD1 | 2.42 | 0.49 |
| 1:B:739:LYS:HE2 | 1:B:742:GLN:NE2 | 2.26 | 0.49 |
| 1:C:109:ARG:HE | 1:C:142:ILE:HD12 | 1.78 | 0.49 |
| 1:C:145:ARG:HB2 | 1:C:147:TYR:CE1 | 2.44 | 0.49 |
| 1:C:191:PHE:CE2 | 1:C:197:LEU:HA | 2.48 | 0.49 |
| 1:C:66:ARG:O | 1:C:66:ARG:HD2 | 2.12 | 0.49 |
| 1:A:410:PHE:HB2 | 1:A:683:MET:HE1 | 1.93 | 0.49 |
| 1:A:472:PRO:HA | 1:A:475:ILE:HG13 | 1.94 | 0.49 |
| 1:A:509:SER:HB3 | 1:A:534:SER:HB3 | 1.95 | 0.49 |
| 1:A:51:ASP:OD1 | 1:A:53:TYR:N | 2.44 | 0.49 |
| 1:A:803:PHE:CZ | 1:A:845:CYS:HB3 | 2.47 | 0.49 |
| 1:A:757:GLU:HB2 | 1:A:889:LEU:HD22 | 1.93 | 0.49 |
| 1:A:94:SER:HB3 | 1:A:371:ASN:OD1 | 2.12 | 0.49 |
| 1:B:748:CYS:O | 1:B:752:MET:HG3 | 2.12 | 0.49 |
| 1:C:458:PRO:CG | 1:C:592:MET:SD | 3.01 | 0.49 |
| 1:B:644:THR:HG21 | 1:C:77:ASP:OD2 | 2.12 | 0.49 |
| 1:D:164:ILE:O | 1:D:168:ALA:N | 2.40 | 0.49 |
| 1:D:296:PHE:CD1 | 1:D:297:GLU:N | 2.80 | 0.49 |
| 1:D:405:LYS:O | 1:D:691:PRO:HD3 | 2.13 | 0.49 |
| 1:A:195:LYS:HE2 | 1:A:233:ILE:HG23 | 1.93 | 0.49 |
| 1:A:514:LEU:CD1 | 1:A:526:ILE:HG23 | 2.40 | 0.49 |
| 1:B:374:LYS:C | 1:B:376:GLN:H | 2.16 | 0.49 |
| 1:B:722:GLU:HA | 1:B:722:GLU:OE1 | 2.12 | 0.49 |
| 1:B:808:ILE:O | 1:B:812:ASN:ND2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:180:SER:O | 1:D:182:ILE:N | 2.45 | 0.49 |
| 1:D:533:LEU:HD12 | 1:D:536:LYS:N | 2.27 | 0.49 |
| 3:H:105:DC:C6 | 3:H:106:DT:H72 | 2.47 | 0.49 |
| 3:L:111:DT:H2" | 3:L:112:DT:C6 | 2.47 | 0.49 |
| 1:A:511:ASP:OD2 | 1:A:512:GLU:N | 2.45 | 0.49 |
| 1:A:747:GLU:OE2 | 1:A:747:GLU:HA | 2.13 | 0.49 |
| 1:A:782:VAL:CG1 | 1:A:783:SER:N | 2.75 | 0.49 |
| 1:B:273:TYR:CZ | 1:B:340:PHE:HB2 | 2.48 | 0.49 |
| 1:B:727:ILE:HG21 | 1:B:732:THR:CG2 | 2.42 | 0.49 |
| 1:B:773:GLN:H | 1:B:773:GLN:NE2 | 2.10 | 0.49 |
| 1:C:83:LEU:HD22 | 1:C:83:LEU:N | 2.28 | 0.49 |
| 1:D:223:ILE:HB | 1:D:224:PRO:CD | 2.40 | 0.49 |
| 1:D:289:SER:O | 1:D:293:ILE:HG13 | 2.13 | 0.49 |
| 2:G:4:CTG:H2' | 2:G:5:DG:C8 | 2.47 | 0.49 |
| 3:L:110:DA:H1' | 3:L:111:DT:H5" | 1.93 | 0.49 |
| 1:B:876:PHE:O | 1:B:879:PRO:HG2 | 2.11 | 0.49 |
| 1:C:110:VAL:HB | 1:C:141:SER:HB3 | 1.94 | 0.49 |
| 1:D:180:SER:HA | 1:D:183:ILE:HG13 | 1.95 | 0.49 |
| 1:D:162:TRP:CZ3 | 1:D:188:TYR:HB2 | 2.48 | 0.49 |
| 1:D:795:GLY:HA3 | 1:D:813:ARG:HD3 | 1.94 | 0.49 |
| 1:A:730:LEU:HB3 | 1:A:883:PHE:HZ | 1.75 | 0.49 |
| 1:B:233:ILE:O | 1:B:233:ILE:HG22 | 2.12 | 0.49 |
| 1:B:217:ASN:N | 1:B:274:ILE:HG21 | 2.16 | 0.49 |
| 1:B:278:LYS:HE2 | 1:B:288:TYR:CD2 | 2.47 | 0.49 |
| 1:B:362:ILE:HG12 | 2:G:3:DT:C5' | 2.43 | 0.49 |
| 1:B:858:ILE:HB | 1:B:862:VAL:HG23 | 1.94 | 0.49 |
| 1:C:171:GLN:C | 1:C:173:GLN:H | 2.16 | 0.49 |
| 1:C:726:LYS:HG3 | 1:C:728:MET:CE | 2.42 | 0.49 |
| 1:D:157:GLY:O | 1:D:313:ARG:NH1 | 2.46 | 0.49 |
| 1:D:41:CYS:HB3 | 1:D:57:CYS:CA | 2.40 | 0.49 |
| 1:D:491:ALA:O | 1:D:495:ASN:HB2 | 2.13 | 0.49 |
| 1:D:668:ARG:HG2 | 1:D:679:HIS:ND1 | 2.28 | 0.49 |
| 1:B:530:ILE:HG13 | 1:B:531:LYS:N | 2.28 | 0.49 |
| 1:B:398:GLU:OE2 | 1:B:705:LYS:HE3 | 2.13 | 0.49 |
| 1:C:495:ASN:HB3 | 1:C:522:PHE:CD2 | 2.48 | 0.49 |
| 1:D:419:ILE:HG23 | 1:D:589:PHE:CD1 | 2.48 | 0.49 |
| 1:A:97:TYR:O | 1:A:352:LYS:HE3 | 2.13 | 0.48 |
| 1:B:130:LYS:HB2 | 1:B:130:LYS:NZ | 2.28 | 0.48 |
| 1:B:139:TYR:CG | 1:B:140:ASP:N | 2.80 | 0.48 |
| 1:B:270:VAL:HG13 | 1:B:270:VAL:O | 2.12 | 0.48 |
| 1:C:182:ILE:HD13 | 1:C:329:TYR:CG | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:324:ASN:O | 1:C:328:VAL:HG23 | 2.13 | 0.48 |
| 1:C:691:PRO:HD3 | 1:C:699:GLY:HA3 | 1.94 | 0.48 |
| 1:D:514:LEU:CD1 | 1:D:541:MET:HE1 | 2.43 | 0.48 |
| 1:D:810:THR:O | 1:D:841:PHE:HE1 | 1.95 | 0.48 |
| 1:A:4:PHE:N | 1:A:4:PHE:HD1 | 2.11 | 0.48 |
| 1:C:482:ARG:CZ | 1:C:560:LYS:HB2 | 2.43 | 0.48 |
| 1:D:582:ASN:O | 1:D:585:ALA:HB3 | 2.12 | 0.48 |
| 3:L:104:DG:C2' | 3:L:105:DC:H5'' | 2.39 | 0.48 |
| 1:A:380:ILE:HD12 | 1:A:576:ARG:NE | 2.27 | 0.48 |
| 1:B:273:TYR:HA | 1:B:276:LEU:HD12 | 1.95 | 0.48 |
| 1:C:203:ASN:HA | 1:C:206:GLN:HG2 | 1.94 | 0.48 |
| 1:C:831:TYR:CE2 | 1:C:851:GLY:N | 2.80 | 0.48 |
| 1:D:506:PRO:O | 1:D:507:ASN:ND2 | 2.44 | 0.48 |
| 1:A:6:LEU:CD1 | 1:A:26:GLU:HG3 | 2.43 | 0.48 |
| 1:A:296:PHE:HD2 | 1:A:297:GLU:CG | 2.26 | 0.48 |
| 1:A:303:LEU:HB2 | 1:A:323:TYR:HD1 | 1.78 | 0.48 |
| 1:A:702:TRP:NE1 | 1:A:708:TYR:HD1 | 2.11 | 0.48 |
| 1:B:110:VAL:H | 1:B:141:SER:HB3 | 1.79 | 0.48 |
| 1:B:313:ARG:HG2 | 1:B:314:GLU:OE1 | 2.12 | 0.48 |
| 1:B:775:ASN:ND2 | 1:B:777:ILE:H | 2.12 | 0.48 |
| 1:D:144:ASP:OD1 | 1:D:185:LYS:HE3 | 2.14 | 0.48 |
| 1:D:2:LYS:HG2 | 1:D:3:GLU:H | 1.78 | 0.48 |
| 1:D:559:ARG:O | 1:D:562:LEU:HB3 | 2.14 | 0.48 |
| 1:D:36:SER:HB3 | 1:D:59:ARG:NH1 | 2.28 | 0.48 |
| 1:A:506:PRO:HB2 | 1:A:535:ALA:CB | 2.43 | 0.48 |
| 1:A:796:PHE:HB3 | 1:A:797:PRO:HD2 | 1.95 | 0.48 |
| 1:A:870:VAL:O | 1:A:874:LYS:HG2 | 2.14 | 0.48 |
| 1:B:268:ILE:HG22 | 1:B:269:SER:N | 2.29 | 0.48 |
| 1:B:499:ILE:HG21 | 1:B:530:ILE:HD12 | 1.95 | 0.48 |
| 1:B:771:PHE:HD1 | 1:B:774:LEU:HD12 | 1.79 | 0.48 |
| 1:C:204:PHE:O | 1:C:208:LYS:HB2 | 2.14 | 0.48 |
| 1:C:426:SER:OG | 1:C:427:PRO:HD2 | 2.14 | 0.48 |
| 1:D:273:TYR:HA | 1:D:276:LEU:HD12 | 1.95 | 0.48 |
| 1:D:360:SER:HB2 | 1:D:363:LYS:HB3 | 1.95 | 0.48 |
| 1:B:362:ILE:HG12 | 2:G:3:DT:H5' | 1.94 | 0.48 |
| 2:G:8:DT:H2' | 2:G:9:DG:C8 | 2.48 | 0.48 |
| 1:A:126:PRO:HA | 1:A:225:TYR:CD1 | 2.49 | 0.48 |
| 1:B:856:ASP:HA | 1:B:859:LYS:HB3 | 1.95 | 0.48 |
| 1:D:848:TRP:CB | 1:D:854:ILE:HB | 2.44 | 0.48 |
| 1:A:63:ALA:HB3 | 1:A:67:ASP:OD1 | 2.14 | 0.48 |
| 1:A:836:ARG:HH12 | 1:A:865:TRP:HA | 1.73 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:119:SER:CB | 1:B:124:PRO:HG3 | 2.44 | 0.48 |
| 1:B:324:ASN:O | 1:B:327:ALA:HB3 | 2.14 | 0.48 |
| 1:B:52:ILE:HD12 | 1:B:428:GLU:HB3 | 1.94 | 0.48 |
| 1:C:148:VAL:C | 1:C:149:PHE:CD1 | 2.87 | 0.48 |
| 1:C:499:ILE:HG21 | 1:C:542:LEU:HB2 | 1.94 | 0.48 |
| 1:D:402:ASN:CG | 1:D:403:ARG:N | 2.66 | 0.48 |
| 3:F:105:DC:H2'' | 3:F:106:DT:O5' | 2.14 | 0.48 |
| 1:A:195:LYS:HE2 | 1:A:233:ILE:CG2 | 2.44 | 0.48 |
| 1:A:482:ARG:HE | 1:A:556:GLN:HE21 | 1.61 | 0.48 |
| 1:A:737:THR:O | 1:A:738:PRO:O | 2.31 | 0.48 |
| 1:B:428:GLU:N | 1:B:428:GLU:OE2 | 2.39 | 0.48 |
| 1:B:486:LYS:HB3 | 1:B:556:GLN:NE2 | 2.28 | 0.48 |
| 1:B:772:ARG:CZ | 1:B:868:TYR:HB2 | 2.44 | 0.48 |
| 1:B:796:PHE:HD1 | 1:B:813:ARG:NH1 | 2.10 | 0.48 |
| 1:B:835:LEU:HA | 1:B:866:MET:HA | 1.95 | 0.48 |
| 1:C:176:ASP:O | 1:C:177:GLU:CB | 2.60 | 0.48 |
| 1:C:109:ARG:HH11 | 1:C:208:LYS:HA | 1.78 | 0.48 |
| 1:D:805:ILE:O | 1:D:809:LEU:HG | 2.14 | 0.48 |
| 1:D:835:LEU:HD13 | 1:D:839:ASN:OD1 | 2.14 | 0.48 |
| 1:B:312:LEU:HD12 | 1:B:320:TYR:HD1 | 1.78 | 0.48 |
| 1:B:713:TRP:CZ3 | 1:B:723:PRO:HD3 | 2.48 | 0.48 |
| 1:B:837:GLU:CG | 1:B:838:GLY:N | 2.76 | 0.48 |
| 1:B:894:LYS:CB | 1:B:894:LYS:NZ | 2.67 | 0.48 |
| 1:C:319:ARG:O | 1:C:322:SER:N | 2.46 | 0.48 |
| 1:C:85:MET:CA | 1:C:380:ILE:HD11 | 2.42 | 0.48 |
| 1:D:437:ALA:HB3 | 1:D:442:TYR:CZ | 2.49 | 0.48 |
| 3:J:105:DC:H2' | 3:J:106:DT:C5 | 2.48 | 0.48 |
| 1:A:19:TYR:CE1 | 1:A:29:ARG:HG2 | 2.49 | 0.48 |
| 1:A:41:CYS:HB2 | 1:A:42:PRO:CD | 2.43 | 0.48 |
| 1:A:641:PHE:HA | 1:A:646:HIS:CD2 | 2.48 | 0.48 |
| 1:A:830:VAL:HA | 1:A:848:TRP:O | 2.14 | 0.48 |
| 1:B:142:ILE:HD12 | 1:B:142:ILE:N | 2.29 | 0.48 |
| 1:B:51:ASP:OD1 | 1:B:51:ASP:C | 2.51 | 0.48 |
| 1:B:727:ILE:HG21 | 1:B:732:THR:HG21 | 1.96 | 0.48 |
| 1:B:898:PHE:HA | 1:B:901:PHE:CD1 | 2.49 | 0.48 |
| 1:C:343:LEU:HD11 | 1:C:558:ASN:ND2 | 2.29 | 0.48 |
| 1:D:136:ILE:HD11 | 1:D:201:TYR:CE1 | 2.49 | 0.48 |
| 1:D:9:GLU:O | 1:D:15:ILE:HA | 2.14 | 0.48 |
| 1:D:159:VAL:CG1 | 1:D:160:GLU:H | 2.20 | 0.48 |
| 1:D:368:ILE:HD11 | 1:D:562:LEU:HD11 | 1.96 | 0.48 |
| 1:D:727:ILE:HG23 | 1:D:730:LEU:HD12 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:776:TYR:O | 1:D:779:ILE:CD1 | 2.61 | 0.48 |
| 1:A:708:TYR:HD2 | 1:A:708:TYR:C | 2.18 | 0.47 |
| 1:A:846:ILE:HG13 | 1:A:846:ILE:O | 2.14 | 0.47 |
| 1:B:901:PHE:CZ | 1:D:650:PHE:HZ | 2.32 | 0.47 |
| 1:B:901:PHE:HZ | 1:D:650:PHE:HZ | 1.59 | 0.47 |
| 1:C:109:ARG:NH1 | 1:C:208:LYS:HD2 | 2.29 | 0.47 |
| 1:C:115:ILE:HG13 | 1:C:116:GLU:N | 2.27 | 0.47 |
| 1:C:87:ASP:OD2 | 1:C:90:LEU:HD13 | 2.13 | 0.47 |
| 1:A:280:PHE:CD2 | 1:A:343:LEU:HD21 | 2.49 | 0.47 |
| 1:A:780:ALA:HA | 1:A:833:LEU:CD2 | 2.44 | 0.47 |
| 1:B:693:LEU:HA | 4:B:938:HOH:O | 2.14 | 0.47 |
| 1:B:405:LYS:HA | 1:B:698:ILE:O | 2.14 | 0.47 |
| 1:B:841:PHE:HE1 | 1:B:858:ILE:HG21 | 1.79 | 0.47 |
| 1:C:454:TYR:HB3 | 1:C:463:TYR:O | 2.14 | 0.47 |
| 1:D:218:VAL:HG12 | 1:D:223:ILE:HG13 | 1.97 | 0.47 |
| 1:D:410:PHE:HB3 | 1:D:683:MET:HG2 | 1.96 | 0.47 |
| 1:D:420:ILE:HD12 | 1:D:420:ILE:N | 2.29 | 0.47 |
| 1:D:461:MET:HA | 1:D:461:MET:HE3 | 1.95 | 0.47 |
| 1:D:597:ILE:HG21 | 1:D:683:MET:CE | 2.44 | 0.47 |
| 1:D:815:ILE:CG2 | 1:D:858:ILE:HD13 | 2.41 | 0.47 |
| 1:A:606:ASN:HD21 | 1:A:613:GLY:HA2 | 1.76 | 0.47 |
| 1:A:846:ILE:HD12 | 1:A:847:ALA:N | 2.29 | 0.47 |
| 1:A:868:TYR:O | 1:A:871:LEU:N | 2.46 | 0.47 |
| 1:B:228:ASN:HA | 1:B:231:LYS:HE3 | 1.95 | 0.47 |
| 1:B:466:ASP:OD2 | 1:B:467:ARG:N | 2.47 | 0.47 |
