# Full wwPDB EM Validation Report

Apr 27, 2024 – 05:24 pm BST

| | | |
|---|---|---|
| PDB ID | : | 2Y7H |
| EMDB ID | : | EMD-1534 |
| Title | : | Atomic model of the DNA-bound methylase complex from the Type I restriction-modification enzyme EcoKI (M2S1). Based on fitting into EM map 1534. |
| Authors | : | Kennaway, C.K.; Obarska-Kosinska, A.; White, J.H.; Tuszynska, I.; Cooper, L.P.; Bujnicki, J.M.; Trinick, J.; Dryden, D.T.F. |
| Deposited on | : | 2011-01-31 |
| Resolution | : | 18.00 Å(reported) |
| Based on initial models | : | 2AR0, 1YF2, 1S7Z |

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

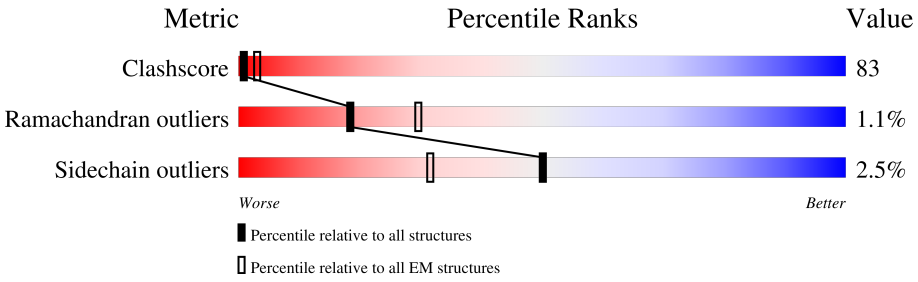
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 18.00 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) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 464 | 52% 24% 71% 5% |
| 2 | B | 529 | 47% 38% 59% · |
| 2 | C | 529 | 47% 37% 61% · |
| 3 | D | 20 | 50% 25% 70% 5% |
| 4 | E | 20 | 50% 30% 70% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 5 | SAM | B | 530 | - | - | X | - |
| 5 | SAM | C | 530 | - | - | X | - |

# 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called TYPE-1 RESTRICTION ENZYME ECOKI SPECIFICITY PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 464 | Total | C | N | O | S | 0 | 0 |
| | | | 3622 | 2298 | 644 | 671 | 9 | | |

- Molecule 2 is a protein called TYPE I RESTRICTION ENZYME ECOKI M PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 529 | Total | C | N | O | S | 0 | 0 |
| | | | 4175 | 2612 | 730 | 816 | 17 | | |
| 2 | C | 529 | Total | C | N | O | S | 0 | 0 |
| | | | 4175 | 2612 | 730 | 816 | 17 | | |

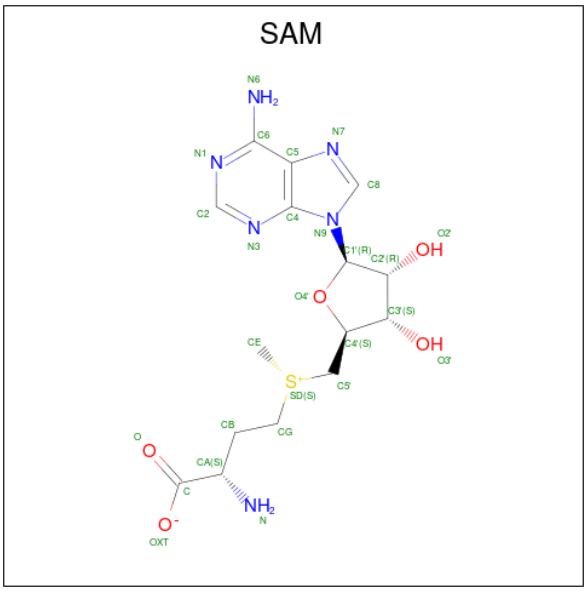
- Molecule 3 is a DNA chain called 5'-D(*GP*TP*TP*CP*AP*AP*CP*GP*TP*CP*GP*AP*CP*GP *TP*GP*CP*AP*AP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | D | 20 | Total | C | N | O | P | 0 | 0 |
| | | | 409 | 194 | 76 | 119 | 20 | | |

- Molecule 4 is a DNA chain called 5'-D(*GP*TP*TP*GP*CP*AP*CP*GP*TP*CP*GP*AP*CP*GP *TP*TP*GP*AP*AP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | E | 20 | Total | C | N | O | P | 0 | 0 |
| | | | 411 | 195 | 75 | 121 | 20 | | |

- Molecule 5 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



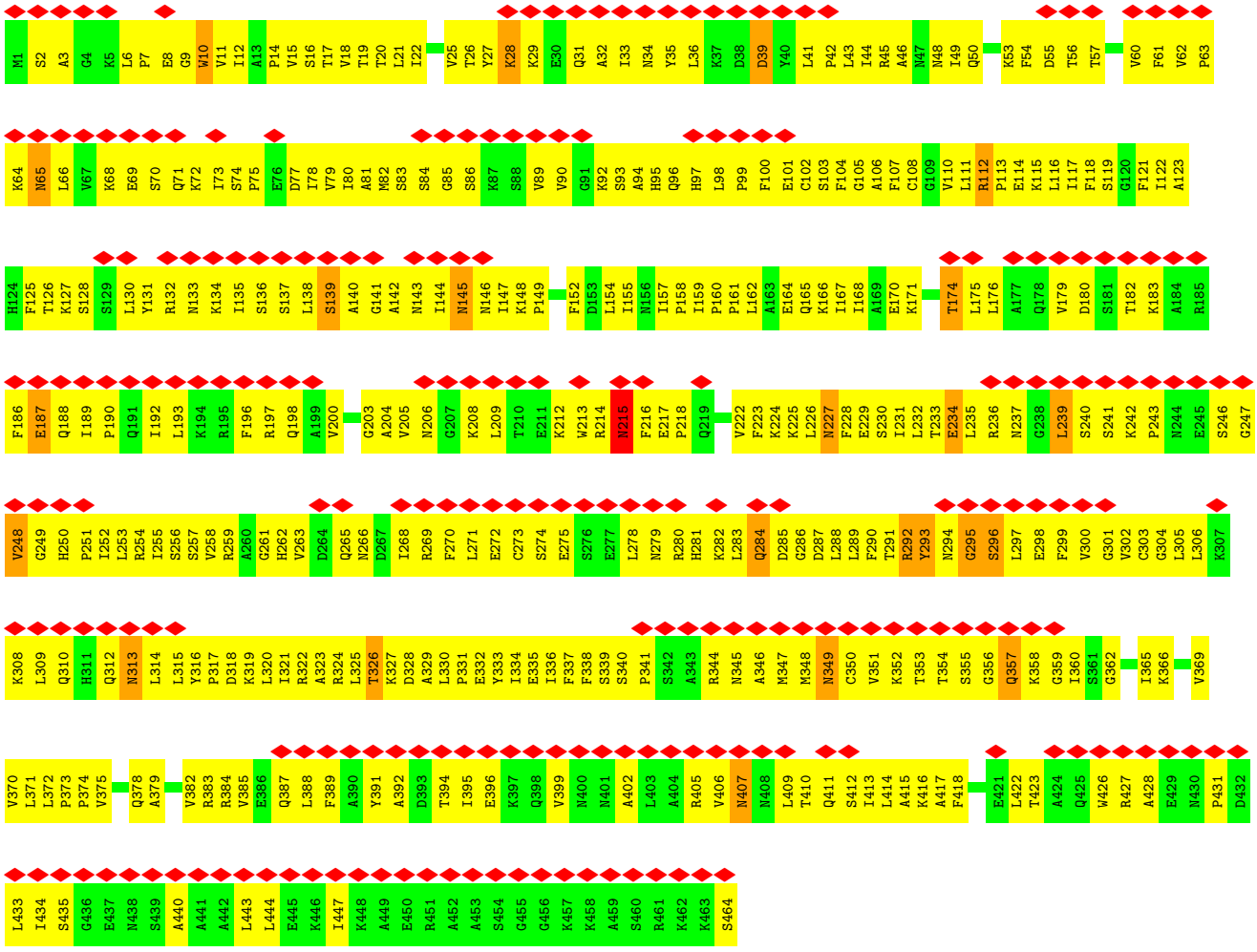

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 5 | B | 1 | Total | C | N | O | S | 0 |
| | | | 27 | 15 | 6 | 5 | 1 | |
| 5 | C | 1 | Total | C | N | O | S | 0 |
| | | | 27 | 15 | 6 | 5 | 1 | |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

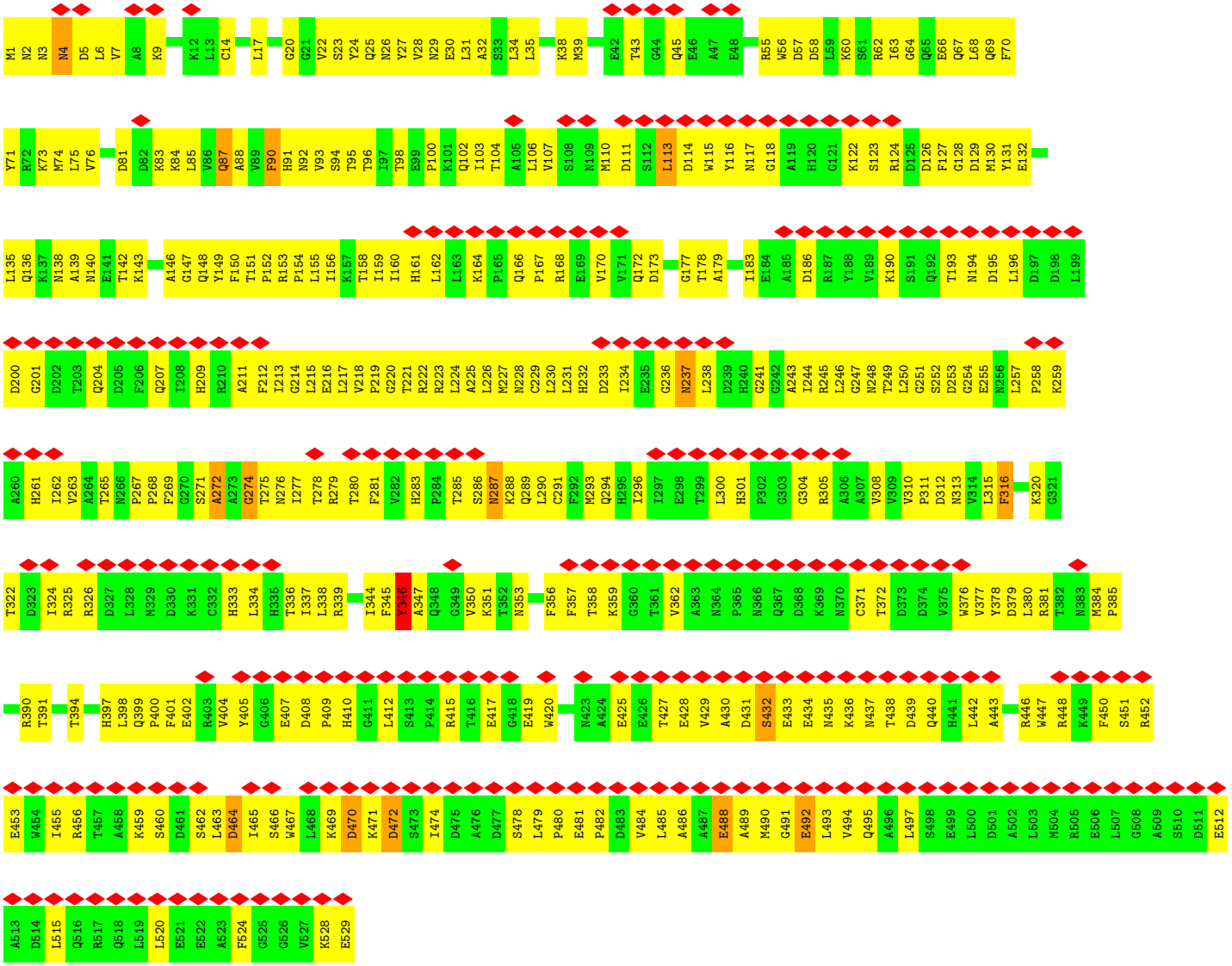
• Molecule 1: TYPE-1 RESTRICTION ENZYME ECOKI SPECIFICITY PROTEIN

Chain A:

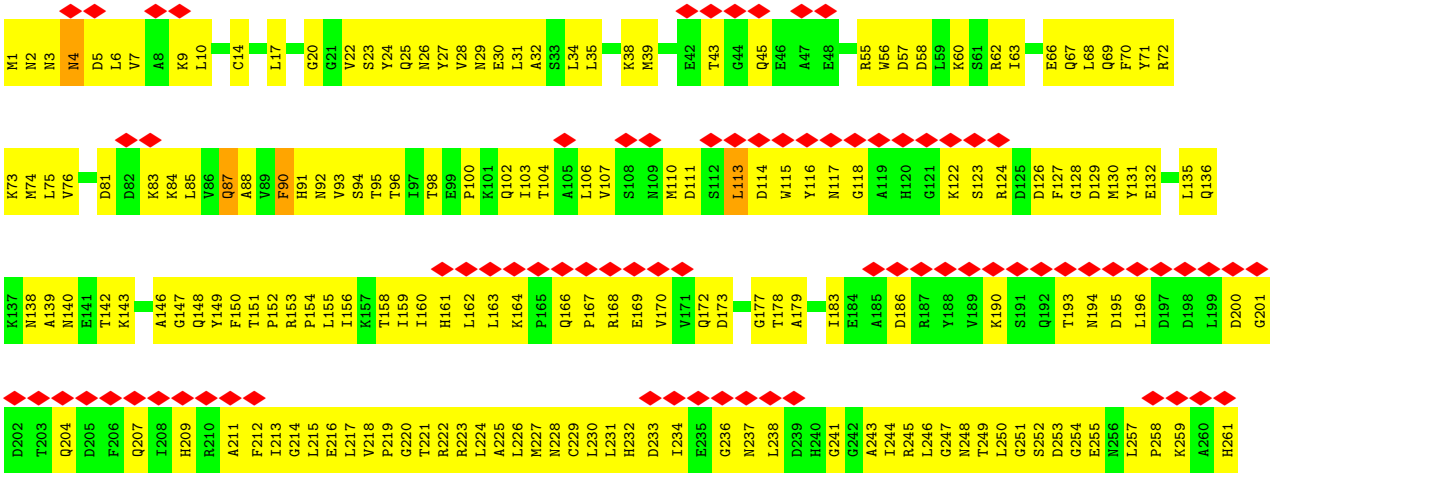

• Molecule 2: TYPE I RESTRICTION ENZYME ECOKI M PROTEIN

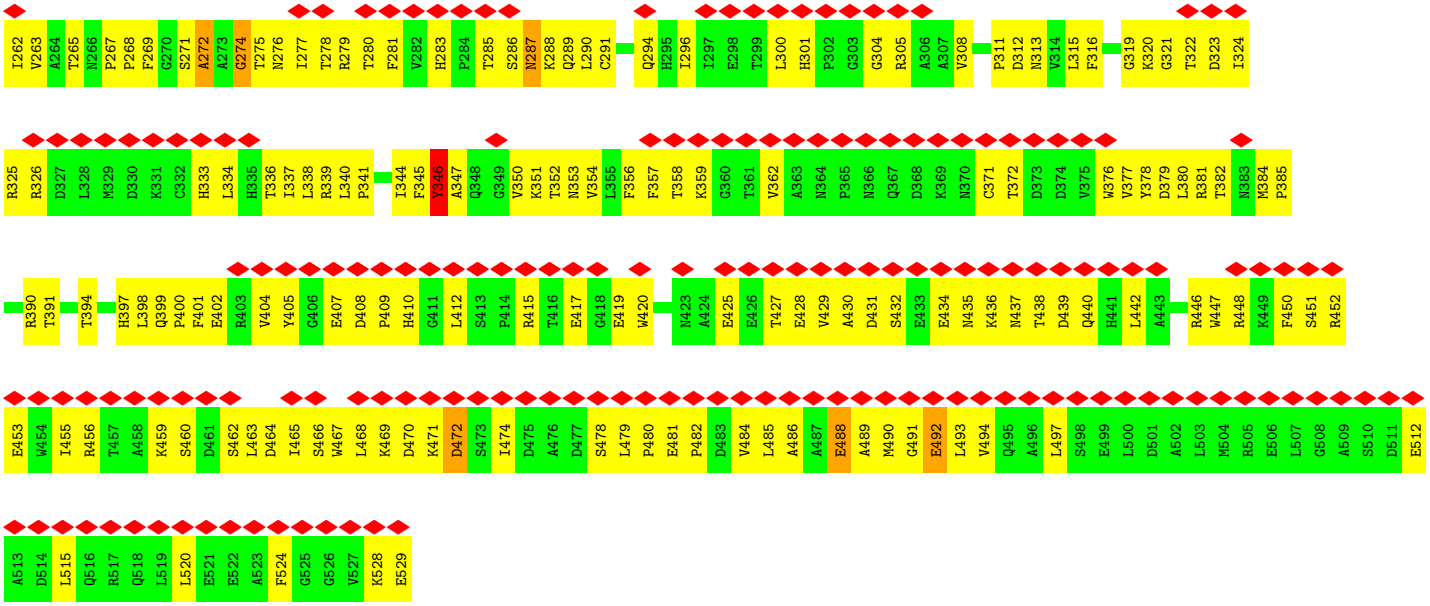
Chain B:



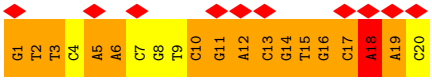
• Molecule 2: TYPE I RESTRICTION ENZYME ECOKI M PROTEIN

Chain C:

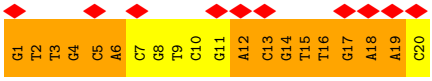






• Molecule 3: 5'-D(*GP*TP*TP*CP*AP*AP*CP*GP*TP*CP*GP*AP*CP*GP *TP*GP*CP* AP*AP*C)-3'


• Molecule 4: 5'-D(*GP*TP*TP*GP*CP*AP*CP*GP*TP*CP*GP*AP*CP*GP *TP*TP*GP* AP*AP*C)-3'

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 17807 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | FILTERED AT FIRST ZERO | Depositor |
| Microscope | JEOL 1200EX | Depositor |
| Voltage (kV) | 80 | Depositor |
| Electron dose ($e^-/Å^2$) | 25 | Depositor |
| Minimum defocus (nm) | 275 | Depositor |
| Maximum defocus (nm) | 870 | Depositor |
| Magnification | 39500 | Depositor |
| Image detector | KODAK SO-163 FILM | Depositor |
| Maximum map value | 13.363 | Depositor |
| Minimum map value | -3.137 | Depositor |
| Average map value | -0.105 | Depositor |
| Map value standard deviation | 2.517 | Depositor |
| Recommended contour level | 6.41 | Depositor |
| Map size (Å) | 150, 150, 150 | wwPDB |
| Map dimensions | 48, 48, 48 | wwPDB |
| Map angles (°) | 90, 90, 90 | wwPDB |
| Pixel spacing (Å) | 3.125, 3.125, 3.125 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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 | 0.98 | 2/3685 (0.1%) | 1.05 | 3/4968 (0.1%) |
| 2 | B | 0.94 | 0/4262 | 1.05 | 3/5773 (0.1%) |
| 2 | C | 0.94 | 0/4262 | 1.02 | 2/5773 (0.0%) |
| 3 | D | 3.89 | 80/458 (17.5%) | 5.67 | 167/704 (23.7%) |
| 4 | E | 3.95 | 79/460 (17.2%) | 5.69 | 171/708 (24.2%) |
| All | All | 1.39 | 161/13127 (1.2%) | 1.88 | 346/17926 (1.9%) |

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 | B | 0 | 1 |
| 3 | D | 1 | 1 |
| All | All | 1 | 3 |

All (161) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 292 | ARG | C-N | 15.10 | 1.68 | 1.34 |
| 3 | D | 14 | DG | N3-C4 | 13.28 | 1.44 | 1.35 |
| 3 | D | 11 | DG | N3-C4 | 13.10 | 1.44 | 1.35 |
| 3 | D | 16 | DG | N3-C4 | 13.07 | 1.44 | 1.35 |
| 4 | E | 1 | DG | N3-C4 | 13.03 | 1.44 | 1.35 |
| 3 | D | 1 | DG | N3-C4 | 13.01 | 1.44 | 1.35 |
| 4 | E | 11 | DG | N3-C4 | 13.00 | 1.44 | 1.35 |
| 4 | E | 8 | DG | N3-C4 | 12.91 | 1.44 | 1.35 |
| 4 | E | 14 | DG | N3-C4 | 12.90 | 1.44 | 1.35 |
| 3 | D | 8 | DG | N3-C4 | 12.87 | 1.44 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 17 | DG | N3-C4 | 12.87 | 1.44 | 1.35 |
| 4 | E | 4 | DG | N3-C4 | 12.85 | 1.44 | 1.35 |
| 3 | D | 13 | DC | C2-N3 | 11.56 | 1.45 | 1.35 |
| 4 | E | 20 | DC | C2-N3 | 11.47 | 1.45 | 1.35 |
| 4 | E | 7 | DC | C2-N3 | 11.46 | 1.45 | 1.35 |
| 3 | D | 20 | DC | C2-N3 | 11.45 | 1.45 | 1.35 |
| 3 | D | 7 | DC | C2-N3 | 11.42 | 1.44 | 1.35 |
| 4 | E | 10 | DC | C2-N3 | 11.38 | 1.44 | 1.35 |
| 3 | D | 17 | DC | C2-N3 | 11.29 | 1.44 | 1.35 |
| 3 | D | 10 | DC | C2-N3 | 11.24 | 1.44 | 1.35 |
| 4 | E | 5 | DC | C2-N3 | 11.23 | 1.44 | 1.35 |
| 4 | E | 13 | DC | C2-N3 | 11.18 | 1.44 | 1.35 |
| 3 | D | 4 | DC | C2-N3 | 11.05 | 1.44 | 1.35 |
| 4 | E | 5 | DC | O3'-P | 10.91 | 1.74 | 1.61 |
| 4 | E | 4 | DG | N9-C8 | -10.62 | 1.30 | 1.37 |
| 4 | E | 17 | DG | N9-C8 | -10.35 | 1.30 | 1.37 |
| 4 | E | 14 | DG | N9-C8 | -10.14 | 1.30 | 1.37 |
| 3 | D | 8 | DG | N9-C8 | -10.11 | 1.30 | 1.37 |
| 4 | E | 1 | DG | N9-C8 | -10.05 | 1.30 | 1.37 |
| 3 | D | 11 | DG | N9-C8 | -9.97 | 1.30 | 1.37 |
| 4 | E | 11 | DG | N9-C8 | -9.93 | 1.30 | 1.37 |
| 4 | E | 8 | DG | N9-C8 | -9.87 | 1.30 | 1.37 |
| 3 | D | 1 | DG | N9-C8 | -9.86 | 1.30 | 1.37 |
| 3 | D | 16 | DG | N9-C8 | -9.75 | 1.31 | 1.37 |
| 3 | D | 5 | DA | O3'-P | 9.36 | 1.72 | 1.61 |
| 4 | E | 5 | DC | N3-C4 | -9.28 | 1.27 | 1.33 |
| 3 | D | 6 | DA | N7-C5 | -9.17 | 1.33 | 1.39 |
| 3 | D | 4 | DC | N3-C4 | -9.14 | 1.27 | 1.33 |
| 3 | D | 17 | DC | N3-C4 | -9.09 | 1.27 | 1.33 |
| 4 | E | 13 | DC | N3-C4 | -9.06 | 1.27 | 1.33 |
| 4 | E | 20 | DC | N3-C4 | -9.04 | 1.27 | 1.33 |
| 4 | E | 7 | DC | N3-C4 | -8.99 | 1.27 | 1.33 |
| 3 | D | 13 | DC | N3-C4 | -8.97 | 1.27 | 1.33 |
| 3 | D | 10 | DC | N3-C4 | -8.97 | 1.27 | 1.33 |
| 3 | D | 20 | DC | N3-C4 | -8.96 | 1.27 | 1.33 |
| 3 | D | 7 | DC | N3-C4 | -8.93 | 1.27 | 1.33 |
| 4 | E | 10 | DC | N3-C4 | -8.76 | 1.27 | 1.33 |
| 3 | D | 5 | DA | N7-C5 | -8.76 | 1.33 | 1.39 |
| 3 | D | 12 | DA | N7-C5 | -8.56 | 1.34 | 1.39 |
| 3 | D | 14 | DG | N9-C8 | -8.46 | 1.31 | 1.37 |
| 3 | D | 1 | DG | N7-C5 | 8.45 | 1.44 | 1.39 |
| 4 | E | 12 | DA | N9-C8 | -8.44 | 1.31 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 8 | DG | N9-C4 | -8.39 | 1.31 | 1.38 |
| 4 | E | 1 | DG | N7-C5 | 8.37 | 1.44 | 1.39 |
| 4 | E | 12 | DA | N7-C5 | -8.36 | 1.34 | 1.39 |
| 3 | D | 18 | DA | N7-C5 | -8.35 | 1.34 | 1.39 |
| 4 | E | 17 | DG | N7-C5 | 8.33 | 1.44 | 1.39 |
| 4 | E | 17 | DG | N9-C4 | -8.33 | 1.31 | 1.38 |
| 3 | D | 8 | DG | N9-C4 | -8.32 | 1.31 | 1.38 |
| 4 | E | 4 | DG | N7-C5 | 8.32 | 1.44 | 1.39 |
| 3 | D | 12 | DA | N9-C8 | -8.31 | 1.31 | 1.37 |
| 4 | E | 18 | DA | N9-C8 | -8.30 | 1.31 | 1.37 |
| 3 | D | 8 | DG | N7-C5 | 8.29 | 1.44 | 1.39 |
| 4 | E | 11 | DG | N9-C4 | -8.28 | 1.31 | 1.38 |
| 4 | E | 19 | DA | N9-C8 | -8.28 | 1.31 | 1.37 |
| 3 | D | 19 | DA | N7-C5 | -8.27 | 1.34 | 1.39 |
| 4 | E | 11 | DG | N7-C5 | 8.26 | 1.44 | 1.39 |
| 4 | E | 18 | DA | N7-C5 | -8.23 | 1.34 | 1.39 |
| 4 | E | 6 | DA | N7-C5 | -8.23 | 1.34 | 1.39 |
| 4 | E | 8 | DG | N7-C5 | 8.22 | 1.44 | 1.39 |
| 4 | E | 19 | DA | N7-C5 | -8.22 | 1.34 | 1.39 |
| 3 | D | 19 | DA | N9-C8 | -8.20 | 1.31 | 1.37 |
| 4 | E | 1 | DG | N9-C4 | -8.20 | 1.31 | 1.38 |
| 4 | E | 4 | DG | N9-C4 | -8.20 | 1.31 | 1.38 |
| 3 | D | 1 | DG | N9-C4 | -8.17 | 1.31 | 1.38 |
| 3 | D | 18 | DA | N9-C8 | -8.16 | 1.31 | 1.37 |
| 3 | D | 6 | DA | N9-C8 | -8.12 | 1.31 | 1.37 |
| 3 | D | 11 | DG | N7-C5 | 8.11 | 1.44 | 1.39 |
| 3 | D | 16 | DG | N9-C4 | -8.06 | 1.31 | 1.38 |
| 3 | D | 16 | DG | N7-C5 | 8.05 | 1.44 | 1.39 |
| 4 | E | 14 | DG | N9-C4 | -8.02 | 1.31 | 1.38 |
| 4 | E | 14 | DG | N7-C5 | 7.94 | 1.44 | 1.39 |
| 3 | D | 11 | DG | N9-C4 | -7.93 | 1.31 | 1.38 |
| 4 | E | 6 | DA | N9-C8 | -7.87 | 1.31 | 1.37 |
| 3 | D | 5 | DA | N9-C8 | -7.66 | 1.31 | 1.37 |
| 4 | E | 11 | DG | O3'-P | 7.63 | 1.70 | 1.61 |
| 3 | D | 14 | DG | N9-C4 | -7.55 | 1.31 | 1.38 |
| 3 | D | 16 | DG | O3'-P | 7.38 | 1.70 | 1.61 |
| 3 | D | 14 | DG | N7-C5 | 7.22 | 1.43 | 1.39 |
| 3 | D | 11 | DG | C8-N7 | -7.22 | 1.26 | 1.30 |
| 4 | E | 14 | DG | C8-N7 | -7.19 | 1.26 | 1.30 |
| 3 | D | 8 | DG | C8-N7 | -7.11 | 1.26 | 1.30 |
| 4 | E | 4 | DG | C8-N7 | -7.03 | 1.26 | 1.30 |
| 4 | E | 11 | DG | C8-N7 | -7.02 | 1.26 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | D | 16 | DG | C8-N7 | -6.98 | 1.26 | 1.30 |
| 1 | A | 295 | GLY | C-N | -6.93 | 1.18 | 1.34 |
| 4 | E | 17 | DG | C5-C4 | -6.89 | 1.33 | 1.38 |
| 3 | D | 16 | DG | C5-C4 | -6.85 | 1.33 | 1.38 |
| 3 | D | 17 | DC | O3'-P | 6.82 | 1.69 | 1.61 |
| 4 | E | 8 | DG | C8-N7 | -6.81 | 1.26 | 1.30 |
| 3 | D | 1 | DG | C8-N7 | -6.80 | 1.26 | 1.30 |
| 3 | D | 11 | DG | C5-C4 | -6.80 | 1.33 | 1.38 |
| 4 | E | 17 | DG | C8-N7 | -6.76 | 1.26 | 1.30 |
| 3 | D | 15 | DT | O3'-P | 6.75 | 1.69 | 1.61 |
| 4 | E | 13 | DC | C4-C5 | 6.72 | 1.48 | 1.43 |
| 4 | E | 1 | DG | C8-N7 | -6.71 | 1.26 | 1.30 |
| 3 | D | 1 | DG | C5-C4 | -6.70 | 1.33 | 1.38 |
| 4 | E | 11 | DG | C5-C4 | -6.70 | 1.33 | 1.38 |
| 4 | E | 4 | DG | C5-C4 | -6.68 | 1.33 | 1.38 |
| 4 | E | 8 | DG | C5-C4 | -6.67 | 1.33 | 1.38 |
| 4 | E | 1 | DG | C5-C4 | -6.66 | 1.33 | 1.38 |
| 3 | D | 8 | DG | C5-C4 | -6.65 | 1.33 | 1.38 |
| 4 | E | 16 | DT | O3'-P | 6.63 | 1.69 | 1.61 |
| 3 | D | 5 | DA | C8-N7 | -6.62 | 1.26 | 1.31 |
| 4 | E | 14 | DG | C5-C4 | -6.60 | 1.33 | 1.38 |
| 4 | E | 20 | DC | C4-C5 | 6.55 | 1.48 | 1.43 |
| 3 | D | 7 | DC | C4-C5 | 6.55 | 1.48 | 1.43 |
| 3 | D | 13 | DC | C4-C5 | 6.54 | 1.48 | 1.43 |
| 4 | E | 7 | DC | C4-C5 | 6.51 | 1.48 | 1.43 |
| 3 | D | 20 | DC | C4-C5 | 6.49 | 1.48 | 1.43 |
| 4 | E | 5 | DC | C4-C5 | 6.47 | 1.48 | 1.43 |
| 4 | E | 17 | DG | O3'-P | 6.45 | 1.68 | 1.61 |
| 3 | D | 17 | DC | C4-C5 | 6.45 | 1.48 | 1.43 |
| 3 | D | 14 | DG | C8-N7 | -6.44 | 1.27 | 1.30 |
| 4 | E | 10 | DC | C4-C5 | 6.38 | 1.48 | 1.43 |
| 3 | D | 10 | DC | C4-C5 | 6.38 | 1.48 | 1.43 |
| 3 | D | 18 | DA | C8-N7 | -6.32 | 1.27 | 1.31 |
| 4 | E | 7 | DC | O3'-P | 6.32 | 1.68 | 1.61 |
| 4 | E | 18 | DA | C8-N7 | -6.29 | 1.27 | 1.31 |
| 4 | E | 19 | DA | C8-N7 | -6.20 | 1.27 | 1.31 |
| 4 | E | 17 | DG | C2-N3 | -6.20 | 1.27 | 1.32 |
| 3 | D | 12 | DA | C8-N7 | -6.16 | 1.27 | 1.31 |
| 3 | D | 19 | DA | C8-N7 | -6.10 | 1.27 | 1.31 |
| 4 | E | 12 | DA | C8-N7 | -6.07 | 1.27 | 1.31 |
| 3 | D | 14 | DG | C2-N3 | -6.06 | 1.27 | 1.32 |
| 3 | D | 3 | DT | O3'-P | 6.06 | 1.68 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | D | 8 | DG | C2-N3 | -6.06 | 1.27 | 1.32 |
| 4 | E | 8 | DG | C2-N3 | -6.04 | 1.27 | 1.32 |
| 3 | D | 6 | DA | O3'-P | 6.02 | 1.68 | 1.61 |
| 4 | E | 11 | DG | C2-N3 | -5.95 | 1.27 | 1.32 |
| 4 | E | 1 | DG | C2-N3 | -5.90 | 1.28 | 1.32 |
| 3 | D | 16 | DG | C2-N3 | -5.87 | 1.28 | 1.32 |
| 3 | D | 4 | DC | C4-C5 | 5.86 | 1.47 | 1.43 |
| 3 | D | 1 | DG | C2-N3 | -5.85 | 1.28 | 1.32 |
| 4 | E | 14 | DG | C2-N3 | -5.85 | 1.28 | 1.32 |
| 4 | E | 6 | DA | C8-N7 | -5.85 | 1.27 | 1.31 |
| 4 | E | 4 | DG | C2-N3 | -5.79 | 1.28 | 1.32 |
| 3 | D | 11 | DG | C2-N3 | -5.75 | 1.28 | 1.32 |
| 4 | E | 3 | DT | O3'-P | 5.69 | 1.68 | 1.61 |
| 3 | D | 4 | DC | N1-C2 | -5.67 | 1.34 | 1.40 |
| 3 | D | 6 | DA | C8-N7 | -5.65 | 1.27 | 1.31 |
| 4 | E | 15 | DT | O3'-P | 5.61 | 1.67 | 1.61 |
| 3 | D | 14 | DG | C6-N1 | -5.54 | 1.35 | 1.39 |
| 4 | E | 4 | DG | O3'-P | 5.49 | 1.67 | 1.61 |
| 4 | E | 6 | DA | O3'-P | 5.37 | 1.67 | 1.61 |
| 3 | D | 7 | DC | O3'-P | 5.36 | 1.67 | 1.61 |
| 3 | D | 11 | DG | O3'-P | 5.25 | 1.67 | 1.61 |
| 3 | D | 14 | DG | C5-C4 | -5.18 | 1.34 | 1.38 |
| 3 | D | 9 | DT | O3'-P | -5.15 | 1.54 | 1.61 |
| 3 | D | 11 | DG | C6-N1 | -5.04 | 1.36 | 1.39 |
| 4 | E | 2 | DT | O3'-P | 5.03 | 1.67 | 1.61 |

All (346) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | E | 4 | DG | C4-C5-N7 | -24.73 | 100.91 | 110.80 |
| 3 | D | 1 | DG | C4-C5-N7 | -24.21 | 101.12 | 110.80 |
| 4 | E | 8 | DG | C4-C5-N7 | -24.19 | 101.12 | 110.80 |
| 4 | E | 17 | DG | C4-C5-N7 | -24.18 | 101.13 | 110.80 |
| 4 | E | 11 | DG | C4-C5-N7 | -24.05 | 101.18 | 110.80 |
| 3 | D | 8 | DG | C4-C5-N7 | -23.95 | 101.22 | 110.80 |
| 4 | E | 1 | DG | C4-C5-N7 | -23.87 | 101.25 | 110.80 |
| 4 | E | 14 | DG | C4-C5-N7 | -23.83 | 101.27 | 110.80 |
| 3 | D | 16 | DG | C4-C5-N7 | -23.73 | 101.31 | 110.80 |
| 3 | D | 11 | DG | C4-C5-N7 | -23.50 | 101.40 | 110.80 |
| 3 | D | 14 | DG | C4-C5-N7 | -22.48 | 101.81 | 110.80 |
| 3 | D | 11 | DG | N3-C4-C5 | -19.57 | 118.81 | 128.60 |
| 3 | D | 16 | DG | N3-C4-C5 | -19.24 | 118.98 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | E | 14 | DG | N3-C4-C5 | -19.15 | 119.02 | 128.60 |
| 4 | E | 11 | DG | N3-C4-C5 | -18.91 | 119.14 | 128.60 |
| 4 | E | 4 | DG | N3-C4-C5 | -18.88 | 119.16 | 128.60 |
| 3 | D | 1 | DG | N3-C4-C5 | -18.77 | 119.21 | 128.60 |
| 4 | E | 8 | DG | N3-C4-C5 | -18.70 | 119.25 | 128.60 |
| 3 | D | 14 | DG | N3-C4-C5 | -18.57 | 119.31 | 128.60 |
| 4 | E | 1 | DG | N3-C4-C5 | -18.56 | 119.32 | 128.60 |
| 3 | D | 8 | DG | N3-C4-C5 | -18.48 | 119.36 | 128.60 |
| 3 | D | 14 | DG | N9-C4-C5 | 18.47 | 112.79 | 105.40 |
| 4 | E | 17 | DG | N3-C4-C5 | -18.32 | 119.44 | 128.60 |
| 3 | D | 14 | DG | C2-N3-C4 | 17.51 | 120.65 | 111.90 |
| 4 | E | 6 | DA | C2-N3-C4 | 17.50 | 119.35 | 110.60 |
| 2 | B | 470 | ASP | O-C-N | -17.15 | 95.26 | 122.70 |
| 4 | E | 14 | DG | C2-N3-C4 | 16.93 | 120.36 | 111.90 |
| 3 | D | 1 | DG | C2-N3-C4 | 16.89 | 120.34 | 111.90 |
| 3 | D | 16 | DG | C2-N3-C4 | 16.89 | 120.34 | 111.90 |
| 4 | E | 11 | DG | C2-N3-C4 | 16.84 | 120.32 | 111.90 |
| 4 | E | 8 | DG | C2-N3-C4 | 16.72 | 120.26 | 111.90 |
| 3 | D | 11 | DG | C2-N3-C4 | 16.72 | 120.26 | 111.90 |
| 4 | E | 17 | DG | C2-N3-C4 | 16.71 | 120.25 | 111.90 |
| 3 | D | 6 | DA | C2-N3-C4 | 16.68 | 118.94 | 110.60 |
| 4 | E | 1 | DG | C2-N3-C4 | 16.67 | 120.24 | 111.90 |
| 4 | E | 4 | DG | C2-N3-C4 | 16.56 | 120.18 | 111.90 |
| 3 | D | 8 | DG | C2-N3-C4 | 16.54 | 120.17 | 111.90 |
| 3 | D | 6 | DA | N1-C2-N3 | -16.50 | 121.05 | 129.30 |
| 4 | E | 6 | DA | N1-C2-N3 | -16.34 | 121.13 | 129.30 |
| 3 | D | 18 | DA | C2-N3-C4 | 15.98 | 118.59 | 110.60 |
| 3 | D | 19 | DA | C2-N3-C4 | 15.95 | 118.57 | 110.60 |
| 4 | E | 18 | DA | C2-N3-C4 | 15.91 | 118.56 | 110.60 |
| 4 | E | 19 | DA | C2-N3-C4 | 15.75 | 118.47 | 110.60 |
| 3 | D | 5 | DA | C2-N3-C4 | 15.67 | 118.44 | 110.60 |
| 3 | D | 1 | DG | N9-C4-C5 | 15.52 | 111.61 | 105.40 |
| 4 | E | 8 | DG | N9-C4-C5 | 15.51 | 111.60 | 105.40 |
| 3 | D | 16 | DG | N9-C4-C5 | 15.32 | 111.53 | 105.40 |
| 3 | D | 12 | DA | C2-N3-C4 | 15.30 | 118.25 | 110.60 |
| 4 | E | 17 | DG | N9-C4-C5 | 15.29 | 111.52 | 105.40 |
| 3 | D | 5 | DA | N1-C2-N3 | -15.25 | 121.67 | 129.30 |
| 4 | E | 1 | DG | N9-C4-C5 | 15.23 | 111.49 | 105.40 |
| 4 | E | 4 | DG | N9-C4-C5 | 15.22 | 111.49 | 105.40 |
| 3 | D | 4 | DC | N3-C4-C5 | -15.21 | 115.82 | 121.90 |
| 3 | D | 14 | DG | C5-C6-O6 | -15.15 | 119.51 | 128.60 |
| 4 | E | 19 | DA | N1-C2-N3 | -15.11 | 121.75 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 19 | DA | N1-C2-N3 | -15.10 | 121.75 | 129.30 |
| 3 | D | 8 | DG | N9-C4-C5 | 15.07 | 111.43 | 105.40 |
| 4 | E | 11 | DG | N9-C4-C5 | 15.01 | 111.40 | 105.40 |
| 4 | E | 14 | DG | N9-C4-C5 | 14.99 | 111.39 | 105.40 |
| 4 | E | 12 | DA | C2-N3-C4 | 14.91 | 118.06 | 110.60 |
| 3 | D | 18 | DA | N1-C2-N3 | -14.86 | 121.87 | 129.30 |
| 4 | E | 18 | DA | N1-C2-N3 | -14.81 | 121.89 | 129.30 |
| 3 | D | 11 | DG | N9-C4-C5 | 14.67 | 111.27 | 105.40 |
| 3 | D | 12 | DA | N1-C2-N3 | -13.87 | 122.37 | 129.30 |
| 4 | E | 17 | DG | C6-C5-N7 | 13.86 | 138.71 | 130.40 |
| 3 | D | 1 | DG | C6-C5-N7 | 13.58 | 138.55 | 130.40 |
| 4 | E | 4 | DG | C6-C5-N7 | 13.55 | 138.53 | 130.40 |
| 4 | E | 12 | DA | N1-C2-N3 | -13.55 | 122.53 | 129.30 |
| 3 | D | 8 | DG | C6-C5-N7 | 13.54 | 138.52 | 130.40 |
| 3 | D | 11 | DG | C5-C6-O6 | -13.50 | 120.50 | 128.60 |
| 3 | D | 14 | DG | C6-C5-N7 | 13.50 | 138.50 | 130.40 |
| 4 | E | 8 | DG | C6-C5-N7 | 13.49 | 138.49 | 130.40 |
| 4 | E | 1 | DG | C6-C5-N7 | 13.45 | 138.47 | 130.40 |
| 4 | E | 11 | DG | C6-C5-N7 | 13.39 | 138.44 | 130.40 |
| 3 | D | 8 | DG | C5-C6-O6 | -13.06 | 120.76 | 128.60 |
| 4 | E | 8 | DG | C5-C6-O6 | -12.97 | 120.82 | 128.60 |
| 4 | E | 11 | DG | C5-C6-O6 | -12.94 | 120.83 | 128.60 |
| 4 | E | 14 | DG | C6-C5-N7 | 12.91 | 138.15 | 130.40 |
| 4 | E | 17 | DG | C5-C6-O6 | -12.90 | 120.86 | 128.60 |
| 3 | D | 16 | DG | C6-C5-N7 | 12.87 | 138.12 | 130.40 |
| 4 | E | 14 | DG | C5-C6-O6 | -12.80 | 120.92 | 128.60 |
| 4 | E | 1 | DG | C5-C6-O6 | -12.76 | 120.95 | 128.60 |
| 4 | E | 4 | DG | C5-C6-O6 | -12.70 | 120.98 | 128.60 |
| 3 | D | 16 | DG | C5-C6-O6 | -12.69 | 120.99 | 128.60 |
| 3 | D | 1 | DG | C5-C6-O6 | -12.40 | 121.16 | 128.60 |
| 3 | D | 11 | DG | C6-C5-N7 | 12.31 | 137.78 | 130.40 |
| 3 | D | 12 | DA | C5-N7-C8 | 12.31 | 110.05 | 103.90 |
| 4 | E | 6 | DA | C5-N7-C8 | 12.22 | 110.01 | 103.90 |
| 3 | D | 18 | DA | C5-N7-C8 | 12.05 | 109.92 | 103.90 |
| 3 | D | 6 | DA | C5-N7-C8 | 12.03 | 109.91 | 103.90 |
| 3 | D | 13 | DC | N3-C4-C5 | -11.95 | 117.12 | 121.90 |
| 4 | E | 12 | DA | C5-N7-C8 | 11.88 | 109.84 | 103.90 |
| 4 | E | 18 | DA | C5-N7-C8 | 11.87 | 109.83 | 103.90 |
| 4 | E | 6 | DA | C4-C5-C6 | 11.80 | 122.90 | 117.00 |
| 3 | D | 19 | DA | C5-N7-C8 | 11.66 | 109.73 | 103.90 |
| 3 | D | 5 | DA | C4-C5-C6 | 11.64 | 122.82 | 117.00 |
| 3 | D | 20 | DC | N3-C4-C5 | -11.49 | 117.30 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 7 | DC | N3-C4-C5 | -11.46 | 117.32 | 121.90 |
| 4 | E | 19 | DA | C5-N7-C8 | 11.45 | 109.63 | 103.90 |
| 4 | E | 6 | DA | N3-C4-C5 | -11.45 | 118.79 | 126.80 |
| 4 | E | 10 | DC | N3-C4-C5 | -11.42 | 117.33 | 121.90 |
| 4 | E | 20 | DC | N3-C4-C5 | -11.32 | 117.37 | 121.90 |
| 3 | D | 17 | DC | N3-C4-C5 | -11.32 | 117.37 | 121.90 |
| 3 | D | 6 | DA | C4-C5-C6 | 11.31 | 122.66 | 117.00 |
| 4 | E | 7 | DC | N3-C4-C5 | -11.21 | 117.42 | 121.90 |
| 3 | D | 18 | DA | C4-C5-C6 | 11.20 | 122.60 | 117.00 |
| 3 | D | 5 | DA | C5-N7-C8 | 11.15 | 109.48 | 103.90 |
| 4 | E | 18 | DA | C4-C5-C6 | 11.10 | 122.55 | 117.00 |
| 4 | E | 6 | DA | C4-C5-N7 | -11.07 | 105.16 | 110.70 |
| 4 | E | 13 | DC | N3-C4-C5 | -11.06 | 117.48 | 121.90 |
| 3 | D | 12 | DA | C4-C5-C6 | 11.05 | 122.53 | 117.00 |
| 3 | D | 6 | DA | C4-C5-N7 | -11.00 | 105.20 | 110.70 |
| 3 | D | 6 | DA | N3-C4-C5 | -10.88 | 119.18 | 126.80 |
| 4 | E | 5 | DC | N3-C4-C5 | -10.87 | 117.55 | 121.90 |
| 4 | E | 19 | DA | C4-C5-C6 | 10.85 | 122.42 | 117.00 |
| 3 | D | 12 | DA | C4-C5-N7 | -10.83 | 105.28 | 110.70 |
| 3 | D | 19 | DA | C4-C5-C6 | 10.83 | 122.41 | 117.00 |
| 3 | D | 18 | DA | C4-C5-N7 | -10.82 | 105.29 | 110.70 |
| 3 | D | 18 | DA | N3-C4-C5 | -10.79 | 119.25 | 126.80 |
| 3 | D | 10 | DC | N3-C4-C5 | -10.71 | 117.61 | 121.90 |
| 4 | E | 18 | DA | N3-C4-C5 | -10.68 | 119.33 | 126.80 |
| 4 | E | 18 | DA | C4-C5-N7 | -10.66 | 105.37 | 110.70 |
| 3 | D | 19 | DA | C4-C5-N7 | -10.62 | 105.39 | 110.70 |
| 4 | E | 4 | DG | C5-N7-C8 | 10.61 | 109.60 | 104.30 |
| 3 | D | 15 | DT | O4'-C1'-N1 | 10.56 | 115.39 | 108.00 |
| 4 | E | 12 | DA | C4-C5-N7 | -10.56 | 105.42 | 110.70 |
| 3 | D | 19 | DA | N3-C4-C5 | -10.52 | 119.43 | 126.80 |
| 3 | D | 12 | DA | N3-C4-C5 | -10.50 | 119.45 | 126.80 |
| 4 | E | 12 | DA | C4-C5-C6 | 10.47 | 122.24 | 117.00 |
| 3 | D | 5 | DA | N3-C4-C5 | -10.45 | 119.48 | 126.80 |
| 4 | E | 19 | DA | C4-C5-N7 | -10.38 | 105.51 | 110.70 |
| 4 | E | 19 | DA | N3-C4-C5 | -10.36 | 119.55 | 126.80 |
| 4 | E | 11 | DG | C5-N7-C8 | 10.32 | 109.46 | 104.30 |
| 3 | D | 2 | DT | O4'-C1'-N1 | 10.27 | 115.19 | 108.00 |
| 3 | D | 1 | DG | C5-N7-C8 | 10.15 | 109.38 | 104.30 |
| 4 | E | 8 | DG | C5-N7-C8 | 10.15 | 109.38 | 104.30 |
| 4 | E | 17 | DG | C5-N7-C8 | 10.08 | 109.34 | 104.30 |
| 4 | E | 12 | DA | N3-C4-C5 | -10.08 | 119.74 | 126.80 |
| 4 | E | 14 | DG | C5-N7-C8 | 10.02 | 109.31 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 11 | DG | C5-N7-C8 | 9.96 | 109.28 | 104.30 |
| 3 | D | 16 | DG | C5-N7-C8 | 9.96 | 109.28 | 104.30 |
| 3 | D | 8 | DG | C5-N7-C8 | 9.94 | 109.27 | 104.30 |
| 4 | E | 1 | DG | C5-N7-C8 | 9.80 | 109.20 | 104.30 |
| 3 | D | 5 | DA | C4-C5-N7 | -9.76 | 105.82 | 110.70 |
| 3 | D | 17 | DC | OP1-P-OP2 | -9.61 | 105.18 | 119.60 |
| 4 | E | 17 | DG | OP1-P-OP2 | -9.61 | 105.19 | 119.60 |
| 3 | D | 2 | DT | C2-N3-C4 | -9.46 | 121.52 | 127.20 |
| 3 | D | 3 | DT | OP1-P-OP2 | -9.30 | 105.64 | 119.60 |
| 4 | E | 9 | DT | C2-N3-C4 | -9.26 | 121.64 | 127.20 |
| 4 | E | 2 | DT | C2-N3-C4 | -9.25 | 121.65 | 127.20 |
| 3 | D | 3 | DT | C2-N3-C4 | -9.24 | 121.65 | 127.20 |
| 4 | E | 3 | DT | OP1-P-OP2 | -9.24 | 105.74 | 119.60 |
| 4 | E | 3 | DT | C2-N3-C4 | -9.18 | 121.69 | 127.20 |
| 1 | A | 174 | THR | CA-CB-CG2 | -9.17 | 99.56 | 112.40 |
| 4 | E | 15 | DT | O4'-C1'-N1 | 9.17 | 114.42 | 108.00 |
| 3 | D | 9 | DT | C2-N3-C4 | -9.16 | 121.70 | 127.20 |
| 4 | E | 15 | DT | C2-N3-C4 | -9.07 | 121.76 | 127.20 |
| 4 | E | 6 | DA | N3-C4-N9 | 8.99 | 134.59 | 127.40 |
| 4 | E | 16 | DT | C2-N3-C4 | -8.90 | 121.86 | 127.20 |
| 4 | E | 18 | DA | OP1-P-OP2 | -8.89 | 106.26 | 119.60 |
| 3 | D | 18 | DA | OP1-P-OP2 | -8.89 | 106.27 | 119.60 |
| 3 | D | 14 | DG | N1-C6-O6 | 8.87 | 125.22 | 119.90 |
| 3 | D | 15 | DT | C2-N3-C4 | -8.79 | 121.93 | 127.20 |
| 4 | E | 18 | DA | N3-C4-N9 | 8.64 | 134.31 | 127.40 |
| 3 | D | 18 | DA | N3-C4-N9 | 8.64 | 134.31 | 127.40 |
| 3 | D | 5 | DA | N1-C6-N6 | 8.61 | 123.77 | 118.60 |
| 3 | D | 4 | DC | C4-C5-C6 | 8.56 | 121.68 | 117.40 |
| 3 | D | 5 | DA | N3-C4-N9 | 8.53 | 134.22 | 127.40 |
| 3 | D | 17 | DC | O4'-C1'-N1 | 8.48 | 113.94 | 108.00 |
| 3 | D | 12 | DA | N3-C4-N9 | 8.43 | 134.15 | 127.40 |
| 3 | D | 14 | DG | OP1-P-OP2 | -8.42 | 106.97 | 119.60 |
| 3 | D | 5 | DA | OP1-P-OP2 | -8.40 | 107.01 | 119.60 |
| 3 | D | 19 | DA | N3-C4-N9 | 8.35 | 134.08 | 127.40 |
| 4 | E | 19 | DA | N3-C4-N9 | 8.32 | 134.06 | 127.40 |
| 3 | D | 6 | DA | N3-C4-N9 | 8.17 | 133.93 | 127.40 |
| 3 | D | 7 | DC | O4'-C1'-N1 | 8.15 | 113.71 | 108.00 |
| 4 | E | 12 | DA | N3-C4-N9 | 8.13 | 133.91 | 127.40 |
| 3 | D | 1 | DG | O4'-C1'-N9 | 8.08 | 113.66 | 108.00 |
| 4 | E | 14 | DG | OP1-P-OP2 | -7.89 | 107.76 | 119.60 |
| 4 | E | 7 | DC | O4'-C1'-N1 | 7.79 | 113.45 | 108.00 |
| 3 | D | 2 | DT | C5-C4-O4 | -7.63 | 119.56 | 124.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 2 | DT | C5-C6-N1 | -7.58 | 119.15 | 123.70 |
| 3 | D | 14 | DG | C5-C6-N1 | 7.53 | 115.27 | 111.50 |
| 3 | D | 4 | DC | N1-C2-O2 | 7.52 | 123.41 | 118.90 |
| 3 | D | 3 | DT | C5-C4-O4 | -7.51 | 119.64 | 124.90 |
| 4 | E | 17 | DG | C5-C6-N1 | 7.50 | 115.25 | 111.50 |
| 4 | E | 3 | DT | N1-C2-N3 | 7.50 | 119.10 | 114.60 |
| 4 | E | 11 | DG | C5-C6-N1 | 7.48 | 115.24 | 111.50 |
| 3 | D | 1 | DG | C5-C6-N1 | 7.47 | 115.23 | 111.50 |
| 4 | E | 6 | DA | N1-C6-N6 | 7.45 | 123.07 | 118.60 |
| 4 | E | 15 | DT | N1-C2-N3 | 7.45 | 119.07 | 114.60 |
| 1 | A | 292 | ARG | O-C-N | -7.42 | 110.82 | 122.70 |
| 3 | D | 9 | DT | C5-C4-O4 | -7.41 | 119.72 | 124.90 |
| 3 | D | 11 | DG | N1-C6-O6 | 7.41 | 124.34 | 119.90 |
| 4 | E | 9 | DT | C5-C4-O4 | -7.41 | 119.72 | 124.90 |
| 3 | D | 16 | DG | C5-C6-N1 | 7.39 | 115.20 | 111.50 |
| 3 | D | 8 | DG | C5-C6-N1 | 7.38 | 115.19 | 111.50 |
| 4 | E | 16 | DT | C5-C4-O4 | -7.38 | 119.73 | 124.90 |
| 4 | E | 1 | DG | C5-C6-N1 | 7.34 | 115.17 | 111.50 |
| 4 | E | 10 | DC | N3-C4-N4 | 7.32 | 123.12 | 118.00 |
| 3 | D | 11 | DG | C5-C6-N1 | 7.31 | 115.16 | 111.50 |
| 4 | E | 8 | DG | C5-C6-N1 | 7.30 | 115.15 | 111.50 |
| 4 | E | 19 | DA | N1-C6-N6 | 7.30 | 122.98 | 118.60 |
| 4 | E | 14 | DG | C5-C6-N1 | 7.29 | 115.14 | 111.50 |
| 4 | E | 3 | DT | C5-C4-O4 | -7.28 | 119.80 | 124.90 |
| 3 | D | 13 | DC | N3-C4-N4 | 7.28 | 123.09 | 118.00 |
| 4 | E | 2 | DT | C5-C4-O4 | -7.27 | 119.81 | 124.90 |
| 3 | D | 2 | DT | N1-C2-N3 | 7.25 | 118.95 | 114.60 |
| 4 | E | 16 | DT | N1-C2-N3 | 7.25 | 118.95 | 114.60 |
| 4 | E | 15 | DT | C5-C4-O4 | -7.23 | 119.84 | 124.90 |
| 3 | D | 13 | DC | C4-C5-C6 | 7.21 | 121.01 | 117.40 |
| 3 | D | 15 | DT | N1-C2-N3 | 7.21 | 118.93 | 114.60 |
| 3 | D | 7 | DC | N3-C4-N4 | 7.20 | 123.04 | 118.00 |
| 4 | E | 9 | DT | N1-C2-N3 | 7.18 | 118.91 | 114.60 |
| 3 | D | 17 | DC | N3-C4-N4 | 7.18 | 123.02 | 118.00 |
| 3 | D | 4 | DC | N3-C4-N4 | 7.17 | 123.02 | 118.00 |
| 4 | E | 4 | DG | N7-C8-N9 | -7.15 | 109.52 | 113.10 |
| 4 | E | 6 | DA | C6-N1-C2 | 7.15 | 122.89 | 118.60 |
| 3 | D | 3 | DT | N1-C2-N3 | 7.14 | 118.89 | 114.60 |
| 3 | D | 5 | DA | C6-N1-C2 | 7.13 | 122.88 | 118.60 |
| 3 | D | 15 | DT | C5-C4-O4 | -7.13 | 119.91 | 124.90 |
| 4 | E | 11 | DG | N7-C8-N9 | -7.13 | 109.54 | 113.10 |
| 3 | D | 1 | DG | OP1-P-OP2 | -7.12 | 108.91 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 10 | DC | N3-C4-N4 | 7.11 | 122.97 | 118.00 |
| 3 | D | 20 | DC | N3-C4-N4 | 7.08 | 122.96 | 118.00 |
| 4 | E | 7 | DC | N3-C4-N4 | 7.07 | 122.95 | 118.00 |
| 4 | E | 18 | DA | N1-C6-N6 | 7.05 | 122.83 | 118.60 |
| 3 | D | 19 | DA | N1-C6-N6 | 7.04 | 122.83 | 118.60 |
| 4 | E | 20 | DC | N3-C4-N4 | 7.04 | 122.93 | 118.00 |
| 3 | D | 6 | DA | C6-N1-C2 | 7.03 | 122.82 | 118.60 |
| 3 | D | 18 | DA | N1-C6-N6 | 7.03 | 122.82 | 118.60 |
| 3 | D | 9 | DT | N1-C2-N3 | 7.02 | 118.81 | 114.60 |
| 4 | E | 13 | DC | N3-C4-N4 | 7.02 | 122.91 | 118.00 |
| 4 | E | 2 | DT | N1-C2-N3 | 7.01 | 118.81 | 114.60 |
| 4 | E | 4 | DG | C5-C6-N1 | 7.01 | 115.00 | 111.50 |
| 4 | E | 2 | DT | O4'-C1'-N1 | 7.00 | 112.90 | 108.00 |
| 3 | D | 12 | DA | N1-C6-N6 | 6.98 | 122.79 | 118.60 |
| 4 | E | 17 | DG | N7-C8-N9 | -6.95 | 109.63 | 113.10 |
| 4 | E | 5 | DC | N3-C4-N4 | 6.93 | 122.85 | 118.00 |
| 3 | D | 8 | DG | N1-C6-O6 | 6.91 | 124.05 | 119.90 |
| 4 | E | 8 | DG | N1-C6-O6 | 6.88 | 124.03 | 119.90 |
| 4 | E | 8 | DG | N7-C8-N9 | -6.88 | 109.66 | 113.10 |
| 3 | D | 20 | DC | C4-C5-C6 | 6.87 | 120.84 | 117.40 |
| 4 | E | 4 | DG | N1-C6-O6 | 6.86 | 124.01 | 119.90 |
| 3 | D | 1 | DG | N7-C8-N9 | -6.82 | 109.69 | 113.10 |
| 3 | D | 17 | DC | C4-C5-C6 | 6.82 | 120.81 | 117.40 |
| 4 | E | 12 | DA | N1-C6-N6 | 6.80 | 122.68 | 118.60 |
| 4 | E | 14 | DG | N1-C6-O6 | 6.72 | 123.93 | 119.90 |
| 3 | D | 6 | DA | N1-C6-N6 | 6.71 | 122.63 | 118.60 |
| 4 | E | 11 | DG | N1-C6-O6 | 6.71 | 123.93 | 119.90 |
| 4 | E | 13 | DC | C4-C5-C6 | 6.71 | 120.76 | 117.40 |
| 3 | D | 7 | DC | C4-C5-C6 | 6.68 | 120.74 | 117.40 |
| 3 | D | 13 | DC | N3-C2-O2 | -6.66 | 117.24 | 121.90 |
| 4 | E | 20 | DC | C4-C5-C6 | 6.66 | 120.73 | 117.40 |
| 3 | D | 13 | DC | N1-C2-O2 | 6.66 | 122.89 | 118.90 |
| 4 | E | 17 | DG | N1-C6-O6 | 6.65 | 123.89 | 119.90 |
| 4 | E | 1 | DG | N1-C6-O6 | 6.64 | 123.88 | 119.90 |
| 3 | D | 8 | DG | N7-C8-N9 | -6.63 | 109.79 | 113.10 |
| 3 | D | 11 | DG | N7-C8-N9 | -6.60 | 109.80 | 113.10 |
| 4 | E | 11 | DG | O4'-C1'-N9 | 6.59 | 112.62 | 108.00 |
| 3 | D | 11 | DG | OP1-P-OP2 | -6.57 | 109.74 | 119.60 |
| 4 | E | 1 | DG | N7-C8-N9 | -6.57 | 109.81 | 113.10 |
| 3 | D | 16 | DG | N7-C8-N9 | -6.55 | 109.83 | 113.10 |
| 4 | E | 19 | DA | C6-N1-C2 | 6.55 | 122.53 | 118.60 |
| 4 | E | 9 | DT | O4'-C1'-N1 | 6.54 | 112.58 | 108.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 11 | DG | N3-C4-N9 | 6.53 | 129.92 | 126.00 |
| 3 | D | 10 | DC | C4-C5-C6 | 6.53 | 120.67 | 117.40 |
| 3 | D | 4 | DC | N3-C2-O2 | -6.53 | 117.33 | 121.90 |
| 3 | D | 16 | DG | N1-C6-O6 | 6.52 | 123.81 | 119.90 |
| 4 | E | 2 | DT | C5-C6-N1 | -6.50 | 119.80 | 123.70 |
| 4 | E | 7 | DC | N3-C2-O2 | -6.43 | 117.40 | 121.90 |
| 4 | E | 10 | DC | C4-C5-C6 | 6.43 | 120.61 | 117.40 |
| 3 | D | 19 | DA | C6-N1-C2 | 6.41 | 122.45 | 118.60 |
| 4 | E | 14 | DG | N7-C8-N9 | -6.41 | 109.90 | 113.10 |
| 3 | D | 13 | DC | O4'-C1'-N1 | 6.40 | 112.48 | 108.00 |
| 4 | E | 7 | DC | N1-C2-O2 | 6.37 | 122.72 | 118.90 |
| 3 | D | 2 | DT | P-O3'-C3' | 6.31 | 127.27 | 119.70 |
| 4 | E | 10 | DC | N1-C2-O2 | 6.31 | 122.69 | 118.90 |
| 4 | E | 20 | DC | N1-C2-O2 | 6.30 | 122.68 | 118.90 |
| 4 | E | 9 | DT | C5-C6-N1 | -6.30 | 119.92 | 123.70 |
| 3 | D | 7 | DC | N1-C2-O2 | 6.29 | 122.67 | 118.90 |
| 4 | E | 7 | DC | C4-C5-C6 | 6.27 | 120.54 | 117.40 |
| 4 | E | 3 | DT | C5-C6-N1 | -6.26 | 119.94 | 123.70 |
| 3 | D | 9 | DT | C5-C6-N1 | -6.26 | 119.95 | 123.70 |
| 3 | D | 20 | DC | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 4 | E | 18 | DA | C6-N1-C2 | 6.23 | 122.34 | 118.60 |
| 3 | D | 18 | DA | C6-N1-C2 | 6.22 | 122.33 | 118.60 |
| 3 | D | 12 | DA | OP1-P-OP2 | -6.22 | 110.27 | 119.60 |
| 3 | D | 10 | DC | N1-C2-O2 | 6.19 | 122.61 | 118.90 |
| 3 | D | 1 | DG | N1-C6-O6 | 6.17 | 123.60 | 119.90 |
| 4 | E | 20 | DC | N3-C2-O2 | -6.16 | 117.59 | 121.90 |
| 4 | E | 5 | DC | C4-C5-C6 | 6.15 | 120.48 | 117.40 |
| 3 | D | 7 | DC | N3-C2-O2 | -6.14 | 117.60 | 121.90 |
| 3 | D | 3 | DT | C5-C6-N1 | -6.12 | 120.03 | 123.70 |
| 3 | D | 17 | DC | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 3 | D | 20 | DC | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 4 | E | 13 | DC | N3-C2-O2 | -6.11 | 117.62 | 121.90 |
| 3 | D | 13 | DC | P-O3'-C3' | 6.09 | 127.00 | 119.70 |
| 3 | D | 15 | DT | C5-C6-N1 | -6.08 | 120.05 | 123.70 |
| 4 | E | 5 | DC | N3-C2-O2 | -6.06 | 117.66 | 121.90 |
| 4 | E | 15 | DT | C5-C6-N1 | -6.04 | 120.08 | 123.70 |
| 3 | D | 5 | DA | C5-C6-N1 | -6.01 | 114.69 | 117.70 |
| 3 | D | 14 | DG | C5-N7-C8 | 6.01 | 107.31 | 104.30 |
| 3 | D | 17 | DC | N1-C2-O2 | 6.01 | 122.50 | 118.90 |
| 3 | D | 10 | DC | N3-C2-O2 | -5.99 | 117.70 | 121.90 |
| 3 | D | 14 | DG | N1-C2-N3 | -5.97 | 120.32 | 123.90 |
| 4 | E | 14 | DG | N3-C4-N9 | 5.97 | 129.58 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | E | 5 | DC | N1-C2-O2 | 5.90 | 122.44 | 118.90 |
| 4 | E | 10 | DC | N3-C2-O2 | -5.86 | 117.80 | 121.90 |
| 2 | B | 346 | TYR | CB-CG-CD2 | -5.83 | 117.50 | 121.00 |
| 3 | D | 16 | DG | N3-C4-N9 | 5.82 | 129.49 | 126.00 |
| 4 | E | 13 | DC | N1-C2-O2 | 5.79 | 122.38 | 118.90 |
| 2 | C | 346 | TYR | CB-CG-CD2 | -5.77 | 117.54 | 121.00 |
| 3 | D | 4 | DC | C2-N3-C4 | 5.76 | 122.78 | 119.90 |
| 4 | E | 11 | DG | N3-C4-N9 | 5.75 | 129.45 | 126.00 |
| 4 | E | 1 | DG | OP1-P-OP2 | -5.71 | 111.04 | 119.60 |
| 3 | D | 15 | DT | OP1-P-OP2 | -5.69 | 111.06 | 119.60 |
| 4 | E | 15 | DT | OP1-P-OP2 | -5.67 | 111.09 | 119.60 |
| 4 | E | 1 | DG | O4'-C1'-N9 | 5.67 | 111.97 | 108.00 |
| 4 | E | 4 | DG | N3-C4-N9 | 5.59 | 129.35 | 126.00 |
| 2 | B | 90 | PHE | CA-CB-CG | -5.57 | 100.53 | 113.90 |
| 2 | C | 90 | PHE | CA-CB-CG | -5.56 | 100.56 | 113.90 |
| 3 | D | 12 | DA | N7-C8-N9 | -5.55 | 111.03 | 113.80 |
| 4 | E | 6 | DA | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 4 | E | 17 | DG | O4'-C1'-N9 | 5.52 | 111.86 | 108.00 |
| 4 | E | 16 | DT | C5-C6-N1 | -5.50 | 120.40 | 123.70 |
| 4 | E | 2 | DT | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 4 | E | 12 | DA | N7-C8-N9 | -5.44 | 111.08 | 113.80 |
| 3 | D | 12 | DA | C6-N1-C2 | 5.43 | 121.86 | 118.60 |
| 3 | D | 8 | DG | N3-C4-N9 | 5.35 | 129.21 | 126.00 |
| 4 | E | 6 | DA | N7-C8-N9 | -5.32 | 111.14 | 113.80 |
| 4 | E | 4 | DG | O4'-C1'-N9 | -5.31 | 104.28 | 108.00 |
| 4 | E | 1 | DG | N3-C4-N9 | 5.31 | 129.18 | 126.00 |
| 3 | D | 1 | DG | N3-C4-N9 | 5.30 | 129.18 | 126.00 |
| 4 | E | 8 | DG | N3-C4-N9 | 5.25 | 129.15 | 126.00 |
| 4 | E | 3 | DT | O4'-C1'-N1 | 5.19 | 111.63 | 108.00 |
| 4 | E | 16 | DT | O3'-P-O5' | 5.18 | 113.84 | 104.00 |
| 4 | E | 4 | DG | C8-N9-C4 | 5.17 | 108.47 | 106.40 |
| 3 | D | 18 | DA | N7-C8-N9 | -5.17 | 111.21 | 113.80 |
| 4 | E | 18 | DA | N7-C8-N9 | -5.12 | 111.24 | 113.80 |
| 4 | E | 13 | DC | O4'-C1'-N1 | 5.08 | 111.55 | 108.00 |
| 3 | D | 6 | DA | OP1-P-OP2 | -5.07 | 111.99 | 119.60 |
| 4 | E | 17 | DG | N3-C4-N9 | 5.07 | 129.04 | 126.00 |
| 4 | E | 12 | DA | C6-N1-C2 | 5.06 | 121.64 | 118.60 |
| 1 | A | 39 | ASP | CA-CB-CG | -5.06 | 102.26 | 113.40 |
| 4 | E | 11 | DG | C8-N9-C4 | 5.05 | 108.42 | 106.40 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 3 | D | 15 | DT | C4' |

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 293 | TYR | Sidechain |
| 2 | B | 470 | ASP | Mainchain |
| 3 | D | 18 | DA | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 3622 | 0 | 3738 | 1029 | 0 |
| 2 | B | 4175 | 0 | 4050 | 560 | 0 |
| 2 | C | 4175 | 0 | 4050 | 582 | 0 |
| 3 | D | 409 | 0 | 225 | 91 | 0 |
| 4 | E | 411 | 0 | 226 | 80 | 0 |
| 5 | B | 27 | 0 | 22 | 28 | 0 |
| 5 | C | 27 | 0 | 22 | 30 | 0 |
| All | All | 12846 | 0 | 12333 | 2091 | 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 83.