| 1:C:55:LYS:HE2 | 1:C:55:LYS:N | 2.29 | 0.47 |
| 1:D:116:GLU:HG2 | 1:D:324:ASN:OD1 | 2.14 | 0.47 |
| 1:D:37:LEU:HD11 | 1:D:72:ILE:HD11 | 1.96 | 0.47 |
| 1:D:498:ILE:O | 1:D:498:ILE:HG22 | 2.14 | 0.47 |
| 1:D:412:LEU:HB2 | 1:D:623:ASP:HB2 | 1.96 | 0.47 |
| 1:B:900:MET:O | 1:D:635:LYS:HE3 | 2.14 | 0.47 |
| 3:J:112:DT:H2' | 3:J:113:DC:C6 | 2.50 | 0.47 |
| 1:A:24:GLY:HA3 | 1:A:107:LYS:HE3 | 1.96 | 0.47 |
| 1:A:43:GLU:N | 1:A:43:GLU:OE2 | 2.47 | 0.47 |
| 1:A:864:HIS:HD2 | 1:A:865:TRP:NE1 | 2.12 | 0.47 |
| 1:B:109:ARG:HD2 | 1:B:140:ASP:OD2 | 2.14 | 0.47 |
| 1:B:491:ALA:O | 1:B:495:ASN:N | 2.45 | 0.47 |
| 1:D:489:MET:O | 1:D:493:GLN:HG2 | 2.13 | 0.47 |
| 1:D:833:LEU:HD22 | 1:D:834:PRO:HD2 | 1.96 | 0.47 |
| 1:C:188:TYR:C | 1:C:189:MET:HG3 | 2.34 | 0.47 |
| 1:D:647:TRP:CZ3 | 1:D:651:LEU:HD12 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:522:PHE:HB2 | 1:A:527:LYS:HE3 | 1.96 | 0.47 |
| 1:B:145:ARG:HG2 | 1:B:187:ILE:HD12 | 1.96 | 0.47 |
| 1:B:309:ILE:HA | 1:B:312:LEU:HB2 | 1.96 | 0.47 |
| 1:B:486:LYS:O | 1:B:490:LEU:HB2 | 2.15 | 0.47 |
| 1:B:594:LEU:HD11 | 1:B:625:ILE:CG2 | 2.45 | 0.47 |
| 1:C:51:ASP:OD2 | 1:C:51:ASP:C | 2.52 | 0.47 |
| 1:D:113:PHE:CZ | 1:D:222:ALA:HB1 | 2.49 | 0.47 |
| 1:D:330:ARG:HD3 | 1:D:333:GLN:OE1 | 2.15 | 0.47 |
| 1:D:578:TYR:CD1 | 1:D:579:ASP:N | 2.82 | 0.47 |
| 3:L:105:DC:H2' | 3:L:106:DT:H72 | 1.97 | 0.47 |
| 1:B:103:TYR:CD1 | 1:B:103:TYR:N | 2.81 | 0.47 |
| 1:B:186:ILE:HG22 | 1:B:187:ILE:H | 1.79 | 0.47 |
| 1:B:330:ARG:HA | 1:B:333:GLN:OE1 | 2.14 | 0.47 |
| 1:B:471:VAL:N | 1:B:472:PRO:HD2 | 2.30 | 0.47 |
| 1:B:891:TYR:N | 1:B:891:TYR:CD2 | 2.82 | 0.47 |
| 1:C:134:ASP:O | 1:C:135:ALA:HB2 | 2.15 | 0.47 |
| 1:C:118:THR:OG1 | 1:C:313:ARG:HG3 | 2.15 | 0.47 |
| 1:D:117:VAL:HG21 | 1:D:225:TYR:CE1 | 2.50 | 0.47 |
| 1:D:413:THR:O | 1:D:414:SER:C | 2.52 | 0.47 |
| 1:D:514:LEU:H | 1:D:541:MET:CE | 2.27 | 0.47 |
| 1:D:741:VAL:HG13 | 1:D:876:PHE:HD1 | 1.80 | 0.47 |
| 1:A:255:ASN:ND2 | 1:A:257:TYR:HD2 | 2.12 | 0.47 |
| 1:A:602:ASN:HD21 | 1:A:616:PHE:H | 1.62 | 0.47 |
| 1:A:404:TYR:CE1 | 1:A:618:LEU:HD13 | 2.50 | 0.47 |
| 1:B:247:LYS:HE3 | 1:B:266:PHE:CZ | 2.50 | 0.47 |
| 1:C:789:ALA:O | 1:C:791:TYR:N | 2.48 | 0.47 |
| 1:D:469:GLY:HA3 | 1:D:472:PRO:HD2 | 1.96 | 0.47 |
| 1:D:874:LYS:HG3 | 1:D:875:THR:N | 2.29 | 0.47 |
| 1:A:191:PHE:HA | 4:A:928:HOH:O | 2.15 | 0.47 |
| 1:A:217:ASN:HA | 1:A:272:ASP:OD2 | 2.14 | 0.47 |
| 1:A:458:PRO:HG3 | 1:A:592:MET:SD | 2.54 | 0.47 |
| 1:B:260:ARG:HH11 | 1:B:260:ARG:HG2 | 1.80 | 0.47 |
| 1:B:654:PHE:CE1 | 1:B:659:MET:HG3 | 2.50 | 0.47 |
| 1:C:572:ASN:HD21 | 1:C:574:TRP:HB2 | 1.80 | 0.47 |
| 1:C:726:LYS:HE2 | 1:C:728:MET:HE1 | 1.96 | 0.47 |
| 1:D:113:PHE:HE1 | 1:D:218:VAL:HG13 | 1.79 | 0.47 |
| 1:D:508:LEU:CD2 | 1:D:534:SER:HB2 | 2.45 | 0.47 |
| 1:D:698:ILE:HG12 | 1:D:752:MET:O | 2.15 | 0.47 |
| 1:D:825:VAL:HB | 1:D:828:GLU:HG2 | 1.97 | 0.47 |
| 3:L:110:DA:C2' | 3:L:111:DT:C5' | 2.91 | 0.47 |
| 1:A:105:HIS:ND1 | 1:A:106:THR:N | 2.63 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:21:ASP:OD1 | 1:A:25:ARG:NH1 | 2.48 | 0.47 |
| 1:A:408:MET:HE2 | 1:A:685:ARG:HD2 | 1.97 | 0.47 |
| 1:A:433:THR:HA | 1:A:460:GLY:O | 2.15 | 0.47 |
| 1:A:37:LEU:CD1 | 1:A:72:ILE:HD11 | 2.44 | 0.47 |
| 1:A:786:ASN:N | 1:A:786:ASN:HD22 | 2.12 | 0.47 |
| 1:A:83:LEU:HD12 | 1:A:83:LEU:H | 1.77 | 0.47 |
| 1:B:124:PRO:O | 1:B:125:GLU:C | 2.53 | 0.47 |
| 1:B:472:PRO:O | 1:B:475:ILE:HG22 | 2.15 | 0.47 |
| 1:B:898:PHE:N | 1:B:898:PHE:CD1 | 2.83 | 0.47 |
| 1:C:606:ASN:HB3 | 1:C:611:THR:O | 2.15 | 0.47 |
| 1:C:659:MET:O | 1:C:660:GLU:C | 2.53 | 0.47 |
| 1:C:782:VAL:HG12 | 1:C:783:SER:N | 2.30 | 0.47 |
| 1:D:277:TYR:HE1 | 1:D:338:ARG:CZ | 2.28 | 0.47 |
| 1:D:345:LEU:HD23 | 1:D:355:ILE:HG21 | 1.95 | 0.47 |
| 1:D:777:ILE:HD11 | 1:D:853:GLU:HA | 1.95 | 0.47 |
| 1:D:892:GLU:O | 1:D:894:LYS:HG3 | 2.15 | 0.47 |
| 3:J:105:DC:C2' | 3:J:106:DT:C6 | 2.98 | 0.47 |
| 3:J:110:DA:C2' | 3:J:111:DT:H5" | 2.45 | 0.47 |
| 1:A:231:LYS:HG3 | 1:A:236:GLU:HA | 1.97 | 0.47 |
| 1:A:658:ARG:HH11 | 1:A:658:ARG:HG3 | 1.79 | 0.47 |
| 1:B:644:THR:HG23 | 1:B:645:ASN:H | 1.79 | 0.47 |
| 1:B:800:LYS:O | 1:B:800:LYS:HG2 | 2.14 | 0.47 |
| 1:C:482:ARG:NH1 | 1:C:556:GLN:HE21 | 2.06 | 0.47 |
| 1:D:207:GLN:HG2 | 1:D:208:LYS:HD2 | 1.96 | 0.47 |
| 1:D:290:LEU:C | 1:D:290:LEU:HD23 | 2.35 | 0.47 |
| 1:D:342:ASN:OD1 | 1:D:554:THR:HG21 | 2.15 | 0.47 |
| 1:D:793:VAL:CG2 | 1:D:796:PHE:HB2 | 2.44 | 0.47 |
| 1:A:606:ASN:ND2 | 1:A:613:GLY:N | 2.60 | 0.46 |
| 1:B:197:LEU:O | 1:B:197:LEU:HD23 | 2.15 | 0.46 |
| 1:B:516:VAL:HG13 | 1:B:544:ARG:NH1 | 2.26 | 0.46 |
| 1:C:474:GLU:O | 1:C:477:LYS:N | 2.44 | 0.46 |
| 1:D:414:SER:O | 1:D:417:PRO:HD2 | 2.14 | 0.46 |
| 1:D:482:ARG:C | 1:D:484:GLU:N | 2.68 | 0.46 |
| 3:H:110:DA:H2" | 3:H:111:DT:H5" | 1.97 | 0.46 |
| 1:A:406:TYR:CD2 | 1:A:633:ILE:HG13 | 2.50 | 0.46 |
| 1:A:653:LYS:HD3 | 1:A:657:GLU:OE2 | 2.15 | 0.46 |
| 1:A:785:ALA:C | 1:A:786:ASN:HD22 | 2.19 | 0.46 |
| 1:A:836:ARG:CD | 1:A:866:MET:O | 2.64 | 0.46 |
| 1:B:731:GLU:HA | 1:B:734:LYS:HG2 | 1.97 | 0.46 |
| 1:C:708:TYR:CZ | 1:C:728:MET:HG3 | 2.50 | 0.46 |
| 1:D:154:SER:HB3 | 1:D:155:PRO:HD2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:6:LEU:HG | 1:D:19:TYR:HA | 1.97 | 0.46 |
| 1:D:345:LEU:O | 1:D:349:TYR:HD1 | 1.98 | 0.46 |
| 1:D:373:LEU:CD1 | 1:D:380:ILE:HG22 | 2.43 | 0.46 |
| 1:D:514:LEU:HD12 | 1:D:541:MET:HE1 | 1.98 | 0.46 |
| 2:G:17:DC:H2" | 2:G:18:DG:O5' | 2.15 | 0.46 |
| 1:A:493:GLN:O | 1:A:497:GLU:HG2 | 2.15 | 0.46 |
| 1:B:197:LEU:HD23 | 1:B:197:LEU:C | 2.36 | 0.46 |
| 1:B:271:LEU:HB3 | 1:B:276:LEU:CD1 | 2.39 | 0.46 |
| 1:B:48:LYS:O | 1:B:377:ASN:HB3 | 2.15 | 0.46 |
| 1:B:655:ALA:HA | 1:B:659:MET:HB2 | 1.98 | 0.46 |
| 1:B:790:LYS:HE3 | 1:B:791:TYR:CZ | 2.50 | 0.46 |
| 1:D:280:PHE:HE1 | 1:D:561:LEU:HD11 | 1.80 | 0.46 |
| 1:D:764:PHE:CE1 | 1:D:876:PHE:HE2 | 2.33 | 0.46 |
| 1:A:411:ASP:CG | 1:A:686:GLU:HG3 | 2.36 | 0.46 |
| 1:A:409:SER:O | 1:A:686:GLU:HB2 | 2.14 | 0.46 |
| 1:B:205:TRP:NE1 | 1:B:242:LEU:O | 2.48 | 0.46 |
| 1:C:199:MET:O | 1:C:202:LEU:HB3 | 2.16 | 0.46 |
| 1:C:671:CYS:SG | 1:C:676:ASN:HB2 | 2.55 | 0.46 |
| 1:D:725:LEU:H | 1:D:725:LEU:HD22 | 1.81 | 0.46 |
| 1:D:95:ASP:O | 1:D:97:TYR:N | 2.49 | 0.46 |
| 1:A:159:VAL:HG21 | 1:A:317:HIS:CD2 | 2.51 | 0.46 |
| 1:A:294:SER:O | 1:A:298:LEU:CD1 | 2.63 | 0.46 |
| 1:A:607:GLU:C | 1:A:609:CYS:H | 2.19 | 0.46 |
| 1:A:741:VAL:C | 1:A:743:LYS:N | 2.69 | 0.46 |
| 1:B:415:LEU:HD11 | 1:B:419:ILE:HD11 | 1.98 | 0.46 |
| 1:B:516:VAL:HG22 | 1:B:517:ASP:H | 1.80 | 0.46 |
| 1:D:109:ARG:HH21 | 1:D:208:LYS:HB3 | 1.70 | 0.46 |
| 1:A:150:ASP:CG | 1:A:317:HIS:HE2 | 2.18 | 0.46 |
| 1:A:692:PRO:HD2 | 1:A:695:SER:OG | 2.16 | 0.46 |
| 1:A:878:LYS:N | 1:A:879:PRO:HD2 | 2.30 | 0.46 |
| 1:B:231:LYS:HB2 | 1:B:239:ALA:HB2 | 1.97 | 0.46 |
| 1:B:533:LEU:HG | 1:B:534:SER:H | 1.80 | 0.46 |
| 1:B:831:TYR:HD2 | 1:B:848:TRP:NE1 | 2.13 | 0.46 |
| 1:C:214:THR:HG21 | 1:C:341:ILE:CD1 | 2.45 | 0.46 |
| 1:C:594:LEU:O | 1:C:597:ILE:HG22 | 2.16 | 0.46 |
| 1:D:218:VAL:HA | 1:D:222:ALA:CB | 2.41 | 0.46 |
| 1:D:469:GLY:CA | 1:D:472:PRO:HD2 | 2.46 | 0.46 |
| 1:A:362:ILE:HD12 | 1:A:569:ALA:CB | 2.45 | 0.46 |
| 1:B:146:PHE:CD1 | 1:B:146:PHE:N | 2.83 | 0.46 |
| 1:C:707:ARG:HB3 | 1:C:730:LEU:HD23 | 1.98 | 0.46 |
| 1:D:202:LEU:HD11 | 1:D:241:ARG:HB3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:361:PRO:HB3 | 1:D:565:SER:HB2 | 1.97 | 0.46 |
| 1:A:653:LYS:HD2 | 1:A:653:LYS:C | 2.36 | 0.46 |
| 1:C:17:GLU:HG2 | 1:C:18:ARG:N | 2.30 | 0.46 |
| 1:C:139:TYR:CD2 | 1:C:332:LEU:HD21 | 2.51 | 0.46 |
| 1:C:559:ARG:HA | 1:C:559:ARG:HD3 | 1.78 | 0.46 |
| 1:D:218:VAL:CG1 | 1:D:223:ILE:HG13 | 2.46 | 0.46 |
| 1:D:230:ILE:HG21 | 1:D:239:ALA:HA | 1.97 | 0.46 |
| 1:A:113:PHE:CE2 | 1:A:222:ALA:HB1 | 2.51 | 0.46 |
| 1:A:129:ALA:HB1 | 1:A:229:ARG:HG2 | 1.98 | 0.46 |
| 1:A:218:VAL:HG22 | 1:A:223:ILE:HG13 | 1.97 | 0.46 |
| 1:A:36:SER:O | 1:A:37:LEU:HD23 | 2.15 | 0.46 |
| 1:A:426:SER:OG | 1:A:427:PRO:HD2 | 2.16 | 0.46 |
| 1:A:685:ARG:HD2 | 1:A:688:ILE:HD11 | 1.97 | 0.46 |
| 1:B:505:ASN:HB3 | 1:B:535:ALA:HB3 | 1.97 | 0.46 |
| 1:B:846:ILE:HD11 | 1:B:858:ILE:HD12 | 1.98 | 0.46 |
| 1:B:887:ALA:CB | 1:B:889:LEU:HD12 | 2.46 | 0.46 |
| 1:D:849:PRO:HG2 | 1:D:852:THR:HG1 | 1.80 | 0.46 |
| 2:E:16:DG:H2" | 2:E:17:DC:H5" | 1.98 | 0.46 |
| 1:A:293:ILE:O | 1:A:293:ILE:HG22 | 2.15 | 0.46 |
| 1:A:296:PHE:HD2 | 1:A:297:GLU:HG2 | 1.81 | 0.46 |
| 1:B:41:CYS:HB2 | 1:B:42:PRO:HD2 | 1.98 | 0.46 |
| 1:B:654:PHE:O | 1:B:658:ARG:HB2 | 2.16 | 0.46 |
| 1:C:109:ARG:HH11 | 1:C:208:LYS:CA | 2.29 | 0.46 |
| 1:C:17:GLU:OE1 | 1:C:97:TYR:OH | 2.23 | 0.46 |
| 1:D:560:LYS:O | 1:D:563:ILE:N | 2.49 | 0.46 |
| 1:B:901:PHE:CD2 | 1:D:608:VAL:HG12 | 2.51 | 0.46 |
| 1:D:74:ARG:O | 1:D:77:ASP:HB2 | 2.16 | 0.46 |
| 1:A:6:LEU:HD12 | 1:A:26:GLU:HG3 | 1.98 | 0.45 |
| 1:A:602:ASN:HD22 | 1:A:616:PHE:HB2 | 1.80 | 0.45 |
| 1:A:643:ASP:HA | 1:A:693:LEU:HD23 | 1.97 | 0.45 |
| 1:B:168:ALA:HA | 1:B:178:VAL:HG12 | 1.97 | 0.45 |