All (2091) 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:A:292:ARG:C | 1:A:293:TYR:N | 1.68 | 1.43 |
| 1:A:209:LEU:HB2 | 1:A:216:PHE:CZ | 1.60 | 1.36 |
| 1:A:3:ALA:O | 2:B:488:GLU:HG3 | 1.22 | 1.28 |
| 1:A:412:SER:HB2 | 2:B:495:GLN:CG | 1.68 | 1.23 |
| 2:C:512:GLU:HB2 | 2:C:515:LEU:HD23 | 1.20 | 1.17 |
| 2:B:1:MET:HE1 | 2:B:129:ASP:HA | 1.23 | 1.16 |
| 1:A:3:ALA:O | 2:B:488:GLU:CG | 1.93 | 1.15 |
| 1:A:193:LEU:HG | 1:A:388:LEU:HD13 | 1.19 | 1.14 |
| 1:A:70:SER:HB2 | 3:D:2:DT:C7 | 1.76 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:234:GLU:HG3 | 4:E:2:DT:H3' | 1.20 | 1.14 |
| 2:B:512:GLU:HB2 | 2:B:515:LEU:HD23 | 1.20 | 1.13 |
| 2:C:440:GLN:HB2 | 2:C:484:VAL:HG21 | 1.30 | 1.13 |
| 1:A:209:LEU:CB | 1:A:216:PHE:CZ | 2.32 | 1.12 |
| 1:A:415:ALA:HB2 | 2:B:492:GLU:CG | 1.80 | 1.12 |
| 1:A:412:SER:HB2 | 2:B:495:GLN:HG3 | 1.21 | 1.11 |
| 1:A:6:LEU:HD21 | 1:A:10:TRP:HB2 | 1.26 | 1.10 |
| 1:A:325:LEU:HD13 | 1:A:329:ALA:HB3 | 1.32 | 1.10 |
| 1:A:189:ILE:HG23 | 1:A:190:PRO:HD3 | 1.33 | 1.10 |
| 2:B:269:PHE:HB2 | 3:D:6:DA:C8 | 1.88 | 1.09 |
| 2:C:139:ALA:HB1 | 2:C:150:PHE:HB2 | 1.29 | 1.09 |
| 1:A:412:SER:HB2 | 2:B:495:GLN:CD | 1.73 | 1.08 |
| 2:C:269:PHE:HB2 | 4:E:6:DA:C8 | 1.87 | 1.08 |
| 1:A:265:GLN:HG3 | 1:A:269:ARG:HH21 | 1.12 | 1.08 |
| 1:A:234:GLU:HG3 | 4:E:2:DT:C3' | 1.83 | 1.07 |
| 2:B:93:VAL:HG12 | 2:B:223:ARG:HD3 | 1.32 | 1.07 |
| 2:C:122:LYS:HD3 | 2:C:124:ARG:HE | 1.13 | 1.07 |
| 1:A:143:ASN:HB2 | 2:B:313:ASN:HA | 1.11 | 1.06 |
| 1:A:279:ASN:O | 4:E:1:DG:P | 2.13 | 1.06 |
| 2:B:139:ALA:HB1 | 2:B:150:PHE:HB2 | 1.29 | 1.06 |
| 2:B:122:LYS:HD3 | 2:B:124:ARG:HE | 1.13 | 1.06 |
| 2:C:163:LEU:HD11 | 2:C:262:ILE:HD13 | 1.34 | 1.06 |
| 2:B:440:GLN:HB2 | 2:B:484:VAL:HG21 | 1.31 | 1.06 |
| 2:C:440:GLN:HB2 | 2:C:484:VAL:CG2 | 1.84 | 1.06 |
| 1:A:75:PRO:HG2 | 1:A:111:LEU:HD21 | 1.38 | 1.05 |
| 1:A:294:ASN:ND2 | 3:D:13:DC:H2" | 1.69 | 1.05 |
| 1:A:175:LEU:HG | 1:A:406:VAL:HG22 | 1.38 | 1.05 |
| 1:A:289:LEU:HD11 | 1:A:320:LEU:HD11 | 1.37 | 1.05 |
| 2:C:93:VAL:HG12 | 2:C:223:ARG:HD3 | 1.33 | 1.05 |
| 1:A:139:SER:HB2 | 2:B:466:SER:HB3 | 1.33 | 1.05 |
| 1:A:25:VAL:HG13 | 1:A:71:GLN:HA | 1.37 | 1.05 |
| 1:A:294:ASN:HD21 | 3:D:13:DC:H2" | 0.88 | 1.04 |
| 1:A:355:SER:HB3 | 2:C:316:PHE:HE1 | 1.22 | 1.04 |
| 2:B:440:GLN:HB2 | 2:B:484:VAL:CG2 | 1.85 | 1.04 |
| 5:C:530:SAM:CE | 4:E:6:DA:N6 | 2.19 | 1.04 |
| 1:A:239:LEU:HD22 | 1:A:241:SER:H | 1.18 | 1.03 |
| 1:A:160:PRO:HG2 | 1:A:165:GLN:HG2 | 1.35 | 1.03 |
| 2:B:350:VAL:CG1 | 3:D:6:DA:H4' | 1.88 | 1.02 |
| 1:A:83:SER:HA | 1:A:147:ILE:HG22 | 1.41 | 1.02 |
| 1:A:415:ALA:HB2 | 2:B:492:GLU:HG3 | 1.40 | 1.02 |
| 1:A:252:ILE:HG13 | 1:A:317:PRO:HD3 | 1.41 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1:MET:HE2 | 2:B:132:GLU:HG3 | 1.42 | 1.01 |
| 1:A:71:GLN:HG2 | 1:A:102:CYS:HB3 | 1.41 | 1.01 |
| 1:A:428:ALA:HB1 | 1:A:433:LEU:HD12 | 1.39 | 1.01 |
| 1:A:412:SER:CB | 2:B:495:GLN:HG3 | 1.90 | 1.00 |
| 2:B:285:THR:HG22 | 2:B:287:ASN:H | 1.22 | 1.00 |
| 5:B:530:SAM:CE | 3:D:6:DA:N6 | 2.25 | 1.00 |
| 1:A:209:LEU:HB2 | 1:A:216:PHE:HZ | 1.23 | 1.00 |
| 2:C:24:TYR:HA | 2:C:27:TYR:CE2 | 1.97 | 1.00 |
| 2:B:24:TYR:HA | 2:B:27:TYR:CE2 | 1.97 | 1.00 |
| 2:C:285:THR:HG22 | 2:C:287:ASN:H | 1.22 | 0.99 |
| 1:A:28:LYS:H | 1:A:28:LYS:HD3 | 1.27 | 0.99 |
| 1:A:196:PHE:CZ | 1:A:384:ARG:HD2 | 1.97 | 0.99 |
| 1:A:209:LEU:HB2 | 1:A:216:PHE:CE2 | 1.98 | 0.99 |
| 5:C:530:SAM:HE3 | 4:E:6:DA:N6 | 1.78 | 0.99 |
| 2:C:276:ASN:HD22 | 2:C:278:THR:HG23 | 1.26 | 0.99 |
| 3:D:12:DA:H2" | 3:D:13:DC:H5' | 1.45 | 0.99 |
| 1:A:70:SER:HB2 | 3:D:2:DT:H72 | 1.43 | 0.98 |
| 1:A:85:GLY:HA2 | 4:E:14:DG:C8 | 1.99 | 0.98 |
| 1:A:62:VAL:HG12 | 1:A:64:LYS:H | 1.28 | 0.98 |
| 1:A:355:SER:HB3 | 2:C:316:PHE:CE1 | 1.99 | 0.98 |
| 2:C:220:GLY:HA2 | 2:C:223:ARG:HE | 1.27 | 0.98 |
| 2:B:220:GLY:HA2 | 2:B:223:ARG:HE | 1.28 | 0.97 |
| 1:A:39:ASP:HB3 | 1:A:60:VAL:HG12 | 1.42 | 0.97 |
| 1:A:70:SER:HB2 | 3:D:2:DT:H71 | 1.45 | 0.97 |
| 2:C:430:ALA:HB2 | 2:C:469:LYS:HG3 | 1.46 | 0.97 |
| 2:B:276:ASN:HD22 | 2:B:278:THR:HG23 | 1.26 | 0.97 |
| 1:A:251:PRO:HA | 1:A:269:ARG:HG2 | 1.45 | 0.97 |
| 1:A:234:GLU:CG | 4:E:2:DT:H3' | 1.95 | 0.97 |
| 1:A:283:LEU:HD22 | 1:A:322:ARG:HD2 | 1.46 | 0.97 |
| 2:B:448:ARG:HD3 | 2:B:467:TRP:CE2 | 2.01 | 0.96 |
| 1:A:283:LEU:HD11 | 1:A:316:TYR:CE1 | 2.00 | 0.96 |
| 2:C:128:GLY:HA3 | 2:C:231:LEU:HD22 | 1.46 | 0.96 |
| 1:A:215:ASN:HD21 | 2:C:492:GLU:CB | 1.77 | 0.96 |
| 1:A:293:TYR:HB2 | 1:A:319:LYS:HD2 | 1.47 | 0.96 |
| 2:C:448:ARG:HD3 | 2:C:467:TRP:CE2 | 2.01 | 0.96 |
| 1:A:196:PHE:CZ | 1:A:200:VAL:HG21 | 2.00 | 0.96 |
| 1:A:209:LEU:HD22 | 1:A:216:PHE:HE2 | 1.26 | 0.96 |
| 2:C:93:VAL:HG12 | 2:C:223:ARG:CD | 1.96 | 0.95 |
| 1:A:143:ASN:CB | 2:B:313:ASN:HA | 1.95 | 0.95 |
| 2:C:28:VAL:HB | 2:C:131:TYR:CZ | 2.02 | 0.95 |
| 1:A:19:THR:HG21 | 1:A:22:ILE:HD11 | 1.49 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:269:PHE:CD1 | 4:E:6:DA:C5 | 2.54 | 0.95 |
| 1:A:334:ILE:HG12 | 1:A:338:PHE:CE2 | 2.01 | 0.95 |
| 2:C:84:LYS:HA | 2:C:87:GLN:HG2 | 1.49 | 0.94 |
| 2:B:93:VAL:HG12 | 2:B:223:ARG:CD | 1.96 | 0.94 |
| 5:B:530:SAM:HE3 | 3:D:6:DA:N6 | 1.81 | 0.94 |
| 1:A:142:ALA:CA | 2:B:312:ASP:HB3 | 1.98 | 0.94 |
| 2:C:322:THR:HA | 2:C:325:ARG:HE | 1.33 | 0.94 |
| 1:A:271:LEU:HD22 | 1:A:273:CYS:H | 1.30 | 0.94 |
| 2:B:128:GLY:HA3 | 2:B:231:LEU:HD22 | 1.46 | 0.94 |
| 1:A:209:LEU:CB | 1:A:216:PHE:CE2 | 2.50 | 0.94 |
| 2:B:28:VAL:HB | 2:B:131:TYR:CZ | 2.02 | 0.94 |
| 2:C:257:LEU:HD12 | 2:C:258:PRO:HD2 | 1.47 | 0.94 |
| 1:A:292:ARG:HH12 | 4:E:3:DT:C7 | 1.81 | 0.94 |
| 2:B:257:LEU:HD12 | 2:B:258:PRO:HD2 | 1.47 | 0.94 |
| 1:A:46:ALA:HB1 | 1:A:82:MET:HE1 | 1.50 | 0.93 |
| 1:A:223:PHE:CE1 | 1:A:369:VAL:HG13 | 2.04 | 0.93 |
| 2:B:250:LEU:HD13 | 2:B:277:ILE:HG12 | 1.50 | 0.93 |
| 1:A:427:ARG:HB3 | 1:A:447:ILE:HD12 | 1.50 | 0.93 |
| 2:C:268:PRO:HG3 | 5:C:530:SAM:C8 | 1.97 | 0.93 |
| 1:A:142:ALA:HA | 2:B:312:ASP:HB3 | 1.50 | 0.93 |
| 2:B:268:PRO:HG3 | 5:B:530:SAM:C8 | 1.99 | 0.93 |
| 2:B:350:VAL:HG12 | 3:D:6:DA:H4' | 1.46 | 0.93 |
| 1:A:325:LEU:HD13 | 1:A:329:ALA:CB | 1.98 | 0.93 |
| 1:A:319:LYS:HE3 | 3:D:15:DT:H4' | 1.49 | 0.92 |
| 2:C:440:GLN:CG | 2:C:484:VAL:HB | 1.98 | 0.92 |
| 1:A:212:LYS:HE3 | 1:A:223:PHE:HB2 | 1.49 | 0.92 |
| 2:B:84:LYS:HA | 2:B:87:GLN:HG2 | 1.49 | 0.92 |
| 1:A:215:ASN:OD1 | 2:C:489:ALA:HA | 1.70 | 0.92 |
| 1:A:212:LYS:CE | 1:A:223:PHE:HB2 | 1.99 | 0.92 |
| 1:A:290:PHE:HB3 | 1:A:321:ILE:CG2 | 1.98 | 0.92 |
| 2:B:20:GLY:HA2 | 2:B:102:GLN:HG3 | 1.51 | 0.92 |
| 2:B:440:GLN:CG | 2:B:484:VAL:HB | 1.99 | 0.92 |
| 1:A:428:ALA:CB | 1:A:433:LEU:HD12 | 1.98 | 0.91 |
| 2:B:149:TYR:HD1 | 5:B:530:SAM:HO3' | 0.92 | 0.91 |
| 1:A:90:VAL:HG13 | 1:A:132:ARG:HD2 | 1.49 | 0.91 |
| 1:A:168:ILE:CD1 | 1:A:417:ALA:HB1 | 2.00 | 0.91 |
| 1:A:232:LEU:CG | 1:A:321:ILE:HD11 | 2.01 | 0.91 |
| 2:C:71:TYR:CE2 | 2:C:75:LEU:HD11 | 2.06 | 0.91 |
| 2:B:71:TYR:CE2 | 2:B:75:LEU:HD11 | 2.06 | 0.91 |
| 2:C:20:GLY:HA2 | 2:C:102:GLN:HG3 | 1.51 | 0.90 |
| 4:E:12:DA:H2" | 4:E:13:DC:H5" | 1.53 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:250:LEU:HD13 | 2:C:277:ILE:HG12 | 1.50 | 0.90 |
| 1:A:71:GLN:CG | 1:A:102:CYS:HB3 | 2.01 | 0.90 |
| 1:A:112:ARG:HB2 | 1:A:117:ILE:HG23 | 1.50 | 0.90 |
| 1:A:168:ILE:HG23 | 1:A:413:ILE:CD1 | 2.00 | 0.90 |
| 1:A:280:ARG:HB2 | 1:A:315:LEU:HD11 | 1.51 | 0.90 |
| 2:B:1:MET:CE | 2:B:129:ASP:HA | 2.00 | 0.90 |
| 1:A:248:VAL:HG11 | 1:A:269:ARG:CB | 2.01 | 0.90 |
| 1:A:348:MET:SD | 2:C:469:LYS:HG2 | 2.12 | 0.90 |
| 2:B:84:LYS:HA | 2:B:87:GLN:CG | 2.01 | 0.89 |
| 1:A:209:LEU:HD22 | 1:A:216:PHE:CE2 | 2.07 | 0.89 |
| 1:A:285:ASP:HB3 | 1:A:308:LYS:HG2 | 1.55 | 0.89 |
| 1:A:294:ASN:HA | 3:D:14:DG:C8 | 2.07 | 0.89 |
| 2:B:269:PHE:CD1 | 3:D:6:DA:C5 | 2.61 | 0.89 |
| 2:C:84:LYS:HA | 2:C:87:GLN:CG | 2.01 | 0.89 |
| 2:C:439:ASP:HA | 2:C:485:LEU:CD2 | 2.02 | 0.89 |
| 2:B:6:LEU:HB3 | 2:B:130:MET:SD | 2.13 | 0.89 |
| 2:C:394:THR:H | 2:C:397:HIS:HD2 | 1.20 | 0.89 |
| 2:B:439:ASP:HA | 2:B:485:LEU:CD2 | 2.02 | 0.89 |
| 1:A:168:ILE:HG23 | 1:A:413:ILE:HD11 | 1.52 | 0.89 |
| 2:B:394:THR:H | 2:B:397:HIS:HD2 | 1.20 | 0.89 |
| 2:B:215:LEU:HD13 | 2:B:245:ARG:HE | 1.38 | 0.88 |
| 2:B:217:LEU:HD22 | 2:B:275:THR:HG22 | 1.55 | 0.88 |
| 1:A:300:VAL:HG13 | 1:A:344:ARG:HD2 | 1.55 | 0.88 |
| 1:A:32:ALA:HB3 | 1:A:35:TYR:CD2 | 2.08 | 0.88 |
| 1:A:75:PRO:HA | 1:A:100:PHE:CD2 | 2.08 | 0.88 |
| 1:A:426:TRP:CZ2 | 1:A:444:LEU:HG | 2.08 | 0.88 |
| 1:A:196:PHE:CE1 | 1:A:384:ARG:HD2 | 2.09 | 0.88 |
| 1:A:352:LYS:HE2 | 2:C:468:LEU:H | 1.39 | 0.88 |
| 2:B:115:TRP:HH2 | 2:B:122:LYS:HE2 | 1.39 | 0.88 |
| 2:C:217:LEU:HD22 | 2:C:275:THR:HG22 | 1.55 | 0.88 |
| 2:C:6:LEU:HB3 | 2:C:130:MET:SD | 2.13 | 0.87 |
| 2:C:149:TYR:HA | 5:C:530:SAM:SD | 2.14 | 0.87 |
| 2:C:217:LEU:HD22 | 2:C:275:THR:CG2 | 2.03 | 0.87 |
| 1:A:215:ASN:ND2 | 1:A:216:PHE:H | 1.71 | 0.87 |
| 1:A:215:ASN:HD21 | 2:C:492:GLU:HB2 | 1.40 | 0.87 |
| 2:B:217:LEU:HD22 | 2:B:275:THR:CG2 | 2.03 | 0.87 |
| 2:C:115:TRP:HH2 | 2:C:122:LYS:HE2 | 1.39 | 0.87 |
| 1:A:292:ARG:HH12 | 4:E:3:DT:H72 | 1.39 | 0.87 |
| 2:B:149:TYR:HA | 5:B:530:SAM:SD | 2.15 | 0.86 |
| 1:A:415:ALA:HB2 | 2:B:492:GLU:HG2 | 1.57 | 0.86 |
| 2:C:3:ASN:HD22 | 2:C:7:VAL:HG11 | 1.39 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:220:GLY:HA2 | 2:C:223:ARG:NE | 1.90 | 0.86 |
| 1:A:326:THR:HG23 | 1:A:327:LYS:H | 1.38 | 0.86 |
| 2:B:440:GLN:HG2 | 2:B:484:VAL:HB | 1.57 | 0.86 |
| 2:C:283:HIS:H | 2:C:294:GLN:HE22 | 1.24 | 0.86 |
| 1:A:39:ASP:HB2 | 1:A:62:VAL:CG2 | 2.06 | 0.86 |
| 1:A:143:ASN:HB2 | 2:B:313:ASN:CA | 2.02 | 0.86 |
| 1:A:85:GLY:HA2 | 4:E:14:DG:H8 | 1.38 | 0.86 |
| 1:A:320:LEU:HD23 | 1:A:321:ILE:N | 1.90 | 0.86 |
| 2:C:440:GLN:HG2 | 2:C:484:VAL:HB | 1.56 | 0.86 |
| 3:D:12:DA:H2" | 3:D:13:DC:C5' | 2.06 | 0.86 |
| 1:A:98:LEU:HB3 | 1:A:99:PRO:HD2 | 1.56 | 0.86 |
| 2:C:84:LYS:HD3 | 2:C:87:GLN:HG2 | 1.58 | 0.86 |
| 2:C:207:GLN:HA | 2:C:211:ALA:HB2 | 1.58 | 0.86 |
| 2:B:24:TYR:HB3 | 2:B:138:ASN:HD21 | 1.41 | 0.86 |
| 1:A:232:LEU:HD23 | 1:A:233:THR:N | 1.91 | 0.85 |
| 1:A:215:ASN:ND2 | 2:C:492:GLU:HB2 | 1.89 | 0.85 |
| 1:A:215:ASN:ND2 | 1:A:216:PHE:N | 2.23 | 0.85 |
| 1:A:46:ALA:HA | 1:A:107:PHE:CZ | 2.11 | 0.85 |
| 1:A:280:ARG:CB | 1:A:315:LEU:HD11 | 2.06 | 0.85 |
| 1:A:428:ALA:HB2 | 1:A:443:LEU:HD21 | 1.57 | 0.85 |
| 1:A:303:CYS:SG | 1:A:335:GLU:HG3 | 2.16 | 0.85 |
| 2:B:220:GLY:HA2 | 2:B:223:ARG:NE | 1.91 | 0.85 |
| 1:A:49:ILE:HG13 | 1:A:107:PHE:HE2 | 1.40 | 0.85 |
| 1:A:433:LEU:HD13 | 1:A:443:LEU:HD13 | 1.58 | 0.85 |
| 2:B:222:ARG:NH1 | 2:B:226:LEU:HD11 | 1.91 | 0.85 |
| 1:A:6:LEU:HD23 | 1:A:7:PRO:N | 1.90 | 0.85 |
| 2:C:350:VAL:HG12 | 4:E:6:DA:H4' | 1.59 | 0.85 |
| 1:A:252:ILE:CG2 | 1:A:268:ILE:HG23 | 2.06 | 0.85 |
| 1:A:299:PHE:CE2 | 1:A:347:MET:HG2 | 2.12 | 0.85 |
| 2:C:215:LEU:HD13 | 2:C:245:ARG:HE | 1.38 | 0.84 |
| 1:A:118:PHE:CZ | 1:A:166:LYS:HE3 | 2.12 | 0.84 |
| 2:B:207:GLN:HA | 2:B:211:ALA:HB2 | 1.58 | 0.84 |
| 2:C:222:ARG:NH1 | 2:C:226:LEU:HD11 | 1.91 | 0.84 |
| 1:A:133:ASN:HD21 | 2:B:430:ALA:HA | 1.39 | 0.84 |
| 2:C:122:LYS:HD3 | 2:C:124:ARG:NE | 1.93 | 0.84 |
| 2:B:84:LYS:HD3 | 2:B:87:GLN:HG2 | 1.58 | 0.84 |
| 2:B:115:TRP:CH2 | 2:B:122:LYS:HE2 | 2.12 | 0.84 |
| 2:C:24:TYR:HB3 | 2:C:138:ASN:HD21 | 1.41 | 0.84 |
| 1:A:235:LEU:HD23 | 1:A:236:ARG:N | 1.92 | 0.84 |
| 1:A:347:MET:HE1 | 1:A:360:ILE:HD12 | 1.59 | 0.84 |
| 1:A:348:MET:HB3 | 2:C:469:LYS:HZ2 | 1.43 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:163:LEU:CD1 | 2:C:262:ILE:HD13 | 2.06 | 0.84 |
| 1:A:77:ASP:HA | 1:A:95:HIS:NE2 | 1.91 | 0.84 |
| 2:B:481:GLU:HB2 | 2:B:482:PRO:HD3 | 1.60 | 0.84 |
| 5:C:530:SAM:HE3 | 4:E:6:DA:H62 | 1.38 | 0.84 |
| 1:A:143:ASN:HD21 | 3:D:5:DA:P | 2.01 | 0.84 |
| 1:A:290:PHE:HB3 | 1:A:321:ILE:HG23 | 1.58 | 0.84 |
| 2:B:339:ARG:HD3 | 2:B:381:ARG:NH2 | 1.93 | 0.84 |
| 1:A:75:PRO:HA | 1:A:100:PHE:CE2 | 2.12 | 0.83 |
| 2:B:439:ASP:HA | 2:B:485:LEU:HD22 | 1.60 | 0.83 |
| 2:C:115:TRP:CH2 | 2:C:122:LYS:HE2 | 2.12 | 0.83 |
| 1:A:73:ILE:CG2 | 1:A:100:PHE:HB3 | 2.07 | 0.83 |
| 1:A:289:LEU:HD11 | 1:A:320:LEU:CD1 | 2.08 | 0.83 |
| 2:C:149:TYR:HD1 | 5:C:530:SAM:O3' | 1.60 | 0.83 |
| 1:A:39:ASP:OD1 | 1:A:62:VAL:HA | 1.78 | 0.83 |
| 2:C:38:LYS:HD3 | 2:C:56:TRP:CZ2 | 2.13 | 0.83 |
| 1:A:196:PHE:CE2 | 1:A:200:VAL:HG21 | 2.12 | 0.83 |
| 1:A:254:ARG:NH2 | 1:A:256:SER:HB2 | 1.93 | 0.83 |
| 1:A:236:ARG:HA | 1:A:318:ASP:OD2 | 1.78 | 0.83 |
| 2:B:38:LYS:HD3 | 2:B:56:TRP:CZ2 | 2.13 | 0.83 |
| 1:A:348:MET:HB3 | 2:C:469:LYS:NZ | 1.94 | 0.83 |
| 1:A:248:VAL:HG13 | 1:A:270:PHE:C | 1.98 | 0.83 |
| 2:B:122:LYS:HD3 | 2:B:124:ARG:NE | 1.93 | 0.83 |
| 2:B:3:ASN:HD22 | 2:B:7:VAL:HG11 | 1.41 | 0.83 |
| 2:C:439:ASP:HA | 2:C:485:LEU:HD22 | 1.58 | 0.83 |
| 2:C:319:GLY:O | 2:C:322:THR:HG22 | 1.77 | 0.83 |
| 1:A:70:SER:OG | 3:D:1:DG:H2' | 1.79 | 0.83 |
| 1:A:315:LEU:HD23 | 1:A:316:TYR:N | 1.93 | 0.83 |
| 2:B:1:MET:HE2 | 2:B:132:GLU:CG | 2.08 | 0.83 |
| 4:E:1:DG:C8 | 4:E:2:DT:H72 | 2.14 | 0.83 |
| 1:A:391:TYR:O | 1:A:394:THR:HG22 | 1.79 | 0.82 |
| 1:A:415:ALA:CB | 2:B:492:GLU:CG | 2.57 | 0.82 |
| 2:B:431:ASP:OD2 | 2:B:488:GLU:HB3 | 1.79 | 0.82 |
| 1:A:10:TRP:CE2 | 1:A:418:PHE:HA | 2.15 | 0.82 |
| 1:A:253:LEU:HD11 | 1:A:263:VAL:HG21 | 1.59 | 0.82 |
| 2:B:283:HIS:H | 2:B:294:GLN:HE22 | 1.24 | 0.82 |
| 2:C:442:LEU:HG | 2:C:448:ARG:NH1 | 1.94 | 0.82 |
| 1:A:142:ALA:CB | 2:B:312:ASP:HB3 | 2.09 | 0.82 |
| 1:A:75:PRO:HG3 | 1:A:111:LEU:HD11 | 1.60 | 0.82 |
| 1:A:83:SER:HA | 1:A:147:ILE:CG2 | 2.08 | 0.82 |
| 1:A:10:TRP:CH2 | 1:A:161:PRO:HD2 | 2.15 | 0.82 |
| 2:C:480:PRO:HG3 | 2:C:520:LEU:HD21 | 1.62 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:481:GLU:HB2 | 2:C:482:PRO:HD3 | 1.60 | 0.82 |
| 1:A:25:VAL:CG1 | 1:A:71:GLN:HA | 2.10 | 0.82 |
| 1:A:6:LEU:HD21 | 1:A:10:TRP:CB | 2.10 | 0.81 |
| 1:A:10:TRP:CZ2 | 1:A:161:PRO:HD2 | 2.15 | 0.81 |
| 1:A:270:PHE:HD2 | 1:A:274:SER:HB3 | 1.44 | 0.81 |
| 2:B:372:THR:O | 2:B:452:ARG:HD2 | 1.81 | 0.81 |
| 2:B:442:LEU:HG | 2:B:448:ARG:NH1 | 1.95 | 0.81 |
| 1:A:25:VAL:HG11 | 1:A:71:GLN:HG3 | 1.62 | 0.81 |
| 2:C:372:THR:O | 2:C:452:ARG:HD2 | 1.80 | 0.81 |
| 2:C:431:ASP:OD2 | 2:C:488:GLU:HB3 | 1.79 | 0.81 |
| 2:B:6:LEU:HB2 | 2:B:117:ASN:CG | 2.01 | 0.81 |
| 1:A:45:ARG:HA | 1:A:104:PHE:CE1 | 2.14 | 0.81 |
| 1:A:46:ALA:HB1 | 1:A:82:MET:CE | 2.09 | 0.81 |
| 1:A:285:ASP:CB | 1:A:308:LYS:HG2 | 2.11 | 0.81 |
| 1:A:270:PHE:CE2 | 1:A:275:GLU:HB3 | 2.15 | 0.81 |
| 1:A:319:LYS:HD2 | 3:D:15:DT:OP2 | 1.80 | 0.81 |
| 1:A:42:PRO:HB3 | 1:A:57:THR:HG21 | 1.63 | 0.81 |
| 2:C:3:ASN:ND2 | 2:C:7:VAL:HG11 | 1.96 | 0.81 |
| 1:A:6:LEU:HD13 | 1:A:12:ILE:HD11 | 1.62 | 0.80 |
| 1:A:39:ASP:HB2 | 1:A:62:VAL:HG23 | 1.61 | 0.80 |
| 1:A:179:VAL:O | 1:A:182:THR:HG22 | 1.81 | 0.80 |
| 1:A:235:LEU:HD23 | 1:A:236:ARG:H | 1.45 | 0.80 |
| 1:A:215:ASN:HD22 | 1:A:216:PHE:N | 1.79 | 0.80 |
| 1:A:223:PHE:HE1 | 1:A:369:VAL:HG13 | 1.45 | 0.80 |
| 1:A:225:LYS:HB2 | 1:A:228:PHE:CE1 | 2.16 | 0.80 |
| 2:B:91:HIS:HB3 | 2:B:222:ARG:NH2 | 1.95 | 0.80 |
| 1:A:283:LEU:HD22 | 1:A:322:ARG:CD | 2.10 | 0.80 |
| 1:A:352:LYS:CG | 2:C:466:SER:HB3 | 2.12 | 0.80 |
| 2:C:32:ALA:HB1 | 2:C:227:MET:SD | 2.22 | 0.80 |
| 2:C:91:HIS:HB3 | 2:C:222:ARG:NH2 | 1.95 | 0.80 |
| 1:A:294:ASN:HB2 | 3:D:14:DG:H5” | 1.62 | 0.80 |
| 2:B:480:PRO:HG3 | 2:B:520:LEU:HD21 | 1.62 | 0.80 |
| 1:A:50:GLN:HG3 | 4:E:14:DG:OP1 | 1.82 | 0.80 |
| 1:A:352:LYS:CD | 2:C:466:SER:HB3 | 2.10 | 0.80 |
| 2:C:6:LEU:HB2 | 2:C:117:ASN:CG | 2.01 | 0.80 |
| 2:C:350:VAL:CG1 | 4:E:6:DA:H4’ | 2.12 | 0.80 |
| 1:A:250:HIS:HE1 | 1:A:282:LYS:HE3 | 1.47 | 0.80 |
| 1:A:281:HIS:O | 1:A:315:LEU:HG | 1.79 | 0.80 |
| 1:A:314:LEU:HD23 | 1:A:315:LEU:N | 1.97 | 0.80 |
| 1:A:296:SER:OG | 1:A:300:VAL:HB | 1.82 | 0.80 |
| 2:B:32:ALA:HB1 | 2:B:227:MET:SD | 2.22 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:122:LYS:NZ | 2:C:124:ARG:HG2 | 1.97 | 0.79 |
| 1:A:282:LYS:C | 1:A:283:LEU:HD23 | 2.02 | 0.79 |
| 2:C:471:LYS:HD2 | 2:C:472:ASP:H | 1.47 | 0.79 |
| 1:A:188:GLN:HE22 | 1:A:192:ILE:HG13 | 1.47 | 0.79 |
| 1:A:112:ARG:HB2 | 1:A:117:ILE:CG2 | 2.11 | 0.79 |
| 2:B:471:LYS:HD2 | 2:B:472:ASP:H | 1.47 | 0.79 |
| 1:A:189:ILE:CG2 | 1:A:190:PRO:HD3 | 2.13 | 0.79 |
| 1:A:208:LYS:C | 1:A:209:LEU:HD12 | 2.03 | 0.79 |
| 1:A:319:LYS:CE | 3:D:15:DT:H4' | 2.12 | 0.79 |
| 2:C:480:PRO:O | 2:C:484:VAL:HG13 | 1.83 | 0.79 |
| 1:A:209:LEU:CD2 | 1:A:216:PHE:CE2 | 2.66 | 0.79 |
| 1:A:131:TYR:CZ | 1:A:135:ILE:HD11 | 2.18 | 0.79 |
| 1:A:239:LEU:CD2 | 1:A:241:SER:H | 1.96 | 0.79 |
| 1:A:248:VAL:HG11 | 1:A:269:ARG:HB3 | 1.65 | 0.79 |
| 1:A:160:PRO:HG2 | 1:A:165:GLN:CG | 2.13 | 0.79 |
| 1:A:248:VAL:HG12 | 1:A:250:HIS:H | 1.49 | 0.78 |
| 2:C:149:TYR:HD1 | 5:C:530:SAM:HO3' | 0.79 | 0.78 |
| 2:C:163:LEU:HD11 | 2:C:262:ILE:CD1 | 2.11 | 0.78 |
| 1:A:26:THR:CG2 | 1:A:70:SER:HB3 | 2.13 | 0.78 |
| 1:A:373:PRO:HG2 | 1:A:378:GLN:HG2 | 1.65 | 0.78 |
| 2:B:6:LEU:HB3 | 2:B:130:MET:HE3 | 1.64 | 0.78 |
| 2:B:122:LYS:NZ | 2:B:124:ARG:HG2 | 1.97 | 0.78 |
| 2:B:480:PRO:O | 2:B:484:VAL:HG13 | 1.83 | 0.78 |
| 2:C:322:THR:HB | 2:C:325:ARG:HH21 | 1.49 | 0.78 |
| 1:A:49:ILE:HD12 | 1:A:82:MET:HG3 | 1.66 | 0.78 |
| 1:A:374:PRO:O | 1:A:378:GLN:HG3 | 1.83 | 0.78 |
| 2:B:394:THR:H | 2:B:397:HIS:CD2 | 2.01 | 0.78 |
| 1:A:283:LEU:HD11 | 1:A:316:TYR:CD1 | 2.19 | 0.78 |
| 2:C:3:ASN:HB2 | 2:C:7:VAL:HB | 1.65 | 0.78 |
| 1:A:78:ILE:HA | 1:A:112:ARG:HH12 | 1.47 | 0.78 |
| 1:A:164:GLU:HG3 | 1:A:423:THR:HA | 1.65 | 0.78 |
| 5:C:530:SAM:HE2 | 4:E:6:DA:N6 | 1.98 | 0.78 |
| 1:A:434:ILE:O | 1:A:440:ALA:HB2 | 1.84 | 0.78 |
| 2:B:146:ALA:O | 2:B:149:TYR:HD2 | 1.65 | 0.78 |
| 2:C:394:THR:H | 2:C:397:HIS:CD2 | 2.01 | 0.78 |
| 1:A:294:ASN:HD21 | 3:D:13:DC:C2' | 1.84 | 0.78 |
| 1:A:3:ALA:O | 2:B:488:GLU:CD | 2.21 | 0.78 |
| 1:A:3:ALA:C | 2:B:488:GLU:HG3 | 2.03 | 0.78 |
| 2:B:481:GLU:O | 2:B:485:LEU:HG | 1.84 | 0.78 |
| 1:A:148:LYS:CG | 1:A:149:PRO:HD2 | 2.13 | 0.78 |
| 1:A:247:GLY:O | 1:A:271:LEU:HB2 | 1.83 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:41:LEU:HD23 | 1:A:42:PRO:N | 1.98 | 0.77 |
| 2:B:3:ASN:ND2 | 2:B:7:VAL:HG11 | 1.98 | 0.77 |
| 2:C:200:ASP:O | 2:C:204:GLN:HG3 | 1.85 | 0.77 |
| 2:C:481:GLU:O | 2:C:485:LEU:HG | 1.84 | 0.77 |
| 1:A:236:ARG:HD2 | 4:E:2:DT:O4 | 1.83 | 0.77 |
| 1:A:289:LEU:CD1 | 1:A:320:LEU:HD21 | 2.15 | 0.77 |
| 2:B:268:PRO:HG3 | 5:B:530:SAM:H8 | 1.64 | 0.77 |
| 2:C:83:LYS:H | 2:C:83:LYS:HD3 | 1.50 | 0.77 |
| 1:A:35:TYR:CD1 | 1:A:65:ASN:HA | 2.20 | 0.77 |
| 1:A:46:ALA:HA | 1:A:107:PHE:CE1 | 2.19 | 0.77 |
| 2:B:384:MET:HB3 | 2:B:385:PRO:HD2 | 1.67 | 0.77 |
| 4:E:16:DT:H2" | 4:E:17:DG:C8 | 2.18 | 0.77 |
| 2:B:149:TYR:HD1 | 5:B:530:SAM:O3' | 1.66 | 0.77 |
| 2:B:200:ASP:O | 2:B:204:GLN:HG3 | 1.84 | 0.77 |
| 2:B:334:LEU:HD12 | 2:B:356:PHE:O | 1.85 | 0.77 |
| 1:A:141:GLY:HA2 | 2:B:464:ASP:OD2 | 1.85 | 0.77 |
| 1:A:271:LEU:HD23 | 1:A:272:GLU:N | 1.99 | 0.77 |
| 5:B:530:SAM:HE2 | 3:D:6:DA:H61 | 1.47 | 0.77 |
| 2:C:6:LEU:HB3 | 2:C:130:MET:HE3 | 1.66 | 0.77 |
| 1:A:283:LEU:CD2 | 1:A:322:ARG:HD2 | 2.15 | 0.77 |
| 1:A:392:ALA:O | 1:A:395:ILE:HG22 | 1.85 | 0.77 |
| 2:B:83:LYS:HD3 | 2:B:83:LYS:H | 1.50 | 0.77 |
| 1:A:253:LEU:HD22 | 1:A:320:LEU:CD1 | 2.15 | 0.77 |
| 1:A:289:LEU:CD1 | 1:A:320:LEU:HD11 | 2.12 | 0.77 |
| 1:A:10:TRP:NE1 | 1:A:418:PHE:HA | 2.00 | 0.76 |
| 1:A:70:SER:CB | 3:D:2:DT:H72 | 2.14 | 0.76 |
| 1:A:271:LEU:CD2 | 1:A:273:CYS:H | 1.97 | 0.76 |
| 2:C:490:MET:O | 2:C:494:VAL:HG23 | 1.85 | 0.76 |
| 1:A:46:ALA:CB | 4:E:14:DG:H5' | 2.15 | 0.76 |
| 2:C:268:PRO:HG3 | 5:C:530:SAM:H8 | 1.66 | 0.76 |
| 2:B:179:ALA:O | 2:B:183:ILE:HD13 | 1.85 | 0.76 |
| 2:C:9:LYS:NZ | 2:C:113:LEU:HB2 | 2.01 | 0.76 |
| 1:A:39:ASP:HB3 | 1:A:60:VAL:CG1 | 2.15 | 0.76 |
| 1:A:426:TRP:CE2 | 1:A:444:LEU:HG | 2.21 | 0.76 |
| 2:B:490:MET:O | 2:B:494:VAL:HG23 | 1.85 | 0.76 |
| 5:B:530:SAM:CE | 3:D:6:DA:H61 | 1.96 | 0.76 |
| 1:A:232:LEU:HG | 1:A:321:ILE:HD11 | 1.68 | 0.76 |
| 2:B:113:LEU:HD23 | 2:B:113:LEU:O | 1.86 | 0.76 |
| 2:B:350:VAL:HG11 | 3:D:6:DA:C4' | 2.16 | 0.76 |
| 2:C:20:GLY:CA | 2:C:102:GLN:HG3 | 2.15 | 0.76 |
| 2:C:384:MET:HB3 | 2:C:385:PRO:HD2 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:512:GLU:HB2 | 2:C:515:LEU:CD2 | 2.11 | 0.76 |
| 1:A:10:TRP:CE2 | 1:A:160:PRO:HA | 2.21 | 0.76 |
| 1:A:168:ILE:HD13 | 1:A:417:ALA:HB1 | 1.66 | 0.76 |
| 2:B:271:SER:O | 2:B:288:LYS:HG3 | 1.86 | 0.76 |
| 2:C:271:SER:O | 2:C:288:LYS:HG3 | 1.86 | 0.76 |
| 2:C:478:SER:C | 2:C:479:LEU:HD12 | 2.05 | 0.76 |
| 1:A:35:TYR:HB3 | 1:A:65:ASN:OD1 | 1.85 | 0.76 |
| 2:C:71:TYR:HE2 | 2:C:95:THR:HB | 1.50 | 0.76 |
| 1:A:270:PHE:CZ | 1:A:315:LEU:HD13 | 2.20 | 0.75 |
| 1:A:25:VAL:HG12 | 1:A:26:THR:H | 1.48 | 0.75 |
| 1:A:225:LYS:HB2 | 1:A:228:PHE:CD1 | 2.20 | 0.75 |
| 2:B:478:SER:C | 2:B:479:LEU:HD12 | 2.05 | 0.75 |
| 2:B:6:LEU:HB3 | 2:B:130:MET:CE | 2.16 | 0.75 |
| 1:A:352:LYS:CE | 2:C:468:LEU:H | 1.99 | 0.75 |
| 1:A:427:ARG:HB3 | 1:A:447:ILE:CD1 | 2.14 | 0.75 |
| 1:A:78:ILE:HD12 | 1:A:111:LEU:HD21 | 1.68 | 0.75 |
| 1:A:133:ASN:ND2 | 2:B:430:ALA:HA | 2.02 | 0.75 |
| 2:B:222:ARG:CD | 2:B:246:LEU:HB2 | 2.17 | 0.75 |
| 2:C:113:LEU:O | 2:C:113:LEU:HD23 | 1.86 | 0.75 |
| 1:A:294:ASN:O | 1:A:358:LYS:HD2 | 1.86 | 0.75 |
| 2:C:131:TYR:OH | 2:C:224:LEU:HG | 1.87 | 0.75 |
| 1:A:90:VAL:HG13 | 1:A:132:ARG:CD | 2.16 | 0.75 |
| 2:B:71:TYR:HE2 | 2:B:95:THR:HB | 1.52 | 0.75 |
| 2:C:6:LEU:HB3 | 2:C:130:MET:CE | 2.17 | 0.75 |
| 2:C:100:PRO:O | 2:C:103:ILE:HG22 | 1.86 | 0.75 |
| 2:C:471:LYS:CD | 2:C:472:ASP:H | 2.00 | 0.75 |
| 1:A:42:PRO:HB2 | 1:A:101:GLU:OE2 | 1.87 | 0.75 |
| 1:A:333:TYR:O | 1:A:336:ILE:HG22 | 1.87 | 0.75 |
| 2:B:305:ARG:HD3 | 2:B:410:HIS:CE1 | 2.22 | 0.75 |
| 2:C:1:MET:SD | 2:C:132:GLU:HB2 | 2.26 | 0.75 |
| 1:A:139:SER:HB2 | 2:B:466:SER:CB | 2.16 | 0.75 |
| 2:B:20:GLY:CA | 2:B:102:GLN:HG3 | 2.15 | 0.75 |
| 5:C:530:SAM:HE2 | 4:E:6:DA:H61 | 1.49 | 0.75 |
| 2:B:128:GLY:HA3 | 2:B:231:LEU:CD2 | 2.18 | 0.74 |
| 1:A:137:SER:HB3 | 2:B:432:SER:HB3 | 1.69 | 0.74 |
| 2:B:9:LYS:NZ | 2:B:113:LEU:HB2 | 2.01 | 0.74 |
| 1:A:239:LEU:HD22 | 1:A:241:SER:N | 1.98 | 0.74 |
| 2:C:305:ARG:HD3 | 2:C:410:HIS:CE1 | 2.22 | 0.74 |
| 1:A:118:PHE:HZ | 1:A:166:LYS:HE3 | 1.52 | 0.74 |
| 1:A:253:LEU:O | 1:A:317:PRO:HD2 | 1.87 | 0.74 |
| 2:B:6:LEU:HB2 | 2:B:117:ASN:CB | 2.18 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:91:HIS:HB3 | 2:B:222:ARG:HH21 | 1.51 | 0.74 |
| 2:C:179:ALA:O | 2:C:183:ILE:HD13 | 1.85 | 0.74 |
| 3:D:16:DG:H2" | 3:D:17:DC:C5 | 2.22 | 0.74 |
| 1:A:148:LYS:HG3 | 1:A:149:PRO:HD2 | 1.69 | 0.74 |
| 2:C:334:LEU:HD12 | 2:C:356:PHE:O | 1.86 | 0.74 |
| 1:A:19:THR:HG21 | 1:A:22:ILE:CD1 | 2.17 | 0.74 |
| 1:A:176:LEU:O | 1:A:179:VAL:HG22 | 1.86 | 0.74 |
| 1:A:371:LEU:HD23 | 1:A:371:LEU:H | 1.52 | 0.74 |
| 4:E:12:DA:H2" | 4:E:13:DC:C5' | 2.17 | 0.74 |
| 1:A:49:ILE:HG23 | 1:A:94:ALA:HB2 | 1.69 | 0.74 |
| 1:A:234:GLU:O | 4:E:2:DT:OP2 | 2.06 | 0.74 |
| 1:A:272:GLU:O | 1:A:275:GLU:HG2 | 1.87 | 0.74 |
| 1:A:309:LEU:CD2 | 1:A:310:GLN:H | 2.01 | 0.74 |
| 2:C:222:ARG:CD | 2:C:246:LEU:HB2 | 2.17 | 0.74 |
| 1:A:255:ILE:HD13 | 3:D:14:DG:H5' | 1.69 | 0.73 |
| 1:A:319:LYS:HG3 | 3:D:15:DT:OP1 | 1.88 | 0.73 |
| 1:A:334:ILE:HG12 | 1:A:338:PHE:HE2 | 1.53 | 0.73 |
| 2:B:131:TYR:OH | 2:B:224:LEU:HG | 1.87 | 0.73 |
| 2:C:91:HIS:HB3 | 2:C:222:ARG:HH21 | 1.51 | 0.73 |
| 1:A:252:ILE:CD1 | 1:A:315:LEU:HD22 | 2.18 | 0.73 |
| 1:A:253:LEU:CD1 | 1:A:263:VAL:HG21 | 2.18 | 0.73 |
| 2:C:24:TYR:CD2 | 2:C:27:TYR:HE2 | 2.06 | 0.73 |
| 1:A:112:ARG:HD2 | 1:A:119:SER:OG | 1.88 | 0.73 |
| 1:A:142:ALA:HB1 | 2:B:312:ASP:HB3 | 1.70 | 0.73 |
| 1:A:133:ASN:OD1 | 2:B:431:ASP:HB2 | 1.89 | 0.73 |
| 1:A:285:ASP:HB3 | 1:A:308:LYS:CG | 2.17 | 0.73 |
| 1:A:26:THR:CG2 | 1:A:69:GLU:HG2 | 2.18 | 0.73 |
| 1:A:62:VAL:HG12 | 1:A:64:LYS:N | 2.04 | 0.73 |
| 1:A:250:HIS:O | 1:A:269:ARG:HB3 | 1.88 | 0.73 |
| 1:A:415:ALA:CB | 2:B:492:GLU:HG3 | 2.17 | 0.73 |
| 2:B:6:LEU:HB2 | 2:B:117:ASN:HB2 | 1.70 | 0.73 |
| 2:B:24:TYR:CD2 | 2:B:27:TYR:HE2 | 2.06 | 0.73 |
| 2:B:100:PRO:O | 2:B:103:ILE:HG22 | 1.86 | 0.73 |
| 2:B:350:VAL:CG1 | 3:D:6:DA:C4' | 2.65 | 0.73 |
| 2:B:471:LYS:CD | 2:B:472:ASP:H | 2.00 | 0.73 |
| 1:A:123:ALA:O | 1:A:126:THR:HG22 | 1.89 | 0.73 |
| 1:A:84:SER:HA | 1:A:146:ASN:HD22 | 1.52 | 0.73 |
| 2:B:435:ASN:HD21 | 2:B:467:TRP:HB2 | 1.52 | 0.73 |
| 1:A:32:ALA:HB3 | 1:A:35:TYR:CE2 | 2.22 | 0.73 |
| 1:A:175:LEU:CG | 1:A:406:VAL:HG22 | 2.16 | 0.73 |
| 1:A:407:ASN:O | 1:A:410:THR:HG22 | 1.88 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:45:ARG:HA | 1:A:104:PHE:HE1 | 1.53 | 0.73 |
| 1:A:186:PHE:HD1 | 1:A:395:ILE:HG21 | 1.53 | 0.73 |
| 2:B:512:GLU:HB2 | 2:B:515:LEU:CD2 | 2.10 | 0.73 |
| 2:C:263:VAL:HG23 | 2:C:300:LEU:HD21 | 1.71 | 0.73 |
| 2:C:275:THR:HG21 | 5:C:530:SAM:N6 | 2.04 | 0.73 |
| 1:A:154:LEU:HD23 | 1:A:154:LEU:O | 1.89 | 0.72 |
| 1:A:271:LEU:HD23 | 1:A:272:GLU:H | 1.53 | 0.72 |
| 2:C:6:LEU:HB2 | 2:C:117:ASN:CB | 2.19 | 0.72 |
| 2:B:275:THR:HG21 | 5:B:530:SAM:N6 | 2.05 | 0.72 |
| 2:C:128:GLY:HA3 | 2:C:231:LEU:CD2 | 2.17 | 0.72 |
| 1:A:196:PHE:CE1 | 1:A:200:VAL:HG21 | 2.23 | 0.72 |
| 2:C:220:GLY:O | 2:C:224:LEU:HD13 | 1.89 | 0.72 |
| 1:A:6:LEU:HD13 | 1:A:12:ILE:CD1 | 2.18 | 0.72 |
| 1:A:349:ASN:HD21 | 2:C:467:TRP:HA | 1.53 | 0.72 |
| 2:B:220:GLY:O | 2:B:224:LEU:HD13 | 1.89 | 0.72 |
| 2:C:69:GLN:O | 2:C:72:ARG:HG2 | 1.88 | 0.72 |
| 2:C:149:TYR:CD1 | 5:C:530:SAM:O3' | 2.38 | 0.72 |
| 1:A:285:ASP:CG | 1:A:308:LYS:HG2 | 2.10 | 0.72 |
| 2:B:433:GLU:HA | 2:B:436:LYS:HB2 | 1.72 | 0.72 |
| 2:B:1:MET:HE3 | 2:B:132:GLU:HB2 | 1.70 | 0.72 |
| 2:B:263:VAL:HG23 | 2:B:300:LEU:HD21 | 1.71 | 0.72 |
| 5:B:530:SAM:HE2 | 3:D:6:DA:N6 | 2.04 | 0.72 |
| 1:A:111:LEU:HD22 | 1:A:112:ARG:HH22 | 1.55 | 0.72 |
| 1:A:231:ILE:O | 1:A:323:ALA:HA | 1.90 | 0.72 |
| 2:B:362:VAL:HG21 | 2:B:412:LEU:HD11 | 1.71 | 0.72 |
| 2:C:146:ALA:O | 2:C:149:TYR:HD2 | 1.71 | 0.72 |
| 1:A:78:ILE:HG13 | 1:A:111:LEU:HD23 | 1.70 | 0.72 |
| 1:A:253:LEU:HD22 | 1:A:320:LEU:HD12 | 1.72 | 0.72 |
| 1:A:257:SER:HB2 | 1:A:266:ASN:ND2 | 2.05 | 0.71 |
| 1:A:330:LEU:HD22 | 1:A:333:TYR:H | 1.54 | 0.71 |
| 1:A:339:SER:HA | 1:A:344:ARG:NH2 | 2.05 | 0.71 |
| 2:B:92:ASN:CB | 2:B:219:PRO:HB3 | 2.20 | 0.71 |
| 2:C:276:ASN:ND2 | 2:C:278:THR:HG23 | 2.04 | 0.71 |
| 1:A:331:PRO:O | 1:A:334:ILE:HG22 | 1.90 | 0.71 |
| 1:A:293:TYR:CB | 1:A:319:LYS:HD2 | 2.20 | 0.71 |
| 1:A:315:LEU:HD23 | 1:A:316:TYR:H | 1.53 | 0.71 |
| 1:A:330:LEU:CD1 | 1:A:379:ALA:HA | 2.20 | 0.71 |
| 2:C:92:ASN:CB | 2:C:219:PRO:HB3 | 2.20 | 0.71 |
| 2:C:362:VAL:HG21 | 2:C:412:LEU:HD11 | 1.72 | 0.71 |
| 1:A:137:SER:CB | 2:B:432:SER:HB3 | 2.20 | 0.71 |
| 1:A:288:LEU:HD11 | 1:A:303:CYS:SG | 2.31 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:350:VAL:HG11 | 3:D:6:DA:H4' | 1.71 | 0.71 |
| 2:C:90:PHE:HA | 2:C:93:VAL:HG11 | 1.73 | 0.71 |
| 1:A:388:LEU:HD23 | 1:A:388:LEU:O | 1.90 | 0.71 |
| 1:A:119:SER:O | 1:A:122:ILE:HG22 | 1.91 | 0.71 |
| 1:A:353:THR:HG23 | 2:C:351:LYS:CE | 2.20 | 0.71 |
| 2:C:322:THR:HA | 2:C:325:ARG:NE | 2.03 | 0.71 |
| 1:A:29:LYS:HE3 | 1:A:31:GLN:HB3 | 1.72 | 0.71 |
| 1:A:197:ARG:HD3 | 1:A:341:PRO:HD2 | 1.71 | 0.71 |
| 1:A:28:LYS:HG3 | 1:A:65:ASN:OD1 | 1.90 | 0.71 |
| 1:A:253:LEU:HB2 | 1:A:314:LEU:HD11 | 1.73 | 0.71 |
| 1:A:289:LEU:HD12 | 1:A:320:LEU:HD21 | 1.73 | 0.71 |
| 2:B:399:GLN:O | 2:B:402:GLU:HG2 | 1.90 | 0.71 |
| 2:B:439:ASP:HA | 2:B:485:LEU:HD23 | 1.73 | 0.71 |
| 2:C:399:GLN:HB2 | 2:C:400:PRO:HD3 | 1.72 | 0.71 |
| 1:A:15:VAL:HG23 | 1:A:155:ILE:HG23 | 1.71 | 0.71 |
| 1:A:111:LEU:HD22 | 1:A:112:ARG:NH2 | 2.05 | 0.71 |
| 1:A:295:GLY:HA3 | 1:A:358:LYS:HA | 1.71 | 0.71 |
| 1:A:357:GLN:OE1 | 1:A:358:LYS:HG2 | 1.91 | 0.71 |
| 2:B:245:ARG:NH2 | 2:B:253:ASP:HB3 | 2.06 | 0.71 |
| 2:B:39:MET:HA | 2:B:39:MET:HE2 | 1.73 | 0.71 |
| 1:A:35:TYR:HD1 | 1:A:65:ASN:HA | 1.53 | 0.70 |
| 1:A:212:LYS:HB3 | 1:A:215:ASN:O | 1.91 | 0.70 |
| 1:A:319:LYS:CD | 3:D:15:DT:OP2 | 2.39 | 0.70 |
| 2:C:170:VAL:H | 2:C:261:HIS:HD2 | 1.39 | 0.70 |
| 2:B:3:ASN:HB2 | 2:B:7:VAL:HB | 1.73 | 0.70 |
| 5:B:530:SAM:HE3 | 3:D:6:DA:H62 | 1.52 | 0.70 |
| 2:C:6:LEU:HB2 | 2:C:117:ASN:HB2 | 1.72 | 0.70 |
| 1:A:270:PHE:CZ | 1:A:275:GLU:HB3 | 2.26 | 0.70 |
| 1:A:319:LYS:HG3 | 3:D:15:DT:P | 2.31 | 0.70 |
| 2:B:90:PHE:HA | 2:B:93:VAL:HG11 | 1.73 | 0.70 |
| 2:C:5:ASP:CB | 2:C:116:TYR:HE2 | 2.05 | 0.70 |
| 1:A:294:ASN:ND2 | 3:D:14:DG:H8 | 1.88 | 0.70 |
| 2:B:350:VAL:HG11 | 3:D:6:DA:C1' | 2.22 | 0.70 |
| 1:A:78:ILE:HG22 | 1:A:96:GLN:HG2 | 1.74 | 0.70 |
| 1:A:144:ILE:CG2 | 1:A:146:ASN:H | 2.05 | 0.70 |
| 1:A:193:LEU:HG | 1:A:388:LEU:CD1 | 2.11 | 0.70 |
| 1:A:232:LEU:CD2 | 1:A:321:ILE:HD11 | 2.22 | 0.70 |
| 2:B:6:LEU:CB | 2:B:130:MET:HE3 | 2.20 | 0.70 |
| 2:B:69:GLN:OE1 | 2:C:76:VAL:HG13 | 1.92 | 0.70 |
| 2:C:321:GLY:O | 2:C:325:ARG:HG3 | 1.91 | 0.70 |
| 1:A:197:ARG:NE | 1:A:340:SER:HA | 2.07 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:293:TYR:CD1 | 1:A:319:LYS:HD3 | 2.26 | 0.70 |
| 2:B:5:ASP:CB | 2:B:116:TYR:HE2 | 2.05 | 0.70 |
| 2:B:399:GLN:HB2 | 2:B:400:PRO:HD3 | 1.72 | 0.70 |
| 2:C:6:LEU:CB | 2:C:130:MET:HE3 | 2.22 | 0.70 |
| 1:A:252:ILE:HA | 1:A:315:LEU:O | 1.92 | 0.69 |
| 2:C:245:ARG:NH2 | 2:C:253:ASP:HB3 | 2.06 | 0.69 |
| 2:C:399:GLN:O | 2:C:402:GLU:HG2 | 1.90 | 0.69 |
| 2:B:147:GLY:HA3 | 2:B:346:TYR:CG | 2.28 | 0.69 |
| 1:A:282:LYS:O | 1:A:283:LEU:HD23 | 1.92 | 0.69 |
| 2:B:28:VAL:HB | 2:B:131:TYR:CE1 | 2.27 | 0.69 |
| 1:A:20:THR:CG2 | 1:A:111:LEU:HB2 | 2.23 | 0.69 |
| 2:B:339:ARG:HD3 | 2:B:381:ARG:CZ | 2.23 | 0.69 |
| 1:A:28:LYS:HD3 | 1:A:28:LYS:N | 2.04 | 0.69 |
| 1:A:144:ILE:HG12 | 2:B:316:PHE:CZ | 2.26 | 0.69 |
| 1:A:175:LEU:HD13 | 1:A:175:LEU:O | 1.92 | 0.69 |
| 1:A:209:LEU:HB3 | 1:A:216:PHE:CZ | 2.27 | 0.69 |
| 2:C:149:TYR:O | 5:C:530:SAM:HB2 | 1.93 | 0.69 |
| 2:C:222:ARG:HD3 | 2:C:246:LEU:HB2 | 1.75 | 0.69 |
| 2:C:269:PHE:CB | 4:E:6:DA:C8 | 2.73 | 0.69 |
| 1:A:270:PHE:CE1 | 1:A:315:LEU:HD13 | 2.28 | 0.69 |
| 1:A:345:ASN:HA | 2:C:469:LYS:CE | 2.22 | 0.69 |
| 1:A:352:LYS:HE3 | 2:C:466:SER:HB3 | 1.75 | 0.69 |
| 1:A:362:GLY:O | 1:A:365:ILE:HG22 | 1.93 | 0.69 |
| 2:B:170:VAL:H | 2:B:261:HIS:HD2 | 1.39 | 0.69 |
| 2:C:257:LEU:CD1 | 2:C:258:PRO:HD2 | 2.21 | 0.69 |
| 1:A:341:PRO:HA | 1:A:344:ARG:HG2 | 1.75 | 0.69 |
| 2:B:146:ALA:O | 2:B:149:TYR:CD2 | 2.45 | 0.69 |
| 1:A:70:SER:OG | 3:D:1:DG:H3' | 1.93 | 0.69 |
| 1:A:349:ASN:HB2 | 2:C:431:ASP:N | 2.08 | 0.69 |
| 2:B:222:ARG:HD3 | 2:B:246:LEU:HB2 | 1.74 | 0.69 |
| 2:C:110:MET:O | 2:C:113:LEU:HD22 | 1.93 | 0.69 |
| 1:A:39:ASP:CB | 1:A:60:VAL:HG12 | 2.20 | 0.68 |
| 2:C:147:GLY:HA3 | 2:C:346:TYR:CG | 2.27 | 0.68 |
| 1:A:14:PRO:O | 1:A:17:THR:HG22 | 1.93 | 0.68 |
| 1:A:193:LEU:O | 1:A:193:LEU:HD23 | 1.92 | 0.68 |
| 1:A:250:HIS:CE1 | 1:A:282:LYS:HE3 | 2.28 | 0.68 |
| 1:A:44:ILE:HG12 | 1:A:102:CYS:O | 1.93 | 0.68 |
| 1:A:80:ILE:CD1 | 1:A:107:PHE:HD2 | 2.06 | 0.68 |
| 2:C:135:LEU:O | 2:C:135:LEU:HD23 | 1.93 | 0.68 |
| 1:A:49:ILE:HG13 | 1:A:107:PHE:CE2 | 2.27 | 0.68 |
| 1:A:75:PRO:CG | 1:A:111:LEU:HD11 | 2.24 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:118:PHE:HZ | 1:A:162:LEU:HD11 | 1.57 | 0.68 |
| 1:A:270:PHE:CD2 | 1:A:274:SER:HB3 | 2.27 | 0.68 |
| 1:A:345:ASN:HA | 2:C:469:LYS:HE2 | 1.76 | 0.68 |
| 2:B:28:VAL:HG23 | 2:B:224:LEU:HD21 | 1.75 | 0.68 |
| 1:A:75:PRO:HG2 | 1:A:111:LEU:CD2 | 2.21 | 0.68 |
| 1:A:255:ILE:HG21 | 3:D:14:DG:H5' | 1.76 | 0.68 |
| 2:B:110:MET:O | 2:B:113:LEU:HD22 | 1.93 | 0.68 |
| 2:C:440:GLN:OE1 | 2:C:440:GLN:O | 2.12 | 0.68 |
| 1:A:198:GLN:OE1 | 1:A:198:GLN:O | 2.12 | 0.68 |
| 2:B:135:LEU:HD23 | 2:B:135:LEU:O | 1.93 | 0.68 |
| 2:C:28:VAL:HB | 2:C:131:TYR:CE1 | 2.27 | 0.68 |
| 2:C:28:VAL:HG23 | 2:C:224:LEU:HD21 | 1.75 | 0.68 |
| 1:A:232:LEU:HD21 | 1:A:321:ILE:HD11 | 1.76 | 0.68 |
| 1:A:73:ILE:HG23 | 1:A:100:PHE:HB3 | 1.75 | 0.68 |
| 1:A:283:LEU:HD11 | 1:A:316:TYR:HE1 | 1.55 | 0.68 |
| 1:A:79:VAL:HB | 1:A:110:VAL:CG1 | 2.24 | 0.68 |
| 2:B:276:ASN:ND2 | 2:B:278:THR:HG23 | 2.04 | 0.68 |
| 1:A:25:VAL:O | 1:A:105:GLY:HA2 | 1.93 | 0.67 |
| 1:A:236:ARG:HG2 | 1:A:237:ASN:N | 2.09 | 0.67 |
| 1:A:292:ARG:HB3 | 1:A:319:LYS:O | 1.93 | 0.67 |
| 2:B:1:MET:CE | 2:B:132:GLU:HB2 | 2.24 | 0.67 |
| 1:A:35:TYR:HB3 | 1:A:65:ASN:CG | 2.14 | 0.67 |
| 1:A:164:GLU:O | 1:A:167:ILE:HG22 | 1.94 | 0.67 |
| 1:A:252:ILE:HG22 | 1:A:268:ILE:O | 1.95 | 0.67 |
| 2:B:149:TYR:O | 5:B:530:SAM:HB2 | 1.94 | 0.67 |
| 1:A:130:LEU:HD23 | 1:A:130:LEU:O | 1.95 | 0.67 |
| 1:A:293:TYR:O | 1:A:294:ASN:HB3 | 1.95 | 0.67 |
| 2:C:269:PHE:HB3 | 4:E:6:DA:H5" | 1.76 | 0.67 |
| 2:C:439:ASP:HA | 2:C:485:LEU:HD23 | 1.75 | 0.67 |
| 1:A:209:LEU:CD2 | 1:A:216:PHE:HE2 | 2.00 | 0.67 |
| 2:B:218:VAL:HG12 | 2:B:220:GLY:H | 1.60 | 0.67 |
| 2:C:9:LYS:HZ1 | 2:C:113:LEU:HB2 | 1.60 | 0.67 |
| 2:C:322:THR:CB | 2:C:325:ARG:HH21 | 2.07 | 0.67 |
| 1:A:25:VAL:HG12 | 1:A:26:THR:N | 2.10 | 0.67 |
| 1:A:193:LEU:CG | 1:A:388:LEU:HD13 | 2.12 | 0.67 |
| 1:A:292:ARG:NH1 | 4:E:3:DT:H72 | 2.09 | 0.67 |
| 2:B:380:LEU:O | 2:B:384:MET:HG3 | 1.95 | 0.67 |
| 2:B:481:GLU:O | 2:B:484:VAL:HG22 | 1.95 | 0.67 |
| 1:A:292:ARG:HH12 | 4:E:3:DT:H71 | 1.59 | 0.66 |
| 2:B:440:GLN:OE1 | 2:B:440:GLN:O | 2.12 | 0.66 |
| 2:C:22:VAL:HG22 | 2:C:96:THR:OG1 | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:17:DC:H2" | 3:D:18:DA:N7 | 2.10 | 0.66 |
| 1:A:152:PHE:O | 1:A:155:ILE:HG22 | 1.94 | 0.66 |
| 1:A:232:LEU:CD1 | 1:A:321:ILE:HD11 | 2.25 | 0.66 |
| 1:A:349:ASN:HB3 | 2:C:432:SER:HB3 | 1.76 | 0.66 |
| 3:D:16:DG:H2" | 3:D:17:DC:C6 | 2.31 | 0.66 |
| 1:A:25:VAL:CG1 | 1:A:71:GLN:HG3 | 2.24 | 0.66 |
| 1:A:316:TYR:CD2 | 1:A:320:LEU:HB3 | 2.30 | 0.66 |
| 2:C:486:ALA:HB3 | 2:C:489:ALA:CB | 2.26 | 0.66 |
| 1:A:77:ASP:HA | 1:A:95:HIS:CE1 | 2.30 | 0.66 |
| 2:C:380:LEU:O | 2:C:384:MET:HG3 | 1.94 | 0.66 |
| 2:C:486:ALA:HB1 | 2:C:488:GLU:OE2 | 1.95 | 0.66 |
| 2:B:339:ARG:HA | 2:B:353:ASN:HD22 | 1.59 | 0.66 |
| 2:B:486:ALA:HB1 | 2:B:488:GLU:OE2 | 1.95 | 0.66 |
| 2:C:39:MET:HE2 | 2:C:39:MET:HA | 1.76 | 0.66 |
| 1:A:112:ARG:CB | 1:A:117:ILE:HG23 | 2.24 | 0.66 |
| 1:A:204:ALA:HB3 | 1:A:218:PRO:HG3 | 1.76 | 0.66 |
| 1:A:248:VAL:HG12 | 1:A:249:GLY:N | 2.11 | 0.66 |
| 1:A:352:LYS:CE | 2:C:466:SER:HB3 | 2.25 | 0.66 |
| 2:B:257:LEU:CD1 | 2:B:258:PRO:HD2 | 2.21 | 0.66 |
| 1:A:142:ALA:HB1 | 2:B:312:ASP:O | 1.96 | 0.66 |
| 1:A:233:THR:CG2 | 1:A:322:ARG:HB3 | 2.26 | 0.66 |
| 1:A:28:LYS:HZ1 | 1:A:43:LEU:HD21 | 1.61 | 0.66 |
| 2:B:148:GLN:O | 5:B:530:SAM:HE3 | 1.96 | 0.66 |
| 2:B:350:VAL:HG11 | 3:D:6:DA:H1' | 1.78 | 0.66 |
| 1:A:198:GLN:OE1 | 1:A:198:GLN:C | 2.33 | 0.65 |
| 1:A:372:LEU:HD13 | 1:A:373:PRO:O | 1.96 | 0.65 |
| 2:C:344:ILE:HG13 | 2:C:345:PHE:CD1 | 2.31 | 0.65 |
| 2:C:481:GLU:O | 2:C:484:VAL:HG22 | 1.95 | 0.65 |
| 1:A:196:PHE:O | 1:A:200:VAL:HG23 | 1.95 | 0.65 |
| 1:A:289:LEU:HD21 | 1:A:320:LEU:HD11 | 1.78 | 0.65 |
| 1:A:345:ASN:HA | 2:C:469:LYS:NZ | 2.11 | 0.65 |
| 1:A:250:HIS:CD2 | 1:A:270:PHE:HE1 | 2.14 | 0.65 |
| 1:A:282:LYS:HE2 | 1:A:313:ASN:OD1 | 1.96 | 0.65 |
| 2:C:6:LEU:HG | 2:C:10:LEU:CD1 | 2.26 | 0.65 |
| 2:C:163:LEU:HG | 2:C:262:ILE:HG21 | 1.79 | 0.65 |
| 1:A:230:SER:OG | 1:A:323:ALA:HB1 | 1.96 | 0.65 |
| 1:A:305:LEU:HD23 | 1:A:306:LEU:N | 2.11 | 0.65 |
| 1:A:352:LYS:HG3 | 2:C:466:SER:HB3 | 1.77 | 0.65 |
| 2:B:344:ILE:HG13 | 2:B:345:PHE:CD1 | 2.32 | 0.65 |
| 2:C:24:TYR:HB3 | 2:C:138:ASN:ND2 | 2.10 | 0.65 |
| 1:A:46:ALA:HB1 | 4:E:14:DG:H5' | 1.76 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:339:ARG:HA | 2:C:353:ASN:HD22 | 1.62 | 0.65 |
| 2:B:22:VAL:HG22 | 2:B:96:THR:OG1 | 1.95 | 0.65 |
| 2:B:269:PHE:CD2 | 2:B:311:PRO:HB3 | 2.31 | 0.65 |
| 2:C:5:ASP:HB3 | 2:C:116:TYR:HE2 | 1.61 | 0.65 |
| 2:C:71:TYR:CE2 | 2:C:95:THR:HB | 2.31 | 0.65 |
| 2:C:269:PHE:HB2 | 4:E:6:DA:N9 | 2.10 | 0.65 |
| 1:A:10:TRP:N | 1:A:10:TRP:HE3 | 1.93 | 0.65 |
| 1:A:44:ILE:HD11 | 1:A:103:SER:HB2 | 1.79 | 0.65 |
| 1:A:265:GLN:HG3 | 1:A:269:ARG:NH2 | 1.98 | 0.65 |
| 2:C:218:VAL:HG12 | 2:C:220:GLY:H | 1.60 | 0.65 |
| 1:A:410:THR:O | 1:A:413:ILE:HG22 | 1.96 | 0.65 |
| 1:A:20:THR:O | 1:A:21:LEU:HD23 | 1.97 | 0.65 |
| 1:A:355:SER:H | 2:C:312:ASP:CB | 2.10 | 0.65 |
| 2:B:90:PHE:C | 2:B:93:VAL:HG13 | 2.17 | 0.65 |
| 2:B:448:ARG:HD3 | 2:B:467:TRP:CD2 | 2.32 | 0.65 |
| 1:A:39:ASP:HB2 | 1:A:62:VAL:HG22 | 1.78 | 0.64 |
| 1:A:61:PHE:CZ | 1:A:66:LEU:HA | 2.32 | 0.64 |
| 2:B:24:TYR:HB3 | 2:B:138:ASN:ND2 | 2.10 | 0.64 |
| 2:C:28:VAL:CG2 | 2:C:224:LEU:HD21 | 2.27 | 0.64 |
| 1:A:70:SER:OG | 3:D:1:DG:C2' | 2.45 | 0.64 |
| 1:A:140:ALA:HB1 | 2:B:351:LYS:NZ | 2.13 | 0.64 |
| 1:A:164:GLU:HG3 | 1:A:423:THR:CA | 2.27 | 0.64 |
| 1:A:300:VAL:HG12 | 1:A:301:GLY:N | 2.12 | 0.64 |
| 2:B:5:ASP:HB3 | 2:B:116:TYR:HE2 | 1.61 | 0.64 |
| 2:C:90:PHE:C | 2:C:93:VAL:HG13 | 2.17 | 0.64 |
| 2:B:29:ASN:HD22 | 2:B:224:LEU:CD1 | 2.11 | 0.64 |
| 2:C:269:PHE:CE1 | 4:E:6:DA:C6 | 2.85 | 0.64 |
| 2:C:442:LEU:HG | 2:C:448:ARG:HH12 | 1.62 | 0.64 |
| 1:A:282:LYS:HE2 | 1:A:313:ASN:CG | 2.18 | 0.64 |
| 2:B:440:GLN:OE1 | 2:B:440:GLN:C | 2.36 | 0.64 |
| 1:A:261:GLY:O | 1:A:263:VAL:HG13 | 1.98 | 0.64 |
| 1:A:330:LEU:HD23 | 1:A:332:GLU:H | 1.62 | 0.64 |
| 2:B:106:LEU:CD2 | 2:B:110:MET:HE3 | 2.28 | 0.64 |
| 2:B:229:CYS:HB3 | 2:B:234:ILE:HB | 1.80 | 0.64 |
| 2:B:269:PHE:CE1 | 3:D:6:DA:C6 | 2.85 | 0.64 |