| 1:B:61:LEU:CD2 | 1:B:62:PHE:H | 2.29 | 0.45 |
| 1:C:488:TYR:HB3 | 1:C:519:ARG:HG2 | 1.98 | 0.45 |
| 1:C:642:ARG:CD | 1:C:642:ARG:N | 2.71 | 0.45 |
| 1:D:14:SER:HA | 1:D:32:GLU:HA | 1.98 | 0.45 |
| 1:A:213:LEU:HD12 | 1:A:223:ILE:HD11 | 1.99 | 0.45 |
| 1:A:402:ASN:HB3 | 1:A:404:TYR:CE2 | 2.50 | 0.45 |
| 1:A:685:ARG:HH11 | 1:A:688:ILE:HG13 | 1.79 | 0.45 |
| 1:B:170:LEU:HD12 | 1:B:170:LEU:N | 2.31 | 0.45 |
| 1:C:136:ILE:HG22 | 1:C:137:THR:N | 2.31 | 0.45 |
| 1:C:151:LEU:CD2 | 1:C:154:SER:HB3 | 2.45 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:116:GLU:HG3 | 1:C:324:ASN:HB2 | 1.98 | 0.45 |
| 1:C:454:TYR:HB2 | 1:C:462:MET:HG2 | 1.98 | 0.45 |
| 1:C:768:GLU:HG2 | 1:C:872:LEU:HD21 | 1.97 | 0.45 |
| 1:D:182:ILE:C | 1:D:182:ILE:HD13 | 2.36 | 0.45 |
| 1:D:214:THR:HG22 | 1:D:273:TYR:HB2 | 1.97 | 0.45 |
| 1:D:576:ARG:HB2 | 1:D:576:ARG:CZ | 2.46 | 0.45 |
| 1:D:793:VAL:O | 1:D:793:VAL:HG23 | 2.16 | 0.45 |
| 1:D:815:ILE:HG22 | 1:D:858:ILE:CG2 | 2.30 | 0.45 |
| 1:D:187:ILE:O | 1:D:187:ILE:HG12 | 2.15 | 0.45 |
| 1:D:596:TRP:CE2 | 1:D:670:MET:HB2 | 2.51 | 0.45 |
| 1:A:126:PRO:HG3 | 1:A:221:PHE:CD1 | 2.51 | 0.45 |
| 1:A:42:PRO:O | 1:A:45:GLN:N | 2.43 | 0.45 |
| 1:A:835:LEU:HD12 | 1:A:844:LYS:C | 2.36 | 0.45 |
| 1:A:87:ASP:OD1 | 1:A:363:LYS:NZ | 2.32 | 0.45 |
| 1:B:132:PRO:HA | 1:B:194:GLU:OE1 | 2.16 | 0.45 |
| 1:B:168:ALA:HA | 1:B:178:VAL:CG1 | 2.46 | 0.45 |
| 1:B:736:SER:HA | 1:B:782:VAL:HB | 1.98 | 0.45 |
| 1:C:130:LYS:O | 1:C:229:ARG:NH1 | 2.49 | 0.45 |
| 1:C:441:ASP:HB3 | 1:C:447:ALA:HB2 | 1.98 | 0.45 |
| 1:C:745:LEU:HA | 1:C:745:LEU:HD23 | 1.73 | 0.45 |
| 1:D:482:ARG:HG2 | 1:D:559:ARG:CB | 2.46 | 0.45 |
| 1:D:644:THR:HG21 | 1:D:713:TRP:CZ2 | 2.52 | 0.45 |
| 1:A:186:ILE:HG22 | 1:A:187:ILE:N | 2.30 | 0.45 |
| 1:A:221:PHE:O | 1:A:222:ALA:C | 2.54 | 0.45 |
| 1:A:337:LYS:O | 1:A:339:GLN:OE1 | 2.35 | 0.45 |
| 1:A:780:ALA:HA | 1:A:833:LEU:HD21 | 1.98 | 0.45 |
| 1:B:123:PHE:CE2 | 1:B:126:PRO:HD3 | 2.51 | 0.45 |
| 1:B:231:LYS:CG | 1:B:236:GLU:HA | 2.39 | 0.45 |
| 1:C:142:ILE:HG22 | 1:C:143:ASP:OD1 | 2.17 | 0.45 |
| 1:C:572:ASN:ND2 | 1:C:574:TRP:H | 2.15 | 0.45 |
| 1:D:420:ILE:HD11 | 1:D:586:ILE:HD13 | 1.98 | 0.45 |
| 1:D:406:TYR:CE2 | 1:D:691:PRO:HD2 | 2.51 | 0.45 |
| 2:I:6:DA:H2" | 2:I:7:DA:C5' | 2.43 | 0.45 |
| 1:A:112:ASN:ND2 | 1:A:214:THR:HG23 | 2.31 | 0.45 |
| 1:A:680:LEU:HA | 1:A:682:PHE:CZ | 2.52 | 0.45 |
| 1:B:355:ILE:O | 1:B:358:VAL:HG13 | 2.16 | 0.45 |
| 1:B:389:GLN:OE1 | 1:B:390:PRO:HD2 | 2.16 | 0.45 |
| 1:B:445:ALA:HA | 1:B:673:TYR:CE2 | 2.51 | 0.45 |
| 1:B:751:ARG:O | 1:B:756:GLY:N | 2.33 | 0.45 |
| 1:C:109:ARG:NH1 | 1:C:208:LYS:CA | 2.78 | 0.45 |
| 1:C:132:PRO:HB3 | 1:C:229:ARG:HH21 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:145:ARG:HD3 | 1:C:185:LYS:HB3 | 1.99 | 0.45 |
| 1:C:274:ILE:CG2 | 1:C:275:ASP:N | 2.78 | 0.45 |
| 1:C:465:LYS:HZ3 | 1:C:675:ASN:ND2 | 2.14 | 0.45 |
| 1:C:458:PRO:HG3 | 1:C:592:MET:SD | 2.57 | 0.45 |
| 1:D:180:SER:O | 1:D:183:ILE:HG13 | 2.17 | 0.45 |
| 1:D:250:VAL:HG22 | 1:D:263:ILE:HG13 | 1.98 | 0.45 |
| 1:D:422:GLN:OE1 | 1:D:681:MET:HG2 | 2.17 | 0.45 |
| 1:D:443:ILE:HG22 | 1:D:443:ILE:O | 2.17 | 0.45 |
| 1:D:706:LYS:NZ | 1:D:706:LYS:HB2 | 2.31 | 0.45 |
| 1:A:406:TYR:CB | 1:A:629:ALA:HB3 | 2.47 | 0.45 |
| 1:A:441:ASP:HB3 | 1:A:447:ALA:HB2 | 1.99 | 0.45 |
| 1:A:819:ILE:O | 1:A:819:ILE:HG13 | 2.17 | 0.45 |
| 1:B:362:ILE:HD11 | 1:B:572:ASN:CB | 2.47 | 0.45 |
| 1:B:867:ASP:OD1 | 1:B:870:VAL:HB | 2.17 | 0.45 |
| 1:C:251:LYS:N | 1:C:262:ILE:O | 2.50 | 0.45 |
| 1:C:351:ALA:O | 1:C:352:LYS:HB2 | 2.17 | 0.45 |
| 1:D:162:TRP:HZ3 | 1:D:188:TYR:HB2 | 1.81 | 0.45 |
| 1:D:132:PRO:N | 1:D:229:ARG:HH21 | 2.14 | 0.45 |
| 1:D:401:PRO:O | 1:D:402:ASN:HB2 | 2.16 | 0.45 |
| 1:D:62:PHE:CD2 | 1:D:68:ALA:HA | 2.51 | 0.45 |
| 1:A:412:LEU:HG | 1:A:683:MET:HG2 | 1.98 | 0.45 |
| 1:A:467:ARG:HH11 | 1:A:467:ARG:CG | 2.28 | 0.45 |
| 1:A:559:ARG:NH1 | 1:A:559:ARG:CG | 2.74 | 0.45 |
| 1:A:597:ILE:HB | 1:A:667:PHE:CZ | 2.51 | 0.45 |
| 1:A:731:GLU:OE1 | 1:A:731:GLU:N | 2.48 | 0.45 |
| 1:B:597:ILE:O | 1:B:601:VAL:HG23 | 2.17 | 0.45 |
| 1:C:112:ASN:HA | 1:C:214:THR:O | 2.17 | 0.45 |
| 1:C:197:LEU:C | 1:C:197:LEU:HD23 | 2.37 | 0.45 |
| 1:C:223:ILE:CB | 1:C:224:PRO:HD3 | 2.46 | 0.45 |
| 1:C:391:TYR:HB2 | 1:C:392:PRO:HD2 | 1.99 | 0.45 |
| 1:C:811:TYR:O | 1:C:815:ILE:HG12 | 2.17 | 0.45 |
| 1:D:216:TRP:CB | 1:D:290:LEU:HD12 | 2.46 | 0.45 |
| 1:D:296:PHE:HD1 | 1:D:297:GLU:N | 2.15 | 0.45 |
| 1:D:353:ILE:HG13 | 1:D:354:GLN:O | 2.17 | 0.45 |
| 1:D:777:ILE:CG2 | 1:D:831:TYR:HE1 | 2.30 | 0.45 |
| 1:B:218:VAL:HG13 | 1:B:223:ILE:HG13 | 1.99 | 0.45 |
| 1:B:413:THR:O | 1:B:414:SER:C | 2.55 | 0.45 |
| 1:B:421:ARG:HB3 | 1:B:680:LEU:HD12 | 1.98 | 0.45 |
| 1:D:486:LYS:O | 1:D:490:LEU:HB2 | 2.17 | 0.45 |
| 1:D:605:LEU:CD2 | 1:D:632:ILE:HD11 | 2.47 | 0.45 |
| 1:D:663:ILE:O | 1:D:664:ASP:C | 2.54 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:686:GLU:HB3 | 1:D:715:MET:CE | 2.47 | 0.45 |
| 3:F:109:DC:H2" | 3:F:110:DA:H5' | 1.98 | 0.45 |
| 2:G:11:DC:H2" | 2:G:12:DA:C5' | 2.45 | 0.45 |
| 1:A:511:ASP:OD1 | 1:A:533:LEU:HD22 | 2.16 | 0.45 |
| 1:A:503:LEU:CD1 | 1:A:538:LEU:HB3 | 2.46 | 0.45 |
| 1:A:548:THR:O | 1:A:551:ALA:N | 2.50 | 0.45 |
| 1:B:202:LEU:HD21 | 1:B:241:ARG:CB | 2.47 | 0.45 |
| 1:B:50:PHE:O | 1:B:378:LYS:HA | 2.17 | 0.45 |
| 1:B:530:ILE:HG13 | 1:B:531:LYS:H | 1.82 | 0.45 |
| 1:B:685:ARG:NH2 | 1:B:714:ASP:OD1 | 2.50 | 0.45 |
| 1:C:189:MET:O | 1:C:191:PHE:HE1 | 1.99 | 0.45 |
| 1:C:376:GLN:HB2 | 1:C:378:LYS:HG3 | 1.99 | 0.45 |
| 1:D:482:ARG:O | 1:D:484:GLU:N | 2.50 | 0.45 |
| 1:D:513:PRO:HA | 1:D:541:MET:HE1 | 1.99 | 0.45 |
| 1:D:658:ARG:NH1 | 1:D:658:ARG:HG3 | 2.30 | 0.45 |
| 1:D:835:LEU:HD23 | 1:D:846:ILE:HG23 | 1.99 | 0.45 |
| 2:I:6:DA:H1' | 2:I:7:DA:H5" | 1.99 | 0.45 |
| 1:A:2:LYS:HE3 | 3:L:101:DG:O5' | 2.17 | 0.44 |
| 1:B:167:ALA:O | 1:B:178:VAL:HG12 | 2.17 | 0.44 |
| 1:B:188:TYR:HE2 | 1:B:190:PRO:HB3 | 1.80 | 0.44 |
| 1:B:475:ILE:C | 1:B:475:ILE:HD13 | 2.38 | 0.44 |
| 1:B:700:GLY:HA3 | 1:B:710:LEU:HD23 | 1.98 | 0.44 |
| 1:B:810:THR:HG23 | 1:B:813:ARG:NH2 | 2.32 | 0.44 |
| 1:C:614:GLU:OE1 | 1:C:631:LYS:NZ | 2.49 | 0.44 |
| 1:D:647:TRP:HZ3 | 1:D:651:LEU:HD12 | 1.81 | 0.44 |
| 1:D:815:ILE:O | 1:D:815:ILE:HD12 | 2.17 | 0.44 |
| 1:A:280:PHE:CD2 | 1:A:343:LEU:CD2 | 3.00 | 0.44 |
| 1:A:423:VAL:HG12 | 1:A:423:VAL:O | 2.17 | 0.44 |
| 1:A:691:PRO:HD3 | 1:A:699:GLY:HA3 | 1.99 | 0.44 |
| 1:A:835:LEU:HD12 | 1:A:844:LYS:O | 2.16 | 0.44 |
| 1:B:265:LEU:N | 1:B:265:LEU:HD12 | 2.32 | 0.44 |
| 1:B:567:TYR:O | 1:B:571:GLY:N | 2.49 | 0.44 |
| 1:B:403:ARG:HA | 1:B:701:PHE:HA | 1.98 | 0.44 |
| 1:B:797:PRO:HG3 | 1:B:806:ARG:CZ | 2.46 | 0.44 |
| 1:B:92:TYR:O | 1:B:96:THR:HB | 2.17 | 0.44 |
| 1:C:597:ILE:HD12 | 1:C:597:ILE:HA | 1.90 | 0.44 |
| 1:C:5:TYR:O | 1:C:6:LEU:HD23 | 2.17 | 0.44 |
| 1:C:81:GLU:HB3 | 4:C:925:HOH:O | 2.16 | 0.44 |
| 1:D:109:ARG:NH2 | 1:D:208:LYS:CB | 2.76 | 0.44 |
| 1:D:128:GLN:HB3 | 1:D:128:GLN:HE21 | 1.59 | 0.44 |
| 1:D:535:ALA:HA | 1:D:538:LEU:HB2 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:110:DA:H2" | 3:J:111:DT:H5" | 1.99 | 0.44 |
| 1:A:249:ARG:HB3 | 1:A:264:THR:HB | 2.00 | 0.44 |
| 1:A:506:PRO:HB2 | 1:A:535:ALA:HB2 | 1.99 | 0.44 |
| 1:B:250:VAL:O | 1:B:250:VAL:HG23 | 2.16 | 0.44 |
| 1:B:776:TYR:OH | 1:B:853:GLU:HB3 | 2.18 | 0.44 |
| 1:C:19:TYR:CE1 | 1:C:27:ARG:HB2 | 2.51 | 0.44 |
| 1:C:465:LYS:HZ2 | 1:C:675:ASN:ND2 | 2.15 | 0.44 |
| 1:D:578:TYR:C | 1:D:578:TYR:CD1 | 2.90 | 0.44 |
| 1:D:728:MET:SD | 3:L:113:DC:H5' | 2.57 | 0.44 |
| 1:D:96:THR:HB | 1:D:97:TYR:CD1 | 2.53 | 0.44 |
| 2:G:10:DA:H2" | 2:G:11:DC:H5' | 1.97 | 0.44 |
| 1:A:152:LEU:O | 1:A:158:ASN:HA | 2.17 | 0.44 |
| 1:B:126:PRO:HG3 | 1:B:221:PHE:CD1 | 2.50 | 0.44 |
| 1:B:329:TYR:O | 1:B:330:ARG:C | 2.55 | 0.44 |
| 1:C:255:ASN:HD22 | 1:C:255:ASN:HA | 1.58 | 0.44 |
| 1:C:833:LEU:HD13 | 1:C:866:MET:HE3 | 1.98 | 0.44 |
| 1:D:475:ILE:O | 1:D:479:PHE:HB2 | 2.16 | 0.44 |
| 1:D:597:ILE:CD1 | 1:D:663:ILE:HG23 | 2.44 | 0.44 |
| 1:D:864:HIS:C | 1:D:866:MET:N | 2.67 | 0.44 |
| 1:A:162:TRP:HB3 | 1:A:188:TYR:CE1 | 2.53 | 0.44 |
| 1:A:61:LEU:HD22 | 1:A:61:LEU:C | 2.38 | 0.44 |
| 1:C:819:ILE:O | 1:C:819:ILE:HG23 | 2.17 | 0.44 |
| 1:D:359:PHE:O | 1:D:361:PRO:HD3 | 2.18 | 0.44 |
| 1:D:660:GLU:CB | 1:D:661:PRO:HD3 | 2.47 | 0.44 |
| 1:D:660:GLU:HB2 | 1:D:661:PRO:HD3 | 1.99 | 0.44 |
| 1:D:710:LEU:HD12 | 1:D:726:LYS:HB3 | 1.99 | 0.44 |
| 1:D:3:GLU:HB3 | 1:D:99:TYR:OH | 2.16 | 0.44 |
| 1:A:280:PHE:N | 1:A:280:PHE:HD1 | 2.14 | 0.44 |
| 1:A:397:LYS:O | 1:A:399:PRO:HD3 | 2.17 | 0.44 |
| 1:A:478:VAL:HG13 | 1:A:559:ARG:HD2 | 1.98 | 0.44 |
| 1:A:868:TYR:O | 1:A:869:THR:C | 2.55 | 0.44 |
| 1:D:252:VAL:O | 1:D:252:VAL:HG23 | 2.18 | 0.44 |
| 1:D:91:ALA:HA | 1:D:370:PHE:HE1 | 1.83 | 0.44 |
| 1:D:510:VAL:O | 1:D:532:LYS:O | 2.36 | 0.44 |
| 1:D:599:ARG:NH2 | 1:D:600:LYS:HE2 | 2.33 | 0.44 |
| 1:D:406:TYR:HE2 | 1:D:647:TRP:CZ2 | 2.36 | 0.44 |
| 1:A:138:HIS:C | 1:A:138:HIS:CD2 | 2.90 | 0.44 |
| 1:A:145:ARG:HB2 | 1:A:147:TYR:CE1 | 2.52 | 0.44 |
| 1:A:526:ILE:O | 1:A:526:ILE:HG22 | 2.18 | 0.44 |
| 1:A:542:LEU:O | 1:A:546:GLN:HG3 | 2.18 | 0.44 |
| 1:A:8:VAL:O | 1:A:354:GLN:NE2 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:110:VAL:H | 1:B:141:SER:CB | 2.31 | 0.44 |
| 1:B:534:SER:CB | 1:B:537:SER:HB2 | 2.48 | 0.44 |
| 1:B:606:ASN:HD21 | 1:B:613:GLY:N | 2.15 | 0.44 |
| 1:C:147:TYR:N | 1:C:147:TYR:CD1 | 2.85 | 0.44 |
| 1:C:97:TYR:O | 1:C:99:TYR:N | 2.50 | 0.44 |
| 1:D:216:TRP:CZ3 | 1:D:290:LEU:N | 2.86 | 0.44 |
| 1:D:483:LYS:HG2 | 1:D:483:LYS:O | 2.18 | 0.44 |
| 1:D:485:HIS:HB3 | 1:D:556:GLN:HB3 | 1.99 | 0.44 |
| 3:J:104:DG:H2" | 3:J:105:DC:C6 | 2.52 | 0.44 |
| 1:A:410:PHE:N | 1:A:410:PHE:HD1 | 2.16 | 0.44 |
| 1:A:685:ARG:HH21 | 1:A:717:GLY:N | 2.15 | 0.44 |
| 1:B:166:ILE:HG22 | 1:B:175:GLY:HA2 | 2.00 | 0.44 |
| 1:B:775:ASN:ND2 | 1:B:777:ILE:HB | 2.27 | 0.44 |
| 1:C:124:PRO:HB2 | 1:C:225:TYR:CE2 | 2.52 | 0.44 |
| 1:C:347:MET:HE3 | 1:C:562:LEU:HD13 | 1.98 | 0.44 |
| 1:C:495:ASN:HB3 | 1:C:522:PHE:CE2 | 2.52 | 0.44 |
| 1:C:878:LYS:HB3 | 1:C:879:PRO:HD3 | 2.00 | 0.44 |
| 1:D:119:SER:HA | 1:D:120:PRO:HD3 | 1.80 | 0.44 |
| 1:D:496:GLY:HA2 | 1:D:499:ILE:CD1 | 2.47 | 0.44 |
| 1:A:402:ASN:HA | 1:A:886:ALA:O | 2.18 | 0.44 |
| 1:A:797:PRO:HB3 | 1:A:806:ARG:HG3 | 2.00 | 0.44 |
| 1:A:75:MET:HE3 | 1:A:80:LEU:O | 2.18 | 0.44 |
| 1:A:846:ILE:HD11 | 1:A:854:ILE:HD11 | 2.00 | 0.44 |
| 1:B:25:ARG:NH1 | 1:B:25:ARG:HG2 | 2.31 | 0.44 |
| 1:B:285:GLN:HG3 | 1:B:292:TYR:CE2 | 2.53 | 0.44 |
| 1:B:475:ILE:HD13 | 1:B:475:ILE:O | 2.18 | 0.44 |
| 1:B:700:GLY:HA2 | 1:B:753:LEU:CD2 | 2.44 | 0.44 |
| 1:C:343:LEU:CD1 | 1:C:558:ASN:ND2 | 2.81 | 0.44 |
| 1:C:686:GLU:OE1 | 1:C:716:GLU:CG | 2.65 | 0.44 |
| 1:D:96:THR:C | 1:D:97:TYR:CD1 | 2.91 | 0.44 |
| 1:A:804:HIS:NE2 | 3:F:110:DA:OP1 | 2.38 | 0.44 |
| 1:A:514:LEU:HD22 | 1:A:529:LYS:HE2 | 1.99 | 0.43 |
| 1:A:536:LYS:C | 1:A:536:LYS:HD3 | 2.38 | 0.43 |
| 1:A:811:TYR:OH | 1:A:815:ILE:HD13 | 2.18 | 0.43 |
| 1:B:143:ASP:O | 1:B:144:ASP:HB3 | 2.18 | 0.43 |
| 1:B:115:ILE:HD11 | 1:B:221:PHE:CD2 | 2.53 | 0.43 |
| 1:C:194:GLU:O | 1:C:195:LYS:C | 2.55 | 0.43 |
| 1:C:475:ILE:CG2 | 1:C:476:THR:N | 2.79 | 0.43 |
| 1:C:10:GLN:OE1 | 1:C:65:MET:HE3 | 2.18 | 0.43 |
| 1:C:840:PRO:HD2 | 1:C:865:TRP:CD1 | 2.53 | 0.43 |
| 1:C:761:GLN:HE22 | 1:C:893:LYS:HA | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:365:TRP:CE2 | 1:B:566:LEU:HD13 | 2.53 | 0.43 |
| 1:B:52:ILE:O | 1:B:428:GLU:HG3 | 2.18 | 0.43 |
| 1:B:85:MET:HE3 | 1:B:576:ARG:HH22 | 1.83 | 0.43 |
| 1:B:96:THR:HG22 | 1:B:96:THR:O | 2.18 | 0.43 |
| 1:C:7:THR:CG2 | 1:C:211:VAL:HG13 | 2.48 | 0.43 |
| 1:C:606:ASN:OD1 | 1:C:614:GLU:HB2 | 2.18 | 0.43 |
| 1:C:839:ASN:HB2 | 1:C:840:PRO:HD2 | 2.00 | 0.43 |
| 1:D:428:GLU:OE1 | 1:D:469:GLY:HA2 | 2.18 | 0.43 |
| 1:D:50:PHE:N | 1:D:50:PHE:CD1 | 2.87 | 0.43 |
| 1:D:779:ILE:HD13 | 1:D:780:ALA:N | 2.33 | 0.43 |
| 1:A:159:VAL:HG21 | 1:A:317:HIS:CG | 2.53 | 0.43 |
| 1:A:240:LYS:O | 1:A:246:ARG:HA | 2.18 | 0.43 |
| 1:A:782:VAL:O | 1:A:783:SER:HB2 | 2.17 | 0.43 |
| 1:A:831:TYR:N | 1:A:848:TRP:O | 2.51 | 0.43 |
| 1:A:871:LEU:O | 1:A:875:THR:OG1 | 2.34 | 0.43 |
| 1:A:878:LYS:HB3 | 1:A:879:PRO:HD3 | 1.99 | 0.43 |
| 1:B:517:ASP:OD1 | 1:B:519:ARG:CB | 2.64 | 0.43 |
| 1:B:685:ARG:CG | 1:B:685:ARG:HH11 | 2.32 | 0.43 |
| 1:B:744:ALA:O | 1:B:747:GLU:HB3 | 2.19 | 0.43 |
| 1:C:151:LEU:HD11 | 1:C:153:ASN:O | 2.18 | 0.43 |
| 1:D:317:HIS:CE1 | 1:D:321:ILE:HD13 | 2.53 | 0.43 |
| 1:D:326:ILE:HG22 | 1:D:330:ARG:HE | 1.82 | 0.43 |
| 1:D:33:TYR:CE2 | 1:D:35:PRO:HA | 2.52 | 0.43 |
| 1:A:2:LYS:CE | 1:A:2:LYS:HA | 2.48 | 0.43 |
| 1:A:431:ALA:N | 1:A:462:MET:O | 2.44 | 0.43 |
| 1:A:643:ASP:CA | 1:A:693:LEU:HD23 | 2.48 | 0.43 |
| 1:A:702:TRP:NE1 | 1:A:708:TYR:CD1 | 2.86 | 0.43 |
| 1:A:869:THR:O | 1:A:873:GLU:HB2 | 2.18 | 0.43 |
| 1:A:741:VAL:HG11 | 1:A:875:THR:O | 2.19 | 0.43 |
| 1:B:150:ASP:HB3 | 1:B:188:TYR:CE1 | 2.53 | 0.43 |
| 1:B:771:PHE:CD1 | 1:B:774:LEU:HD12 | 2.52 | 0.43 |
| 1:C:661:PRO:O | 1:C:662:ALA:C | 2.55 | 0.43 |
| 1:D:236:GLU:O | 1:D:240:LYS:HG2 | 2.18 | 0.43 |
| 1:D:285:GLN:HE21 | 1:D:285:GLN:N | 2.15 | 0.43 |
| 1:D:709:ALA:HB2 | 1:D:730:LEU:HD11 | 1.99 | 0.43 |
| 1:D:771:PHE:CE2 | 1:D:872:LEU:HB2 | 2.53 | 0.43 |
| 1:A:6:LEU:HG | 1:A:19:TYR:HA | 2.01 | 0.43 |
| 1:B:233:ILE:N | 1:B:233:ILE:CD1 | 2.82 | 0.43 |
| 1:C:312:LEU:O | 1:C:313:ARG:C | 2.55 | 0.43 |
| 1:C:412:LEU:HG | 1:C:683:MET:HE3 | 2.00 | 0.43 |
| 1:C:607:GLU:O | 1:C:609:CYS:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:898:PHE:N | 1:C:898:PHE:CD2 | 2.85 | 0.43 |
| 1:D:212:ILE:CD1 | 1:D:345:LEU:HD21 | 2.43 | 0.43 |
| 1:D:839:ASN:ND2 | 1:D:839:ASN:O | 2.51 | 0.43 |
| 1:A:45:GLN:O | 1:A:46:ALA:C | 2.56 | 0.43 |
| 1:A:5:TYR:HA | 1:A:19:TYR:CB | 2.49 | 0.43 |
| 1:A:745:LEU:CD1 | 1:A:876:PHE:CD1 | 3.01 | 0.43 |
| 1:A:775:ASN:O | 1:A:778:SER:N | 2.44 | 0.43 |
| 1:A:825:VAL:HG22 | 1:A:826:GLU:N | 2.33 | 0.43 |
| 1:C:164:ILE:HG13 | 1:C:183:ILE:HD11 | 2.01 | 0.43 |
| 1:C:271:LEU:HD21 | 1:C:356:GLN:HA | 2.01 | 0.43 |
| 1:D:113:PHE:CE1 | 1:D:218:VAL:HG13 | 2.54 | 0.43 |
| 1:D:253:ILE:HG13 | 1:D:253:ILE:O | 2.18 | 0.43 |
| 1:D:493:GLN:CG | 1:D:494:ARG:H | 2.14 | 0.43 |
| 1:B:396:VAL:HB | 2:G:7:DA:OP1 | 2.19 | 0.43 |
| 1:A:109:ARG:HD2 | 1:A:209:THR:O | 2.19 | 0.43 |
| 1:A:279:LYS:HB3 | 1:A:280:PHE:CE1 | 2.54 | 0.43 |
| 1:A:389:GLN:HB3 | 1:A:389:GLN:HE21 | 1.54 | 0.43 |
| 1:A:529:LYS:NZ | 1:A:529:LYS:HB3 | 2.34 | 0.43 |
| 1:B:330:ARG:O | 1:B:334:ILE:HG13 | 2.19 | 0.43 |
| 1:C:202:LEU:CD2 | 1:C:241:ARG:HH21 | 2.31 | 0.43 |
| 1:C:458:PRO:HG2 | 1:C:592:MET:SD | 2.59 | 0.43 |
| 1:D:133:ILE:HG12 | 1:D:229:ARG:CD | 2.38 | 0.43 |
| 1:D:491:ALA:HB1 | 1:D:521:ASP:OD1 | 2.18 | 0.43 |
| 1:D:687:ALA:HA | 1:D:714:ASP:O | 2.19 | 0.43 |
| 2:G:15:DC:H2' | 2:G:16:DG:C8 | 2.53 | 0.43 |
| 1:A:835:LEU:O | 1:A:837:GLU:N | 2.52 | 0.43 |
| 1:B:130:LYS:NZ | 1:B:130:LYS:CB | 2.81 | 0.43 |
| 1:B:211:VAL:HG12 | 1:B:211:VAL:O | 2.17 | 0.43 |
| 1:B:443:ILE:HD13 | 1:B:595:GLN:HB3 | 2.00 | 0.43 |
| 1:B:446:VAL:O | 1:B:446:VAL:CG2 | 2.60 | 0.43 |
| 1:C:251:LYS:O | 1:C:261:GLU:HA | 2.19 | 0.43 |
| 1:C:496:GLY:O | 1:C:500:LYS:HG3 | 2.18 | 0.43 |
| 1:C:412:LEU:HG | 1:C:683:MET:HE2 | 1.99 | 0.43 |
| 1:C:702:TRP:CZ3 | 1:C:710:LEU:HD21 | 2.53 | 0.43 |
| 1:D:109:ARG:NH2 | 1:D:140:ASP:OD2 | 2.52 | 0.43 |
| 3:F:110:DA:C2' | 3:F:111:DT:C5' | 2.94 | 0.43 |
| 1:A:779:ILE:O | 1:A:871:LEU:HD21 | 2.18 | 0.43 |
| 1:B:727:ILE:HG23 | 1:B:730:LEU:HD12 | 2.01 | 0.43 |
| 1:C:133:ILE:HG13 | 1:C:229:ARG:HG2 | 2.01 | 0.43 |
| 1:D:132:PRO:CA | 1:D:229:ARG:NH2 | 2.79 | 0.43 |
| 1:D:19:TYR:CD1 | 1:D:19:TYR:N | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:230:ILE:CG2 | 1:D:239:ALA:HA | 2.49 | 0.43 |
| 1:D:417:PRO:O | 1:D:420:ILE:N | 2.52 | 0.43 |
| 1:D:62:PHE:HZ | 1:D:71:TRP:CE3 | 2.37 | 0.43 |
| 1:A:120:PRO:HG2 | 1:A:156:TYR:HE1 | 1.81 | 0.43 |
| 1:B:135:ALA:HB1 | 1:B:324:ASN:HD22 | 1.84 | 0.43 |
| 1:B:170:LEU:CD1 | 1:B:170:LEU:N | 2.82 | 0.43 |
| 1:B:186:ILE:O | 1:B:187:ILE:CG1 | 2.67 | 0.43 |
| 1:B:412:LEU:HB2 | 1:B:623:ASP:HB2 | 2.01 | 0.43 |
| 1:B:441:ASP:HB3 | 1:B:447:ALA:HB2 | 2.00 | 0.43 |
| 1:B:517:ASP:C | 1:B:519:ARG:H | 2.22 | 0.43 |
| 1:B:555:ALA:O | 1:B:559:ARG:HD3 | 2.18 | 0.43 |
| 1:B:880:LEU:O | 1:B:884:THR:HG23 | 2.19 | 0.43 |
| 1:C:271:LEU:HB3 | 1:C:276:LEU:HD21 | 2.00 | 0.43 |
| 1:C:154:SER:OG | 1:C:313:ARG:NH2 | 2.52 | 0.43 |
| 1:C:836:ARG:NH1 | 1:C:836:ARG:HG3 | 2.34 | 0.43 |
| 1:D:573:VAL:HA | 1:D:578:TYR:CD2 | 2.54 | 0.43 |
| 1:D:73:LYS:O | 1:D:77:ASP:OD2 | 2.36 | 0.43 |
| 1:D:825:VAL:HB | 1:D:828:GLU:HG3 | 2.00 | 0.43 |
| 1:A:294:SER:O | 1:A:298:LEU:HD12 | 2.19 | 0.42 |
| 1:A:299:ASN:O | 1:A:300:VAL:HB | 2.18 | 0.42 |
| 1:A:45:GLN:O | 1:A:47:THR:HG23 | 2.18 | 0.42 |
| 1:A:562:LEU:O | 1:A:563:ILE:C | 2.56 | 0.42 |
| 1:B:186:ILE:CG2 | 1:B:187:ILE:H | 2.32 | 0.42 |
| 1:B:145:ARG:HG2 | 1:B:187:ILE:CD1 | 2.48 | 0.42 |
| 1:B:214:THR:OG1 | 1:B:273:TYR:HD2 | 2.02 | 0.42 |
| 1:B:331:VAL:O | 1:B:334:ILE:HB | 2.19 | 0.42 |
| 1:C:461:MET:SD | 1:C:581:ARG:HB3 | 2.59 | 0.42 |
| 1:D:125:GLU:HG3 | 1:D:127:SER:HB3 | 2.00 | 0.42 |
| 1:D:803:PHE:O | 1:D:806:ARG:HB2 | 2.19 | 0.42 |
| 1:A:656:ARG:HA | 1:A:660:GLU:CG | 2.48 | 0.42 |
| 1:A:741:VAL:C | 1:A:743:LYS:H | 2.22 | 0.42 |
| 1:A:745:LEU:O | 1:A:749:ILE:HG13 | 2.19 | 0.42 |
| 1:B:76:GLU:OE1 | 1:B:382:GLN:NE2 | 2.52 | 0.42 |
| 1:B:597:ILE:CD1 | 1:B:683:MET:SD | 3.07 | 0.42 |
| 1:B:685:ARG:CZ | 1:B:688:ILE:HD11 | 2.48 | 0.42 |
| 1:B:751:ARG:NE | 1:B:763:TYR:HB2 | 2.34 | 0.42 |
| 1:C:323:TYR:O | 1:C:326:ILE:N | 2.52 | 0.42 |
| 1:C:413:THR:O | 1:C:414:SER:C | 2.57 | 0.42 |
| 1:C:453:VAL:CG2 | 1:C:454:TYR:N | 2.82 | 0.42 |
| 1:D:597:ILE:CG2 | 1:D:598:GLU:N | 2.82 | 0.42 |
| 1:A:120:PRO:CG | 1:A:156:TYR:CE1 | 3.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:502:ALA:O | 1:A:503:LEU:HD12 | 2.19 | 0.42 |
| 1:B:120:PRO:HG2 | 1:B:156:TYR:HE2 | 1.82 | 0.42 |
| 1:B:840:PRO:HD3 | 1:B:865:TRP:CE2 | 2.55 | 0.42 |
| 1:C:135:ALA:C | 1:C:136:ILE:HG13 | 2.38 | 0.42 |