| 2:C:216:GLU:O | 2:C:246:LEU:HD22 | 1.98 | 0.64 |
| 1:A:214:ARG:HD2 | 1:A:369:VAL:CG1 | 2.28 | 0.64 |
| 1:A:248:VAL:HG11 | 1:A:269:ARG:HB2 | 1.79 | 0.64 |
| 2:B:269:PHE:CB | 3:D:6:DA:C8 | 2.76 | 0.64 |
| 2:C:6:LEU:HD23 | 2:C:130:MET:CB | 2.27 | 0.64 |
| 2:C:229:CYS:HB3 | 2:C:234:ILE:HB | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:286:GLY:HA2 | 1:A:305:LEU:HD21 | 1.79 | 0.64 |
| 2:C:263:VAL:HG23 | 2:C:300:LEU:CD2 | 2.28 | 0.64 |
| 1:A:28:LYS:HB2 | 1:A:65:ASN:HD21 | 1.63 | 0.63 |
| 1:A:413:ILE:HG12 | 1:A:417:ALA:HB2 | 1.80 | 0.63 |
| 1:A:35:TYR:HE1 | 1:A:68:LYS:HD2 | 1.63 | 0.63 |
| 1:A:44:ILE:HG22 | 1:A:54:PHE:CZ | 2.33 | 0.63 |
| 1:A:70:SER:CB | 3:D:2:DT:C7 | 2.66 | 0.63 |
| 1:A:300:VAL:HG12 | 1:A:301:GLY:H | 1.63 | 0.63 |
| 2:C:448:ARG:HD3 | 2:C:467:TRP:CD2 | 2.33 | 0.63 |
| 1:A:426:TRP:CE3 | 1:A:447:ILE:HB | 2.33 | 0.63 |
| 2:B:6:LEU:HD23 | 2:B:130:MET:CB | 2.28 | 0.63 |
| 2:B:216:GLU:O | 2:B:246:LEU:HD22 | 1.98 | 0.63 |
| 2:C:29:ASN:HD22 | 2:C:224:LEU:CD1 | 2.11 | 0.63 |
| 1:A:15:VAL:O | 1:A:19:THR:HG22 | 1.99 | 0.63 |
| 1:A:175:LEU:HG | 1:A:406:VAL:CG2 | 2.24 | 0.63 |
| 1:A:232:LEU:HD12 | 1:A:365:ILE:HG21 | 1.80 | 0.63 |
| 1:A:265:GLN:HG2 | 1:A:266:ASN:N | 2.13 | 0.63 |
| 2:B:304:GLY:O | 2:B:358:THR:HG23 | 1.99 | 0.63 |
| 2:B:92:ASN:HB3 | 2:B:219:PRO:HB3 | 1.81 | 0.63 |
| 2:C:304:GLY:O | 2:C:358:THR:HG23 | 1.99 | 0.63 |
| 2:C:486:ALA:HB3 | 2:C:489:ALA:HB3 | 1.80 | 0.63 |
| 1:A:115:LYS:O | 1:A:162:LEU:HD23 | 1.99 | 0.63 |
| 1:A:253:LEU:HD23 | 1:A:254:ARG:O | 1.99 | 0.63 |
| 2:B:28:VAL:CG2 | 2:B:224:LEU:HD21 | 2.28 | 0.63 |
| 2:B:24:TYR:HA | 2:B:27:TYR:CD2 | 2.34 | 0.63 |
| 2:C:68:LEU:HD23 | 2:C:68:LEU:O | 1.99 | 0.63 |
| 2:C:440:GLN:OE1 | 2:C:440:GLN:C | 2.36 | 0.63 |
| 2:B:71:TYR:CE2 | 2:B:95:THR:HB | 2.33 | 0.62 |
| 2:B:68:LEU:O | 2:B:68:LEU:HD23 | 1.99 | 0.62 |
| 2:C:263:VAL:CG2 | 2:C:300:LEU:HD21 | 2.30 | 0.62 |
| 1:A:41:LEU:HD23 | 1:A:42:PRO:CD | 2.28 | 0.62 |
| 1:A:188:GLN:NE2 | 1:A:192:ILE:HG13 | 2.14 | 0.62 |
| 2:B:84:LYS:HA | 2:B:87:GLN:HG3 | 1.81 | 0.62 |
| 2:C:84:LYS:HA | 2:C:87:GLN:HG3 | 1.82 | 0.62 |
| 2:C:146:ALA:O | 2:C:149:TYR:CD2 | 2.52 | 0.62 |
| 1:A:9:GLY:C | 1:A:10:TRP:HE3 | 2.02 | 0.62 |
| 1:A:326:THR:HG23 | 1:A:327:LYS:N | 2.13 | 0.62 |
| 1:A:371:LEU:H | 1:A:371:LEU:CD2 | 2.12 | 0.62 |
| 3:D:2:DT:H2" | 3:D:3:DT:H72 | 1.80 | 0.62 |
| 1:A:78:ILE:HA | 1:A:112:ARG:NH1 | 2.13 | 0.62 |
| 1:A:232:LEU:HD11 | 1:A:321:ILE:HD11 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:299:PHE:CZ | 1:A:347:MET:HE2 | 2.34 | 0.62 |
| 2:B:263:VAL:HG23 | 2:B:300:LEU:CD2 | 2.28 | 0.62 |
| 2:B:83:LYS:HD3 | 2:B:83:LYS:N | 2.14 | 0.62 |
| 2:C:55:ARG:NE | 2:C:57:ASP:HB2 | 2.15 | 0.62 |
| 1:A:28:LYS:NZ | 1:A:43:LEU:HD21 | 2.15 | 0.62 |
| 1:A:284:GLN:CD | 1:A:322:ARG:HH22 | 2.03 | 0.62 |
| 1:A:294:ASN:CB | 3:D:14:DG:H5" | 2.29 | 0.62 |
| 1:A:383:ARG:O | 1:A:387:GLN:HG2 | 2.00 | 0.62 |
| 1:A:131:TYR:CE2 | 1:A:135:ILE:HD11 | 2.33 | 0.62 |
| 2:B:149:TYR:O | 5:B:530:SAM:CB | 2.47 | 0.62 |
| 1:A:125:PHE:HE1 | 1:A:418:PHE:HZ | 1.47 | 0.61 |
| 1:A:333:TYR:HA | 1:A:382:VAL:HG22 | 1.81 | 0.61 |
| 2:B:263:VAL:CG2 | 2:B:300:LEU:HD21 | 2.30 | 0.61 |
| 2:C:24:TYR:HA | 2:C:27:TYR:CD2 | 2.34 | 0.61 |
| 2:C:70:PHE:HE2 | 2:C:74:MET:HE1 | 1.65 | 0.61 |
| 2:C:83:LYS:HD3 | 2:C:83:LYS:N | 2.14 | 0.61 |
| 1:A:12:ILE:HD12 | 1:A:12:ILE:N | 2.15 | 0.61 |
| 1:A:157:ILE:O | 1:A:157:ILE:HD12 | 1.99 | 0.61 |
| 1:A:214:ARG:HD2 | 1:A:369:VAL:HG11 | 1.82 | 0.61 |
| 2:B:322:THR:HA | 2:B:325:ARG:NH2 | 2.16 | 0.61 |
| 2:C:92:ASN:HB2 | 2:C:219:PRO:HB3 | 1.82 | 0.61 |
| 1:A:248:VAL:HG13 | 1:A:270:PHE:O | 2.00 | 0.61 |
| 1:A:274:SER:O | 1:A:278:LEU:HD23 | 2.00 | 0.61 |
| 1:A:319:LYS:HE3 | 3:D:15:DT:C4' | 2.27 | 0.61 |
| 2:B:249:THR:O | 2:B:254:GLY:HA3 | 2.01 | 0.61 |
| 2:C:38:LYS:HB2 | 2:C:56:TRP:CZ3 | 2.35 | 0.61 |
| 2:C:92:ASN:HB3 | 2:C:219:PRO:HB3 | 1.81 | 0.61 |
| 1:A:35:TYR:HD1 | 1:A:65:ASN:CA | 2.13 | 0.61 |
| 1:A:186:PHE:CD1 | 1:A:395:ILE:HG21 | 2.35 | 0.61 |
| 1:A:234:GLU:CB | 4:E:2:DT:H3' | 2.30 | 0.61 |
| 1:A:330:LEU:HD23 | 1:A:331:PRO:HD2 | 1.81 | 0.61 |
| 2:C:227:MET:O | 2:C:231:LEU:HD13 | 2.01 | 0.61 |
| 1:A:85:GLY:CA | 4:E:14:DG:C8 | 2.80 | 0.61 |
| 1:A:427:ARG:O | 1:A:447:ILE:HD11 | 2.00 | 0.61 |
| 1:A:217:GLU:CG | 1:A:218:PRO:HD2 | 2.30 | 0.61 |
| 1:A:353:THR:C | 2:C:351:LYS:HE2 | 2.21 | 0.61 |
| 2:B:92:ASN:HB2 | 2:B:219:PRO:HB3 | 1.82 | 0.61 |
| 2:C:215:LEU:CD1 | 2:C:245:ARG:HE | 2.13 | 0.61 |
| 1:A:118:PHE:CE2 | 1:A:162:LEU:HD22 | 2.35 | 0.61 |
| 1:A:270:PHE:HE2 | 1:A:275:GLU:HB3 | 1.63 | 0.61 |
| 2:B:5:ASP:HB3 | 2:B:116:TYR:CE2 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:339:ARG:HH22 | 2:C:464:ASP:HA | 1.66 | 0.61 |
| 1:A:128:SER:O | 1:A:131:TYR:HB3 | 2.01 | 0.61 |
| 2:B:38:LYS:HB2 | 2:B:56:TRP:CZ3 | 2.35 | 0.61 |
| 2:B:486:ALA:HB3 | 2:B:489:ALA:CB | 2.31 | 0.61 |
| 2:C:71:TYR:HE2 | 2:C:75:LEU:HD11 | 1.66 | 0.61 |
| 2:C:149:TYR:O | 5:C:530:SAM:CB | 2.49 | 0.61 |
| 1:A:74:SER:OG | 1:A:78:ILE:HD13 | 2.01 | 0.61 |
| 1:A:78:ILE:HD12 | 1:A:111:LEU:CD2 | 2.30 | 0.61 |
| 1:A:347:MET:CE | 1:A:360:ILE:HD12 | 2.29 | 0.61 |
| 2:B:215:LEU:CD1 | 2:B:245:ARG:HE | 2.13 | 0.61 |
| 1:A:15:VAL:HA | 1:A:18:VAL:HG22 | 1.83 | 0.61 |
| 1:A:209:LEU:HD12 | 1:A:209:LEU:N | 2.16 | 0.61 |
| 2:B:55:ARG:NE | 2:B:57:ASP:HB2 | 2.15 | 0.61 |
| 2:B:315:LEU:O | 2:B:325:ARG:HD3 | 2.01 | 0.61 |
| 2:C:249:THR:O | 2:C:254:GLY:HA3 | 2.01 | 0.61 |
| 1:A:39:ASP:O | 1:A:60:VAL:HG11 | 2.00 | 0.60 |
| 2:C:287:ASN:HB3 | 2:C:290:LEU:HB2 | 1.84 | 0.60 |
| 2:C:456:ARG:O | 2:C:460:SER:HA | 2.00 | 0.60 |
| 1:A:294:ASN:HB2 | 3:D:14:DG:C5' | 2.31 | 0.60 |
| 2:B:35:LEU:O | 2:B:39:MET:HG2 | 2.02 | 0.60 |
| 2:C:93:VAL:CG1 | 2:C:223:ARG:HD3 | 2.21 | 0.60 |
| 1:A:164:GLU:O | 1:A:168:ILE:HG13 | 2.02 | 0.60 |
| 1:A:209:LEU:HG | 1:A:218:PRO:HA | 1.83 | 0.60 |
| 1:A:248:VAL:HG12 | 1:A:249:GLY:H | 1.66 | 0.60 |
| 1:A:297:LEU:O | 1:A:298:GLU:HG2 | 2.01 | 0.60 |
| 2:B:90:PHE:O | 2:B:93:VAL:HG13 | 2.01 | 0.60 |
| 1:A:328:ASP:OD1 | 1:A:375:VAL:HG22 | 2.02 | 0.60 |
| 2:B:287:ASN:HB3 | 2:B:290:LEU:HB2 | 1.84 | 0.60 |
| 2:C:90:PHE:O | 2:C:93:VAL:HG13 | 2.01 | 0.60 |
| 1:A:233:THR:HG22 | 1:A:322:ARG:HB3 | 1.81 | 0.60 |
| 2:B:118:GLY:HA2 | 2:B:123:SER:HB2 | 1.83 | 0.60 |
| 2:C:106:LEU:HD23 | 2:C:106:LEU:O | 2.01 | 0.60 |
| 2:B:106:LEU:O | 2:B:106:LEU:HD23 | 2.02 | 0.60 |
| 2:B:227:MET:O | 2:B:231:LEU:HD13 | 2.00 | 0.60 |
| 1:A:101:GLU:HG2 | 1:A:102:CYS:H | 1.65 | 0.60 |
| 2:C:163:LEU:O | 2:C:163:LEU:HD13 | 2.01 | 0.60 |
| 1:A:143:ASN:ND2 | 3:D:5:DA:P | 2.74 | 0.60 |
| 1:A:160:PRO:CG | 1:A:165:GLN:HG2 | 2.21 | 0.60 |
| 1:A:25:VAL:HB | 1:A:104:PHE:O | 2.02 | 0.60 |
| 1:A:83:SER:CA | 1:A:147:ILE:HG22 | 2.24 | 0.60 |
| 1:A:162:LEU:HD13 | 1:A:162:LEU:O | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:236:ARG:HA | 1:A:318:ASP:CG | 2.22 | 0.60 |
| 1:A:319:LYS:HE2 | 3:D:16:DG:N7 | 2.16 | 0.60 |
| 2:C:244:ILE:N | 2:C:244:ILE:HD12 | 2.17 | 0.60 |
| 2:C:275:THR:HG21 | 5:C:530:SAM:HN61 | 1.67 | 0.60 |
| 1:A:209:LEU:HB3 | 1:A:216:PHE:CE2 | 2.33 | 0.59 |
| 1:A:232:LEU:HD12 | 1:A:365:ILE:CG2 | 2.32 | 0.59 |
| 1:A:357:GLN:CD | 1:A:358:LYS:HG2 | 2.23 | 0.59 |
| 2:B:149:TYR:CD1 | 5:B:530:SAM:O3' | 2.46 | 0.59 |
| 2:C:5:ASP:HB3 | 2:C:116:TYR:CE2 | 2.35 | 0.59 |
| 1:A:46:ALA:HA | 1:A:107:PHE:HZ | 1.65 | 0.59 |
| 2:C:90:PHE:O | 2:C:93:VAL:HG22 | 2.03 | 0.59 |
| 1:A:309:LEU:HD22 | 1:A:310:GLN:H | 1.65 | 0.59 |
| 2:B:90:PHE:O | 2:B:93:VAL:HG22 | 2.03 | 0.59 |
| 2:C:35:LEU:O | 2:C:39:MET:HG2 | 2.02 | 0.59 |
| 2:C:334:LEU:HA | 2:C:357:PHE:HB3 | 1.84 | 0.59 |
| 1:A:263:VAL:HG23 | 1:A:263:VAL:O | 2.03 | 0.59 |
| 1:A:280:ARG:HB3 | 1:A:315:LEU:HD11 | 1.85 | 0.59 |
| 2:B:55:ARG:HE | 2:B:57:ASP:HB2 | 1.67 | 0.59 |
| 2:C:489:ALA:O | 2:C:493:LEU:HD23 | 2.02 | 0.59 |
| 2:B:269:PHE:CD1 | 3:D:6:DA:C6 | 2.90 | 0.59 |
| 2:B:524:PHE:CE2 | 2:B:528:LYS:HD2 | 2.37 | 0.59 |
| 2:C:269:PHE:CD1 | 4:E:6:DA:C4 | 2.90 | 0.59 |
| 1:A:70:SER:OG | 3:D:1:DG:C3' | 2.51 | 0.59 |
| 1:A:349:ASN:HB2 | 2:C:430:ALA:CB | 2.32 | 0.59 |
| 1:A:353:THR:HG23 | 2:C:351:LYS:HE2 | 1.85 | 0.59 |
| 2:B:70:PHE:HE2 | 2:B:74:MET:HE3 | 1.67 | 0.59 |
| 1:A:319:LYS:HZ1 | 3:D:15:DT:H4' | 1.68 | 0.59 |
| 4:E:16:DT:H2" | 4:E:17:DG:N7 | 2.18 | 0.59 |
| 1:A:32:ALA:HB3 | 1:A:35:TYR:HD2 | 1.62 | 0.59 |
| 2:C:269:PHE:CB | 4:E:6:DA:O4' | 2.50 | 0.59 |
| 2:C:524:PHE:CE2 | 2:C:528:LYS:HD2 | 2.37 | 0.59 |
| 1:A:20:THR:HG23 | 1:A:21:LEU:N | 2.17 | 0.59 |
| 1:A:131:TYR:HE1 | 1:A:155:ILE:CD1 | 2.16 | 0.59 |
| 1:A:215:ASN:HD21 | 2:C:492:GLU:CG | 2.14 | 0.59 |
| 1:A:226:LEU:CD2 | 1:A:365:ILE:HG12 | 2.32 | 0.59 |
| 2:B:290:LEU:HD13 | 2:B:324:ILE:HD12 | 1.85 | 0.59 |
| 2:C:269:PHE:CD1 | 4:E:6:DA:C6 | 2.91 | 0.59 |
| 1:A:6:LEU:CD2 | 1:A:10:TRP:HB2 | 2.17 | 0.58 |
| 1:A:83:SER:OG | 1:A:146:ASN:HB3 | 2.02 | 0.58 |
| 1:A:412:SER:CB | 2:B:495:GLN:CD | 2.62 | 0.58 |
| 2:B:76:VAL:HG13 | 2:C:69:GLN:OE1 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:143:ASN:OD1 | 3:D:5:DA:OP2 | 2.20 | 0.58 |
| 1:A:144:ILE:N | 2:B:316:PHE:HZ | 2.00 | 0.58 |
| 1:A:284:GLN:H | 1:A:322:ARG:NH2 | 2.00 | 0.58 |
| 2:B:269:PHE:CE2 | 2:B:311:PRO:HB3 | 2.37 | 0.58 |
| 2:B:334:LEU:HA | 2:B:357:PHE:HB3 | 1.85 | 0.58 |
| 2:B:489:ALA:O | 2:B:493:LEU:HD23 | 2.02 | 0.58 |
| 2:C:72:ARG:HG3 | 2:C:73:LYS:N | 2.18 | 0.58 |
| 1:A:3:ALA:O | 2:B:488:GLU:OE1 | 2.21 | 0.58 |
| 1:A:143:ASN:ND2 | 3:D:5:DA:OP1 | 2.36 | 0.58 |
| 1:A:351:VAL:HG12 | 1:A:352:LYS:O | 2.04 | 0.58 |
| 2:C:6:LEU:HG | 2:C:10:LEU:HD13 | 1.85 | 0.58 |
| 2:C:123:SER:HB3 | 2:C:126:ASP:CG | 2.23 | 0.58 |
| 1:A:49:ILE:CG1 | 1:A:107:PHE:HE2 | 2.13 | 0.58 |
| 1:A:186:PHE:HD1 | 1:A:395:ILE:CG2 | 2.15 | 0.58 |
| 1:A:253:LEU:H | 1:A:316:TYR:HA | 1.68 | 0.58 |
| 1:A:312:GLN:HG2 | 1:A:313:ASN:N | 2.19 | 0.58 |
| 2:B:275:THR:HG21 | 5:B:530:SAM:HN61 | 1.68 | 0.58 |
| 2:C:6:LEU:O | 2:C:10:LEU:HD13 | 2.02 | 0.58 |
| 2:C:494:VAL:HA | 2:C:497:LEU:HD13 | 1.85 | 0.58 |
| 4:E:2:DT:H2" | 4:E:3:DT:H71 | 1.84 | 0.58 |
| 1:A:36:LEU:HD22 | 1:A:36:LEU:N | 2.18 | 0.58 |
| 1:A:139:SER:CB | 2:B:466:SER:HB3 | 2.22 | 0.58 |
| 1:A:225:LYS:HB2 | 1:A:228:PHE:HE1 | 1.66 | 0.58 |
| 2:B:244:ILE:HD12 | 2:B:244:ILE:N | 2.17 | 0.58 |
| 2:B:268:PRO:HD3 | 5:B:530:SAM:C5' | 2.33 | 0.58 |
| 2:C:106:LEU:CD2 | 2:C:110:MET:HE2 | 2.33 | 0.58 |
| 1:A:209:LEU:HB3 | 1:A:217:GLU:O | 2.03 | 0.58 |
| 1:A:345:ASN:HD22 | 2:C:469:LYS:HE2 | 1.67 | 0.58 |
| 2:B:6:LEU:HD23 | 2:B:130:MET:HB2 | 1.86 | 0.58 |
| 2:B:156:ILE:O | 2:B:160:ILE:HD13 | 2.03 | 0.58 |
| 2:B:218:VAL:HG12 | 2:B:220:GLY:N | 2.19 | 0.58 |
| 2:C:118:GLY:HA2 | 2:C:123:SER:HB2 | 1.83 | 0.58 |
| 4:E:1:DG:H2' | 4:E:2:DT:C7 | 2.34 | 0.58 |
| 2:C:55:ARG:HE | 2:C:57:ASP:HB2 | 1.67 | 0.58 |
| 2:C:156:ILE:O | 2:C:160:ILE:HD13 | 2.03 | 0.58 |
| 2:C:268:PRO:HD3 | 5:C:530:SAM:C5' | 2.34 | 0.58 |
| 1:A:231:ILE:HG22 | 1:A:324:ARG:HB3 | 1.84 | 0.58 |
| 1:A:265:GLN:CG | 1:A:269:ARG:HH21 | 2.03 | 0.58 |
| 1:A:345:ASN:HA | 2:C:469:LYS:HZ1 | 1.67 | 0.58 |
| 1:A:348:MET:HE2 | 2:C:469:LYS:HA | 1.85 | 0.58 |
| 1:A:412:SER:CA | 2:B:495:GLN:HG3 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:123:SER:HB3 | 2:B:126:ASP:CG | 2.23 | 0.58 |
| 1:A:11:VAL:HG12 | 1:A:12:ILE:N | 2.19 | 0.58 |
| 1:A:26:THR:HG23 | 1:A:69:GLU:HG2 | 1.84 | 0.58 |
| 1:A:306:LEU:N | 1:A:306:LEU:HD12 | 2.19 | 0.58 |
| 1:A:349:ASN:HB2 | 2:C:430:ALA:HB1 | 1.85 | 0.58 |
| 2:C:17:LEU:HB2 | 2:C:27:TYR:CD1 | 2.39 | 0.58 |
| 1:A:46:ALA:HB3 | 4:E:14:DG:H5' | 1.86 | 0.57 |
| 1:A:279:ASN:HB3 | 4:E:1:DG:OP1 | 2.04 | 0.57 |
| 1:A:294:ASN:ND2 | 3:D:14:DG:H5" | 2.18 | 0.57 |
| 2:C:275:THR:CG2 | 5:C:530:SAM:N6 | 2.67 | 0.57 |
| 2:B:153:ARG:HB3 | 2:B:154:PRO:HD3 | 1.86 | 0.57 |
| 2:C:222:ARG:CZ | 2:C:226:LEU:HD11 | 2.34 | 0.57 |
| 1:A:182:THR:HG21 | 1:A:399:VAL:HG22 | 1.85 | 0.57 |
| 1:A:305:LEU:HD22 | 1:A:306:LEU:O | 2.04 | 0.57 |
| 2:B:39:MET:HA | 2:B:39:MET:CE | 2.33 | 0.57 |
| 2:B:93:VAL:CG1 | 2:B:223:ARG:HD3 | 2.20 | 0.57 |
| 2:B:494:VAL:HA | 2:B:497:LEU:HD13 | 1.85 | 0.57 |
| 2:C:39:MET:HA | 2:C:39:MET:CE | 2.33 | 0.57 |
| 1:A:241:SER:O | 1:A:243:PRO:HD3 | 2.04 | 0.57 |
| 1:A:293:TYR:HE2 | 4:E:5:DC:H41 | 1.52 | 0.57 |
| 2:B:222:ARG:CZ | 2:B:226:LEU:HD11 | 2.34 | 0.57 |
| 2:B:401:PHE:O | 2:B:404:VAL:HG22 | 2.05 | 0.57 |
| 2:C:148:GLN:O | 5:C:530:SAM:CE | 2.52 | 0.57 |
| 1:A:85:GLY:CA | 4:E:14:DG:H8 | 2.15 | 0.57 |
| 1:A:188:GLN:HE22 | 1:A:192:ILE:CG1 | 2.16 | 0.57 |
| 1:A:53:LYS:CE | 1:A:97:HIS:HE1 | 2.17 | 0.57 |
| 1:A:270:PHE:HE2 | 1:A:275:GLU:CA | 2.17 | 0.57 |
| 1:A:355:SER:H | 2:C:312:ASP:HB3 | 1.69 | 0.57 |
| 2:C:122:LYS:HZ1 | 2:C:124:ARG:HG2 | 1.69 | 0.57 |
| 1:A:234:GLU:OE2 | 4:E:3:DT:H71 | 2.03 | 0.57 |
| 1:A:274:SER:O | 1:A:278:LEU:HB2 | 2.04 | 0.57 |
| 2:C:38:LYS:HB2 | 2:C:56:TRP:CH2 | 2.40 | 0.57 |
| 2:C:218:VAL:HG12 | 2:C:220:GLY:N | 2.19 | 0.57 |
| 1:A:233:THR:HG23 | 1:A:316:TYR:OH | 2.04 | 0.57 |
| 2:B:9:LYS:HZ1 | 2:B:113:LEU:HB2 | 1.68 | 0.57 |
| 3:D:10:DC:O2 | 3:D:11:DG:H1' | 2.04 | 0.57 |
| 1:A:74:SER:O | 1:A:100:PHE:HA | 2.05 | 0.57 |
| 1:A:86:SER:OG | 1:A:90:VAL:HB | 2.05 | 0.57 |
| 2:B:106:LEU:HD21 | 2:B:110:MET:HE3 | 1.87 | 0.57 |
| 2:B:148:GLN:O | 5:B:530:SAM:CE | 2.53 | 0.57 |
| 2:B:432:SER:O | 2:B:436:LYS:HB2 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:28:VAL:HG23 | 2:C:29:ASN:N | 2.19 | 0.57 |
| 2:C:290:LEU:HD13 | 2:C:324:ILE:HD12 | 1.87 | 0.57 |
| 1:A:251:PRO:HG3 | 1:A:269:ARG:CZ | 2.35 | 0.56 |
| 2:C:153:ARG:HB3 | 2:C:154:PRO:HD3 | 1.86 | 0.56 |
| 2:B:17:LEU:HB2 | 2:B:27:TYR:CD1 | 2.39 | 0.56 |
| 1:A:222:VAL:HG12 | 1:A:223:PHE:N | 2.18 | 0.56 |
| 1:A:305:LEU:HD23 | 1:A:306:LEU:H | 1.68 | 0.56 |
| 1:A:314:LEU:HD23 | 1:A:314:LEU:C | 2.25 | 0.56 |
| 1:A:346:ALA:HA | 2:C:431:ASP:O | 2.04 | 0.56 |
| 2:C:350:VAL:CG1 | 4:E:6:DA:C4' | 2.83 | 0.56 |
| 1:A:26:THR:HG22 | 1:A:70:SER:HB3 | 1.86 | 0.56 |
| 1:A:45:ARG:CA | 1:A:104:PHE:HE1 | 2.18 | 0.56 |
| 1:A:61:PHE:HE2 | 1:A:66:LEU:HB2 | 1.71 | 0.56 |
| 1:A:412:SER:HB2 | 2:B:495:GLN:NE2 | 2.18 | 0.56 |
| 2:C:34:LEU:HB3 | 2:C:110:MET:SD | 2.44 | 0.56 |
| 2:C:94:SER:H | 2:C:223:ARG:NH1 | 2.04 | 0.56 |
| 2:C:153:ARG:HB3 | 2:C:154:PRO:CD | 2.36 | 0.56 |
| 4:E:1:DG:H2' | 4:E:2:DT:H73 | 1.88 | 0.56 |
| 1:A:33:ILE:HG23 | 1:A:34:ASN:N | 2.20 | 0.56 |
| 1:A:168:ILE:HD11 | 1:A:417:ALA:HB1 | 1.86 | 0.56 |
| 1:A:433:LEU:HD13 | 1:A:443:LEU:CD1 | 2.34 | 0.56 |
| 2:B:28:VAL:HG23 | 2:B:29:ASN:N | 2.19 | 0.56 |
| 2:B:34:LEU:HB3 | 2:B:110:MET:SD | 2.44 | 0.56 |
| 2:B:358:THR:HG22 | 2:B:359:LYS:N | 2.21 | 0.56 |
| 2:C:279:ARG:HH21 | 2:C:281:PHE:HZ | 1.54 | 0.56 |
| 1:A:259:ARG:HD3 | 3:D:14:DG:OP1 | 2.05 | 0.56 |
| 1:A:274:SER:HA | 1:A:278:LEU:HD23 | 1.87 | 0.56 |
| 1:A:302:VAL:HG12 | 1:A:303:CYS:N | 2.20 | 0.56 |
| 2:B:248:ASN:O | 2:B:253:ASP:HB2 | 2.06 | 0.56 |
| 2:C:142:THR:HG23 | 2:C:143:LYS:N | 2.21 | 0.56 |
| 1:A:248:VAL:HG11 | 1:A:269:ARG:C | 2.26 | 0.56 |
| 1:A:319:LYS:NZ | 3:D:15:DT:H4' | 2.20 | 0.56 |
| 1:A:378:GLN:O | 1:A:382:VAL:HG23 | 2.05 | 0.56 |
| 1:A:104:PHE:CE1 | 1:A:107:PHE:CE1 | 2.94 | 0.56 |
| 1:A:239:LEU:HD23 | 1:A:240:SER:N | 2.21 | 0.56 |
| 1:A:444:LEU:HD23 | 1:A:444:LEU:O | 2.06 | 0.56 |
| 2:B:71:TYR:HE2 | 2:B:75:LEU:HD11 | 1.64 | 0.56 |
| 1:A:348:MET:CE | 2:C:470:ASP:H | 2.19 | 0.56 |
| 1:A:26:THR:HG23 | 1:A:69:GLU:CG | 2.35 | 0.55 |
| 2:C:401:PHE:O | 2:C:404:VAL:HG22 | 2.05 | 0.55 |
| 1:A:205:VAL:HG23 | 1:A:205:VAL:O | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:365:ILE:HG23 | 1:A:366:LYS:N | 2.21 | 0.55 |
| 2:C:38:LYS:HD3 | 2:C:56:TRP:CE2 | 2.41 | 0.55 |
| 2:C:103:ILE:HG23 | 2:C:104:THR:N | 2.21 | 0.55 |
| 2:C:440:GLN:CB | 2:C:484:VAL:CG2 | 2.74 | 0.55 |
| 2:C:450:PHE:CZ | 2:C:467:TRP:CZ3 | 2.94 | 0.55 |
| 2:B:62:ARG:HD2 | 2:B:70:PHE:CG | 2.41 | 0.55 |
| 1:A:17:THR:HG23 | 1:A:18:VAL:N | 2.21 | 0.55 |
| 1:A:61:PHE:CE2 | 1:A:66:LEU:HA | 2.41 | 0.55 |
| 1:A:217:GLU:HG3 | 1:A:218:PRO:HD2 | 1.89 | 0.55 |
| 2:B:38:LYS:HD3 | 2:B:56:TRP:CE2 | 2.41 | 0.55 |
| 2:B:63:ILE:N | 2:B:67:GLN:HB2 | 2.21 | 0.55 |
| 1:A:236:ARG:HG2 | 1:A:237:ASN:H | 1.72 | 0.55 |
| 1:A:253:LEU:HD23 | 1:A:253:LEU:C | 2.27 | 0.55 |
| 1:A:255:ILE:HG23 | 1:A:256:SER:N | 2.21 | 0.55 |
| 1:A:291:THR:HG23 | 1:A:291:THR:O | 2.05 | 0.55 |
| 2:B:153:ARG:HB3 | 2:B:154:PRO:CD | 2.36 | 0.55 |
| 1:A:164:GLU:CG | 1:A:423:THR:HA | 2.36 | 0.55 |
| 2:B:275:THR:CG2 | 5:B:530:SAM:N6 | 2.68 | 0.55 |
| 2:B:316:PHE:HB3 | 2:B:462:SER:OG | 2.06 | 0.55 |
| 2:B:338:LEU:HD13 | 2:B:401:PHE:CD1 | 2.42 | 0.55 |
| 2:C:94:SER:H | 2:C:223:ARG:HH12 | 1.55 | 0.55 |
| 2:B:38:LYS:HB2 | 2:B:56:TRP:CH2 | 2.40 | 0.55 |
| 2:B:43:THR:CG2 | 2:B:45:GLN:HB2 | 2.37 | 0.55 |
| 2:B:193:THR:O | 2:B:194:ASN:HB2 | 2.06 | 0.55 |
| 2:C:81:ASP:HB2 | 2:C:83:LYS:NZ | 2.22 | 0.55 |
| 1:A:20:THR:HG22 | 1:A:111:LEU:O | 2.07 | 0.55 |
| 1:A:144:ILE:HG12 | 2:B:316:PHE:CE1 | 2.41 | 0.55 |
| 2:B:215:LEU:HD13 | 2:B:245:ARG:NE | 2.17 | 0.55 |
| 2:C:353:ASN:HD21 | 2:C:381:ARG:NH2 | 2.05 | 0.55 |
| 1:A:25:VAL:HG11 | 1:A:103:SER:O | 2.07 | 0.55 |
| 1:A:78:ILE:HG13 | 1:A:110:VAL:O | 2.06 | 0.55 |
| 1:A:103:SER:HG | 1:A:107:PHE:CB | 2.19 | 0.55 |
| 1:A:431:PRO:O | 1:A:434:ILE:HG12 | 2.05 | 0.55 |
| 2:C:248:ASN:O | 2:C:253:ASP:HB2 | 2.06 | 0.55 |
| 1:A:57:THR:HG23 | 1:A:57:THR:O | 2.07 | 0.55 |
| 1:A:144:ILE:HG23 | 1:A:146:ASN:H | 1.72 | 0.55 |
| 1:A:330:LEU:CD2 | 1:A:332:GLU:H | 2.19 | 0.55 |
| 1:A:345:ASN:HD22 | 2:C:469:LYS:CE | 2.20 | 0.55 |
| 1:A:354:THR:OG1 | 2:C:312:ASP:HB3 | 2.07 | 0.55 |
| 2:B:259:LYS:HB2 | 2:B:301:HIS:CE1 | 2.42 | 0.55 |
| 2:B:442:LEU:HG | 2:B:448:ARG:HH12 | 1.69 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:390:ARG:HG3 | 2:C:391:THR:N | 2.22 | 0.55 |
| 1:A:142:ALA:HB1 | 2:B:312:ASP:CB | 2.36 | 0.54 |
| 1:A:254:ARG:HG2 | 1:A:255:ILE:H | 1.72 | 0.54 |
| 2:B:94:SER:H | 2:B:223:ARG:NH1 | 2.05 | 0.54 |
| 2:C:193:THR:O | 2:C:194:ASN:HB2 | 2.06 | 0.54 |
| 2:C:222:ARG:HD3 | 2:C:246:LEU:CB | 2.37 | 0.54 |
| 2:B:427:THR:HG22 | 2:B:428:GLU:N | 2.21 | 0.54 |
| 2:C:265:THR:HG23 | 2:C:267:PRO:HD3 | 1.89 | 0.54 |
| 2:C:269:PHE:HB3 | 4:E:6:DA:C5' | 2.37 | 0.54 |
| 4:E:17:DG:H2" | 4:E:18:DA:N7 | 2.21 | 0.54 |
| 1:A:15:VAL:CG2 | 1:A:155:ILE:HG23 | 2.36 | 0.54 |
| 1:A:143:ASN:CG | 3:D:5:DA:OP2 | 2.46 | 0.54 |
| 1:A:144:ILE:HB | 2:B:316:PHE:CZ | 2.42 | 0.54 |
| 1:A:409:LEU:HD23 | 1:A:409:LEU:C | 2.27 | 0.54 |
| 2:B:103:ILE:HG23 | 2:B:104:THR:N | 2.21 | 0.54 |
| 2:C:358:THR:HG22 | 2:C:359:LYS:N | 2.21 | 0.54 |
| 2:C:436:LYS:HG2 | 2:C:437:ASN:ND2 | 2.22 | 0.54 |
| 1:A:7:PRO:HG2 | 1:A:418:PHE:O | 2.07 | 0.54 |
| 1:A:157:ILE:HD12 | 1:A:157:ILE:C | 2.28 | 0.54 |
| 1:A:289:LEU:CG | 1:A:320:LEU:HD11 | 2.37 | 0.54 |
| 1:A:319:LYS:HE3 | 3:D:15:DT:O5' | 2.07 | 0.54 |
| 1:A:357:GLN:HG2 | 1:A:358:LYS:H | 1.73 | 0.54 |
| 1:A:104:PHE:CE2 | 1:A:106:ALA:HB3 | 2.43 | 0.54 |
| 1:A:251:PRO:HA | 1:A:269:ARG:CG | 2.30 | 0.54 |
| 2:B:17:LEU:HB2 | 2:B:27:TYR:CE1 | 2.43 | 0.54 |
| 2:B:336:THR:HG22 | 2:B:337:ILE:N | 2.23 | 0.54 |
| 2:B:450:PHE:CZ | 2:B:467:TRP:CZ3 | 2.95 | 0.54 |
| 2:C:6:LEU:HD23 | 2:C:130:MET:HB2 | 1.89 | 0.54 |
| 2:C:338:LEU:HD13 | 2:C:401:PHE:CD1 | 2.41 | 0.54 |
| 1:A:144:ILE:CG1 | 2:B:316:PHE:CZ | 2.91 | 0.54 |
| 2:B:1:MET:HB3 | 2:B:129:ASP:OD1 | 2.08 | 0.54 |
| 2:B:71:TYR:CZ | 2:B:75:LEU:HD21 | 2.43 | 0.54 |
| 2:B:230:LEU:C | 2:B:230:LEU:HD13 | 2.28 | 0.54 |
| 2:B:390:ARG:HG3 | 2:B:391:THR:N | 2.23 | 0.54 |
| 2:C:43:THR:CG2 | 2:C:45:GLN:HB2 | 2.37 | 0.54 |
| 2:C:63:ILE:N | 2:C:67:GLN:HB2 | 2.23 | 0.54 |
| 2:C:269:PHE:CE2 | 2:C:311:PRO:HD3 | 2.43 | 0.54 |
| 1:A:168:ILE:HG23 | 1:A:413:ILE:HD13 | 1.88 | 0.54 |
| 1:A:290:PHE:CE2 | 1:A:360:ILE:HG21 | 2.43 | 0.54 |
| 1:A:355:SER:HB2 | 2:C:312:ASP:HB2 | 1.88 | 0.54 |
| 2:C:60:LYS:HE3 | 2:C:111:ASP:OD2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:62:ARG:HD2 | 2:C:70:PHE:CB | 2.37 | 0.54 |
| 2:C:71:TYR:CZ | 2:C:75:LEU:HD21 | 2.43 | 0.54 |
| 2:C:350:VAL:HG11 | 4:E:6:DA:C4' | 2.38 | 0.54 |
| 1:A:270:PHE:HE2 | 1:A:275:GLU:N | 2.06 | 0.54 |
| 2:B:6:LEU:HB3 | 2:B:130:MET:CG | 2.37 | 0.54 |
| 2:B:142:THR:HG23 | 2:B:143:LYS:N | 2.21 | 0.54 |
| 2:C:275:THR:HG21 | 5:C:530:SAM:C6 | 2.38 | 0.54 |
| 1:A:92:LYS:HG3 | 1:A:93:SER:N | 2.23 | 0.54 |
| 1:A:345:ASN:HD21 | 2:C:430:ALA:HA | 1.73 | 0.54 |
| 2:B:60:LYS:HE3 | 2:B:111:ASP:OD2 | 2.07 | 0.54 |
| 2:B:94:SER:H | 2:B:223:ARG:HH12 | 1.56 | 0.54 |
| 1:A:428:ALA:HB2 | 1:A:443:LEU:CD2 | 2.35 | 0.54 |
| 2:B:246:LEU:HD13 | 2:B:246:LEU:C | 2.28 | 0.54 |
| 2:B:434:GLU:OE1 | 2:B:465:ILE:HG23 | 2.08 | 0.54 |
| 2:C:246:LEU:C | 2:C:246:LEU:HD13 | 2.28 | 0.54 |
| 2:C:427:THR:HG22 | 2:C:428:GLU:N | 2.21 | 0.54 |
| 1:A:138:LEU:HD22 | 1:A:138:LEU:N | 2.23 | 0.53 |
| 1:A:212:LYS:HD3 | 1:A:217:GLU:OE1 | 2.08 | 0.53 |
| 1:A:246:SER:O | 1:A:248:VAL:HG23 | 2.08 | 0.53 |
| 1:A:255:ILE:HD13 | 3:D:14:DG:C5' | 2.35 | 0.53 |
| 2:C:313:ASN:ND2 | 4:E:5:DC:H5" | 2.22 | 0.53 |
| 1:A:272:GLU:HG3 | 1:A:275:GLU:OE2 | 2.08 | 0.53 |
| 1:A:293:TYR:HE2 | 4:E:5:DC:N4 | 2.05 | 0.53 |
| 1:A:299:PHE:HE2 | 1:A:347:MET:HG2 | 1.69 | 0.53 |
| 2:B:222:ARG:HD3 | 2:B:246:LEU:CB | 2.37 | 0.53 |
| 2:B:279:ARG:HH21 | 2:B:281:PHE:HZ | 1.54 | 0.53 |
| 2:C:17:LEU:HB2 | 2:C:27:TYR:CE1 | 2.42 | 0.53 |
| 2:C:322:THR:CA | 2:C:325:ARG:HH21 | 2.21 | 0.53 |
| 1:A:77:ASP:HA | 1:A:95:HIS:HE2 | 1.72 | 0.53 |
| 1:A:252:ILE:CG1 | 1:A:317:PRO:HD3 | 2.29 | 0.53 |
| 1:A:254:ARG:HG2 | 1:A:255:ILE:N | 2.22 | 0.53 |
| 1:A:332:GLU:CB | 1:A:382:VAL:HG11 | 2.39 | 0.53 |
| 2:C:2:ASN:ND2 | 2:C:3:ASN:H | 2.07 | 0.53 |
| 2:C:62:ARG:HD2 | 2:C:70:PHE:CG | 2.43 | 0.53 |
| 2:C:92:ASN:HB3 | 2:C:219:PRO:CB | 2.38 | 0.53 |
| 2:C:259:LYS:HB2 | 2:C:301:HIS:CE1 | 2.43 | 0.53 |
| 2:C:336:THR:HG22 | 2:C:337:ILE:N | 2.23 | 0.53 |
| 1:A:35:TYR:O | 1:A:62:VAL:HB | 2.09 | 0.53 |
| 1:A:196:PHE:CD2 | 1:A:200:VAL:HG21 | 2.43 | 0.53 |
| 1:A:395:ILE:HG23 | 1:A:396:GLU:N | 2.23 | 0.53 |
| 1:A:402:ALA:HA | 1:A:405:ARG:HD3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:E:1:DG:N9 | 4:E:2:DT:H72 | 2.23 | 0.53 |
| 1:A:144:ILE:HG22 | 1:A:146:ASN:H | 1.71 | 0.53 |
| 1:A:293:TYR:CD1 | 1:A:319:LYS:CD | 2.91 | 0.53 |
| 2:B:81:ASP:HB2 | 2:B:83:LYS:NZ | 2.22 | 0.53 |
| 2:C:350:VAL:HG11 | 4:E:6:DA:C1' | 2.38 | 0.53 |
| 1:A:35:TYR:OH | 1:A:68:LYS:HD3 | 2.09 | 0.53 |
| 1:A:134:LYS:HA | 2:B:431:ASP:O | 2.08 | 0.53 |
| 1:A:143:ASN:ND2 | 3:D:5:DA:OP2 | 2.41 | 0.53 |
| 1:A:215:ASN:CG | 2:C:492:GLU:HB2 | 2.28 | 0.53 |
| 1:A:223:PHE:HE1 | 1:A:369:VAL:CG1 | 2.20 | 0.53 |
| 1:A:332:GLU:HB3 | 1:A:382:VAL:HG11 | 1.91 | 0.53 |
| 2:B:2:ASN:H | 2:B:129:ASP:CG | 2.11 | 0.53 |
| 2:B:92:ASN:HB3 | 2:B:219:PRO:CB | 2.38 | 0.53 |
| 2:B:440:GLN:HG3 | 2:B:484:VAL:HB | 1.89 | 0.53 |
| 2:C:222:ARG:NE | 2:C:246:LEU:HB2 | 2.23 | 0.53 |
| 2:C:344:ILE:HD11 | 2:C:345:PHE:CE1 | 2.44 | 0.53 |
| 2:C:481:GLU:CB | 2:C:482:PRO:HD3 | 2.37 | 0.53 |
| 1:A:243:PRO:O | 1:A:246:SER:HB3 | 2.09 | 0.53 |
| 1:A:370:VAL:HG22 | 1:A:371:LEU:N | 2.24 | 0.53 |
| 1:A:433:LEU:CB | 1:A:443:LEU:HD22 | 2.38 | 0.53 |
| 2:B:114:ASP:C | 2:B:116:TYR:H | 2.12 | 0.53 |
| 2:B:438:THR:O | 2:B:485:LEU:HA | 2.08 | 0.53 |
| 2:C:6:LEU:HB3 | 2:C:130:MET:CG | 2.39 | 0.53 |
| 2:C:163:LEU:HD13 | 2:C:163:LEU:C | 2.29 | 0.53 |
| 1:A:35:TYR:CE1 | 1:A:68:LYS:HD2 | 2.43 | 0.53 |
| 1:A:196:PHE:HZ | 1:A:384:ARG:HD2 | 1.68 | 0.53 |
| 1:A:316:TYR:HD2 | 1:A:320:LEU:HB3 | 1.74 | 0.53 |
| 2:B:222:ARG:NE | 2:B:246:LEU:HB2 | 2.23 | 0.53 |
| 2:B:440:GLN:CB | 2:B:484:VAL:CG2 | 2.75 | 0.53 |
| 1:A:193:LEU:HD12 | 1:A:388:LEU:HD22 | 1.90 | 0.53 |
| 2:B:6:LEU:HB3 | 2:B:130:MET:HG2 | 1.91 | 0.53 |
| 2:B:122:LYS:HZ1 | 2:B:124:ARG:HG2 | 1.73 | 0.53 |
| 2:B:431:ASP:OD2 | 2:B:488:GLU:CB | 2.56 | 0.53 |
| 2:C:230:LEU:C | 2:C:230:LEU:HD13 | 2.29 | 0.53 |
| 2:C:232:HIS:O | 2:C:233:ASP:HB2 | 2.09 | 0.53 |
| 1:A:327:LYS:HG3 | 1:A:328:ASP:N | 2.25 | 0.52 |
| 1:A:410:THR:O | 1:A:414:LEU:HG | 2.09 | 0.52 |
| 2:B:232:HIS:O | 2:B:233:ASP:HB2 | 2.09 | 0.52 |
| 2:B:305:ARG:NH1 | 2:B:409:PRO:HG2 | 2.24 | 0.52 |
| 1:A:159:ILE:HG23 | 1:A:159:ILE:O | 2.08 | 0.52 |
| 1:A:354:THR:HG23 | 1:A:356:GLY:N | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:372:LEU:HD13 | 1:A:372:LEU:C | 2.29 | 0.52 |
| 2:C:106:LEU:HD21 | 2:C:110:MET:HE2 | 1.91 | 0.52 |
| 1:A:136:SER:HB2 | 2:B:469:LYS:HE3 | 1.90 | 0.52 |
| 2:B:85:LEU:HD21 | 2:B:238:LEU:HD21 | 1.92 | 0.52 |
| 2:C:438:THR:O | 2:C:485:LEU:HA | 2.09 | 0.52 |
| 1:A:309:LEU:HD23 | 1:A:310:GLN:H | 1.72 | 0.52 |
| 2:B:4:ASN:O | 2:B:7:VAL:HG12 | 2.10 | 0.52 |
| 2:B:275:THR:HG21 | 5:B:530:SAM:C6 | 2.39 | 0.52 |
| 2:C:3:ASN:HA | 2:C:130:MET:SD | 2.49 | 0.52 |
| 2:C:62:ARG:CD | 2:C:70:PHE:HB2 | 2.39 | 0.52 |
| 1:A:147:ILE:HG23 | 1:A:147:ILE:O | 2.08 | 0.52 |
| 1:A:252:ILE:HD11 | 1:A:316:TYR:C | 2.29 | 0.52 |
| 2:B:213:ILE:HG22 | 2:B:214:GLY:N | 2.24 | 0.52 |
| 2:C:304:GLY:H | 2:C:359:LYS:HB3 | 1.75 | 0.52 |
| 1:A:80:ILE:O | 1:A:93:SER:HA | 2.09 | 0.52 |
| 1:A:98:LEU:CB | 1:A:99:PRO:HD2 | 2.32 | 0.52 |
| 2:C:285:THR:HG22 | 2:C:286:SER:N | 2.23 | 0.52 |
| 1:A:10:TRP:NE1 | 1:A:418:PHE:CD1 | 2.77 | 0.52 |
| 1:A:10:TRP:N | 1:A:10:TRP:CE3 | 2.77 | 0.52 |
| 1:A:84:SER:CA | 1:A:146:ASN:HD22 | 2.22 | 0.52 |
| 1:A:158:PRO:HG2 | 1:A:418:PHE:CE2 | 2.45 | 0.52 |
| 2:B:344:ILE:HD11 | 2:B:345:PHE:CE1 | 2.44 | 0.52 |
| 1:A:80:ILE:CG2 | 1:A:94:ALA:HB3 | 2.40 | 0.52 |
| 1:A:308:LYS:HB2 | 1:A:312:GLN:O | 2.10 | 0.52 |
| 1:A:348:MET:HE1 | 2:C:470:ASP:H | 1.74 | 0.52 |
| 1:A:394:THR:HG23 | 1:A:395:ILE:N | 2.24 | 0.52 |
| 2:B:285:THR:HG22 | 2:B:286:SER:N | 2.23 | 0.52 |
| 2:C:268:PRO:HD3 | 5:C:530:SAM:O4' | 2.10 | 0.52 |
| 1:A:55:ASP:O | 1:A:98:LEU:HD12 | 2.10 | 0.52 |
| 1:A:235:LEU:HD11 | 1:A:315:LEU:CD2 | 2.40 | 0.52 |
| 1:A:347:MET:HE1 | 1:A:360:ILE:CD1 | 2.36 | 0.52 |
| 1:A:352:LYS:HD3 | 2:C:382:THR:HG21 | 1.91 | 0.52 |
| 2:B:6:LEU:HD22 | 2:B:117:ASN:HB2 | 1.92 | 0.52 |
| 2:C:114:ASP:C | 2:C:116:TYR:H | 2.12 | 0.52 |
| 4:E:15:DT:H3' | 4:E:16:DT:C6 | 2.45 | 0.52 |
| 1:A:101:GLU:HG2 | 1:A:102:CYS:N | 2.25 | 0.52 |
| 1:A:118:PHE:CZ | 1:A:162:LEU:HD11 | 2.42 | 0.52 |
| 1:A:341:PRO:HA | 1:A:344:ARG:CG | 2.39 | 0.52 |
| 2:B:376:TRP:CZ3 | 2:B:447:TRP:NE1 | 2.78 | 0.52 |
| 4:E:15:DT:H5' | 4:E:16:DT:C7 | 2.40 | 0.52 |
| 1:A:179:VAL:HG23 | 1:A:180:ASP:N | 2.24 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:412:SER:N | 2:B:495:GLN:HG3 | 2.24 | 0.51 |
| 2:B:429:VAL:HG11 | 2:B:443:ALA:HB1 | 1.91 | 0.51 |
| 2:C:313:ASN:HB3 | 4:E:5:DC:OP1 | 2.11 | 0.51 |
| 2:B:229:CYS:SG | 2:B:244:ILE:HD11 | 2.50 | 0.51 |
| 2:C:229:CYS:SG | 2:C:244:ILE:HD11 | 2.50 | 0.51 |
| 2:C:305:ARG:NH1 | 2:C:409:PRO:HG2 | 2.24 | 0.51 |
| 2:C:339:ARG:NH2 | 2:C:465:ILE:H | 2.08 | 0.51 |
| 1:A:39:ASP:CG | 1:A:62:VAL:HA | 2.29 | 0.51 |
| 1:A:78:ILE:CG1 | 1:A:111:LEU:HD23 | 2.39 | 0.51 |
| 2:B:62:ARG:HD2 | 2:B:70:PHE:CB | 2.40 | 0.51 |
| 2:C:213:ILE:HG22 | 2:C:214:GLY:N | 2.24 | 0.51 |
| 1:A:143:ASN:HB3 | 2:B:316:PHE:CE1 | 2.45 | 0.51 |
| 1:A:252:ILE:HG21 | 1:A:268:ILE:HG23 | 1.89 | 0.51 |
| 2:C:172:GLN:HG2 | 2:C:173:ASP:N | 2.26 | 0.51 |
| 1:A:28:LYS:CB | 1:A:65:ASN:HD21 | 2.22 | 0.51 |
| 1:A:80:ILE:HD11 | 1:A:107:PHE:HB3 | 1.92 | 0.51 |
| 2:B:98:THR:HG23 | 2:C:94:SER:OG | 2.11 | 0.51 |
| 2:C:313:ASN:HA | 2:C:316:PHE:CE1 | 2.46 | 0.51 |
| 1:A:293:TYR:HB2 | 3:D:15:DT:OP2 | 2.10 | 0.51 |
| 2:B:304:GLY:H | 2:B:359:LYS:HB3 | 1.76 | 0.51 |
| 2:B:455:ILE:O | 2:B:459:LYS:HB2 | 2.10 | 0.51 |
| 2:B:486:ALA:HB3 | 2:B:489:ALA:HB3 | 1.91 | 0.51 |
| 2:C:138:ASN:OD1 | 2:C:146:ALA:HB2 | 2.10 | 0.51 |
| 1:A:61:PHE:CE2 | 1:A:66:LEU:CA | 2.94 | 0.51 |
| 1:A:170:GLU:O | 1:A:174:THR:HG23 | 2.11 | 0.51 |
| 1:A:289:LEU:CD2 | 1:A:320:LEU:HD11 | 2.40 | 0.51 |
| 1:A:312:GLN:HG2 | 1:A:313:ASN:H | 1.76 | 0.51 |
| 1:A:322:ARG:HG2 | 1:A:323:ALA:N | 2.26 | 0.51 |
| 2:B:456:ARG:O | 2:B:460:SER:HA | 2.10 | 0.51 |
| 2:C:85:LEU:HD21 | 2:C:238:LEU:HD21 | 1.91 | 0.51 |
| 1:A:18:VAL:O | 1:A:116:LEU:HD23 | 2.11 | 0.51 |
| 1:A:96:GLN:HG3 | 1:A:96:GLN:O | 2.09 | 0.51 |
| 1:A:118:PHE:CE2 | 1:A:166:LYS:HG3 | 2.45 | 0.51 |
| 1:A:175:LEU:HD13 | 1:A:175:LEU:C | 2.31 | 0.51 |
| 1:A:285:ASP:HB3 | 1:A:308:LYS:CB | 2.40 | 0.51 |
| 1:A:10:TRP:NE1 | 1:A:160:PRO:HB3 | 2.26 | 0.51 |
| 1:A:41:LEU:HD21 | 1:A:101:GLU:HA | 1.93 | 0.51 |
| 1:A:44:ILE:HG23 | 1:A:101:GLU:CD | 2.31 | 0.51 |
| 1:A:167:ILE:HG23 | 1:A:168:ILE:N | 2.24 | 0.51 |
| 1:A:270:PHE:HE2 | 1:A:275:GLU:CB | 2.23 | 0.51 |
| 2:B:138:ASN:OD1 | 2:B:146:ALA:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:268:PRO:HD3 | 5:B:530:SAM:O4' | 2.10 | 0.51 |
| 2:C:217:LEU:O | 2:C:219:PRO:HD3 | 2.11 | 0.51 |
| 2:C:287:ASN:ND2 | 2:C:290:LEU:H | 2.08 | 0.51 |
| 2:C:431:ASP:OD2 | 2:C:488:GLU:CB | 2.57 | 0.51 |
| 1:A:118:PHE:HZ | 1:A:162:LEU:CD1 | 2.24 | 0.51 |
| 1:A:131:TYR:CE2 | 1:A:135:ILE:CD1 | 2.94 | 0.51 |
| 1:A:135:ILE:O | 1:A:138:LEU:HD23 | 2.11 | 0.51 |
| 1:A:137:SER:CB | 2:B:432:SER:CB | 2.88 | 0.51 |
| 1:A:215:ASN:OD1 | 2:C:489:ALA:CA | 2.52 | 0.51 |
| 1:A:248:VAL:HG13 | 1:A:270:PHE:CA | 2.40 | 0.51 |
| 2:B:70:PHE:CE2 | 2:B:74:MET:HE3 | 2.46 | 0.51 |
| 2:B:172:GLN:HG2 | 2:B:173:ASP:N | 2.26 | 0.51 |
| 2:C:283:HIS:H | 2:C:294:GLN:NE2 | 2.02 | 0.51 |
| 1:A:122:ILE:HG23 | 1:A:123:ALA:N | 2.25 | 0.50 |
| 2:B:243:ALA:HB3 | 2:B:244:ILE:HD12 | 1.93 | 0.50 |
| 2:B:515:LEU:HD22 | 2:B:515:LEU:N | 2.26 | 0.50 |
| 2:C:6:LEU:HB3 | 2:C:130:MET:HG2 | 1.93 | 0.50 |
| 2:C:315:LEU:HD22 | 2:C:463:LEU:CB | 2.41 | 0.50 |
| 2:C:376:TRP:CZ3 | 2:C:447:TRP:NE1 | 2.78 | 0.50 |
| 2:B:24:TYR:CD2 | 2:B:27:TYR:CE2 | 2.95 | 0.50 |
| 2:B:265:THR:HG23 | 2:B:267:PRO:HD3 | 1.92 | 0.50 |
| 2:C:1:MET:CE | 2:C:132:GLU:HG3 | 2.41 | 0.50 |
| 2:C:322:THR:HG23 | 2:C:323:ASP:N | 2.26 | 0.50 |
| 1:A:7:PRO:HG2 | 1:A:418:PHE:CB | 2.41 | 0.50 |
| 1:A:61:PHE:HZ | 1:A:66:LEU:HA | 1.76 | 0.50 |
| 1:A:336:ILE:HG23 | 1:A:337:PHE:N | 2.26 | 0.50 |
| 2:B:287:ASN:ND2 | 2:B:290:LEU:H | 2.08 | 0.50 |
| 2:C:305:ARG:HD3 | 2:C:410:HIS:ND1 | 2.26 | 0.50 |
| 1:A:104:PHE:CE2 | 1:A:106:ALA:CB | 2.95 | 0.50 |
| 2:B:3:ASN:HA | 2:B:130:MET:SD | 2.52 | 0.50 |
| 2:B:73:LYS:HA | 2:C:72:ARG:HH12 | 1.76 | 0.50 |
| 2:B:122:LYS:HZ2 | 2:B:124:ARG:HG2 | 1.76 | 0.50 |
| 2:C:63:ILE:HG13 | 2:C:104:THR:HG21 | 1.94 | 0.50 |
| 2:C:243:ALA:HB3 | 2:C:244:ILE:HD12 | 1.94 | 0.50 |
| 2:C:268:PRO:HD3 | 5:C:530:SAM:H5'2 | 1.93 | 0.50 |
| 2:C:515:LEU:HD22 | 2:C:515:LEU:N | 2.26 | 0.50 |
| 1:A:162:LEU:HD13 | 1:A:162:LEU:C | 2.32 | 0.50 |
| 1:A:164:GLU:HA | 1:A:167:ILE:HG22 | 1.93 | 0.50 |
| 2:B:28:VAL:HB | 2:B:131:TYR:OH | 2.12 | 0.50 |
| 2:B:436:LYS:HG2 | 2:B:437:ASN:ND2 | 2.27 | 0.50 |
| 2:C:70:PHE:CE2 | 2:C:74:MET:HE1 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:88:ALA:HB2 | 2:C:241:GLY:CA | 2.42 | 0.50 |
| 1:A:49:ILE:CD1 | 1:A:107:PHE:CE2 | 2.94 | 0.50 |
| 1:A:118:PHE:CZ | 1:A:162:LEU:CD1 | 2.95 | 0.50 |
| 1:A:118:PHE:CE2 | 1:A:162:LEU:CD2 | 2.95 | 0.50 |
| 2:B:3:ASN:HB2 | 2:B:130:MET:SD | 2.52 | 0.50 |
| 2:B:287:ASN:HD22 | 2:B:289:GLN:N | 2.10 | 0.50 |
| 2:C:90:PHE:HA | 2:C:93:VAL:CG1 | 2.41 | 0.50 |
| 1:A:22:ILE:HG23 | 1:A:108:CYS:SG | 2.51 | 0.50 |
| 2:B:217:LEU:O | 2:B:219:PRO:HD3 | 2.11 | 0.50 |
| 2:B:220:GLY:HA2 | 2:B:223:ARG:CZ | 2.41 | 0.50 |
| 2:B:486:ALA:HB3 | 2:B:489:ALA:HB2 | 1.93 | 0.50 |
| 2:C:26:ASN:O | 2:C:30:GLU:HG2 | 2.12 | 0.50 |
| 2:C:29:ASN:HB2 | 2:C:224:LEU:HD11 | 1.94 | 0.50 |
| 2:C:322:THR:O | 2:C:326:ARG:HG3 | 2.11 | 0.50 |
| 2:C:340:LEU:HD12 | 2:C:352:THR:OG1 | 2.12 | 0.50 |
| 1:A:15:VAL:O | 1:A:18:VAL:HG22 | 2.12 | 0.50 |
| 1:A:48:ASN:HB3 | 1:A:54:PHE:CE1 | 2.47 | 0.50 |
| 1:A:131:TYR:CE1 | 1:A:155:ILE:CD1 | 2.94 | 0.50 |
| 2:C:28:VAL:HB | 2:C:131:TYR:OH | 2.12 | 0.50 |
| 2:C:177:GLY:O | 2:C:225:ALA:HB2 | 2.12 | 0.50 |
| 3:D:17:DC:H2" | 3:D:18:DA:C8 | 2.46 | 0.50 |
| 1:A:316:TYR:HE2 | 1:A:320:LEU:O | 1.95 | 0.50 |
| 2:B:88:ALA:HB2 | 2:B:241:GLY:CA | 2.42 | 0.50 |
| 2:C:6:LEU:HD22 | 2:C:117:ASN:HB2 | 1.94 | 0.50 |
| 2:C:55:ARG:HG2 | 2:C:58:ASP:OD2 | 2.11 | 0.50 |
| 2:C:113:LEU:HD23 | 2:C:113:LEU:C | 2.32 | 0.50 |
| 2:C:474:ILE:HG23 | 2:C:474:ILE:O | 2.10 | 0.50 |
| 1:A:44:ILE:HG22 | 1:A:54:PHE:CE1 | 2.46 | 0.49 |
| 1:A:140:ALA:HB1 | 2:B:351:LYS:HZ1 | 1.77 | 0.49 |
| 1:A:290:PHE:HE2 | 1:A:360:ILE:HG21 | 1.77 | 0.49 |
| 1:A:299:PHE:CZ | 1:A:347:MET:CE | 2.95 | 0.49 |
| 2:B:178:THR:O | 2:B:179:ALA:HB3 | 2.12 | 0.49 |
| 2:B:474:ILE:O | 2:B:474:ILE:HG23 | 2.10 | 0.49 |
| 2:C:280:THR:HG22 | 2:C:281:PHE:N | 2.26 | 0.49 |
| 1:A:44:ILE:HG13 | 1:A:103:SER:OG | 2.12 | 0.49 |
| 1:A:44:ILE:CG2 | 1:A:54:PHE:CZ | 2.95 | 0.49 |
| 2:B:55:ARG:HG2 | 2:B:58:ASP:OD2 | 2.12 | 0.49 |
| 2:C:70:PHE:CE2 | 2:C:74:MET:CE | 2.95 | 0.49 |
| 1:A:7:PRO:HG2 | 1:A:418:PHE:HB3 | 1.93 | 0.49 |
| 1:A:103:SER:HG | 1:A:107:PHE:HB2 | 1.77 | 0.49 |
| 1:A:171:LYS:HE2 | 1:A:409:LEU:HD11 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:308:LYS:HE3 | 1:A:312:GLN:O | 2.12 | 0.49 |
| 1:A:334:ILE:HG23 | 1:A:335:GLU:N | 2.26 | 0.49 |
| 1:A:410:THR:HG23 | 1:A:411:GLN:N | 2.27 | 0.49 |
| 1:A:433:LEU:HB2 | 1:A:443:LEU:HD22 | 1.94 | 0.49 |
| 2:B:29:ASN:HB2 | 2:B:224:LEU:HD11 | 1.94 | 0.49 |
| 2:C:287:ASN:HD22 | 2:C:289:GLN:N | 2.09 | 0.49 |
| 2:C:350:VAL:HG11 | 4:E:6:DA:H1' | 1.92 | 0.49 |
| 1:A:320:LEU:HD23 | 1:A:321:ILE:O | 2.12 | 0.49 |
| 1:A:330:LEU:HD23 | 1:A:331:PRO:CD | 2.41 | 0.49 |
| 2:B:5:ASP:HB2 | 2:B:116:TYR:HE2 | 1.76 | 0.49 |
| 2:B:162:LEU:HD22 | 2:B:405:TYR:CD2 | 2.47 | 0.49 |
| 2:B:220:GLY:CA | 2:B:223:ARG:HH21 | 2.25 | 0.49 |
| 2:B:280:THR:HG22 | 2:B:281:PHE:N | 2.26 | 0.49 |
| 2:B:305:ARG:HD3 | 2:B:410:HIS:ND1 | 2.26 | 0.49 |
| 2:C:220:GLY:CA | 2:C:223:ARG:HH21 | 2.26 | 0.49 |
| 2:C:376:TRP:CZ2 | 2:C:415:ARG:HB2 | 2.47 | 0.49 |
| 1:A:215:ASN:ND2 | 2:C:492:GLU:CB | 2.52 | 0.49 |
| 1:A:354:THR:O | 1:A:357:GLN:HB2 | 2.12 | 0.49 |
| 1:A:371:LEU:HG | 1:A:373:PRO:HD3 | 1.93 | 0.49 |
| 2:B:417:GLU:HA | 2:B:447:TRP:HD1 | 1.77 | 0.49 |
| 2:C:417:GLU:HA | 2:C:447:TRP:HD1 | 1.77 | 0.49 |
| 1:A:126:THR:HG23 | 1:A:127:LYS:N | 2.27 | 0.49 |
| 1:A:161:PRO:O | 1:A:165:GLN:HG3 | 2.12 | 0.49 |
| 2:B:113:LEU:HD23 | 2:B:113:LEU:C | 2.32 | 0.49 |
| 2:C:28:VAL:O | 2:C:131:TYR:HE1 | 1.96 | 0.49 |
| 1:A:112:ARG:H | 1:A:112:ARG:NE | 2.11 | 0.49 |
| 1:A:443:LEU:O | 1:A:447:ILE:HG12 | 2.13 | 0.49 |
| 2:C:63:ILE:HG13 | 2:C:104:THR:CG2 | 2.43 | 0.49 |
| 2:C:285:THR:HG22 | 2:C:287:ASN:N | 2.07 | 0.49 |
| 2:C:315:LEU:HD22 | 2:C:463:LEU:HB3 | 1.94 | 0.49 |
| 1:A:144:ILE:CB | 2:B:316:PHE:HZ | 2.25 | 0.49 |
| 1:A:371:LEU:HD23 | 1:A:371:LEU:N | 2.24 | 0.49 |
| 2:B:26:ASN:O | 2:B:30:GLU:HG2 | 2.12 | 0.49 |
| 2:B:268:PRO:CG | 5:B:530:SAM:C8 | 2.83 | 0.49 |
| 1:A:49:ILE:HD12 | 1:A:82:MET:CG | 2.38 | 0.49 |
| 1:A:415:ALA:O | 1:A:418:PHE:HB2 | 2.12 | 0.49 |
| 2:B:9:LYS:HZ2 | 2:B:113:LEU:HB2 | 1.76 | 0.49 |
| 1:A:71:GLN:HG2 | 1:A:102:CYS:CB | 2.28 | 0.49 |
| 1:A:212:LYS:HG2 | 1:A:214:ARG:H | 1.77 | 0.49 |
| 1:A:225:LYS:HB2 | 1:A:228:PHE:HD1 | 1.75 | 0.49 |
| 1:A:232:LEU:HD23 | 1:A:232:LEU:C | 2.32 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:155:LEU:O | 2:B:159:ILE:HG13 | 2.13 | 0.49 |
| 2:B:177:GLY:O | 2:B:225:ALA:HB2 | 2.12 | 0.49 |
| 2:B:344:ILE:HG13 | 2:B:345:PHE:N | 2.28 | 0.49 |
| 2:B:376:TRP:CZ2 | 2:B:415:ARG:HB2 | 2.48 | 0.49 |
| 2:B:529:GLU:OXT | 2:B:529:GLU:HG2 | 2.12 | 0.49 |
| 2:C:6:LEU:HD23 | 2:C:130:MET:CG | 2.42 | 0.49 |
| 2:C:333:HIS:HD2 | 2:C:371:CYS:O | 1.96 | 0.49 |
| 3:D:15:DT:H5" | 3:D:16:DG:P | 2.53 | 0.49 |
| 1:A:43:LEU:HB2 | 1:A:61:PHE:HB2 | 1.95 | 0.48 |
| 2:B:268:PRO:HD3 | 5:B:530:SAM:H5'2 | 1.94 | 0.48 |
| 2:C:106:LEU:HD21 | 2:C:110:MET:CE | 2.43 | 0.48 |
| 2:C:178:THR:O | 2:C:179:ALA:HB3 | 2.12 | 0.48 |
| 3:D:1:DG:C5 | 3:D:2:DT:C7 | 2.95 | 0.48 |
| 1:A:32:ALA:CB | 1:A:35:TYR:CE2 | 2.94 | 0.48 |
| 1:A:197:ARG:CZ | 1:A:341:PRO:HD3 | 2.43 | 0.48 |
| 1:A:252:ILE:HD11 | 1:A:316:TYR:O | 2.12 | 0.48 |
| 2:B:283:HIS:H | 2:B:294:GLN:NE2 | 2.02 | 0.48 |
| 2:B:448:ARG:HD3 | 2:B:467:TRP:CZ2 | 2.44 | 0.48 |
| 2:C:162:LEU:HD22 | 2:C:405:TYR:CD2 | 2.48 | 0.48 |
| 2:C:488:GLU:CD | 2:C:488:GLU:H | 2.17 | 0.48 |
| 1:A:22:ILE:HG12 | 1:A:110:VAL:HG23 | 1.95 | 0.48 |
| 1:A:89:VAL:HG21 | 1:A:135:ILE:HG22 | 1.95 | 0.48 |
| 1:A:235:LEU:HD23 | 1:A:236:ARG:O | 2.14 | 0.48 |
| 1:A:248:VAL:CG1 | 1:A:269:ARG:HB3 | 2.38 | 0.48 |
| 2:B:63:ILE:HG13 | 2:B:104:THR:CG2 | 2.43 | 0.48 |
| 2:B:219:PRO:O | 2:B:223:ARG:HG3 | 2.14 | 0.48 |
| 2:C:6:LEU:HD23 | 2:C:130:MET:HG2 | 1.96 | 0.48 |
| 2:C:167:PRO:O | 2:C:168:ARG:HB2 | 2.14 | 0.48 |
| 2:C:344:ILE:HG13 | 2:C:345:PHE:N | 2.28 | 0.48 |
| 2:B:167:PRO:O | 2:B:168:ARG:HB2 | 2.13 | 0.48 |
| 2:B:338:LEU:HD12 | 2:B:378:TYR:HB3 | 1.95 | 0.48 |
| 2:B:379:ASP:O | 2:B:446:ARG:HD3 | 2.14 | 0.48 |
| 2:B:488:GLU:CD | 2:B:488:GLU:H | 2.17 | 0.48 |
| 2:C:128:GLY:O | 2:C:131:TYR:HB3 | 2.14 | 0.48 |
| 2:C:529:GLU:OXT | 2:C:529:GLU:HG2 | 2.12 | 0.48 |
| 1:A:110:VAL:O | 1:A:110:VAL:HG13 | 2.13 | 0.48 |
| 1:A:235:LEU:HD11 | 1:A:315:LEU:HD21 | 1.94 | 0.48 |
| 1:A:248:VAL:CG1 | 1:A:249:GLY:H | 2.25 | 0.48 |
| 1:A:274:SER:CA | 1:A:278:LEU:HD23 | 2.43 | 0.48 |
| 1:A:349:ASN:HB2 | 2:C:430:ALA:C | 2.33 | 0.48 |
| 1:A:387:GLN:OE1 | 1:A:387:GLN:HA | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2:ASN:ND2 | 2:B:3:ASN:H | 2.10 | 0.48 |
| 2:B:262:ILE:HG22 | 2:B:263:VAL:N | 2.28 | 0.48 |
| 2:B:269:PHE:CB | 3:D:6:DA:O4' | 2.61 | 0.48 |
| 2:C:268:PRO:CG | 5:C:530:SAM:C8 | 2.81 | 0.48 |
| 1:A:234:GLU:CD | 1:A:235:LEU:H | 2.17 | 0.48 |
| 1:A:299:PHE:CE2 | 1:A:347:MET:HE2 | 2.48 | 0.48 |
| 2:B:433:GLU:CA | 2:B:436:LYS:HB2 | 2.42 | 0.48 |
| 2:C:4:ASN:O | 2:C:7:VAL:HG12 | 2.12 | 0.48 |
| 2:C:29:ASN:HD22 | 2:C:224:LEU:HD11 | 1.78 | 0.48 |
| 1:A:235:LEU:HD22 | 1:A:316:TYR:O | 2.14 | 0.48 |
| 2:B:63:ILE:HG13 | 2:B:104:THR:HG21 | 1.94 | 0.48 |
| 2:C:122:LYS:CE | 2:C:124:ARG:HG2 | 2.44 | 0.48 |
| 4:E:15:DT:H5' | 4:E:16:DT:H73 | 1.95 | 0.48 |
| 1:A:142:ALA:HA | 2:B:312:ASP:CB | 2.35 | 0.48 |
| 1:A:281:HIS:HE1 | 4:E:1:DG:H3' | 1.77 | 0.48 |
| 2:B:217:LEU:HD21 | 2:B:274:GLY:O | 2.14 | 0.48 |
| 2:C:163:LEU:HG | 2:C:262:ILE:CG2 | 2.43 | 0.48 |
| 2:C:217:LEU:HD22 | 2:C:275:THR:HG23 | 1.93 | 0.48 |
| 1:A:234:GLU:HB3 | 4:E:2:DT:O5' | 2.14 | 0.48 |
| 1:A:333:TYR:HB2 | 1:A:382:VAL:CG2 | 2.44 | 0.48 |
| 2:B:153:ARG:N | 2:B:154:PRO:HD2 | 2.29 | 0.48 |
| 2:C:220:GLY:HA2 | 2:C:223:ARG:CZ | 2.41 | 0.48 |
| 2:C:346:TYR:CD1 | 2:C:347:ALA:N | 2.82 | 0.48 |
| 1:A:39:ASP:OD1 | 1:A:63:PRO:HD3 | 2.13 | 0.48 |
| 1:A:41:LEU:HD22 | 1:A:42:PRO:O | 2.13 | 0.48 |
| 1:A:270:PHE:HD2 | 1:A:274:SER:CB | 2.22 | 0.48 |
| 1:A:278:LEU:HD22 | 1:A:278:LEU:N | 2.29 | 0.48 |
| 1:A:413:ILE:CG1 | 1:A:417:ALA:HB2 | 2.42 | 0.48 |
| 2:B:90:PHE:HA | 2:B:93:VAL:CG1 | 2.41 | 0.48 |
| 2:B:346:TYR:CD1 | 2:B:347:ALA:N | 2.82 | 0.48 |
| 2:C:6:LEU:HG | 2:C:10:LEU:HD11 | 1.96 | 0.48 |
| 2:C:219:PRO:O | 2:C:223:ARG:HG3 | 2.13 | 0.48 |
| 2:C:486:ALA:HB3 | 2:C:489:ALA:HB2 | 1.95 | 0.48 |
| 1:A:8:GLU:OE2 | 1:A:464:SER:HB3 | 2.14 | 0.47 |
| 1:A:253:LEU:HD11 | 1:A:263:VAL:CG2 | 2.38 | 0.47 |
| 1:A:280:ARG:HB3 | 1:A:315:LEU:HD21 | 1.96 | 0.47 |
| 1:A:316:TYR:HB2 | 1:A:317:PRO:HD2 | 1.95 | 0.47 |
| 2:B:63:ILE:CA | 2:B:67:GLN:HB2 | 2.44 | 0.47 |
| 2:C:207:GLN:HA | 2:C:211:ALA:CB | 2.39 | 0.47 |
| 2:C:338:LEU:HD12 | 2:C:378:TYR:HB3 | 1.95 | 0.47 |
| 1:A:62:VAL:CG1 | 1:A:63:PRO:N | 2.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:148:LYS:HG2 | 1:A:149:PRO:HD2 | 1.92 | 0.47 |
| 1:A:270:PHE:CZ | 1:A:315:LEU:CD1 | 2.95 | 0.47 |
| 1:A:358:LYS:HG3 | 3:D:14:DG:O6 | 2.14 | 0.47 |
| 2:B:28:VAL:O | 2:B:131:TYR:HE1 | 1.97 | 0.47 |
| 2:B:160:ILE:N | 2:B:160:ILE:HD12 | 2.29 | 0.47 |
| 2:B:195:ASP:O | 2:B:196:LEU:HB2 | 2.14 | 0.47 |
| 2:C:153:ARG:N | 2:C:154:PRO:HD2 | 2.29 | 0.47 |
| 2:C:339:ARG:HH21 | 2:C:465:ILE:H | 1.62 | 0.47 |
| 1:A:250:HIS:CD2 | 1:A:270:PHE:CE1 | 2.99 | 0.47 |
| 1:A:270:PHE:HB3 | 1:A:280:ARG:NH1 | 2.29 | 0.47 |
| 1:A:409:LEU:HD23 | 1:A:409:LEU:O | 2.13 | 0.47 |
| 2:B:39:MET:SD | 2:B:115:TRP:CH2 | 3.07 | 0.47 |
| 2:B:94:SER:OG | 2:C:98:THR:HG23 | 2.13 | 0.47 |
| 2:B:230:LEU:HD13 | 2:B:230:LEU:O | 2.14 | 0.47 |
| 2:B:333:HIS:HD2 | 2:B:371:CYS:O | 1.96 | 0.47 |
| 1:A:236:ARG:HB2 | 4:E:2:DT:C7 | 2.45 | 0.47 |
| 1:A:330:LEU:HD21 | 1:A:332:GLU:HB2 | 1.96 | 0.47 |
| 2:B:435:ASN:ND2 | 2:B:467:TRP:HB2 | 2.25 | 0.47 |
| 1:A:39:ASP:OD2 | 1:A:60:VAL:HG12 | 2.14 | 0.47 |
| 2:B:93:VAL:HG23 | 2:B:93:VAL:O | 2.15 | 0.47 |
| 2:C:6:LEU:CG | 2:C:130:MET:HG2 | 2.45 | 0.47 |
| 2:C:24:TYR:CD2 | 2:C:27:TYR:CE2 | 2.95 | 0.47 |
| 3:D:18:DA:C6 | 3:D:19:DA:C6 | 3.03 | 0.47 |
| 1:A:62:VAL:HG12 | 1:A:63:PRO:N | 2.29 | 0.47 |
| 1:A:62:VAL:HG13 | 1:A:63:PRO:HD2 | 1.94 | 0.47 |
| 1:A:225:LYS:HB2 | 1:A:227:ASN:HD21 | 1.80 | 0.47 |
| 1:A:308:LYS:HG3 | 1:A:309:LEU:O | 2.13 | 0.47 |
| 2:B:118:GLY:HA2 | 2:B:123:SER:CB | 2.45 | 0.47 |
| 2:B:305:ARG:HH11 | 2:B:410:HIS:CD2 | 2.32 | 0.47 |
| 2:C:230:LEU:HD13 | 2:C:230:LEU:O | 2.14 | 0.47 |
| 2:C:269:PHE:HB2 | 4:E:6:DA:O4' | 2.13 | 0.47 |
| 2:C:440:GLN:HG3 | 2:C:484:VAL:HB | 1.88 | 0.47 |
| 1:A:10:TRP:HE1 | 1:A:160:PRO:HB3 | 1.79 | 0.47 |
| 1:A:10:TRP:CD2 | 1:A:418:PHE:O | 2.67 | 0.47 |
| 1:A:103:SER:OG | 1:A:107:PHE:HB2 | 2.13 | 0.47 |
| 1:A:145:ASN:ND2 | 1:A:145:ASN:H | 2.13 | 0.47 |
| 1:A:232:LEU:HD13 | 1:A:366:LYS:HE3 | 1.97 | 0.47 |
| 1:A:265:GLN:HG2 | 1:A:266:ASN:H | 1.79 | 0.47 |
| 1:A:353:THR:HG23 | 1:A:353:THR:O | 2.14 | 0.47 |
| 2:B:1:MET:HE2 | 2:B:132:GLU:CB | 2.44 | 0.47 |
| 2:B:6:LEU:CG | 2:B:130:MET:HG2 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:43:THR:HG22 | 2:B:45:GLN:HB2 | 1.97 | 0.47 |
| 2:B:128:GLY:CA | 2:B:231:LEU:HD22 | 2.33 | 0.47 |
| 2:B:269:PHE:CD1 | 2:B:269:PHE:N | 2.83 | 0.47 |
| 2:C:39:MET:SD | 2:C:115:TRP:CH2 | 3.07 | 0.47 |
| 2:C:195:ASP:O | 2:C:196:LEU:HB2 | 2.15 | 0.47 |
| 2:C:209:HIS:O | 2:C:236:GLY:HA2 | 2.14 | 0.47 |
| 2:C:245:ARG:HG2 | 2:C:246:LEU:N | 2.30 | 0.47 |
| 2:C:379:ASP:O | 2:C:446:ARG:HD3 | 2.15 | 0.47 |
| 2:C:438:THR:HG23 | 2:C:442:LEU:HD23 | 1.97 | 0.47 |
| 3:D:15:DT:H5" | 3:D:16:DG:OP2 | 2.14 | 0.47 |
| 1:A:186:PHE:CD1 | 1:A:395:ILE:CG2 | 2.95 | 0.47 |
| 1:A:223:PHE:O | 1:A:224:LYS:HG3 | 2.15 | 0.47 |
| 1:A:250:HIS:HD2 | 1:A:251:PRO:O | 1.98 | 0.47 |
| 1:A:215:ASN:HD21 | 2:C:492:GLU:HG3 | 1.79 | 0.47 |
| 1:A:235:LEU:HD13 | 1:A:316:TYR:O | 2.14 | 0.47 |
| 1:A:239:LEU:HD23 | 1:A:240:SER:H | 1.79 | 0.47 |
| 2:B:106:LEU:HD21 | 2:B:110:MET:CE | 2.43 | 0.47 |
| 2:B:440:GLN:HB2 | 2:B:484:VAL:CB | 2.44 | 0.47 |
| 2:C:155:LEU:O | 2:C:159:ILE:HG13 | 2.14 | 0.47 |
| 2:C:275:THR:CG2 | 5:C:530:SAM:HN61 | 2.28 | 0.47 |
| 1:A:144:ILE:CB | 2:B:316:PHE:CZ | 2.97 | 0.47 |
| 1:A:235:LEU:O | 1:A:318:ASP:HA | 2.15 | 0.47 |
| 1:A:252:ILE:HG23 | 1:A:252:ILE:O | 2.15 | 0.47 |
| 1:A:352:LYS:HE2 | 2:C:468:LEU:N | 2.18 | 0.47 |
| 2:B:25:GLN:HA | 2:B:138:ASN:OD1 | 2.15 | 0.47 |
| 2:B:62:ARG:CD | 2:B:70:PHE:HB2 | 2.45 | 0.47 |
| 2:B:70:PHE:CE2 | 2:B:74:MET:CE | 2.97 | 0.47 |
| 2:B:209:HIS:O | 2:B:236:GLY:HA2 | 2.14 | 0.47 |
| 2:C:313:ASN:HA | 2:C:316:PHE:CZ | 2.49 | 0.47 |
| 2:C:377:VAL:HB | 2:C:467:TRP:HH2 | 1.78 | 0.47 |
| 1:A:39:ASP:CB | 1:A:62:VAL:HG22 | 2.44 | 0.46 |
| 1:A:98:LEU:HB3 | 1:A:99:PRO:CD | 2.37 | 0.46 |
| 1:A:355:SER:H | 2:C:312:ASP:HB2 | 1.80 | 0.46 |
| 2:B:439:ASP:CA | 2:B:485:LEU:HD22 | 2.39 | 0.46 |
| 2:B:450:PHE:HZ | 2:B:467:TRP:CZ3 | 2.31 | 0.46 |
| 2:C:43:THR:HG22 | 2:C:45:GLN:HB2 | 1.97 | 0.46 |
| 2:C:93:VAL:O | 2:C:93:VAL:HG23 | 2.14 | 0.46 |
| 2:C:217:LEU:HD21 | 2:C:274:GLY:O | 2.14 | 0.46 |
| 2:C:271:SER:O | 2:C:272:ALA:HB3 | 2.16 | 0.46 |
| 2:C:455:ILE:O | 2:C:459:LYS:HB2 | 2.15 | 0.46 |
| 1:A:61:PHE:HE2 | 1:A:66:LEU:CB | 2.28 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:80:ILE:HD11 | 1:A:107:PHE:HD2 | 1.80 | 0.46 |
| 1:A:144:ILE:HG23 | 1:A:146:ASN:N | 2.31 | 0.46 |
| 1:A:145:ASN:H | 1:A:145:ASN:HD22 | 1.62 | 0.46 |
| 2:B:122:LYS:CE | 2:B:124:ARG:HG2 | 2.44 | 0.46 |
| 2:B:201:GLY:HA2 | 2:B:204:GLN:OE1 | 2.15 | 0.46 |
| 2:B:245:ARG:HG2 | 2:B:246:LEU:N | 2.30 | 0.46 |
| 2:B:524:PHE:HE2 | 2:B:528:LYS:HD2 | 1.81 | 0.46 |
| 2:C:22:VAL:HG12 | 2:C:23:SER:O | 2.15 | 0.46 |
| 1:A:46:ALA:CA | 1:A:107:PHE:CE1 | 2.95 | 0.46 |
| 1:A:234:GLU:HG3 | 4:E:2:DT:C2' | 2.43 | 0.46 |
| 1:A:313:ASN:C | 1:A:313:ASN:HD22 | 2.19 | 0.46 |
| 2:C:3:ASN:HB2 | 2:C:130:MET:SD | 2.55 | 0.46 |
| 2:C:201:GLY:HA2 | 2:C:204:GLN:OE1 | 2.15 | 0.46 |
| 2:C:296:ILE:HD13 | 2:C:308:VAL:HG21 | 1.96 | 0.46 |
| 1:A:117:ILE:HD13 | 1:A:159:ILE:CD1 | 2.45 | 0.46 |
| 1:A:357:GLN:HG2 | 1:A:358:LYS:N | 2.28 | 0.46 |
| 2:B:459:LYS:O | 2:B:460:SER:HB2 | 2.16 | 0.46 |
| 1:A:89:VAL:CG2 | 1:A:135:ILE:CG2 | 2.93 | 0.46 |
| 1:A:164:GLU:OE2 | 1:A:422:LEU:HB2 | 2.16 | 0.46 |
| 1:A:271:LEU:O | 1:A:274:SER:HB3 | 2.15 | 0.46 |
| 1:A:444:LEU:HD23 | 1:A:444:LEU:C | 2.36 | 0.46 |
| 2:C:148:GLN:O | 5:C:530:SAM:HE3 | 2.14 | 0.46 |
| 2:C:378:TYR:HE1 | 2:C:419:GLU:HG2 | 1.81 | 0.46 |
| 1:A:255:ILE:O | 1:A:258:VAL:HB | 2.16 | 0.46 |
| 1:A:290:PHE:CD2 | 1:A:291:THR:N | 2.83 | 0.46 |
| 1:A:349:ASN:CB | 2:C:430:ALA:CB | 2.94 | 0.46 |
| 2:B:22:VAL:HG12 | 2:B:23:SER:O | 2.15 | 0.46 |
| 2:B:231:LEU:HD12 | 2:B:231:LEU:N | 2.30 | 0.46 |
| 2:B:408:ASP:OD2 | 2:B:410:HIS:HB2 | 2.16 | 0.46 |
| 2:B:459:LYS:HB3 | 2:B:462:SER:H | 1.80 | 0.46 |
| 2:C:305:ARG:HH11 | 2:C:410:HIS:CD2 | 2.32 | 0.46 |
| 1:A:6:LEU:HD23 | 1:A:7:PRO:CD | 2.44 | 0.46 |
| 1:A:53:LYS:HE2 | 1:A:97:HIS:CE1 | 2.51 | 0.46 |
| 1:A:196:PHE:CE1 | 1:A:200:VAL:CG2 | 2.95 | 0.46 |
| 1:A:355:SER:HB3 | 2:C:316:PHE:CZ | 2.50 | 0.46 |
| 2:B:29:ASN:HD22 | 2:B:224:LEU:HD11 | 1.78 | 0.46 |
| 2:C:25:GLN:HA | 2:C:138:ASN:OD1 | 2.15 | 0.46 |
| 2:C:75:LEU:HB3 | 2:C:93:VAL:HG23 | 1.97 | 0.46 |
| 2:C:215:LEU:HD13 | 2:C:245:ARG:NE | 2.17 | 0.46 |
| 2:C:228:ASN:O | 2:C:232:HIS:HD2 | 1.99 | 0.46 |
| 2:C:322:THR:HB | 2:C:325:ARG:NH2 | 2.25 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:182:THR:HG23 | 1:A:183:LYS:N | 2.29 | 0.46 |
| 1:A:197:ARG:HE | 1:A:340:SER:HA | 1.80 | 0.46 |
| 1:A:242:LYS:HA | 1:A:243:PRO:HD2 | 1.82 | 0.46 |
| 1:A:252:ILE:HG22 | 1:A:269:ARG:HA | 1.96 | 0.46 |
| 2:B:287:ASN:HD21 | 2:B:289:GLN:HB2 | 1.81 | 0.46 |
| 2:C:85:LEU:CD2 | 2:C:238:LEU:CD2 | 2.94 | 0.46 |
| 2:C:231:LEU:N | 2:C:231:LEU:HD12 | 2.30 | 0.46 |
| 2:C:344:ILE:HD11 | 2:C:345:PHE:HE1 | 1.81 | 0.46 |
| 1:A:27:TYR:CE1 | 1:A:28:LYS:HE2 | 2.51 | 0.46 |
| 1:A:225:LYS:HD2 | 1:A:228:PHE:HE1 | 1.81 | 0.46 |
| 2:B:269:PHE:CD1 | 3:D:6:DA:C4 | 3.02 | 0.46 |
| 2:B:431:ASP:O | 2:B:432:SER:HB3 | 2.15 | 0.46 |
| 2:C:118:GLY:HA2 | 2:C:123:SER:CB | 2.45 | 0.46 |
| 2:C:160:ILE:HD12 | 2:C:160:ILE:N | 2.29 | 0.46 |
| 3:D:1:DG:C4 | 3:D:2:DT:H71 | 2.51 | 0.46 |
| 4:E:16:DT:C2 | 4:E:17:DG:C6 | 3.04 | 0.46 |
| 2:B:296:ILE:HD13 | 2:B:308:VAL:HG21 | 1.98 | 0.46 |
| 2:C:148:GLN:O | 5:C:530:SAM:HE1 | 2.15 | 0.46 |
| 2:C:222:ARG:O | 2:C:226:LEU:HG | 2.16 | 0.46 |
| 1:A:175:LEU:CD1 | 1:A:406:VAL:HG21 | 2.46 | 0.45 |
| 1:A:252:ILE:HD13 | 1:A:315:LEU:HD22 | 1.96 | 0.45 |
| 1:A:325:LEU:CD1 | 1:A:329:ALA:HB3 | 2.24 | 0.45 |
| 2:B:3:ASN:HD22 | 2:B:7:VAL:CG1 | 2.22 | 0.45 |
| 2:B:271:SER:O | 2:B:272:ALA:HB3 | 2.15 | 0.45 |
| 2:C:1:MET:HE1 | 2:C:132:GLU:HG3 | 1.97 | 0.45 |
| 2:C:430:ALA:HB1 | 2:C:469:LYS:HZ3 | 1.81 | 0.45 |
| 1:A:44:ILE:HD11 | 1:A:103:SER:CB | 2.45 | 0.45 |
| 1:A:227:ASN:H | 1:A:227:ASN:HD22 | 1.63 | 0.45 |
| 1:A:355:SER:N | 2:C:312:ASP:HB2 | 2.31 | 0.45 |
| 2:B:62:ARG:CD | 2:B:70:PHE:CB | 2.95 | 0.45 |
| 2:B:73:LYS:HA | 2:C:72:ARG:NH1 | 2.30 | 0.45 |
| 2:B:275:THR:CG2 | 5:B:530:SAM:HN61 | 2.29 | 0.45 |
| 2:C:6:LEU:CD2 | 2:C:130:MET:HE3 | 2.46 | 0.45 |
| 2:C:29:ASN:HD22 | 2:C:224:LEU:HD12 | 1.80 | 0.45 |
| 2:C:63:ILE:CA | 2:C:67:GLN:HB2 | 2.45 | 0.45 |
| 2:C:85:LEU:CD2 | 2:C:238:LEU:HD22 | 2.46 | 0.45 |
| 2:C:130:MET:HB2 | 2:C:130:MET:HE2 | 1.80 | 0.45 |
| 2:C:305:ARG:HH12 | 2:C:409:PRO:HG2 | 1.82 | 0.45 |
| 2:C:341:PRO:HA | 2:C:381:ARG:HG3 | 1.99 | 0.45 |
| 2:C:482:PRO:HA | 2:C:485:LEU:HG | 1.99 | 0.45 |
| 1:A:79:VAL:HG12 | 1:A:80:ILE:N | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:131:TYR:HE1 | 1:A:155:ILE:HD12 | 1.80 | 0.45 |
| 1:A:215:ASN:ND2 | 2:C:492:GLU:HG3 | 2.30 | 0.45 |
| 1:A:427:ARG:CB | 1:A:447:ILE:HD12 | 2.36 | 0.45 |
| 2:B:75:LEU:HB3 | 2:B:93:VAL:HG23 | 1.97 | 0.45 |
| 2:B:481:GLU:CB | 2:B:482:PRO:HD3 | 2.37 | 0.45 |
| 2:C:5:ASP:HB2 | 2:C:116:TYR:HE2 | 1.76 | 0.45 |
| 2:C:408:ASP:OD2 | 2:C:410:HIS:HB2 | 2.16 | 0.45 |
| 1:A:70:SER:O | 3:D:1:DG:P | 2.75 | 0.45 |
| 1:A:118:PHE:CZ | 1:A:166:LYS:HG3 | 2.51 | 0.45 |
| 2:B:17:LEU:HB3 | 2:B:22:VAL:HB | 1.99 | 0.45 |
| 2:B:186:ASP:HA | 2:B:212:PHE:CZ | 2.51 | 0.45 |
| 2:B:228:ASN:O | 2:B:232:HIS:HD2 | 1.99 | 0.45 |
| 2:B:430:ALA:HB3 | 2:B:467:TRP:O | 2.16 | 0.45 |
| 2:C:106:LEU:CD2 | 2:C:110:MET:CE | 2.95 | 0.45 |
| 2:C:524:PHE:HE2 | 2:C:528:LYS:HD2 | 1.80 | 0.45 |
| 1:A:175:LEU:CD1 | 1:A:406:VAL:CG2 | 2.94 | 0.45 |
| 1:A:248:VAL:HG13 | 1:A:270:PHE:N | 2.32 | 0.45 |
| 1:A:434:ILE:HG13 | 1:A:435:SER:N | 2.32 | 0.45 |
| 2:B:32:ALA:HB2 | 2:B:131:TYR:CE1 | 2.52 | 0.45 |
| 2:B:275:THR:HG21 | 5:B:530:SAM:C5 | 2.47 | 0.45 |
| 2:C:186:ASP:HA | 2:C:212:PHE:CZ | 2.51 | 0.45 |
| 1:A:10:TRP:NE1 | 1:A:160:PRO:HA | 2.31 | 0.45 |
| 1:A:18:VAL:O | 1:A:113:PRO:HG2 | 2.17 | 0.45 |
| 1:A:19:THR:O | 1:A:19:THR:HG23 | 2.15 | 0.45 |
| 1:A:26:THR:HG21 | 1:A:70:SER:HB3 | 1.95 | 0.45 |
| 1:A:253:LEU:C | 1:A:317:PRO:HD2 | 2.37 | 0.45 |
| 1:A:293:TYR:CE2 | 4:E:5:DC:N4 | 2.84 | 0.45 |
| 2:B:85:LEU:CD2 | 2:B:238:LEU:CD2 | 2.94 | 0.45 |
| 2:B:85:LEU:CD2 | 2:B:238:LEU:HD22 | 2.47 | 0.45 |
| 2:B:222:ARG:O | 2:B:226:LEU:HG | 2.16 | 0.45 |
| 2:C:122:LYS:HD3 | 2:C:124:ARG:CG | 2.47 | 0.45 |
| 2:C:128:GLY:CA | 2:C:231:LEU:HD22 | 2.33 | 0.45 |
| 1:A:81:ALA:HA | 1:A:92:LYS:O | 2.17 | 0.45 |
| 1:A:214:ARG:HD2 | 1:A:369:VAL:HG12 | 1.97 | 0.45 |
| 1:A:349:ASN:HB3 | 2:C:431:ASP:C | 2.37 | 0.45 |
| 2:B:345:PHE:CD2 | 3:D:6:DA:C2 | 3.05 | 0.45 |
| 2:B:420:TRP:HB2 | 2:B:425:GLU:OE1 | 2.17 | 0.45 |
| 2:C:28:VAL:CG2 | 2:C:224:LEU:CD2 | 2.95 | 0.45 |
| 1:A:10:TRP:NE1 | 1:A:160:PRO:CA | 2.80 | 0.45 |
| 1:A:63:PRO:O | 1:A:66:LEU:HB3 | 2.17 | 0.45 |
| 1:A:236:ARG:HB2 | 4:E:2:DT:H71 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:314:LEU:HD23 | 1:A:315:LEU:CA | 2.46 | 0.45 |
| 1:A:352:LYS:HD3 | 2:C:382:THR:CG2 | 2.46 | 0.45 |
| 2:B:429:VAL:HG12 | 2:B:430:ALA:N | 2.31 | 0.45 |
| 2:C:269:PHE:CD1 | 2:C:269:PHE:N | 2.83 | 0.45 |
| 2:C:275:THR:HG21 | 5:C:530:SAM:C5 | 2.47 | 0.45 |
| 2:C:287:ASN:HD21 | 2:C:289:GLN:HB2 | 1.81 | 0.45 |
| 1:A:293:TYR:O | 1:A:294:ASN:CB | 2.64 | 0.45 |
| 1:A:355:SER:CB | 2:C:312:ASP:HB2 | 2.47 | 0.45 |
| 2:B:85:LEU:HD23 | 2:B:238:LEU:HD22 | 1.98 | 0.45 |
| 2:B:164:LYS:HE3 | 2:B:407:GLU:O | 2.17 | 0.45 |
| 2:C:85:LEU:HD23 | 2:C:238:LEU:HD22 | 1.99 | 0.45 |
| 2:C:448:ARG:HD3 | 2:C:467:TRP:NE1 | 2.30 | 0.45 |
| 1:A:10:TRP:CH2 | 1:A:164:GLU:OE1 | 2.70 | 0.45 |
| 1:A:212:LYS:HG2 | 1:A:213:TRP:N | 2.32 | 0.45 |
| 1:A:292:ARG:HD3 | 1:A:293:TYR:HE1 | 1.82 | 0.45 |
| 2:B:28:VAL:CG2 | 2:B:224:LEU:CD2 | 2.95 | 0.45 |
| 2:B:29:ASN:HD22 | 2:B:224:LEU:HD12 | 1.80 | 0.45 |
| 2:B:170:VAL:H | 2:B:261:HIS:CD2 | 2.26 | 0.45 |
| 2:C:115:TRP:CH2 | 2:C:122:LYS:CE | 2.94 | 0.45 |
| 1:A:55:ASP:OD1 | 1:A:98:LEU:HG | 2.17 | 0.44 |
| 1:A:248:VAL:HG12 | 1:A:250:HIS:N | 2.26 | 0.44 |
| 1:A:294:ASN:CG | 3:D:14:DG:H5” | 2.38 | 0.44 |
| 1:A:331:PRO:HG2 | 1:A:332:GLU:OE1 | 2.17 | 0.44 |
| 2:B:17:LEU:HD21 | 2:B:106:LEU:CD1 | 2.48 | 0.44 |
| 2:B:122:LYS:HD3 | 2:B:124:ARG:CG | 2.47 | 0.44 |
| 2:B:250:LEU:HA | 2:B:279:ARG:NH2 | 2.33 | 0.44 |
| 2:C:17:LEU:HD21 | 2:C:106:LEU:CD1 | 2.47 | 0.44 |
| 2:C:32:ALA:HB2 | 2:C:131:TYR:CE1 | 2.51 | 0.44 |
| 2:C:39:MET:CE | 2:C:39:MET:CA | 2.95 | 0.44 |
| 2:C:334:LEU:HA | 2:C:357:PHE:CB | 2.46 | 0.44 |
| 2:C:338:LEU:HD13 | 2:C:401:PHE:CE1 | 2.52 | 0.44 |
| 2:C:430:ALA:HB1 | 2:C:469:LYS:NZ | 2.32 | 0.44 |
| 2:C:459:LYS:O | 2:C:460:SER:HB2 | 2.17 | 0.44 |
| 1:A:15:VAL:CA | 1:A:18:VAL:HG22 | 2.46 | 0.44 |
| 1:A:215:ASN:ND2 | 2:C:492:GLU:CG | 2.79 | 0.44 |
| 1:A:254:ARG:HG2 | 1:A:255:ILE:HG22 | 1.98 | 0.44 |
| 1:A:290:PHE:HB3 | 1:A:321:ILE:HG22 | 1.92 | 0.44 |
| 1:A:330:LEU:CD2 | 1:A:332:GLU:HB2 | 2.47 | 0.44 |
| 1:A:360:ILE:HG23 | 1:A:360:ILE:O | 2.17 | 0.44 |
| 2:B:3:ASN:CB | 2:B:130:MET:SD | 3.06 | 0.44 |
| 2:B:43:THR:HG21 | 2:B:45:GLN:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:344:ILE:HD11 | 2:B:345:PHE:HE1 | 1.82 | 0.44 |
| 2:C:420:TRP:HB2 | 2:C:425:GLU:OE1 | 2.17 | 0.44 |
| 1:A:416:LYS:O | 1:A:422:LEU:HG | 2.16 | 0.44 |
| 2:B:106:LEU:CD2 | 2:B:110:MET:CE | 2.95 | 0.44 |
| 2:C:149:TYR:CD1 | 5:C:530:SAM:C3' | 2.99 | 0.44 |
| 2:C:451:SER:O | 2:C:455:ILE:HG13 | 2.17 | 0.44 |
| 3:D:1:DG:C5 | 3:D:2:DT:H73 | 2.52 | 0.44 |
| 4:E:18:DA:C6 | 4:E:19:DA:C6 | 3.06 | 0.44 |
| 1:A:42:PRO:HB3 | 1:A:57:THR:CG2 | 2.42 | 0.44 |
| 1:A:352:LYS:HB2 | 2:C:466:SER:CB | 2.47 | 0.44 |
| 2:B:277:ILE:HD13 | 2:B:291:CYS:SG | 2.57 | 0.44 |
| 2:B:384:MET:CB | 2:B:385:PRO:HD2 | 2.37 | 0.44 |
| 2:C:3:ASN:CB | 2:C:130:MET:SD | 3.05 | 0.44 |
| 2:C:17:LEU:HD22 | 2:C:22:VAL:HG21 | 2.00 | 0.44 |
| 2:C:62:ARG:CD | 2:C:70:PHE:CB | 2.95 | 0.44 |
| 1:A:78:ILE:CD1 | 1:A:111:LEU:CD2 | 2.95 | 0.44 |
| 1:A:257:SER:HB2 | 1:A:266:ASN:HD21 | 1.81 | 0.44 |
| 1:A:294:ASN:HD22 | 3:D:14:DG:H8 | 1.64 | 0.44 |
| 2:B:438:THR:HG23 | 2:B:442:LEU:HD23 | 1.98 | 0.44 |
| 2:C:164:LYS:HE3 | 2:C:407:GLU:O | 2.17 | 0.44 |
| 2:C:279:ARG:NE | 2:C:281:PHE:CZ | 2.86 | 0.44 |
| 1:A:53:LYS:HE2 | 1:A:97:HIS:HE1 | 1.82 | 0.44 |
| 1:A:325:LEU:HD13 | 1:A:329:ALA:HB1 | 1.95 | 0.44 |
| 1:A:385:VAL:HG12 | 1:A:389:PHE:HE1 | 1.82 | 0.44 |
| 2:B:39:MET:CE | 2:B:39:MET:CA | 2.95 | 0.44 |
| 2:B:252:SER:O | 2:B:255:GLU:HG2 | 2.18 | 0.44 |
| 2:C:287:ASN:HD22 | 2:C:290:LEU:H | 1.66 | 0.44 |
| 5:C:530:SAM:CE | 4:E:6:DA:H61 | 2.05 | 0.44 |
| 1:A:15:VAL:CG2 | 1:A:155:ILE:CG2 | 2.95 | 0.44 |
| 1:A:73:ILE:HG22 | 1:A:100:PHE:HB3 | 1.94 | 0.44 |
| 1:A:253:LEU:CD1 | 1:A:263:VAL:CG2 | 2.93 | 0.44 |
| 2:B:115:TRP:CH2 | 2:B:122:LYS:CE | 2.94 | 0.44 |
| 2:B:128:GLY:O | 2:B:131:TYR:HB3 | 2.18 | 0.44 |
| 2:B:149:TYR:O | 5:B:530:SAM:HB1 | 2.18 | 0.44 |
| 2:B:287:ASN:HD22 | 2:B:290:LEU:H | 1.66 | 0.44 |
| 2:B:482:PRO:HA | 2:B:485:LEU:HG | 1.99 | 0.44 |
| 2:B:488:GLU:HG2 | 2:B:489:ALA:N | 2.33 | 0.44 |
| 2:C:158:THR:OG1 | 2:C:398:LEU:HD13 | 2.18 | 0.44 |
| 2:C:277:ILE:HD13 | 2:C:291:CYS:SG | 2.57 | 0.44 |
| 1:A:234:GLU:C | 4:E:2:DT:OP2 | 2.56 | 0.44 |
| 1:A:271:LEU:HD22 | 1:A:273:CYS:N | 2.13 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:410:THR:HA | 1:A:413:ILE:HG22 | 1.99 | 0.44 |
| 2:B:158:THR:OG1 | 2:B:398:LEU:HD13 | 2.18 | 0.44 |
| 2:C:250:LEU:HA | 2:C:279:ARG:NH2 | 2.33 | 0.44 |
| 1:A:118:PHE:CZ | 1:A:166:LYS:CE | 2.95 | 0.44 |
| 1:A:223:PHE:CG | 1:A:224:LYS:N | 2.85 | 0.44 |
| 1:A:254:ARG:HH21 | 1:A:256:SER:HB2 | 1.74 | 0.44 |
| 2:B:17:LEU:HD22 | 2:B:22:VAL:HG21 | 2.00 | 0.44 |
| 2:B:215:LEU:HD22 | 2:B:245:ARG:HH21 | 1.83 | 0.44 |
| 2:C:252:SER:O | 2:C:255:GLU:HG2 | 2.18 | 0.44 |
| 1:A:187:GLU:O | 1:A:190:PRO:HD2 | 2.18 | 0.43 |
| 1:A:262:HIS:HD2 | 1:A:263:VAL:H | 1.66 | 0.43 |
| 1:A:288:LEU:HG | 1:A:289:LEU:N | 2.32 | 0.43 |
| 2:C:459:LYS:HD3 | 2:C:459:LYS:HA | 1.80 | 0.43 |
| 2:C:488:GLU:HG2 | 2:C:489:ALA:N | 2.32 | 0.43 |
| 1:A:10:TRP:CZ2 | 1:A:417:ALA:O | 2.71 | 0.43 |
| 1:A:203:GLY:O | 1:A:204:ALA:HB3 | 2.18 | 0.43 |
| 1:A:225:LYS:HB2 | 1:A:227:ASN:ND2 | 2.33 | 0.43 |
| 1:A:286:GLY:CA | 1:A:305:LEU:HD21 | 2.48 | 0.43 |
| 2:B:6:LEU:HD23 | 2:B:130:MET:CG | 2.48 | 0.43 |
| 2:C:17:LEU:HB3 | 2:C:22:VAL:HB | 1.99 | 0.43 |
| 1:A:196:PHE:CD1 | 1:A:200:VAL:HG21 | 2.54 | 0.43 |
| 1:A:426:TRP:HE3 | 1:A:447:ILE:CB | 2.31 | 0.43 |
| 2:B:6:LEU:CB | 2:B:130:MET:HG2 | 2.47 | 0.43 |
| 2:B:459:LYS:HD3 | 2:B:459:LYS:HA | 1.81 | 0.43 |
| 1:A:16:SER:HA | 1:A:19:THR:HG22 | 2.01 | 0.43 |
| 1:A:45:ARG:HA | 1:A:104:PHE:CD1 | 2.51 | 0.43 |
| 1:A:232:LEU:HD21 | 1:A:321:ILE:CD1 | 2.45 | 0.43 |
| 2:B:207:GLN:HA | 2:B:211:ALA:CB | 2.39 | 0.43 |
| 2:C:17:LEU:CB | 2:C:27:TYR:CD1 | 3.01 | 0.43 |
| 2:C:275:THR:CB | 5:C:530:SAM:HN61 | 2.31 | 0.43 |
| 2:C:439:ASP:CA | 2:C:485:LEU:HD22 | 2.38 | 0.43 |
| 1:A:291:THR:CG2 | 1:A:302:VAL:HB | 2.48 | 0.43 |
| 1:A:291:THR:HG22 | 1:A:302:VAL:HB | 1.99 | 0.43 |
| 2:B:220:GLY:HA2 | 2:B:223:ARG:NH2 | 2.34 | 0.43 |
| 2:B:283:HIS:HB3 | 2:B:320:LYS:HE3 | 2.00 | 0.43 |
| 2:B:315:LEU:HD22 | 2:B:463:LEU:HB3 | 2.00 | 0.43 |
| 2:B:338:LEU:HD13 | 2:B:401:PHE:CE1 | 2.53 | 0.43 |
| 2:C:169:GLU:OE1 | 2:C:262:ILE:HD11 | 2.18 | 0.43 |
| 1:A:44:ILE:CG1 | 1:A:103:SER:CB | 2.96 | 0.43 |
| 1:A:89:VAL:CG2 | 1:A:135:ILE:HG22 | 2.47 | 0.43 |
| 1:A:98:LEU:HD23 | 1:A:98:LEU:HA | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:248:VAL:CG1 | 1:A:270:PHE:N | 2.82 | 0.43 |
| 1:A:300:VAL:CG1 | 1:A:301:GLY:N | 2.80 | 0.43 |
| 1:A:314:LEU:HD23 | 1:A:315:LEU:C | 2.38 | 0.43 |
| 2:B:279:ARG:NE | 2:B:281:PHE:CZ | 2.86 | 0.43 |
| 2:B:322:THR:O | 2:B:326:ARG:HG3 | 2.18 | 0.43 |
| 2:B:376:TRP:CE3 | 2:B:447:TRP:NE1 | 2.87 | 0.43 |
| 2:C:20:GLY:HA2 | 2:C:102:GLN:CG | 2.37 | 0.43 |
| 2:C:43:THR:HG21 | 2:C:45:GLN:HB2 | 2.00 | 0.43 |
| 2:C:269:PHE:CZ | 2:C:311:PRO:HD3 | 2.53 | 0.43 |
| 4:E:1:DG:H2" | 4:E:2:DT:H6 | 1.84 | 0.43 |
| 1:A:48:ASN:HB3 | 1:A:54:PHE:CD1 | 2.54 | 0.43 |
| 1:A:80:ILE:HD11 | 1:A:107:PHE:CD2 | 2.53 | 0.43 |
| 1:A:131:TYR:CE1 | 1:A:155:ILE:HD12 | 2.54 | 0.43 |
| 1:A:252:ILE:HG23 | 1:A:268:ILE:HG23 | 1.92 | 0.43 |
| 1:A:411:GLN:HB3 | 2:B:491:GLY:O | 2.19 | 0.43 |
| 2:B:166:GLN:HB3 | 2:B:167:PRO:HD2 | 2.01 | 0.43 |
| 1:A:133:ASN:HA | 2:B:469:LYS:NZ | 2.34 | 0.43 |
| 1:A:254:ARG:CG | 1:A:255:ILE:H | 2.30 | 0.43 |
| 2:B:14:CYS:SG | 2:B:31:LEU:HD11 | 2.59 | 0.43 |
| 2:B:17:LEU:CB | 2:B:27:TYR:CD1 | 3.01 | 0.43 |
| 2:B:497:LEU:HD12 | 2:B:497:LEU:N | 2.34 | 0.43 |
| 2:C:1:MET:SD | 2:C:129:ASP:HA | 2.58 | 0.43 |
| 2:C:497:LEU:N | 2:C:497:LEU:HD12 | 2.34 | 0.43 |
| 1:A:17:THR:CG2 | 1:A:18:VAL:N | 2.82 | 0.43 |
| 1:A:20:THR:CG2 | 1:A:21:LEU:N | 2.82 | 0.43 |
| 1:A:26:THR:HG21 | 1:A:70:SER:H | 1.84 | 0.43 |
| 1:A:78:ILE:HG22 | 1:A:96:GLN:CG | 2.44 | 0.43 |
| 2:B:380:LEU:O | 2:B:380:LEU:HD23 | 2.19 | 0.43 |
| 2:C:322:THR:CG2 | 2:C:323:ASP:N | 2.82 | 0.43 |
| 1:A:112:ARG:H | 1:A:112:ARG:CD | 2.32 | 0.43 |
| 1:A:155:ILE:HG23 | 1:A:155:ILE:O | 2.19 | 0.43 |
| 1:A:197:ARG:CZ | 1:A:340:SER:HA | 2.48 | 0.43 |
| 1:A:222:VAL:CG1 | 1:A:223:PHE:N | 2.82 | 0.43 |
| 1:A:254:ARG:HA | 1:A:317:PRO:HG2 | 2.01 | 0.43 |
| 1:A:426:TRP:CE3 | 1:A:447:ILE:CB | 3.00 | 0.43 |
| 2:B:62:ARG:HH11 | 2:B:66:GLU:HG2 | 1.84 | 0.43 |
| 2:B:275:THR:CB | 5:B:530:SAM:HN61 | 2.32 | 0.43 |
| 2:B:378:TYR:HE1 | 2:B:419:GLU:HG2 | 1.84 | 0.43 |
| 2:C:115:TRP:CE3 | 2:C:127:PHE:CE1 | 3.07 | 0.43 |
| 1:A:89:VAL:HG22 | 1:A:89:VAL:O | 2.19 | 0.42 |
| 1:A:142:ALA:O | 2:B:316:PHE:CZ | 2.72 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:154:LEU:HD23 | 1:A:154:LEU:C | 2.39 | 0.42 |
| 1:A:365:ILE:CG2 | 1:A:366:LYS:N | 2.82 | 0.42 |
| 1:A:388:LEU:HD23 | 1:A:388:LEU:C | 2.39 | 0.42 |
| 2:B:151:THR:HG22 | 2:B:152:PRO:N | 2.34 | 0.42 |
| 2:B:224:LEU:HD12 | 2:B:224:LEU:N | 2.34 | 0.42 |
| 2:B:269:PHE:CZ | 2:B:311:PRO:HD3 | 2.54 | 0.42 |
| 2:B:305:ARG:HH12 | 2:B:409:PRO:HG2 | 1.82 | 0.42 |
| 2:B:334:LEU:HA | 2:B:357:PHE:CB | 2.46 | 0.42 |
| 2:C:6:LEU:CB | 2:C:117:ASN:HB2 | 2.47 | 0.42 |
| 2:C:122:LYS:HZ2 | 2:C:124:ARG:HG2 | 1.81 | 0.42 |
| 1:A:10:TRP:CE2 | 1:A:418:PHE:CA | 2.94 | 0.42 |
| 1:A:35:TYR:CD1 | 1:A:65:ASN:ND2 | 2.87 | 0.42 |
| 1:A:72:LYS:HB3 | 3:D:1:DG:OP2 | 2.19 | 0.42 |
| 1:A:284:GLN:HE21 | 1:A:284:GLN:HB3 | 1.47 | 0.42 |
| 1:A:287:ASP:HB2 | 1:A:322:ARG:HH21 | 1.84 | 0.42 |
| 1:A:385:VAL:CG1 | 1:A:389:PHE:HE1 | 2.32 | 0.42 |
| 2:B:130:MET:HB2 | 2:B:130:MET:HE2 | 1.75 | 0.42 |
| 2:B:161:HIS:O | 2:B:164:LYS:HG3 | 2.19 | 0.42 |
| 2:B:251:GLY:HA2 | 2:B:278:THR:OG1 | 2.19 | 0.42 |
| 2:C:34:LEU:CB | 2:C:110:MET:SD | 3.07 | 0.42 |
| 2:C:103:ILE:CG2 | 2:C:104:THR:N | 2.82 | 0.42 |
| 2:C:213:ILE:CG2 | 2:C:214:GLY:N | 2.82 | 0.42 |
| 2:C:450:PHE:CE1 | 2:C:467:TRP:CZ3 | 3.07 | 0.42 |
| 2:C:493:LEU:HD22 | 2:C:493:LEU:N | 2.34 | 0.42 |
| 1:A:10:TRP:CE3 | 1:A:418:PHE:O | 2.72 | 0.42 |
| 1:A:104:PHE:CZ | 1:A:106:ALA:HB3 | 2.54 | 0.42 |
| 1:A:117:ILE:HD12 | 1:A:165:GLN:OE1 | 2.19 | 0.42 |
| 1:A:118:PHE:CZ | 1:A:162:LEU:HD21 | 2.53 | 0.42 |
| 1:A:212:LYS:CG | 1:A:213:TRP:N | 2.83 | 0.42 |
| 1:A:224:LYS:O | 1:A:370:VAL:HG12 | 2.20 | 0.42 |
| 1:A:233:THR:O | 1:A:321:ILE:HG13 | 2.19 | 0.42 |
| 1:A:255:ILE:CG2 | 1:A:256:SER:N | 2.83 | 0.42 |
| 1:A:265:GLN:CG | 1:A:266:ASN:N | 2.82 | 0.42 |
| 1:A:347:MET:CE | 1:A:360:ILE:CD1 | 2.96 | 0.42 |
| 2:C:62:ARG:HH11 | 2:C:66:GLU:HG2 | 1.84 | 0.42 |
| 2:C:215:LEU:HD22 | 2:C:245:ARG:HH21 | 1.83 | 0.42 |
| 2:C:269:PHE:CG | 4:E:6:DA:C4 | 3.07 | 0.42 |
| 1:A:41:LEU:HD23 | 1:A:42:PRO:HD2 | 1.98 | 0.42 |
| 1:A:46:ALA:HB1 | 1:A:82:MET:HE3 | 1.97 | 0.42 |
| 1:A:121:PHE:CZ | 1:A:160:PRO:HG3 | 2.55 | 0.42 |
| 1:A:142:ALA:O | 2:B:316:PHE:CE2 | 2.72 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:198:GLN:NE2 | 2:C:491:GLY:HA3 | 2.34 | 0.42 |
| 1:A:254:ARG:CG | 1:A:255:ILE:N | 2.83 | 0.42 |
| 1:A:315:LEU:HD23 | 1:A:316:TYR:O | 2.19 | 0.42 |
| 2:B:277:ILE:O | 2:B:277:ILE:HG22 | 2.20 | 0.42 |
| 2:B:377:VAL:HG12 | 2:B:378:TYR:N | 2.34 | 0.42 |
| 2:C:358:THR:CG2 | 2:C:359:LYS:N | 2.83 | 0.42 |
| 3:D:1:DG:C4 | 3:D:2:DT:C7 | 3.03 | 0.42 |
| 4:E:1:DG:C4 | 4:E:2:DT:H72 | 2.55 | 0.42 |
| 1:A:22:ILE:CG2 | 1:A:108:CYS:SG | 3.07 | 0.42 |
| 1:A:126:THR:CG2 | 1:A:127:LYS:N | 2.83 | 0.42 |
| 1:A:239:LEU:CD2 | 1:A:240:SER:N | 2.82 | 0.42 |
| 1:A:333:TYR:CA | 1:A:382:VAL:HG22 | 2.46 | 0.42 |
| 1:A:395:ILE:CG2 | 1:A:396:GLU:N | 2.83 | 0.42 |
| 1:A:410:THR:CG2 | 1:A:411:GLN:N | 2.83 | 0.42 |
| 1:A:417:ALA:HA | 1:A:422:LEU:HG | 2.00 | 0.42 |
| 2:B:245:ARG:HH22 | 2:B:253:ASP:C | 2.23 | 0.42 |
| 2:B:478:SER:N | 2:B:479:LEU:HD12 | 2.35 | 0.42 |
| 2:C:14:CYS:SG | 2:C:31:LEU:HD11 | 2.59 | 0.42 |
| 2:C:170:VAL:H | 2:C:261:HIS:CD2 | 2.27 | 0.42 |
| 2:C:220:GLY:HA3 | 2:C:223:ARG:HH21 | 1.85 | 0.42 |
| 1:A:15:VAL:HA | 1:A:18:VAL:CG2 | 2.49 | 0.42 |
| 1:A:61:PHE:CE2 | 1:A:66:LEU:HB2 | 2.54 | 0.42 |
| 1:A:144:ILE:HG12 | 2:B:316:PHE:HZ | 1.81 | 0.42 |
| 1:A:167:ILE:CG2 | 1:A:168:ILE:N | 2.83 | 0.42 |
| 1:A:334:ILE:CG2 | 1:A:335:GLU:N | 2.83 | 0.42 |
| 2:B:115:TRP:CE3 | 2:B:127:PHE:CE1 | 3.07 | 0.42 |
| 2:B:269:PHE:HB2 | 3:D:6:DA:N9 | 2.28 | 0.42 |
| 2:C:142:THR:CG2 | 2:C:143:LYS:N | 2.83 | 0.42 |
| 2:C:220:GLY:HA2 | 2:C:223:ARG:NH2 | 2.34 | 0.42 |
| 2:C:262:ILE:HG22 | 2:C:263:VAL:N | 2.34 | 0.42 |
| 2:C:336:THR:CG2 | 2:C:337:ILE:N | 2.83 | 0.42 |
| 1:A:144:ILE:N | 2:B:316:PHE:CZ | 2.83 | 0.42 |
| 1:A:182:THR:CG2 | 1:A:183:LYS:N | 2.83 | 0.42 |
| 1:A:223:PHE:CZ | 1:A:369:VAL:HG13 | 2.49 | 0.42 |
| 1:A:229:GLU:OE2 | 1:A:329:ALA:HB2 | 2.20 | 0.42 |
| 1:A:232:LEU:HG | 1:A:321:ILE:CD1 | 2.46 | 0.42 |
| 2:B:136:GLN:HG2 | 2:B:140:ASN:HD21 | 1.85 | 0.42 |
| 2:B:213:ILE:CG2 | 2:B:214:GLY:N | 2.83 | 0.42 |
| 2:B:285:THR:HG22 | 2:B:287:ASN:N | 2.07 | 0.42 |
| 2:C:85:LEU:HD21 | 2:C:238:LEU:CD2 | 2.50 | 0.42 |
| 2:C:151:THR:HG22 | 2:C:152:PRO:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:166:GLN:HB3 | 2:C:167:PRO:HD2 | 2.00 | 0.42 |
| 2:C:222:ARG:HH12 | 2:C:226:LEU:HD11 | 1.81 | 0.42 |
| 2:C:224:LEU:HD12 | 2:C:224:LEU:N | 2.34 | 0.42 |
| 2:C:354:VAL:CG1 | 2:C:356:PHE:CZ | 3.03 | 0.42 |
| 2:C:478:SER:N | 2:C:479:LEU:HD12 | 2.35 | 0.42 |
| 1:A:54:PHE:CD2 | 1:A:54:PHE:O | 2.73 | 0.42 |
| 1:A:104:PHE:CE1 | 1:A:107:PHE:CD1 | 3.08 | 0.42 |
| 1:A:164:GLU:CG | 1:A:423:THR:CA | 2.95 | 0.42 |
| 1:A:255:ILE:CG2 | 3:D:14:DG:H5' | 2.47 | 0.42 |
| 1:A:330:LEU:HD22 | 1:A:333:TYR:N | 2.30 | 0.42 |
| 1:A:330:LEU:HD23 | 1:A:330:LEU:C | 2.39 | 0.42 |
| 1:A:332:GLU:HB3 | 1:A:382:VAL:CG1 | 2.50 | 0.42 |
| 2:B:22:VAL:HG13 | 2:B:96:THR:OG1 | 2.20 | 0.42 |
| 2:B:123:SER:O | 2:B:127:PHE:HD1 | 2.03 | 0.42 |
| 2:B:479:LEU:HD12 | 2:B:479:LEU:N | 2.33 | 0.42 |
| 2:C:269:PHE:CD1 | 4:E:6:DA:N7 | 2.86 | 0.42 |
| 2:C:435:ASN:HD21 | 2:C:467:TRP:HB2 | 1.84 | 0.42 |
| 1:A:6:LEU:CD1 | 1:A:12:ILE:CD1 | 2.95 | 0.42 |
| 1:A:142:ALA:HB1 | 2:B:312:ASP:CA | 2.50 | 0.42 |
| 1:A:414:LEU:O | 1:A:418:PHE:CD2 | 2.73 | 0.42 |
| 2:B:216:GLU:HG2 | 2:B:221:THR:HB | 2.01 | 0.42 |
| 2:B:305:ARG:HD3 | 2:B:410:HIS:CG | 2.55 | 0.42 |
| 2:B:493:LEU:HD22 | 2:B:493:LEU:N | 2.34 | 0.42 |
| 2:C:3:ASN:HB2 | 2:C:7:VAL:CB | 2.44 | 0.42 |
| 2:C:20:GLY:N | 2:C:102:GLN:HG3 | 2.34 | 0.42 |
| 1:A:122:ILE:CG2 | 1:A:123:ALA:N | 2.83 | 0.42 |
| 1:A:230:SER:HA | 1:A:324:ARG:O | 2.19 | 0.42 |
| 1:A:253:LEU:O | 1:A:316:TYR:HB2 | 2.19 | 0.42 |
| 1:A:289:LEU:HD11 | 1:A:320:LEU:HD21 | 1.97 | 0.42 |
| 1:A:302:VAL:CG1 | 1:A:303:CYS:N | 2.83 | 0.42 |
| 1:A:312:GLN:CG | 1:A:313:ASN:N | 2.82 | 0.42 |
| 2:B:481:GLU:HB2 | 2:B:482:PRO:CD | 2.41 | 0.42 |
| 2:C:72:ARG:CG | 2:C:73:LYS:N | 2.82 | 0.42 |
| 2:C:123:SER:O | 2:C:127:PHE:HD1 | 2.03 | 0.42 |
| 2:C:161:HIS:O | 2:C:164:LYS:HG3 | 2.19 | 0.42 |
| 2:C:376:TRP:CE3 | 2:C:447:TRP:NE1 | 2.87 | 0.42 |
| 2:C:427:THR:CG2 | 2:C:428:GLU:N | 2.83 | 0.42 |
| 2:C:459:LYS:HB3 | 2:C:462:SER:H | 1.85 | 0.42 |
| 1:A:61:PHE:CE1 | 1:A:69:GLU:OE1 | 2.74 | 0.41 |
| 1:A:270:PHE:CD2 | 1:A:271:LEU:O | 2.73 | 0.41 |
| 1:A:415:ALA:CB | 2:B:492:GLU:HG2 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1:MET:CE | 2:B:132:GLU:CB | 2.95 | 0.41 |
| 2:B:451:SER:O | 2:B:455:ILE:HG13 | 2.19 | 0.41 |
| 2:C:149:TYR:CD1 | 5:C:530:SAM:H3' | 2.55 | 0.41 |
| 2:C:172:GLN:CD | 2:C:257:LEU:HD23 | 2.40 | 0.41 |
| 2:C:305:ARG:HD3 | 2:C:410:HIS:CG | 2.55 | 0.41 |
| 1:A:7:PRO:HG3 | 1:A:415:ALA:O | 2.20 | 0.41 |
| 1:A:20:THR:HG23 | 1:A:111:LEU:HB2 | 1.99 | 0.41 |
| 1:A:25:VAL:HB | 1:A:104:PHE:C | 2.40 | 0.41 |
| 1:A:80:ILE:HD13 | 1:A:107:PHE:HD2 | 1.81 | 0.41 |
| 1:A:293:TYR:C | 1:A:295:GLY:H | 2.23 | 0.41 |
| 1:A:336:ILE:CG2 | 1:A:337:PHE:N | 2.83 | 0.41 |
| 2:B:20:GLY:N | 2:B:102:GLN:HG3 | 2.34 | 0.41 |
| 2:B:103:ILE:CG2 | 2:B:104:THR:N | 2.83 | 0.41 |
| 2:B:122:LYS:CD | 2:B:124:ARG:HG2 | 2.50 | 0.41 |
| 2:B:172:GLN:CD | 2:B:257:LEU:HD23 | 2.41 | 0.41 |
| 2:C:22:VAL:HG13 | 2:C:96:THR:OG1 | 2.20 | 0.41 |
| 2:C:263:VAL:CG2 | 2:C:300:LEU:CD2 | 2.95 | 0.41 |
| 2:C:479:LEU:HD12 | 2:C:479:LEU:N | 2.33 | 0.41 |
| 2:C:484:VAL:CG2 | 2:C:485:LEU:N | 2.83 | 0.41 |
| 4:E:1:DG:C4 | 4:E:2:DT:C5 | 3.07 | 0.41 |
| 4:E:16:DT:C2' | 4:E:17:DG:C8 | 2.99 | 0.41 |
| 1:A:10:TRP:CE2 | 1:A:160:PRO:CA | 3.00 | 0.41 |
| 1:A:33:ILE:CG2 | 1:A:34:ASN:N | 2.82 | 0.41 |
| 1:A:70:SER:HA | 3:D:1:DG:H5' | 2.03 | 0.41 |
| 1:A:159:ILE:HA | 1:A:160:PRO:HD2 | 1.83 | 0.41 |
| 1:A:328:ASP:O | 1:A:329:ALA:HB2 | 2.20 | 0.41 |
| 2:B:85:LEU:HD21 | 2:B:238:LEU:CD2 | 2.50 | 0.41 |
| 2:B:142:THR:CG2 | 2:B:143:LYS:N | 2.83 | 0.41 |
| 2:B:217:LEU:HD22 | 2:B:275:THR:HG23 | 1.94 | 0.41 |
| 2:B:269:PHE:CE2 | 2:B:311:PRO:CB | 3.02 | 0.41 |
| 2:C:6:LEU:CB | 2:C:130:MET:HG2 | 2.50 | 0.41 |
| 2:C:122:LYS:CD | 2:C:124:ARG:HG2 | 2.49 | 0.41 |
| 1:A:44:ILE:HG12 | 1:A:103:SER:HA | 2.02 | 0.41 |
| 2:B:293:MET:HE3 | 2:B:310:VAL:HG11 | 2.02 | 0.41 |
| 2:B:336:THR:CG2 | 2:B:337:ILE:N | 2.83 | 0.41 |
| 2:B:344:ILE:CD1 | 2:B:345:PHE:CE1 | 3.03 | 0.41 |
| 2:B:345:PHE:CD2 | 3:D:6:DA:H2 | 2.38 | 0.41 |
| 2:C:277:ILE:O | 2:C:277:ILE:HG22 | 2.20 | 0.41 |
| 1:A:71:GLN:HG3 | 1:A:103:SER:O | 2.19 | 0.41 |
| 1:A:142:ALA:HB1 | 2:B:312:ASP:C | 2.41 | 0.41 |
| 1:A:158:PRO:CG | 1:A:418:PHE:CE2 | 3.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:193:LEU:HD23 | 1:A:193:LEU:C | 2.40 | 0.41 |
| 1:A:416:LYS:O | 1:A:422:LEU:HD23 | 2.20 | 0.41 |
| 2:B:6:LEU:CD2 | 2:B:130:MET:HE3 | 2.50 | 0.41 |
| 1:A:26:THR:HG21 | 3:D:2:DT:H72 | 2.03 | 0.41 |
| 1:A:41:LEU:HD11 | 1:A:73:ILE:HG12 | 2.02 | 0.41 |
| 1:A:61:PHE:CZ | 1:A:66:LEU:CA | 3.00 | 0.41 |
| 2:B:62:ARG:HB3 | 2:B:67:GLN:HA | 2.03 | 0.41 |
| 2:B:220:GLY:HA2 | 2:B:223:ARG:HH21 | 1.85 | 0.41 |
| 2:B:358:THR:CG2 | 2:B:359:LYS:N | 2.83 | 0.41 |
| 2:C:251:GLY:HA2 | 2:C:278:THR:OG1 | 2.19 | 0.41 |
| 2:C:420:TRP:O | 2:C:420:TRP:CD1 | 2.73 | 0.41 |
| 1:A:6:LEU:HA | 1:A:7:PRO:HD2 | 1.79 | 0.41 |
| 1:A:42:PRO:HG2 | 1:A:101:GLU:HG3 | 2.03 | 0.41 |
| 1:A:209:LEU:N | 1:A:209:LEU:CD1 | 2.83 | 0.41 |
| 1:A:316:TYR:CE2 | 1:A:320:LEU:O | 2.74 | 0.41 |
| 1:A:422:LEU:N | 1:A:422:LEU:CD2 | 2.83 | 0.41 |
| 2:B:38:LYS:HA | 2:B:56:TRP:CE3 | 2.56 | 0.41 |
| 2:B:63:ILE:HG12 | 2:B:64:GLY:N | 2.36 | 0.41 |
| 2:B:283:HIS:N | 2:B:294:GLN:HE22 | 2.05 | 0.41 |
| 2:B:484:VAL:CG2 | 2:B:485:LEU:N | 2.83 | 0.41 |
| 2:C:88:ALA:HB2 | 2:C:241:GLY:HA2 | 2.02 | 0.41 |
| 2:C:384:MET:HE3 | 2:C:385:PRO:HD2 | 2.03 | 0.41 |
| 1:A:12:ILE:CD1 | 1:A:12:ILE:N | 2.83 | 0.41 |
| 1:A:126:THR:O | 1:A:131:TYR:CD2 | 2.74 | 0.41 |
| 1:A:136:SER:HB2 | 2:B:469:LYS:CE | 2.51 | 0.41 |
| 1:A:353:THR:CG2 | 2:C:351:LYS:CE | 2.95 | 0.41 |
| 1:A:394:THR:CG2 | 1:A:395:ILE:N | 2.82 | 0.41 |
| 1:A:426:TRP:HE3 | 1:A:447:ILE:HG21 | 1.84 | 0.41 |
| 2:B:190:LYS:HA | 2:B:193:THR:OG1 | 2.21 | 0.41 |
| 2:B:440:GLN:CB | 2:B:484:VAL:HB | 2.50 | 0.41 |
| 2:C:216:GLU:HG2 | 2:C:221:THR:HB | 2.01 | 0.41 |
| 2:C:269:PHE:HD1 | 4:E:6:DA:C5 | 2.25 | 0.41 |
| 2:C:334:LEU:HD12 | 2:C:357:PHE:HB3 | 2.03 | 0.41 |
| 1:A:27:TYR:CE2 | 1:A:28:LYS:O | 2.74 | 0.41 |
| 1:A:41:LEU:CD2 | 1:A:42:PRO:N | 2.78 | 0.41 |
| 1:A:45:ARG:O | 1:A:107:PHE:CZ | 2.74 | 0.41 |
| 1:A:61:PHE:CE1 | 1:A:65:ASN:CG | 2.94 | 0.41 |
| 1:A:133:ASN:CG | 2:B:431:ASP:HB2 | 2.41 | 0.41 |
| 1:A:138:LEU:HD22 | 1:A:138:LEU:H | 1.83 | 0.41 |
| 1:A:316:TYR:CD2 | 1:A:317:PRO:O | 2.74 | 0.41 |
| 2:B:103:ILE:O | 2:B:107:VAL:HG23 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:220:GLY:HA3 | 2:B:223:ARG:HH21 | 1.84 | 0.41 |
| 2:B:427:THR:CG2 | 2:B:428:GLU:N | 2.83 | 0.41 |
| 2:C:148:GLN:OE1 | 4:E:6:DA:C8 | 2.74 | 0.41 |
| 2:C:163:LEU:CG | 2:C:262:ILE:HG21 | 2.48 | 0.41 |
| 2:C:216:GLU:HG3 | 2:C:218:VAL:O | 2.21 | 0.41 |
| 2:C:244:ILE:N | 2:C:244:ILE:CD1 | 2.84 | 0.41 |
| 2:C:245:ARG:HH22 | 2:C:253:ASP:C | 2.23 | 0.41 |
| 2:C:246:LEU:HD13 | 2:C:247:GLY:N | 2.36 | 0.41 |
| 2:C:344:ILE:CD1 | 2:C:345:PHE:CE1 | 3.04 | 0.41 |
| 2:C:377:VAL:HG12 | 2:C:378:TYR:N | 2.35 | 0.41 |
| 2:C:408:ASP:OD1 | 2:C:409:PRO:HD2 | 2.21 | 0.41 |
| 1:A:11:VAL:CG1 | 1:A:12:ILE:N | 2.83 | 0.41 |
| 1:A:36:LEU:N | 1:A:36:LEU:CD2 | 2.83 | 0.41 |
| 1:A:299:PHE:CD2 | 1:A:347:MET:HG2 | 2.54 | 0.41 |
| 1:A:356:GLY:N | 2:C:316:PHE:CZ | 2.89 | 0.41 |
| 1:A:411:GLN:OE1 | 2:B:491:GLY:HA3 | 2.20 | 0.41 |
| 1:A:414:LEU:O | 1:A:418:PHE:CG | 2.74 | 0.41 |
| 2:B:88:ALA:HB2 | 2:B:241:GLY:HA2 | 2.02 | 0.41 |
| 2:C:450:PHE:HZ | 2:C:467:TRP:CZ3 | 2.38 | 0.41 |
| 2:C:515:LEU:HD22 | 2:C:515:LEU:H | 1.86 | 0.41 |
| 1:A:27:TYR:CD2 | 1:A:28:LYS:O | 2.74 | 0.40 |
| 1:A:74:SER:O | 1:A:100:PHE:CD2 | 2.74 | 0.40 |
| 1:A:252:ILE:HG22 | 1:A:268:ILE:C | 2.42 | 0.40 |
| 1:A:268:ILE:HG12 | 1:A:269:ARG:N | 2.36 | 0.40 |
| 1:A:294:ASN:ND2 | 3:D:13:DC:C2' | 2.60 | 0.40 |
| 2:B:28:VAL:CG2 | 2:B:29:ASN:N | 2.85 | 0.40 |
| 2:B:279:ARG:NH2 | 2:B:281:PHE:HZ | 2.19 | 0.40 |
| 2:B:390:ARG:CG | 2:B:391:THR:N | 2.85 | 0.40 |
| 2:B:420:TRP:O | 2:B:420:TRP:CD1 | 2.73 | 0.40 |
| 2:C:136:GLN:HG2 | 2:C:140:ASN:HD21 | 1.86 | 0.40 |
| 2:C:283:HIS:HB3 | 2:C:320:LYS:HE3 | 2.03 | 0.40 |
| 1:A:89:VAL:HG22 | 1:A:135:ILE:HG21 | 2.03 | 0.40 |
| 1:A:236:ARG:CG | 1:A:237:ASN:N | 2.82 | 0.40 |
| 2:B:216:GLU:HG3 | 2:B:218:VAL:O | 2.21 | 0.40 |
| 2:B:237:ASN:HD22 | 2:B:238:LEU:N | 2.19 | 0.40 |
| 2:B:432:SER:HB2 | 2:B:433:GLU:H | 1.62 | 0.40 |
| 2:C:38:LYS:HA | 2:C:56:TRP:CE3 | 2.56 | 0.40 |
| 2:C:62:ARG:HD3 | 2:C:70:PHE:HB2 | 2.02 | 0.40 |
| 2:C:115:TRP:CZ3 | 2:C:127:PHE:CE1 | 3.09 | 0.40 |
| 2:C:390:ARG:CG | 2:C:391:THR:N | 2.84 | 0.40 |
| 1:A:49:ILE:CG1 | 1:A:107:PHE:CE2 | 2.98 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:114:GLU:C | 1:A:116:LEU:H | 2.25 | 0.40 |
| 1:A:232:LEU:HD11 | 1:A:321:ILE:CD1 | 2.48 | 0.40 |
| 1:A:290:PHE:CD1 | 1:A:302:VAL:O | 2.74 | 0.40 |
| 1:A:299:PHE:C | 1:A:300:VAL:HG23 | 2.42 | 0.40 |
| 1:A:303:CYS:SG | 1:A:304:GLY:N | 2.95 | 0.40 |
| 2:C:190:LYS:HA | 2:C:193:THR:OG1 | 2.21 | 0.40 |
| 2:C:440:GLN:HB2 | 2:C:484:VAL:CB | 2.45 | 0.40 |
| 3:D:10:DC:H2" | 3:D:11:DG:O5' | 2.21 | 0.40 |
| 3:D:18:DA:C2 | 4:E:4:DG:N2 | 2.89 | 0.40 |
| 1:A:54:PHE:CE1 | 1:A:56:THR:O | 2.75 | 0.40 |
| 1:A:54:PHE:CE2 | 1:A:101:GLU:OE1 | 2.74 | 0.40 |
| 1:A:125:PHE:CE1 | 1:A:418:PHE:HZ | 2.32 | 0.40 |
| 1:A:137:SER:OG | 1:A:138:LEU:HD22 | 2.21 | 0.40 |
| 1:A:292:ARG:O | 1:A:359:GLY:HA2 | 2.22 | 0.40 |
| 1:A:305:LEU:CD2 | 1:A:306:LEU:N | 2.82 | 0.40 |
| 1:A:350:CYS:N | 2:C:432:SER:HB3 | 2.37 | 0.40 |
| 2:B:34:LEU:CB | 2:B:110:MET:SD | 3.07 | 0.40 |
| 2:B:148:GLN:OE1 | 3:D:6:DA:C8 | 2.74 | 0.40 |
| 2:B:246:LEU:HD13 | 2:B:247:GLY:N | 2.36 | 0.40 |
| 2:B:334:LEU:HD12 | 2:B:357:PHE:HB3 | 2.03 | 0.40 |
| 2:C:103:ILE:O | 2:C:107:VAL:HG23 | 2.21 | 0.40 |
| 2:C:345:PHE:CD2 | 4:E:6:DA:C2 | 3.10 | 0.40 |
| 2:C:429:VAL:HG12 | 2:C:430:ALA:N | 2.37 | 0.40 |
| 3:D:1:DG:C8 | 3:D:2:DT:H71 | 2.56 | 0.40 |
| 1:A:54:PHE:CZ | 1:A:56:THR:O | 2.74 | 0.40 |
| 1:A:75:PRO:HG3 | 1:A:111:LEU:CD1 | 2.41 | 0.40 |
| 1:A:98:LEU:CB | 1:A:99:PRO:CD | 2.99 | 0.40 |
| 1:A:223:PHE:CD1 | 1:A:370:VAL:O | 2.74 | 0.40 |
| 2:B:6:LEU:CB | 2:B:117:ASN:HB2 | 2.45 | 0.40 |
| 2:B:269:PHE:N | 2:B:269:PHE:HD1 | 2.18 | 0.40 |
| 2:B:350:VAL:O | 2:B:350:VAL:HG23 | 2.20 | 0.40 |
| 2:C:38:LYS:CD | 2:C:56:TRP:CE2 | 3.04 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 462/464 (100%) | 433 (94%) | 22 (5%) | 7 (2%) | 10 | 46 |
| 2 | B | 527/529 (100%) | 503 (95%) | 18 (3%) | 6 (1%) | 14 | 52 |
| 2 | C | 527/529 (100%) | 503 (95%) | 20 (4%) | 4 (1%) | 19 | 60 |
| All | All | 1516/1522 (100%) | 1439 (95%) | 60 (4%) | 17 (1%) | 18 | 52 |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 139 | SER |
| 1 | A | 296 | SER |
| 1 | A | 326 | THR |
| 1 | A | 248 | VAL |
| 2 | B | 472 | ASP |
| 2 | C | 472 | ASP |
| 1 | A | 2 | SER |
| 2 | B | 4 | ASN |
| 2 | B | 272 | ALA |
| 2 | B | 432 | SER |
| 2 | C | 4 | ASN |
| 2 | C | 272 | ALA |
| 1 | A | 206 | ASN |
| 1 | A | 215 | ASN |
| 2 | B | 464 | ASP |
| 2 | B | 274 | GLY |
| 2 | C | 274 | GLY |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 398/398 (100%) | 383 (96%) | 15 (4%) | 33 | 57 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | B | 452/452 (100%) | 443 (98%) | 9 (2%) | 55 74 |
| 2 | C | 452/452 (100%) | 443 (98%) | 9 (2%) | 55 74 |
| All | All | 1302/1302 (100%) | 1269 (98%) | 33 (2%) | 50 68 |