| 1:C:254:GLU:HG2 | 1:C:259:SER:HB2 | 2.01 | 0.42 |
| 1:C:321:ILE:O | 1:C:325:ILE:HG13 | 2.19 | 0.42 |
| 1:C:503:LEU:HG | 1:C:538:LEU:HB3 | 2.01 | 0.42 |
| 1:C:9:GLU:HG3 | 1:C:267:GLY:H | 1.85 | 0.42 |
| 1:D:105:HIS:ND1 | 1:D:106:THR:N | 2.67 | 0.42 |
| 1:D:456:CYS:HB3 | 1:D:461:MET:O | 2.19 | 0.42 |
| 1:D:484:GLU:OE1 | 1:D:485:HIS:ND1 | 2.43 | 0.42 |
| 2:E:15:DC:H2'' | 2:E:16:DG:C8 | 2.54 | 0.42 |
| 1:A:621:ASP:HB3 | 3:F:114:DA:C5' | 2.50 | 0.42 |
| 2:G:10:DA:C2' | 2:G:11:DC:H5'' | 2.48 | 0.42 |
| 2:G:6:DA:C2' | 2:G:7:DA:H5'' | 2.49 | 0.42 |
| 2:K:7:DA:H2'' | 2:K:8:DT:OP2 | 2.20 | 0.42 |
| 1:A:397:LYS:HD3 | 1:A:619:TYR:HA | 2.00 | 0.42 |
| 1:A:83:LEU:N | 1:A:83:LEU:CD1 | 2.82 | 0.42 |
| 1:B:422:GLN:HG2 | 1:B:676:ASN:HB3 | 2.00 | 0.42 |
| 1:C:128:GLN:HE21 | 1:C:128:GLN:HB3 | 1.61 | 0.42 |
| 1:C:109:ARG:NH1 | 1:C:208:LYS:CD | 2.79 | 0.42 |
| 1:C:264:THR:O | 1:C:265:LEU:HD23 | 2.20 | 0.42 |
| 1:C:506:PRO:C | 1:C:507:ASN:HD22 | 2.23 | 0.42 |
| 1:C:722:GLU:HA | 1:C:722:GLU:OE1 | 2.20 | 0.42 |
| 1:D:241:ARG:C | 1:D:243:SER:H | 2.23 | 0.42 |
| 1:D:244:PRO:O | 1:D:245:HIS:HD2 | 2.02 | 0.42 |
| 1:D:391:TYR:HB2 | 1:D:392:PRO:CD | 2.42 | 0.42 |
| 1:D:655:ALA:HA | 1:D:659:MET:HB2 | 2.01 | 0.42 |
| 1:D:870:VAL:O | 1:D:874:LYS:HG2 | 2.19 | 0.42 |
| 2:I:3:DT:H5' | 2:I:3:DT:C6 | 2.55 | 0.42 |
| 2:K:8:DT:C2' | 2:K:9:DG:C8 | 3.03 | 0.42 |
| 1:A:206:GLN:OE1 | 1:A:241:ARG:HB3 | 2.19 | 0.42 |
| 1:A:408:MET:HE3 | 1:A:655:ALA:HB2 | 1.99 | 0.42 |
| 1:B:442:TYR:O | 1:B:596:TRP:HZ3 | 2.02 | 0.42 |
| 1:B:408:MET:HE1 | 1:B:685:ARG:HD3 | 2.00 | 0.42 |
| 1:B:757:GLU:O | 1:B:761:GLN:HG3 | 2.19 | 0.42 |
| 1:C:143:ASP:O | 1:C:144:ASP:CB | 2.67 | 0.42 |
| 1:C:635:LYS:HD2 | 1:C:635:LYS:O | 2.19 | 0.42 |
| 1:C:97:TYR:HA | 1:C:99:TYR:CE1 | 2.54 | 0.42 |
| 1:D:616:PHE:O | 1:D:627:VAL:HA | 2.19 | 0.42 |
| 1:D:33:TYR:OH | 1:D:95:ASP:OD2 | 2.31 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2:LYS:NZ | 1:A:2:LYS:CA | 2.74 | 0.42 |
| 1:A:410:PHE:HA | 1:A:684:ASP:O | 2.20 | 0.42 |
| 1:B:273:TYR:O | 1:B:277:TYR:HB2 | 2.20 | 0.42 |
| 1:B:425:ILE:HG23 | 1:B:463:TYR:CZ | 2.54 | 0.42 |
| 1:B:831:TYR:CD2 | 1:B:850:SER:HA | 2.55 | 0.42 |
| 1:B:841:PHE:CE2 | 1:B:862:VAL:HG22 | 2.54 | 0.42 |
| 1:C:249:ARG:HB3 | 1:C:264:THR:HB | 2.02 | 0.42 |
| 1:C:249:ARG:O | 1:C:263:ILE:HA | 2.20 | 0.42 |
| 1:C:285:GLN:O | 1:C:829:LYS:NZ | 2.45 | 0.42 |
| 1:C:28:THR:O | 1:C:28:THR:CG2 | 2.67 | 0.42 |
| 1:C:570:LEU:HD23 | 1:C:575:PHE:HE2 | 1.84 | 0.42 |
| 1:D:535:ALA:HB1 | 1:D:539:ASN:HD21 | 1.82 | 0.42 |
| 1:A:140:ASP:OD1 | 1:A:142:ILE:N | 2.53 | 0.42 |
| 1:A:50:PHE:CD2 | 1:A:56:PRO:HA | 2.54 | 0.42 |
| 1:A:643:ASP:C | 1:A:693:LEU:HD23 | 2.39 | 0.42 |
| 1:A:824:VAL:HG13 | 1:A:849:PRO:CG | 2.47 | 0.42 |
| 1:A:94:SER:HG | 1:A:370:PHE:HE2 | 1.64 | 0.42 |
| 1:C:147:TYR:CB | 1:C:149:PHE:HE1 | 2.30 | 0.42 |
| 1:C:514:LEU:HB3 | 1:C:541:MET:HE1 | 2.00 | 0.42 |
| 1:D:294:SER:C | 1:D:296:PHE:N | 2.73 | 0.42 |
| 1:D:493:GLN:HB3 | 1:D:549:GLU:HG3 | 2.02 | 0.42 |
| 1:A:150:ASP:OD1 | 1:A:317:HIS:NE2 | 2.52 | 0.42 |
| 1:A:277:TYR:HA | 1:A:340:PHE:CE2 | 2.55 | 0.42 |
| 1:A:384:ARG:HG3 | 1:A:386:HIS:CE1 | 2.54 | 0.42 |
| 1:A:606:ASN:ND2 | 1:A:613:GLY:HA2 | 2.35 | 0.42 |
| 1:A:861:ASP:N | 1:A:861:ASP:OD2 | 2.52 | 0.42 |
| 1:B:125:GLU:HA | 1:B:126:PRO:HD3 | 1.90 | 0.42 |
| 1:B:604:TYR:O | 1:B:607:GLU:HB3 | 2.20 | 0.42 |
| 1:B:702:TRP:CZ2 | 1:B:708:TYR:CD2 | 3.08 | 0.42 |
| 1:B:96:THR:HG22 | 1:B:97:TYR:CD2 | 2.55 | 0.42 |
| 1:C:62:PHE:CD2 | 1:C:68:ALA:HA | 2.55 | 0.42 |
| 1:D:101:ILE:O | 1:D:102:LYS:HE3 | 2.20 | 0.42 |
| 1:D:234:PHE:CD1 | 1:D:234:PHE:N | 2.87 | 0.42 |
| 1:D:526:ILE:HG13 | 1:D:526:ILE:O | 2.19 | 0.42 |
| 1:A:171:GLN:HE22 | 1:A:319:ARG:NH1 | 2.10 | 0.42 |
| 1:A:82:ALA:O | 1:A:382:GLN:HB2 | 2.20 | 0.42 |
| 1:A:734:LYS:HB3 | 1:A:737:THR:OG1 | 2.20 | 0.42 |
| 1:A:736:SER:HB2 | 1:A:782:VAL:O | 2.20 | 0.42 |
| 1:A:799:PRO:HD2 | 4:A:920:HOH:O | 2.19 | 0.42 |
| 1:B:151:LEU:HG | 1:B:153:ASN:O | 2.20 | 0.42 |
| 1:B:374:LYS:O | 1:B:376:GLN:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:472:PRO:HA | 1:B:475:ILE:HG22 | 2.01 | 0.42 |
| 1:B:678:GLN:HG2 | 1:B:680:LEU:HG | 2.01 | 0.42 |
| 1:B:761:GLN:OE1 | 1:B:893:LYS:HE3 | 2.19 | 0.42 |
| 1:C:149:PHE:N | 1:C:149:PHE:CD1 | 2.86 | 0.42 |
| 1:C:221:PHE:O | 1:C:222:ALA:C | 2.58 | 0.42 |
| 1:C:457:SER:HA | 1:C:458:PRO:HD3 | 1.86 | 0.42 |
| 1:C:482:ARG:NH1 | 1:C:556:GLN:HG2 | 2.35 | 0.42 |
| 1:C:692:PRO:HD2 | 1:C:695:SER:OG | 2.19 | 0.42 |
| 1:D:147:TYR:CD1 | 1:D:147:TYR:N | 2.87 | 0.42 |
| 1:D:839:ASN:ND2 | 1:D:839:ASN:H | 2.18 | 0.42 |
| 1:D:839:ASN:OD1 | 1:D:843:ASP:O | 2.38 | 0.42 |
| 3:H:110:DA:C2' | 3:H:111:DT:H5'' | 2.50 | 0.42 |
| 1:A:159:VAL:HG23 | 1:A:160:GLU:O | 2.20 | 0.42 |
| 1:A:178:VAL:HA | 1:A:179:PRO:HD3 | 1.84 | 0.42 |
| 1:A:415:LEU:O | 1:A:419:ILE:HG13 | 2.20 | 0.42 |
| 1:B:362:ILE:CD1 | 1:B:575:PHE:HB2 | 2.50 | 0.42 |
| 1:B:499:ILE:HG13 | 1:B:542:LEU:HD13 | 2.02 | 0.42 |
| 1:B:559:ARG:O | 1:B:563:ILE:HG13 | 2.19 | 0.42 |
| 1:B:706:LYS:HE2 | 3:H:113:DC:O2 | 2.20 | 0.42 |
| 1:C:254:GLU:HG2 | 1:C:259:SER:CB | 2.50 | 0.42 |
| 1:D:771:PHE:CD2 | 1:D:872:LEU:HD13 | 2.55 | 0.42 |
| 1:A:621:ASP:HB3 | 3:F:114:DA:H5'' | 2.02 | 0.42 |
| 1:A:150:ASP:OD1 | 1:A:188:TYR:OH | 2.33 | 0.41 |
| 1:A:389:GLN:HA | 1:A:390:PRO:HD3 | 1.83 | 0.41 |
| 1:A:602:ASN:ND2 | 1:A:616:PHE:H | 2.18 | 0.41 |
| 1:B:116:GLU:HA | 1:B:116:GLU:OE1 | 2.19 | 0.41 |
| 1:B:13:ASP:OD2 | 1:B:66:ARG:HB2 | 2.20 | 0.41 |
| 1:B:312:LEU:HD12 | 1:B:320:TYR:CD1 | 2.55 | 0.41 |
| 1:C:292:TYR:O | 1:C:295:GLU:HB3 | 2.19 | 0.41 |
| 1:C:524:ASP:HA | 1:C:527:LYS:HE3 | 2.01 | 0.41 |
| 1:D:423:VAL:HB | 1:D:425:ILE:HG13 | 2.00 | 0.41 |
| 1:B:901:PHE:HB3 | 1:D:608:VAL:CG1 | 2.50 | 0.41 |
| 3:J:112:DT:H2' | 3:J:113:DC:C5 | 2.55 | 0.41 |
| 1:A:297:GLU:C | 1:A:298:LEU:HD12 | 2.41 | 0.41 |
| 1:A:516:VAL:CG1 | 1:A:526:ILE:HG13 | 2.50 | 0.41 |
| 1:A:514:LEU:HD21 | 1:A:529:LYS:HE2 | 2.01 | 0.41 |
| 1:A:618:LEU:HG | 1:A:619:TYR:N | 2.34 | 0.41 |
| 1:A:839:ASN:HB3 | 1:A:865:TRP:CE3 | 2.55 | 0.41 |
| 1:B:248:THR:CG2 | 1:B:265:LEU:HA | 2.44 | 0.41 |
| 1:B:463:TYR:CD1 | 1:B:463:TYR:N | 2.88 | 0.41 |
| 1:B:621:ASP:O | 1:B:623:ASP:N | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:256:MET:HB3 | 1:C:257:TYR:CD1 | 2.55 | 0.41 |
| 1:C:261:GLU:H | 1:C:261:GLU:HG2 | 1.74 | 0.41 |
| 1:D:131:HIS:HB2 | 1:D:225:TYR:OH | 2.20 | 0.41 |
| 1:D:358:VAL:O | 1:D:358:VAL:HG12 | 2.20 | 0.41 |
| 1:D:686:GLU:HA | 1:D:686:GLU:OE1 | 2.20 | 0.41 |
| 2:E:6:DA:C2' | 2:E:7:DA:C5' | 2.84 | 0.41 |
| 1:A:800:LYS:O | 1:A:802:PRO:HD3 | 2.21 | 0.41 |
| 1:A:811:TYR:HH | 1:A:822:PRO:C | 2.23 | 0.41 |
| 1:B:132:PRO:HB3 | 1:B:194:GLU:OE2 | 2.20 | 0.41 |
| 1:B:235:GLY:O | 1:B:236:GLU:C | 2.58 | 0.41 |
| 1:B:61:LEU:HD23 | 1:B:62:PHE:H | 1.85 | 0.41 |
| 1:B:90:LEU:HD12 | 1:B:90:LEU:HA | 1.78 | 0.41 |
| 1:C:303:LEU:HB3 | 1:C:319:ARG:HH11 | 1.85 | 0.41 |
| 1:C:32:GLU:HA | 1:C:32:GLU:OE1 | 2.20 | 0.41 |
| 1:C:752:MET:CE | 1:C:889:LEU:HD12 | 2.50 | 0.41 |
| 1:D:129:ALA:HB1 | 1:D:225:TYR:CE2 | 2.55 | 0.41 |
| 1:D:478:VAL:HG11 | 1:D:562:LEU:HD22 | 2.03 | 0.41 |
| 1:D:496:GLY:HA2 | 1:D:499:ILE:HD12 | 2.03 | 0.41 |
| 1:D:699:GLY:C | 1:D:753:LEU:HD22 | 2.40 | 0.41 |
| 3:L:108:DT:H2'' | 3:L:109:DC:O5' | 2.21 | 0.41 |
| 1:A:279:LYS:HE2 | 1:A:359:PHE:HA | 2.00 | 0.41 |
| 1:A:6:LEU:HD13 | 1:A:211:VAL:HG21 | 2.01 | 0.41 |
| 1:A:776:TYR:CE2 | 1:A:777:ILE:HG13 | 2.56 | 0.41 |
| 1:A:809:LEU:HD23 | 1:A:812:ASN:ND2 | 2.36 | 0.41 |
| 1:A:841:PHE:O | 1:A:842:GLY:C | 2.58 | 0.41 |
| 1:A:776:TYR:CG | 1:A:863:LEU:HD11 | 2.55 | 0.41 |
| 1:B:193:ASN:HB3 | 1:B:196:GLU:CG | 2.50 | 0.41 |
| 1:B:834:PRO:O | 1:B:867:ASP:N | 2.50 | 0.41 |
| 1:C:148:VAL:C | 1:C:149:PHE:HD1 | 2.24 | 0.41 |
| 1:C:520:PHE:O | 1:C:521:ASP:C | 2.58 | 0.41 |
| 1:C:558:ASN:HA | 1:C:558:ASN:HD22 | 1.65 | 0.41 |
| 1:C:811:TYR:CA | 1:C:846:ILE:HD11 | 2.50 | 0.41 |
| 1:C:33:TYR:OH | 1:C:95:ASP:OD1 | 2.32 | 0.41 |
| 1:D:218:VAL:HG12 | 1:D:223:ILE:CD1 | 2.50 | 0.41 |
| 1:D:296:PHE:CD1 | 1:D:296:PHE:C | 2.94 | 0.41 |
| 1:D:421:ARG:CD | 1:D:475:ILE:HG23 | 2.51 | 0.41 |
| 1:D:91:ALA:O | 1:D:94:SER:HB2 | 2.19 | 0.41 |
| 2:E:16:DG:N2 | 3:F:103:DG:C2 | 2.89 | 0.41 |
| 1:A:334:ILE:O | 1:A:337:LYS:HB2 | 2.20 | 0.41 |
| 1:A:471:VAL:HB | 1:A:472:PRO:HD3 | 2.01 | 0.41 |
| 1:A:725:LEU:HD12 | 1:A:746:LYS:HE2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:209:THR:HA | 1:B:210:PRO:HD3 | 1.80 | 0.41 |
| 1:B:280:PHE:N | 1:B:280:PHE:CD1 | 2.88 | 0.41 |
| 1:B:416:TYR:HB2 | 1:B:417:PRO:HD3 | 2.02 | 0.41 |
| 1:B:494:ARG:C | 1:B:496:GLY:H | 2.23 | 0.41 |
| 1:B:546:GLN:O | 1:B:550:VAL:HG23 | 2.21 | 0.41 |
| 1:C:147:TYR:N | 1:C:147:TYR:HD1 | 2.17 | 0.41 |
| 1:C:414:SER:O | 1:C:415:LEU:C | 2.57 | 0.41 |
| 1:C:561:LEU:HA | 1:C:561:LEU:HD12 | 1.82 | 0.41 |
| 1:C:577:TYR:N | 1:C:577:TYR:CD2 | 2.88 | 0.41 |
| 1:C:731:GLU:OE2 | 1:C:879:PRO:HB3 | 2.20 | 0.41 |
| 1:D:18:ARG:HH21 | 1:D:211:VAL:HG22 | 1.84 | 0.41 |
| 1:D:188:TYR:CE2 | 1:D:190:PRO:HB3 | 2.55 | 0.41 |