All (33) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 10 | TRP |
| 1 | A | 28 | LYS |
| 1 | A | 65 | ASN |
| 1 | A | 112 | ARG |
| 1 | A | 145 | ASN |
| 1 | A | 187 | GLU |
| 1 | A | 215 | ASN |
| 1 | A | 227 | ASN |
| 1 | A | 234 | GLU |
| 1 | A | 239 | LEU |
| 1 | A | 284 | GLN |
| 1 | A | 313 | ASN |
| 1 | A | 349 | ASN |
| 1 | A | 357 | GLN |
| 1 | A | 407 | ASN |
| 2 | B | 87 | GLN |
| 2 | B | 113 | LEU |
| 2 | B | 237 | ASN |
| 2 | B | 287 | ASN |
| 2 | B | 316 | PHE |
| 2 | B | 346 | TYR |
| 2 | B | 453 | GLU |
| 2 | B | 488 | GLU |
| 2 | B | 492 | GLU |
| 2 | C | 87 | GLN |
| 2 | C | 113 | LEU |
| 2 | C | 237 | ASN |
| 2 | C | 287 | ASN |
| 2 | C | 346 | TYR |
| 2 | C | 434 | GLU |
| 2 | C | 453 | GLU |
| 2 | C | 488 | GLU |
| 2 | C | 492 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 31 | GLN |
| 1 | A | 34 | ASN |
| 1 | A | 96 | GLN |
| 1 | A | 97 | HIS |
| 1 | A | 133 | ASN |
| 1 | A | 143 | ASN |
| 1 | A | 146 | ASN |
| 1 | A | 156 | ASN |
| 1 | A | 191 | GLN |
| 1 | A | 215 | ASN |
| 1 | A | 227 | ASN |
| 1 | A | 250 | HIS |
| 1 | A | 262 | HIS |
| 1 | A | 265 | GLN |
| 1 | A | 281 | HIS |
| 1 | A | 294 | ASN |
| 1 | A | 313 | ASN |
| 1 | A | 345 | ASN |
| 1 | A | 349 | ASN |
| 1 | A | 368 | GLN |
| 1 | A | 398 | GLN |
| 1 | A | 407 | ASN |
| 2 | B | 2 | ASN |
| 2 | B | 3 | ASN |
| 2 | B | 4 | ASN |
| 2 | B | 29 | ASN |
| 2 | B | 69 | GLN |
| 2 | B | 91 | HIS |
| 2 | B | 92 | ASN |
| 2 | B | 140 | ASN |
| 2 | B | 232 | HIS |
| 2 | B | 237 | ASN |
| 2 | B | 240 | HIS |
| 2 | B | 261 | HIS |
| 2 | B | 276 | ASN |
| 2 | B | 287 | ASN |
| 2 | B | 294 | GLN |
| 2 | B | 301 | HIS |
| 2 | B | 348 | GLN |
| 2 | B | 397 | HIS |
| 2 | B | 399 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 410 | HIS |
| 2 | B | 435 | ASN |
| 2 | B | 437 | ASN |
| 2 | C | 2 | ASN |
| 2 | C | 3 | ASN |
| 2 | C | 4 | ASN |
| 2 | C | 29 | ASN |
| 2 | C | 91 | HIS |
| 2 | C | 92 | ASN |
| 2 | C | 140 | ASN |
| 2 | C | 232 | HIS |
| 2 | C | 237 | ASN |
| 2 | C | 240 | HIS |
| 2 | C | 261 | HIS |
| 2 | C | 276 | ASN |
| 2 | C | 287 | ASN |
| 2 | C | 294 | GLN |
| 2 | C | 301 | HIS |
| 2 | C | 353 | ASN |
| 2 | C | 397 | HIS |
| 2 | C | 399 | GLN |
| 2 | C | 410 | HIS |
| 2 | C | 435 | ASN |
| 2 | C | 437 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands 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 | $\#\|Z\| > 2$ |
| 5 | SAM | B | 530 | - | 24,29,29 | 1.33 | 3 (12%) | 23,42,42 | 1.75 | 5 (21%) |
| 5 | SAM | C | 530 | - | 24,29,29 | 1.32 | 3 (12%) | 23,42,42 | 1.75 | 5 (21%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 5 | SAM | B | 530 | - | - | 2/12/33/33 | 0/3/3/3 |
| 5 | SAM | C | 530 | - | - | 2/12/33/33 | 0/3/3/3 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | C | 530 | SAM | C2-N3 | 4.14 | 1.38 | 1.32 |
| 5 | B | 530 | SAM | C2-N3 | 4.12 | 1.38 | 1.32 |
| 5 | B | 530 | SAM | C2-N1 | 2.79 | 1.39 | 1.33 |
| 5 | C | 530 | SAM | C2-N1 | 2.77 | 1.39 | 1.33 |
| 5 | C | 530 | SAM | OXT-C | -2.34 | 1.22 | 1.30 |
| 5 | B | 530 | SAM | OXT-C | -2.33 | 1.22 | 1.30 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | C | 530 | SAM | N3-C2-N1 | -5.14 | 120.65 | 128.68 |
| 5 | B | 530 | SAM | N3-C2-N1 | -5.11 | 120.69 | 128.68 |
| 5 | C | 530 | SAM | OXT-C-O | -3.65 | 115.81 | 124.09 |
| 5 | B | 530 | SAM | OXT-C-O | -3.62 | 115.87 | 124.09 |
| 5 | B | 530 | SAM | O4'-C1'-C2' | -2.51 | 103.25 | 106.93 |
| 5 | C | 530 | SAM | O4'-C1'-C2' | -2.51 | 103.26 | 106.93 |
| 5 | B | 530 | SAM | C4-C5-N7 | -2.18 | 107.13 | 109.40 |
| 5 | C | 530 | SAM | O2'-C2'-C3' | 2.14 | 118.75 | 111.82 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | C | 530 | SAM | C4-C5-N7 | -2.13 | 107.17 | 109.40 |
| 5 | B | 530 | SAM | O2'-C2'-C3' | 2.12 | 118.67 | 111.82 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | B | 530 | SAM | OXT-C-CA-CB |
| 5 | C | 530 | SAM | OXT-C-CA-CB |
| 5 | B | 530 | SAM | O-C-CA-CB |
| 5 | C | 530 | SAM | O-C-CA-CB |