| 1:D:82:ALA:H | 1:D:382:GLN:CG | 2.33 | 0.41 |
| 1:D:533:LEU:HB3 | 1:D:537:SER:OG | 2.20 | 0.41 |
| 1:D:825:VAL:HG12 | 1:D:826:GLU:H | 1.86 | 0.41 |
| 1:D:890:ASP:N | 1:D:890:ASP:OD2 | 2.51 | 0.41 |
| 1:A:467:ARG:HD3 | 1:A:467:ARG:H | 1.85 | 0.41 |
| 1:A:396:VAL:HG21 | 1:A:706:LYS:NZ | 2.35 | 0.41 |
| 1:A:878:LYS:HB3 | 1:A:879:PRO:CD | 2.51 | 0.41 |
| 1:B:85:MET:HA | 1:B:380:ILE:HD11 | 2.03 | 0.41 |
| 1:B:727:ILE:HB | 1:B:733:GLN:NE2 | 2.36 | 0.41 |
| 1:B:783:SER:O | 1:B:829:LYS:HA | 2.20 | 0.41 |
| 1:C:140:ASP:OD1 | 1:C:142:ILE:HB | 2.21 | 0.41 |
| 1:C:189:MET:O | 1:C:191:PHE:CD1 | 2.74 | 0.41 |
| 1:C:420:ILE:HG21 | 1:C:471:VAL:HG12 | 2.03 | 0.41 |
| 1:C:493:GLN:HA | 1:C:549:GLU:OE2 | 2.21 | 0.41 |
| 1:C:761:GLN:NE2 | 1:C:893:LYS:HA | 2.36 | 0.41 |
| 1:C:97:TYR:N | 1:C:97:TYR:CD1 | 2.89 | 0.41 |
| 1:D:416:TYR:HD2 | 1:D:586:ILE:HG22 | 1.85 | 0.41 |
| 1:D:425:ILE:O | 1:D:426:SER:HB2 | 2.20 | 0.41 |
| 1:D:533:LEU:HD11 | 1:D:536:LYS:HB2 | 2.03 | 0.41 |
| 1:D:602:ASN:HD21 | 1:D:617:VAL:HG22 | 1.86 | 0.41 |
| 2:G:15:DC:H2'' | 2:G:16:DG:C5' | 2.50 | 0.41 |
| 2:G:5:DG:H2'' | 2:G:6:DA:O5' | 2.21 | 0.41 |
| 2:I:12:DA:H2'' | 2:I:13:DG:C5' | 2.50 | 0.41 |
| 1:A:52:ILE:HD12 | 1:A:428:GLU:HB3 | 2.03 | 0.41 |
| 1:A:506:PRO:HB2 | 1:A:535:ALA:CA | 2.50 | 0.41 |
| 1:B:104:ASP:OD2 | 1:B:104:ASP:C | 2.58 | 0.41 |
| 1:B:810:THR:HG22 | 1:B:810:THR:O | 2.21 | 0.41 |
| 1:B:837:GLU:HG2 | 1:B:838:GLY:H | 1.82 | 0.41 |
| 1:C:111:ALA:HB2 | 1:C:210:PRO:HB3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:162:TRP:HB3 | 1:C:188:TYR:CE2 | 2.55 | 0.41 |
| 1:C:516:VAL:HG21 | 1:C:522:PHE:HE1 | 1.82 | 0.41 |
| 1:C:738:PRO:HG2 | 1:C:741:VAL:HB | 2.02 | 0.41 |
| 1:C:839:ASN:C | 1:C:841:PHE:H | 2.24 | 0.41 |
| 1:D:470:VAL:HG13 | 1:D:471:VAL:N | 2.36 | 0.41 |
| 1:D:578:TYR:OH | 1:D:580:LEU:HD13 | 2.21 | 0.41 |
| 1:D:685:ARG:HD2 | 1:D:685:ARG:O | 2.21 | 0.41 |
| 1:A:182:ILE:O | 1:A:186:ILE:HG13 | 2.21 | 0.41 |
| 1:A:194:GLU:CD | 1:A:229:ARG:NH1 | 2.74 | 0.41 |
| 1:A:231:LYS:O | 1:A:235:GLY:N | 2.44 | 0.41 |
| 1:A:175:GLY:O | 1:A:319:ARG:NH2 | 2.53 | 0.41 |
| 1:A:602:ASN:HD21 | 1:A:616:PHE:N | 2.18 | 0.41 |
| 1:A:660:GLU:HB2 | 1:A:661:PRO:CD | 2.49 | 0.41 |
| 1:C:757:GLU:O | 1:C:761:GLN:HG3 | 2.20 | 0.41 |
| 1:D:170:LEU:HD22 | 1:D:177:GLU:OE2 | 2.20 | 0.41 |
| 1:D:216:TRP:O | 1:D:217:ASN:HB2 | 2.21 | 0.41 |
| 1:D:321:ILE:CD1 | 1:D:321:ILE:N | 2.83 | 0.41 |
| 1:D:373:LEU:O | 1:D:378:LYS:HB2 | 2.20 | 0.41 |
| 1:D:2:LYS:CG | 1:D:3:GLU:H | 2.33 | 0.41 |
| 1:D:560:LYS:C | 1:D:562:LEU:N | 2.74 | 0.41 |
| 1:A:119:SER:HA | 1:A:120:PRO:HD3 | 1.93 | 0.41 |
| 1:B:202:LEU:HD11 | 1:B:241:ARG:HB3 | 2.02 | 0.41 |
| 1:B:374:LYS:C | 1:B:376:GLN:N | 2.73 | 0.41 |
| 1:B:457:SER:HA | 1:B:458:PRO:HD3 | 1.86 | 0.41 |
| 1:C:257:TYR:N | 1:C:257:TYR:CD1 | 2.89 | 0.41 |
| 1:D:271:LEU:HB3 | 1:D:276:LEU:HD21 | 2.03 | 0.41 |
| 1:D:367:ALA:O | 1:D:370:PHE:HB3 | 2.21 | 0.41 |
| 2:G:13:DG:H2'' | 2:G:14:DC:O5' | 2.20 | 0.41 |
| 3:J:112:DT:C2' | 3:J:113:DC:C6 | 3.04 | 0.41 |
| 1:B:503:LEU:O | 1:B:504:HIS:C | 2.58 | 0.41 |
| 1:B:703:THR:OG1 | 1:B:704:GLY:N | 2.53 | 0.41 |
| 1:C:253:ILE:O | 1:C:259:SER:HA | 2.21 | 0.41 |
| 1:D:421:ARG:HD2 | 1:D:476:THR:OG1 | 2.20 | 0.41 |
| 1:A:898:PHE:N | 1:A:898:PHE:CD1 | 2.86 | 0.41 |
| 1:B:469:GLY:O | 1:B:472:PRO:HG2 | 2.20 | 0.41 |
| 1:B:771:PHE:O | 1:B:774:LEU:HB2 | 2.20 | 0.41 |
| 1:B:776:TYR:CE2 | 1:B:854:ILE:HG22 | 2.56 | 0.41 |
| 1:B:791:TYR:HE2 | 1:B:800:LYS:O | 2.04 | 0.41 |
| 1:C:256:MET:SD | 1:C:257:TYR:CE1 | 3.14 | 0.41 |
| 1:C:271:LEU:HD11 | 1:C:355:ILE:HG22 | 2.02 | 0.41 |
| 1:C:543:PHE:O | 1:C:547:ARG:HB2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:659:MET:O | 1:C:663:ILE:HG13 | 2.20 | 0.41 |
| 1:D:62:PHE:N | 1:D:62:PHE:CD1 | 2.89 | 0.41 |
| 1:D:597:ILE:CG1 | 1:D:683:MET:HE1 | 2.48 | 0.41 |
| 1:D:883:PHE:N | 1:D:883:PHE:HD2 | 2.18 | 0.41 |
| 2:E:7:DA:H2' | 2:E:8:DT:H72 | 2.02 | 0.41 |
| 1:C:518:TYR:CD1 | 1:C:518:TYR:N | 2.89 | 0.40 |
| 1:C:66:ARG:C | 1:C:66:ARG:HD2 | 2.41 | 0.40 |
| 1:C:83:LEU:H | 1:C:83:LEU:HD22 | 1.86 | 0.40 |
| 1:D:135:ALA:C | 1:D:136:ILE:HG22 | 2.40 | 0.40 |
| 1:D:216:TRP:HZ3 | 1:D:288:TYR:O | 2.03 | 0.40 |
| 1:D:171:GLN:HG2 | 1:D:319:ARG:HH22 | 1.85 | 0.40 |
| 1:D:317:HIS:CE1 | 1:D:321:ILE:CD1 | 3.04 | 0.40 |
| 1:D:835:LEU:HD11 | 1:D:843:ASP:O | 2.21 | 0.40 |
| 1:A:268:ILE:CG2 | 1:A:269:SER:N | 2.84 | 0.40 |
| 1:A:280:PHE:HD2 | 1:A:343:LEU:HD21 | 1.84 | 0.40 |
| 1:A:618:LEU:HD23 | 1:A:626:TYR:O | 2.21 | 0.40 |
| 1:A:685:ARG:NH1 | 1:A:685:ARG:HG2 | 2.37 | 0.40 |
| 1:B:285:GLN:HG2 | 1:B:293:ILE:HD13 | 2.03 | 0.40 |
| 1:B:137:THR:HG22 | 1:B:328:VAL:HG21 | 2.02 | 0.40 |
| 1:B:71:TRP:NE1 | 1:B:75:MET:HE2 | 2.36 | 0.40 |
| 1:B:85:MET:HE3 | 1:B:576:ARG:NH2 | 2.36 | 0.40 |
| 1:C:484:GLU:HG2 | 1:C:488:TYR:CE2 | 2.56 | 0.40 |
| 1:C:540:GLU:HA | 1:C:540:GLU:OE1 | 2.21 | 0.40 |
| 1:C:703:THR:HG22 | 1:C:886:ALA:CB | 2.52 | 0.40 |
| 1:D:348:GLY:HA3 | 1:D:355:ILE:HD13 | 2.03 | 0.40 |
| 1:D:769:LYS:O | 1:D:773:GLN:NE2 | 2.54 | 0.40 |
| 1:A:207:GLN:C | 1:A:208:LYS:HG3 | 2.41 | 0.40 |
| 1:A:218:VAL:CG2 | 1:A:223:ILE:HG13 | 2.52 | 0.40 |
| 1:A:362:ILE:HG12 | 1:A:572:ASN:HD21 | 1.80 | 0.40 |
| 1:A:432:GLY:O | 1:A:462:MET:N | 2.55 | 0.40 |
| 1:A:553:MET:O | 1:A:556:GLN:HG3 | 2.21 | 0.40 |
| 1:B:433:THR:HA | 1:B:460:GLY:O | 2.21 | 0.40 |
| 1:B:508:LEU:CD2 | 1:B:508:LEU:H | 2.23 | 0.40 |
| 1:B:89:LYS:HE3 | 1:B:354:GLN:NE2 | 2.36 | 0.40 |
| 1:D:750:ARG:NH2 | 1:D:755:GLU:OE1 | 2.54 | 0.40 |
| 1:D:887:ALA:O | 1:D:888:LYS:HB2 | 2.21 | 0.40 |
| 1:C:253:ILE:HD13 | 2:I:1:DC:C5 | 2.56 | 0.40 |
| 1:A:113:PHE:CE1 | 1:A:218:VAL:CG2 | 3.05 | 0.40 |
| 1:A:125:GLU:HA | 1:A:126:PRO:HD3 | 1.97 | 0.40 |
| 1:A:221:PHE:C | 1:A:224:PRO:HD2 | 2.42 | 0.40 |
| 1:A:338:ARG:HG3 | 1:A:338:ARG:NH1 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:502:ALA:C | 1:A:503:LEU:HD12 | 2.41 | 0.40 |
| 1:A:546:GLN:HA | 1:A:549:GLU:HB2 | 2.03 | 0.40 |
| 1:B:223:ILE:HB | 1:B:224:PRO:CD | 2.44 | 0.40 |
| 1:B:252:VAL:O | 1:B:253:ILE:C | 2.59 | 0.40 |
| 1:B:626:TYR:CD1 | 1:B:626:TYR:N | 2.89 | 0.40 |
| 1:C:273:TYR:CE2 | 1:C:335:ASP:HB2 | 2.57 | 0.40 |
| 1:C:42:PRO:O | 1:C:43:GLU:C | 2.59 | 0.40 |
| 1:C:537:SER:O | 1:C:541:MET:HG3 | 2.22 | 0.40 |
| 1:C:582:ASN:O | 1:C:585:ALA:HB3 | 2.21 | 0.40 |
| 1:D:202:LEU:C | 1:D:202:LEU:HD23 | 2.41 | 0.40 |
| 1:D:291:ASP:O | 1:D:292:TYR:C | 2.60 | 0.40 |
| 1:D:303:LEU:O | 1:D:304:LYS:C | 2.59 | 0.40 |
| 1:D:458:PRO:HB2 | 1:D:588:THR:HG22 | 2.02 | 0.40 |
| 1:D:456:CYS:HA | 1:D:461:MET:O | 2.21 | 0.40 |
| 1:D:659:MET:O | 1:D:660:GLU:C | 2.59 | 0.40 |
| 3:F:106:DT:H1' | 3:F:107:DG:C5' | 2.44 | 0.40 |
| 3:H:110:DA:H1' | 3:H:111:DT:H5'' | 2.02 | 0.40 |
| 1:A:106:THR:HG22 | 1:A:106:THR:O | 2.20 | 0.40 |
| 1:A:410:PHE:HB2 | 1:A:683:MET:CE | 2.51 | 0.40 |
| 1:B:117:VAL:HG11 | 1:B:225:TYR:OH | 2.21 | 0.40 |
| 1:B:326:ILE:O | 1:B:330:ARG:CG | 2.66 | 0.40 |
| 1:B:355:ILE:HD13 | 1:B:355:ILE:HA | 1.90 | 0.40 |
| 1:B:443:ILE:HD13 | 1:B:595:GLN:CB | 2.51 | 0.40 |
| 1:B:837:GLU:CG | 1:B:838:GLY:H | 2.34 | 0.40 |
| 1:C:332:LEU:O | 1:C:336:ALA:HB2 | 2.22 | 0.40 |
| 1:C:393:GLY:O | 1:C:587:THR:HG23 | 2.22 | 0.40 |
| 1:C:514:LEU:CD2 | 1:C:526:ILE:HG23 | 2.51 | 0.40 |
| 1:C:503:LEU:HD21 | 1:C:538:LEU:HB2 | 2.03 | 0.40 |
| 1:C:365:TRP:CD2 | 1:C:566:LEU:HD13 | 2.56 | 0.40 |
| 1:C:651:LEU:HD23 | 1:C:651:LEU:HA | 1.96 | 0.40 |
| 1:D:302:LYS:HD2 | 1:D:302:LYS:N | 2.37 | 0.40 |
| 1:D:318:GLN:O | 1:D:322:SER:HB2 | 2.21 | 0.40 |
| 1:D:468:ASP:OD2 | 1:D:677:LYS:HE2 | 2.22 | 0.40 |
| 1:D:546:GLN:O | 1:D:549:GLU:HB3 | 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 | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 900/906 (99%) | 745 (83%) | 129 (14%) | 26 (3%) | 4 | 24 |
| 1 | B | 900/906 (99%) | 761 (85%) | 119 (13%) | 20 (2%) | 6 | 31 |
| 1 | C | 899/906 (99%) | 748 (83%) | 125 (14%) | 26 (3%) | 4 | 24 |
| 1 | D | 886/906 (98%) | 710 (80%) | 133 (15%) | 43 (5%) | 2 | 13 |
| All | All | 3585/3624 (99%) | 2964 (83%) | 506 (14%) | 115 (3%) | 4 | 22 |

All (115) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 300 | VAL |
| 1 | A | 790 | LYS |
| 1 | A | 863 | LEU |
| 1 | B | 819 | ILE |
| 1 | C | 177 | GLU |
| 1 | D | 181 | GLU |
| 1 | D | 187 | ILE |
| 1 | D | 192 | ASP |
| 1 | D | 524 | ASP |
| 1 | D | 855 | THR |
| 1 | A | 105 | HIS |
| 1 | A | 169 | LYS |
| 1 | A | 283 | THR |
| 1 | A | 521 | ASP |
| 1 | A | 613 | GLY |
| 1 | A | 772 | ARG |
| 1 | A | 776 | TYR |
| 1 | A | 836 | ARG |
| 1 | A | 841 | PHE |
| 1 | B | 187 | ILE |
| 1 | B | 352 | LYS |
| 1 | B | 392 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 172 | GLU |
| 1 | C | 179 | PRO |
| 1 | C | 315 | SER |
| 1 | C | 790 | LYS |
| 1 | D | 43 | GLU |
| 1 | D | 45 | GLN |
| 1 | D | 96 | THR |
| 1 | D | 272 | ASP |
| 1 | D | 508 | LEU |
| 1 | D | 534 | SER |
| 1 | D | 814 | ALA |
| 1 | D | 822 | PRO |
| 1 | D | 865 | TRP |
| 1 | A | 46 | ALA |
| 1 | A | 738 | PRO |
| 1 | A | 893 | LYS |
| 1 | B | 236 | GLU |
| 1 | B | 237 | SER |
| 1 | B | 375 | GLU |
| 1 | C | 98 | ASN |
| 1 | C | 170 | LEU |
| 1 | C | 314 | GLU |
| 1 | C | 320 | TYR |
| 1 | C | 622 | THR |
| 1 | D | 21 | ASP |
| 1 | D | 44 | SER |
| 1 | D | 98 | ASN |
| 1 | D | 222 | ALA |
| 1 | D | 483 | LYS |
| 1 | D | 532 | LYS |
| 1 | D | 574 | TRP |
| 1 | D | 730 | LEU |
| 1 | A | 394 | ALA |
| 1 | A | 518 | TYR |
| 1 | A | 655 | ALA |
| 1 | A | 898 | PHE |
| 1 | B | 99 | TYR |
| 1 | B | 222 | ALA |
| 1 | B | 252 | VAL |
| 1 | B | 344 | SER |
| 1 | B | 526 | ILE |
| 1 | B | 828 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 222 | ALA |
| 1 | C | 303 | LEU |
| 1 | C | 310 | SER |
| 1 | C | 415 | LEU |
| 1 | C | 514 | LEU |
| 1 | C | 534 | SER |
| 1 | D | 64 | ASN |
| 1 | D | 161 | GLU |
| 1 | D | 186 | ILE |
| 1 | D | 435 | LYS |
| 1 | D | 459 | ASN |
| 1 | D | 528 | GLU |
| 1 | D | 622 | THR |
| 1 | D | 836 | ARG |
| 1 | A | 622 | THR |
| 1 | A | 802 | PRO |
| 1 | B | 300 | VAL |
| 1 | B | 504 | HIS |
| 1 | B | 802 | PRO |
| 1 | C | 430 | ILE |
| 1 | C | 593 | ALA |
| 1 | C | 814 | ALA |
| 1 | D | 240 | LYS |
| 1 | D | 304 | LYS |
| 1 | D | 450 | PRO |
| 1 | D | 512 | GLU |
| 1 | D | 531 | LYS |
| 1 | D | 570 | LEU |
| 1 | D | 630 | ASP |
| 1 | D | 810 | THR |
| 1 | C | 144 | ASP |
| 1 | C | 155 | PRO |
| 1 | C | 414 | SER |
| 1 | D | 300 | VAL |
| 1 | D | 414 | SER |
| 1 | D | 460 | GLY |
| 1 | D | 723 | PRO |
| 1 | B | 142 | ILE |
| 1 | C | 458 | PRO |
| 1 | D | 136 | ILE |
| 1 | C | 510 | VAL |
| 1 | A | 848 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 307 | GLY |
| 1 | C | 840 | PRO |
| 1 | A | 450 | PRO |
| 1 | B | 499 | ILE |
| 1 | C | 608 | VAL |
| 1 | A | 250 | VAL |
| 1 | A | 526 | ILE |
| 1 | A | 608 | VAL |
| 1 | B | 125 | GLU |

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 | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 789/803 (98%) | 715 (91%) | 74 (9%) | 8 | 32 |
| 1 | B | 773/803 (96%) | 717 (93%) | 56 (7%) | 14 | 45 |
| 1 | C | 794/803 (99%) | 745 (94%) | 49 (6%) | 18 | 52 |
| 1 | D | 737/803 (92%) | 672 (91%) | 65 (9%) | 10 | 36 |
| All | All | 3093/3212 (96%) | 2849 (92%) | 244 (8%) | 12 | 41 |

All (244) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 2 | LYS |
| 1 | A | 4 | PHE |
| 1 | A | 25 | ARG |
| 1 | A | 28 | THR |
| 1 | A | 29 | ARG |
| 1 | A | 36 | SER |
| 1 | A | 43 | GLU |
| 1 | A | 58 | THR |
| 1 | A | 59 | ARG |
| 1 | A | 61 | LEU |
| 1 | A | 64 | ASN |
| 1 | A | 73 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 86 | ASP |
| 1 | A | 94 | SER |
| 1 | A | 98 | ASN |
| 1 | A | 105 | HIS |
| 1 | A | 138 | HIS |
| 1 | A | 140 | ASP |
| 1 | A | 196 | GLU |
| 1 | A | 213 | LEU |
| 1 | A | 220 | SER |
| 1 | A | 229 | ARG |
| 1 | A | 242 | LEU |
| 1 | A | 260 | ARG |
| 1 | A | 280 | PHE |
| 1 | A | 285 | GLN |
| 1 | A | 292 | TYR |
| 1 | A | 298 | LEU |
| 1 | A | 304 | LYS |
| 1 | A | 314 | GLU |
| 1 | A | 318 | GLN |
| 1 | A | 339 | GLN |
| 1 | A | 342 | ASN |
| 1 | A | 347 | MET |
| 1 | A | 372 | SER |
| 1 | A | 379 | VAL |
| 1 | A | 408 | MET |
| 1 | A | 410 | PHE |
| 1 | A | 433 | THR |
| 1 | A | 466 | ASP |
| 1 | A | 467 | ARG |
| 1 | A | 475 | ILE |
| 1 | A | 479 | PHE |
| 1 | A | 498 | ILE |
| 1 | A | 543 | PHE |
| 1 | A | 544 | ARG |
| 1 | A | 546 | GLN |
| 1 | A | 548 | THR |
| 1 | A | 556 | GLN |
| 1 | A | 559 | ARG |
| 1 | A | 561 | LEU |
| 1 | A | 587 | THR |
| 1 | A | 602 | ASN |
| 1 | A | 612 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 618 | LEU |
| 1 | A | 653 | LYS |
| 1 | A | 658 | ARG |
| 1 | A | 703 | THR |
| 1 | A | 708 | TYR |
| 1 | A | 731 | GLU |
| 1 | A | 735 | SER |
| 1 | A | 745 | LEU |
| 1 | A | 754 | GLN |
| 1 | A | 758 | GLU |
| 1 | A | 773 | GLN |
| 1 | A | 776 | TYR |
| 1 | A | 806 | ARG |
| 1 | A | 813 | ARG |
| 1 | A | 824 | VAL |
| 1 | A | 846 | ILE |
| 1 | A | 861 | ASP |
| 1 | A | 873 | GLU |
| 1 | A | 880 | LEU |
| 1 | A | 893 | LYS |
| 1 | B | 9 | GLU |
| 1 | B | 22 | SER |
| 1 | B | 47 | THR |
| 1 | B | 61 | LEU |
| 1 | B | 83 | LEU |
| 1 | B | 86 | ASP |
| 1 | B | 90 | LEU |
| 1 | B | 113 | PHE |
| 1 | B | 115 | ILE |
| 1 | B | 116 | GLU |
| 1 | B | 130 | LYS |
| 1 | B | 145 | ARG |
| 1 | B | 146 | PHE |
| 1 | B | 147 | TYR |
| 1 | B | 164 | ILE |
| 1 | B | 177 | GLU |
| 1 | B | 181 | GLU |
| 1 | B | 218 | VAL |
| 1 | B | 248 | THR |
| 1 | B | 249 | ARG |
| 1 | B | 257 | TYR |
| 1 | B | 260 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 274 | ILE |
| 1 | B | 280 | PHE |
| 1 | B | 291 | ASP |
| 1 | B | 316 | ASN |
| 1 | B | 377 | ASN |
| 1 | B | 378 | LYS |
| 1 | B | 386 | HIS |
| 1 | B | 392 | PRO |
| 1 | B | 421 | ARG |
| 1 | B | 451 | SER |
| 1 | B | 468 | ASP |
| 1 | B | 475 | ILE |
| 1 | B | 479 | PHE |
| 1 | B | 489 | MET |
| 1 | B | 495 | ASN |
| 1 | B | 499 | ILE |
| 1 | B | 570 | LEU |
| 1 | B | 632 | ILE |
| 1 | B | 658 | ARG |
| 1 | B | 668 | ARG |
| 1 | B | 685 | ARG |
| 1 | B | 686 | GLU |
| 1 | B | 702 | TRP |
| 1 | B | 708 | TYR |
| 1 | B | 728 | MET |
| 1 | B | 742 | GLN |
| 1 | B | 758 | GLU |
| 1 | B | 766 | GLU |
| 1 | B | 773 | GLN |
| 1 | B | 843 | ASP |
| 1 | B | 856 | ASP |
| 1 | B | 860 | ASP |
| 1 | B | 891 | TYR |
| 1 | B | 899 | ASP |
| 1 | C | 7 | THR |
| 1 | C | 25 | ARG |
| 1 | C | 58 | THR |
| 1 | C | 60 | LYS |
| 1 | C | 61 | LEU |
| 1 | C | 66 | ARG |
| 1 | C | 93 | LEU |
| 1 | C | 138 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 149 | PHE |
| 1 | C | 173 | GLN |
| 1 | C | 192 | ASP |
| 1 | C | 195 | LYS |
| 1 | C | 196 | GLU |
| 1 | C | 200 | GLU |
| 1 | C | 214 | THR |
| 1 | C | 231 | LYS |
| 1 | C | 255 | ASN |
| 1 | C | 256 | MET |
| 1 | C | 257 | TYR |
| 1 | C | 261 | GLU |
| 1 | C | 276 | LEU |
| 1 | C | 284 | ASN |
| 1 | C | 302 | LYS |
| 1 | C | 388 | VAL |
| 1 | C | 399 | PRO |
| 1 | C | 428 | GLU |
| 1 | C | 439 | LEU |
| 1 | C | 473 | THR |
| 1 | C | 474 | GLU |
| 1 | C | 490 | LEU |
| 1 | C | 525 | GLU |
| 1 | C | 556 | GLN |
| 1 | C | 559 | ARG |
| 1 | C | 561 | LEU |
| 1 | C | 562 | LEU |
| 1 | C | 587 | THR |
| 1 | C | 618 | LEU |
| 1 | C | 640 | LYS |
| 1 | C | 642 | ARG |
| 1 | C | 667 | PHE |
| 1 | C | 702 | TRP |
| 1 | C | 731 | GLU |
| 1 | C | 760 | LEU |
| 1 | C | 765 | LYS |
| 1 | C | 770 | GLU |
| 1 | C | 843 | ASP |
| 1 | C | 856 | ASP |
| 1 | C | 880 | LEU |
| 1 | C | 898 | PHE |
| 1 | D | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 10 | GLN |
| 1 | D | 13 | ASP |
| 1 | D | 32 | GLU |
| 1 | D | 41 | CYS |
| 1 | D | 57 | CYS |
| 1 | D | 67 | ASP |
| 1 | D | 86 | ASP |
| 1 | D | 102 | LYS |
| 1 | D | 105 | HIS |
| 1 | D | 113 | PHE |
| 1 | D | 128 | GLN |
| 1 | D | 136 | ILE |
| 1 | D | 152 | LEU |
| 1 | D | 156 | TYR |
| 1 | D | 164 | ILE |
| 1 | D | 182 | ILE |
| 1 | D | 197 | LEU |
| 1 | D | 198 | LEU |
| 1 | D | 200 | GLU |
| 1 | D | 202 | LEU |
| 1 | D | 208 | LYS |
| 1 | D | 213 | LEU |
| 1 | D | 216 | TRP |
| 1 | D | 221 | PHE |
| 1 | D | 225 | TYR |
| 1 | D | 273 | TYR |
| 1 | D | 285 | GLN |
| 1 | D | 302 | LYS |
| 1 | D | 305 | TYR |
| 1 | D | 310 | SER |
| 1 | D | 362 | ILE |
| 1 | D | 363 | LYS |
| 1 | D | 407 | VAL |
| 1 | D | 452 | ASP |
| 1 | D | 456 | CYS |
| 1 | D | 474 | GLU |
| 1 | D | 479 | PHE |
| 1 | D | 484 | GLU |
| 1 | D | 485 | HIS |
| 1 | D | 511 | ASP |
| 1 | D | 518 | TYR |
| 1 | D | 520 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 524 | ASP |
| 1 | D | 540 | GLU |
| 1 | D | 558 | ASN |
| 1 | D | 576 | ARG |
| 1 | D | 591 | GLN |
| 1 | D | 592 | MET |
| 1 | D | 618 | LEU |
| 1 | D | 630 | ASP |
| 1 | D | 658 | ARG |
| 1 | D | 660 | GLU |
| 1 | D | 667 | PHE |
| 1 | D | 674 | MET |
| 1 | D | 702 | TRP |
| 1 | D | 710 | LEU |
| 1 | D | 725 | LEU |
| 1 | D | 731 | GLU |
| 1 | D | 779 | ILE |
| 1 | D | 812 | ASN |
| 1 | D | 839 | ASN |
| 1 | D | 844 | LYS |
| 1 | D | 852 | THR |
| 1 | D | 873 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 10 | GLN |
| 1 | A | 23 | ASN |
| 1 | A | 40 | HIS |
| 1 | A | 64 | ASN |
| 1 | A | 112 | ASN |
| 1 | A | 153 | ASN |
| 1 | A | 171 | GLN |
| 1 | A | 255 | ASN |
| 1 | A | 285 | GLN |
| 1 | A | 342 | ASN |
| 1 | A | 389 | GLN |
| 1 | A | 422 | GLN |
| 1 | A | 495 | ASN |
| 1 | A | 505 | ASN |
| 1 | A | 546 | GLN |
| 1 | A | 556 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 602 | ASN |
| 1 | A | 606 | ASN |
| 1 | A | 646 | HIS |
| 1 | A | 678 | GLN |
| 1 | A | 733 | GLN |
| 1 | A | 773 | GLN |
| 1 | A | 786 | ASN |
| 1 | A | 812 | ASN |
| 1 | A | 818 | ASN |
| 1 | A | 864 | HIS |
| 1 | B | 128 | GLN |
| 1 | B | 138 | HIS |
| 1 | B | 171 | GLN |
| 1 | B | 173 | GLN |
| 1 | B | 193 | ASN |
| 1 | B | 206 | GLN |
| 1 | B | 245 | HIS |
| 1 | B | 284 | ASN |
| 1 | B | 318 | GLN |
| 1 | B | 354 | GLN |
| 1 | B | 376 | GLN |
| 1 | B | 382 | GLN |
| 1 | B | 389 | GLN |
| 1 | B | 495 | ASN |
| 1 | B | 505 | ASN |
| 1 | B | 539 | ASN |
| 1 | B | 556 | GLN |
| 1 | B | 558 | ASN |
| 1 | B | 591 | GLN |
| 1 | B | 646 | HIS |