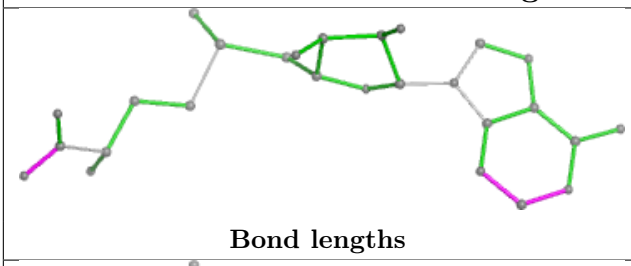
There are no ring outliers.

2 monomers are involved in 58 short contacts:

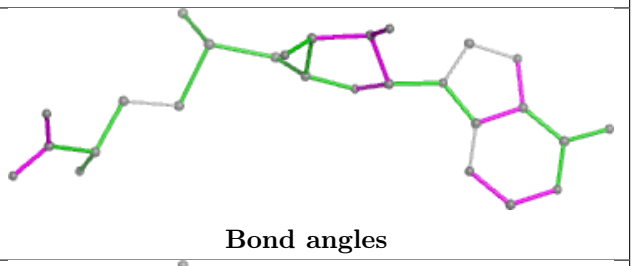
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | B | 530 | SAM | 28 | 0 |
| 5 | C | 530 | SAM | 30 | 0 |