| 1 | B | 733 | GLN |
| 1 | B | 742 | GLN |
| 1 | B | 754 | GLN |
| 1 | B | 773 | GLN |
| 1 | B | 775 | ASN |
| 1 | B | 812 | ASN |
| 1 | B | 818 | ASN |
| 1 | C | 45 | GLN |
| 1 | C | 128 | GLN |
| 1 | C | 171 | GLN |
| 1 | C | 193 | ASN |
| 1 | C | 255 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 284 | ASN |
| 1 | C | 285 | GLN |
| 1 | C | 318 | GLN |
| 1 | C | 440 | HIS |
| 1 | C | 444 | ASN |
| 1 | C | 539 | ASN |
| 1 | C | 556 | GLN |
| 1 | C | 558 | ASN |
| 1 | C | 572 | ASN |
| 1 | C | 646 | HIS |
| 1 | C | 675 | ASN |
| 1 | C | 678 | GLN |
| 1 | C | 711 | ASN |
| 1 | C | 761 | GLN |
| 1 | C | 787 | ASN |
| 1 | C | 818 | ASN |
| 1 | D | 70 | GLN |
| 1 | D | 128 | GLN |
| 1 | D | 171 | GLN |
| 1 | D | 206 | GLN |
| 1 | D | 207 | GLN |
| 1 | D | 245 | HIS |
| 1 | D | 285 | GLN |
| 1 | D | 317 | HIS |
| 1 | D | 318 | GLN |
| 1 | D | 324 | ASN |
| 1 | D | 354 | GLN |
| 1 | D | 382 | GLN |
| 1 | D | 480 | ASN |
| 1 | D | 495 | ASN |
| 1 | D | 505 | ASN |
| 1 | D | 539 | ASN |
| 1 | D | 546 | GLN |
| 1 | D | 676 | ASN |
| 1 | D | 679 | HIS |
| 1 | D | 733 | GLN |
| 1 | D | 742 | GLN |
| 1 | D | 754 | GLN |
| 1 | D | 773 | GLN |
| 1 | D | 812 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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 | CTG | E | 4 | 3,2 | 19,23,24 | 0.81 | 1 (5%) | 21,35,38 | 1.10 | 1 (4%) |
| 2 | CTG | G | 4 | 3,2 | 19,23,24 | 0.91 | 2 (10%) | 21,35,38 | 1.13 | 2 (9%) |
| 2 | CTG | I | 4 | 3,2 | 19,23,24 | 1.07 | 2 (10%) | 21,35,38 | 1.24 | 3 (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 | CTG | E | 4 | 3,2 | - | 1/7/45/46 | 0/2/2/2 |
| 2 | CTG | G | 4 | 3,2 | - | 0/7/45/46 | 0/2/2/2 |
| 2 | CTG | I | 4 | 3,2 | - | 0/7/45/46 | 0/2/2/2 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | I | 4 | CTG | C1'-N1 | 2.76 | 1.49 | 1.45 |
| 2 | E | 4 | CTG | C1'-N1 | 2.42 | 1.48 | 1.45 |
| 2 | I | 4 | CTG | O5'-C5' | -2.28 | 1.39 | 1.44 |
| 2 | G | 4 | CTG | C1'-N1 | 2.27 | 1.48 | 1.45 |
| 2 | G | 4 | CTG | C5-C4 | 2.08 | 1.54 | 1.52 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|-------------|-------|------------------------|---------------------|
| 2 | I | 4 | CTG | C2'-C1'-N1 | -3.59 | 110.74 | 115.59 |
| 2 | E | 4 | CTG | C2'-C1'-N1 | -3.30 | 111.13 | 115.59 |
| 2 | G | 4 | CTG | C2'-C1'-N1 | -3.22 | 111.23 | 115.59 |
| 2 | G | 4 | CTG | N3-C2-N1 | -2.49 | 114.11 | 116.69 |
| 2 | I | 4 | CTG | N3-C2-N1 | -2.15 | 114.46 | 116.69 |
| 2 | I | 4 | CTG | C2'-C3'-C4' | 2.03 | 107.00 | 102.76 |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | E | 4 | CTG | O4'-C4'-C5'-O5' |

There are no ring outliers.

3 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | E | 4 | CTG | 3 | 0 |
| 2 | G | 4 | CTG | 4 | 0 |
| 2 | I | 4 | CTG | 4 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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 | A | 902/906 (99%) | -0.13 | 23 (2%) 57 29 | 29, 63, 155, 176 | 0 |
| 1 | B | 902/906 (99%) | 0.18 | 67 (7%) 14 4 | 30, 84, 172, 189 | 2 (0%) |
| 1 | C | 901/906 (99%) | -0.23 | 6 (0%) 87 69 | 23, 64, 127, 148 | 0 |
| 1 | D | 890/906 (98%) | 0.29 | 61 (6%) 16 5 | 72, 132, 174, 188 | 3 (0%) |
| 2 | E | 17/18 (94%) | 0.13 | 0 100 100 | 75, 106, 144, 148 | 0 |
| 2 | G | 17/18 (94%) | 0.16 | 0 100 100 | 76, 113, 137, 147 | 0 |
| 2 | I | 17/18 (94%) | -0.26 | 0 100 100 | 39, 53, 124, 140 | 0 |
| 2 | K | 14/18 (77%) | 0.52 | 1 (7%) 16 5 | 69, 156, 169, 170 | 0 |
| 3 | F | 14/14 (100%) | -0.11 | 0 100 100 | 85, 125, 157, 161 | 0 |
| 3 | H | 14/14 (100%) | -0.10 | 0 100 100 | 89, 132, 155, 156 | 0 |
| 3 | J | 14/14 (100%) | -0.55 | 0 100 100 | 35, 55, 123, 127 | 0 |
| 3 | L | 13/14 (92%) | 0.48 | 1 (7%) 13 4 | 146, 165, 169, 175 | 0 |
| All | All | 3715/3752 (99%) | 0.02 | 159 (4%) 35 13 | 23, 83, 165, 189 | 5 (0%) |

All (159) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 504 | HIS | 8.2 |
| 1 | D | 847 | ALA | 7.7 |
| 1 | D | 862 | VAL | 7.4 |
| 1 | D | 535 | ALA | 6.5 |
| 1 | B | 503 | LEU | 6.0 |
| 1 | B | 510 | VAL | 6.0 |
| 1 | B | 819 | ILE | 5.7 |
| 1 | D | 858 | ILE | 5.6 |
| 1 | D | 857 | LEU | 5.4 |
| 1 | D | 802 | PRO | 5.3 |
| 1 | B | 505 | ASN | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 865 | TRP | 5.1 |
| 1 | B | 506 | PRO | 5.1 |
| 1 | B | 508 | LEU | 5.0 |
| 1 | D | 793 | VAL | 5.0 |
| 1 | A | 498 | ILE | 4.7 |
| 1 | B | 516 | VAL | 4.6 |
| 1 | B | 846 | ILE | 4.4 |
| 1 | B | 513 | PRO | 4.4 |
| 1 | B | 511 | ASP | 4.4 |
| 1 | B | 793 | VAL | 4.4 |
| 1 | D | 851 | GLY | 4.3 |
| 1 | D | 534 | SER | 4.3 |
| 1 | B | 522 | PHE | 4.2 |
| 1 | B | 821 | ALA | 4.2 |
| 1 | A | 514 | LEU | 4.2 |
| 1 | B | 303 | LEU | 4.2 |
| 1 | B | 315 | SER | 4.1 |
| 1 | B | 523 | SER | 4.1 |
| 1 | B | 509 | SER | 4.0 |
| 1 | D | 834 | PRO | 3.9 |
| 1 | D | 855 | THR | 3.9 |
| 1 | B | 542 | LEU | 3.7 |
| 1 | B | 306 | ASP | 3.6 |
| 1 | D | 819 | ILE | 3.6 |
| 1 | B | 160 | GLU | 3.6 |
| 1 | D | 863 | LEU | 3.6 |
| 1 | B | 502 | ALA | 3.6 |
| 1 | A | 513 | PRO | 3.6 |
| 1 | D | 510 | VAL | 3.5 |
| 1 | D | 794 | GLY | 3.5 |
| 1 | B | 134 | ASP | 3.4 |
| 1 | D | 833 | LEU | 3.4 |
| 1 | D | 778 | SER | 3.3 |
| 1 | B | 532 | LYS | 3.3 |
| 1 | B | 307 | GLY | 3.3 |
| 1 | B | 128 | GLN | 3.2 |
| 1 | D | 393 | GLY | 3.2 |
| 1 | B | 803 | PHE | 3.2 |
| 1 | D | 801 | CYS | 3.2 |
| 1 | B | 173 | GLN | 3.2 |
| 1 | B | 174 | GLY | 3.2 |
| 1 | B | 498 | ILE | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 798 | GLY | 3.2 |
| 1 | D | 511 | ASP | 3.2 |
| 1 | D | 846 | ILE | 3.1 |
| 1 | B | 817 | GLY | 3.1 |
| 1 | D | 771 | PHE | 3.1 |
| 1 | B | 818 | ASN | 3.1 |
| 1 | D | 504 | HIS | 3.1 |
| 1 | A | 505 | ASN | 3.0 |
| 1 | B | 286 | PRO | 3.0 |
| 1 | B | 530 | ILE | 3.0 |
| 1 | B | 129 | ALA | 2.9 |
| 1 | D | 120 | PRO | 2.9 |
| 1 | D | 522 | PHE | 2.9 |
| 1 | B | 492 | ALA | 2.9 |
| 1 | C | 303 | LEU | 2.9 |
| 1 | D | 849 | PRO | 2.9 |
| 1 | D | 792 | ASP | 2.8 |
| 1 | D | 831 | TYR | 2.8 |
| 1 | D | 395 | PHE | 2.8 |
| 1 | A | 786 | ASN | 2.8 |
| 1 | D | 818 | ASN | 2.8 |
| 1 | A | 808 | ILE | 2.8 |
| 1 | A | 504 | HIS | 2.8 |
| 1 | D | 192 | ASP | 2.8 |
| 1 | D | 523 | SER | 2.8 |
| 1 | B | 507 | ASN | 2.8 |
| 3 | L | 113 | DC | 2.8 |
| 1 | D | 832 | VAL | 2.8 |
| 1 | A | 855 | THR | 2.7 |
| 1 | B | 862 | VAL | 2.7 |
| 1 | A | 508 | LEU | 2.7 |
| 1 | B | 861 | ASP | 2.7 |
| 1 | B | 813 | ARG | 2.7 |
| 1 | C | 498 | ILE | 2.7 |
| 1 | C | 513 | PRO | 2.7 |
| 1 | B | 499 | ILE | 2.6 |
| 1 | A | 506 | PRO | 2.6 |
| 1 | C | 508 | LEU | 2.6 |
| 1 | B | 526 | ILE | 2.6 |
| 1 | D | 788 | ILE | 2.6 |
| 1 | B | 127 | SER | 2.6 |
| 1 | D | 505 | ASN | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 155 | PRO | 2.6 |
| 1 | D | 542 | LEU | 2.6 |
| 2 | K | 6 | DA | 2.6 |
| 1 | B | 157 | GLY | 2.6 |
| 1 | B | 179 | PRO | 2.6 |
| 1 | D | 856 | ASP | 2.6 |
| 1 | A | 526 | ILE | 2.6 |
| 1 | D | 183 | ILE | 2.6 |
| 1 | D | 248 | THR | 2.6 |
| 1 | B | 501 | GLU | 2.5 |
| 1 | A | 841 | PHE | 2.5 |
| 1 | A | 512 | GLU | 2.5 |
| 1 | A | 858 | ILE | 2.5 |
| 1 | B | 514 | LEU | 2.5 |
| 1 | A | 524 | ASP | 2.5 |
| 1 | D | 286 | PRO | 2.5 |
| 1 | B | 153 | ASN | 2.5 |
| 1 | B | 539 | ASN | 2.5 |
| 1 | D | 10 | GLN | 2.5 |
| 1 | A | 820 | ASP | 2.4 |
| 1 | D | 820 | ASP | 2.4 |
| 1 | D | 266 | PHE | 2.4 |
| 1 | A | 776 | TYR | 2.4 |
| 1 | B | 340 | PHE | 2.4 |
| 1 | D | 391 | TYR | 2.4 |
| 1 | D | 817 | GLY | 2.3 |
| 1 | B | 175 | GLY | 2.3 |
| 1 | D | 774 | LEU | 2.3 |
| 1 | D | 848 | TRP | 2.3 |
| 1 | B | 797 | PRO | 2.3 |
| 1 | D | 173 | GLN | 2.2 |
| 1 | A | 863 | LEU | 2.2 |
| 1 | A | 515 | ASP | 2.2 |
| 1 | B | 820 | ASP | 2.2 |
| 1 | B | 535 | ALA | 2.2 |
| 1 | D | 850 | SER | 2.2 |
| 1 | D | 507 | ASN | 2.2 |
| 1 | B | 546 | GLN | 2.2 |
| 1 | D | 786 | ASN | 2.2 |
| 1 | B | 497 | GLU | 2.2 |
| 1 | B | 792 | ASP | 2.2 |
| 1 | C | 173 | GLN | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 521 | ASP | 2.2 |
| 1 | B | 799 | PRO | 2.2 |
| 1 | A | 254 | GLU | 2.1 |
| 1 | B | 868 | TYR | 2.1 |
| 1 | D | 812 | ASN | 2.1 |
| 1 | D | 514 | LEU | 2.1 |
| 1 | D | 499 | ILE | 2.1 |
| 1 | D | 539 | ASN | 2.1 |
| 1 | C | 506 | PRO | 2.1 |
| 1 | D | 135 | ALA | 2.1 |
| 1 | D | 777 | ILE | 2.0 |
| 1 | B | 166 | ILE | 2.0 |
| 1 | D | 175 | GLY | 2.0 |
| 1 | B | 538 | LEU | 2.0 |
| 1 | D | 394 | ALA | 2.0 |
| 1 | A | 787 | ASN | 2.0 |
| 1 | B | 118 | THR | 2.0 |
| 1 | D | 546 | GLN | 2.0 |
| 1 | A | 532 | LYS | 2.0 |
| 1 | A | 847 | ALA | 2.0 |
| 1 | D | 157 | GLY | 2.0 |
| 1 | B | 512 | GLU | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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 | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2 | CTG | G | 4 | 22/23 | 0.74 | 0.27 | 122,128,129,129 | 0 |
| 2 | CTG | E | 4 | 22/23 | 0.86 | 0.22 | 109,113,124,125 | 0 |
| 2 | CTG | I | 4 | 22/23 | 0.93 | 0.21 | 72,78,81,81 | 0 |

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.