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

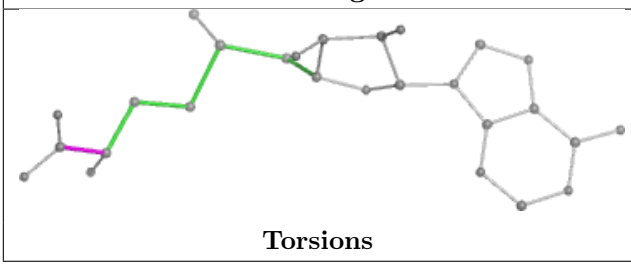
**Ligand SAM B 530**



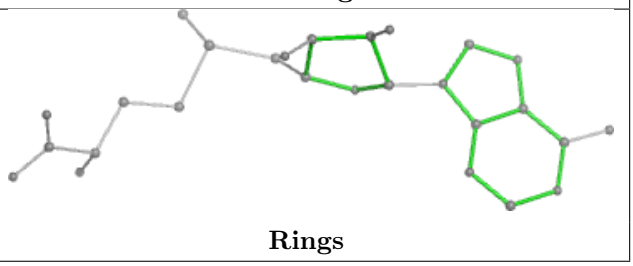
Bond lengths



Bond angles

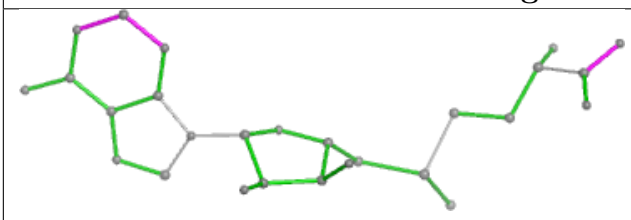


Torsions

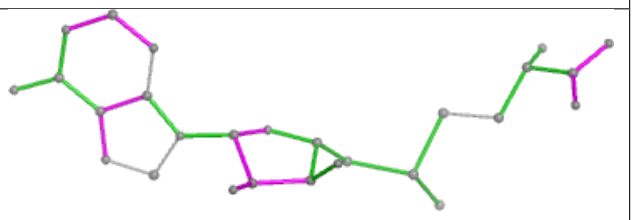


Rings

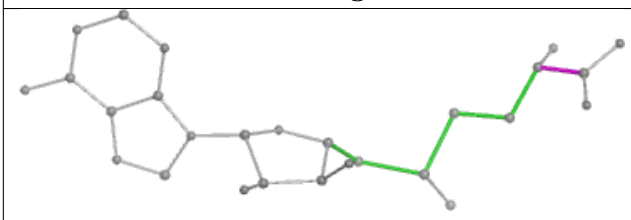
**Ligand SAM C 530**



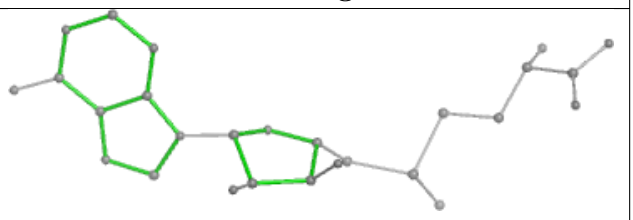
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | A | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 292:ARG | C | 293:TYR | N | 1.68 |
| 1 | A | 295:GLY | C | 296:SER | N | 1.18 |

# 6 Map visualisation

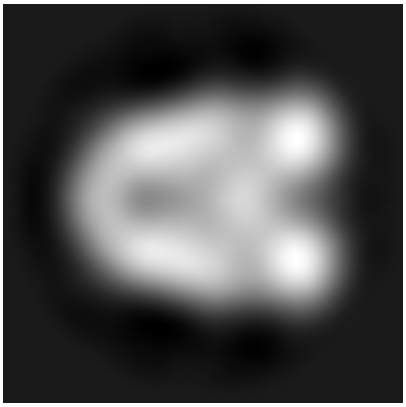
This section contains visualisations of the EMDB entry EMD-1534. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

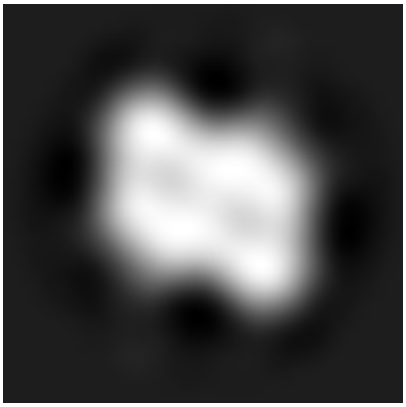
## 6.1 Orthogonal projections

### 6.1.1 Primary map

X



Y



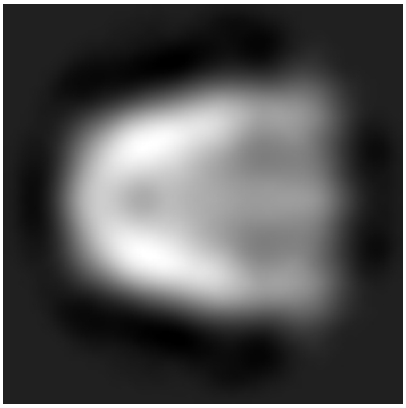
Z

The images above show the map projected in three orthogonal directions.

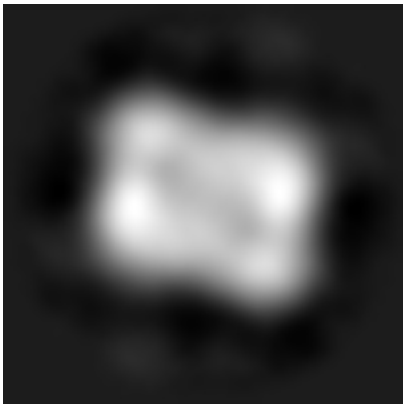
## 6.2 Central slices

### 6.2.1 Primary map

X Index: 24



Y Index: 24

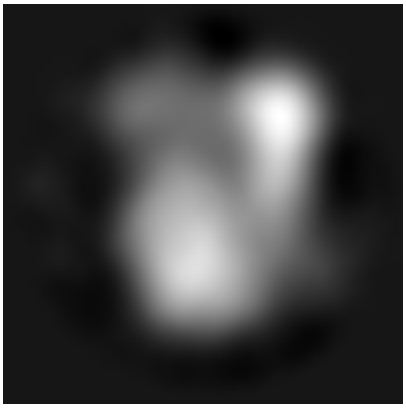


Z Index: 24

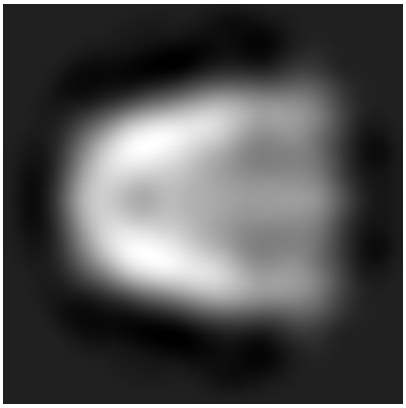
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

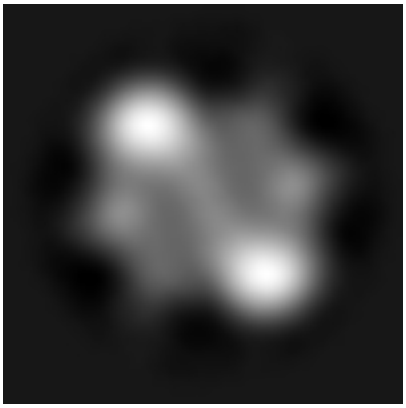
### 6.3.1 Primary map



X Index: 18



Y Index: 24

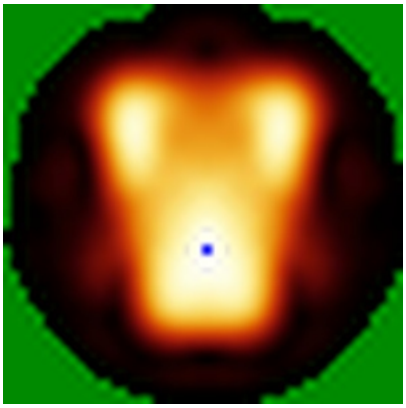


Z Index: 33

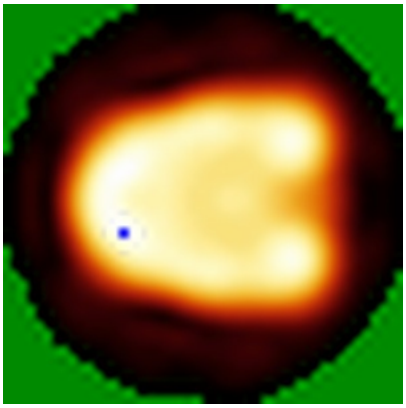
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

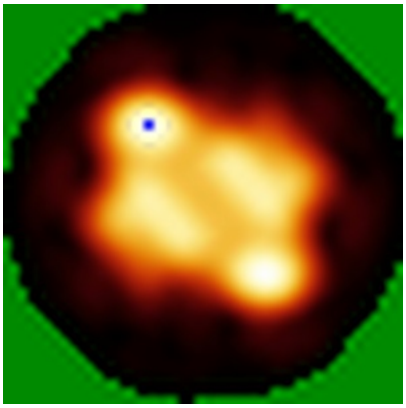
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.41. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

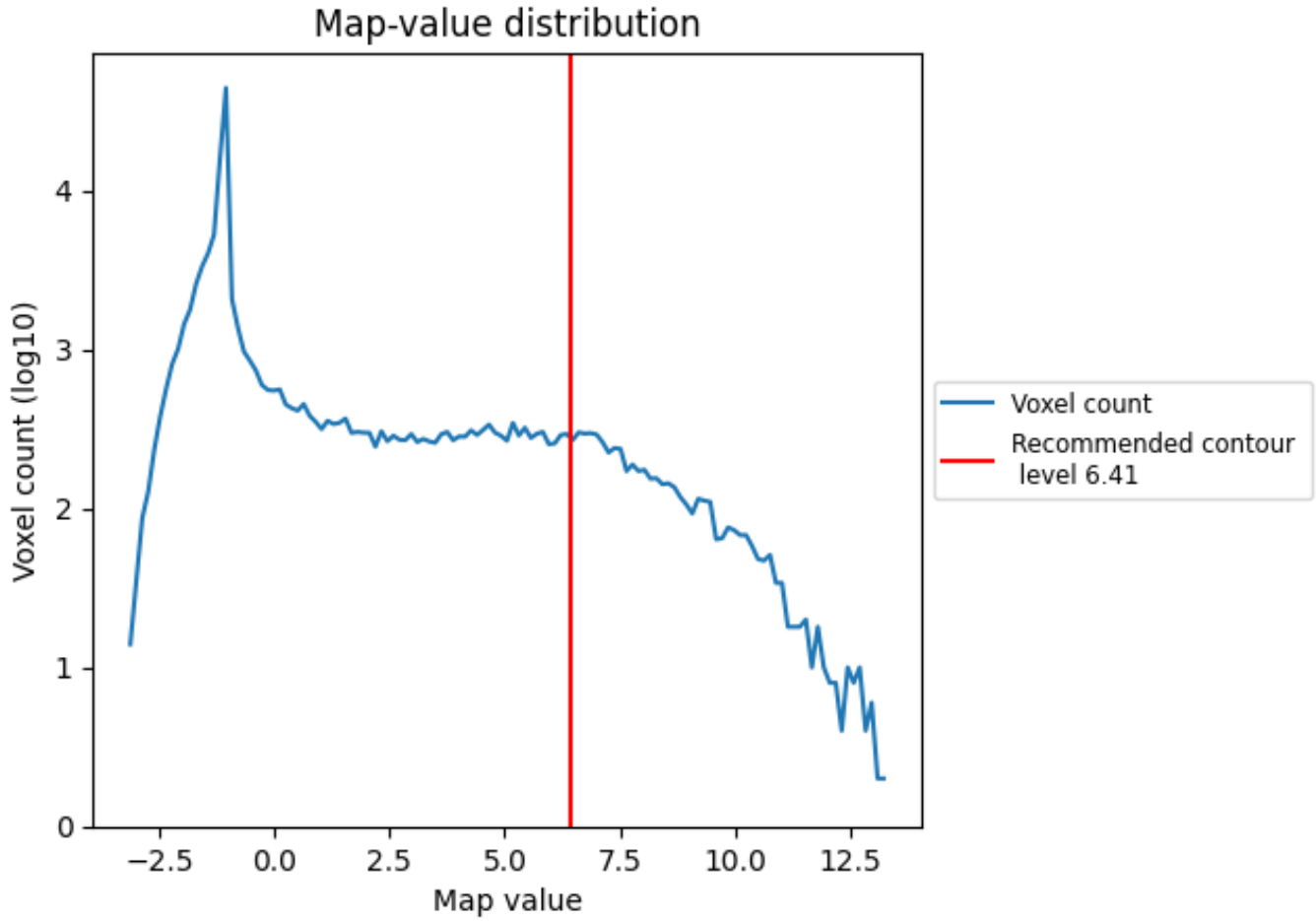
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

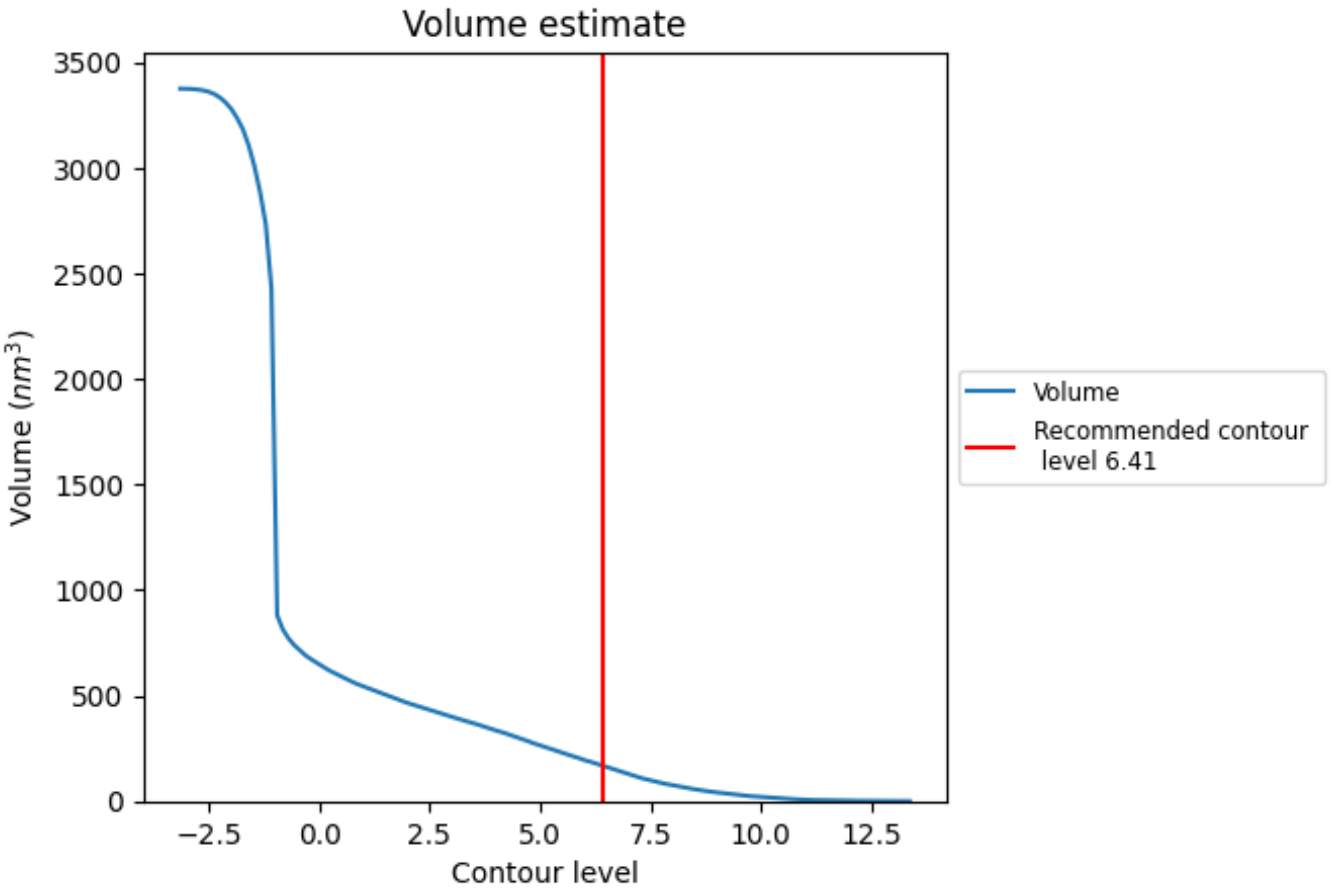
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

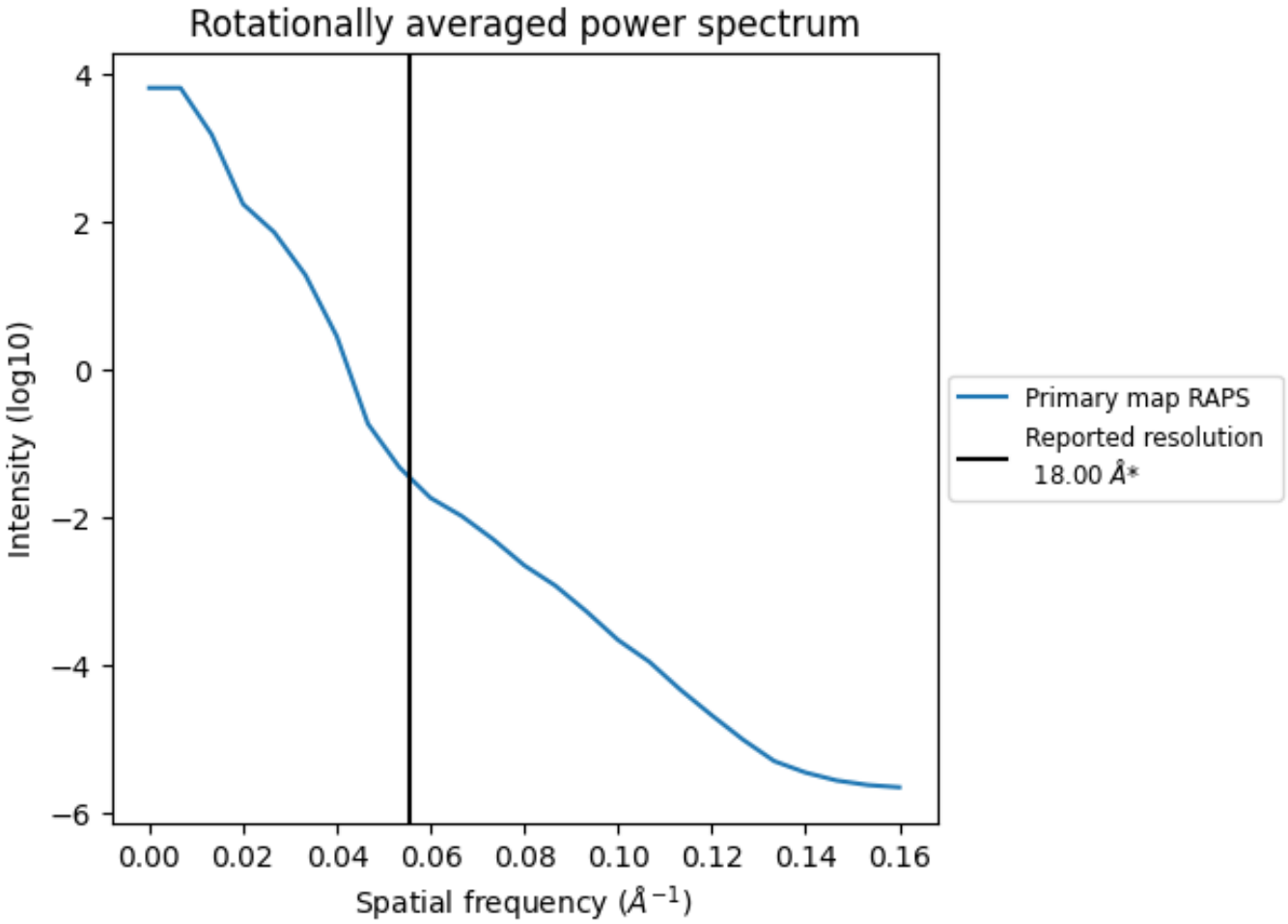
## 7.2 Volume estimate




The volume at the recommended contour level is 169 $nm^3$; this corresponds to an approximate mass of 152 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.056 Å$^{-1}$

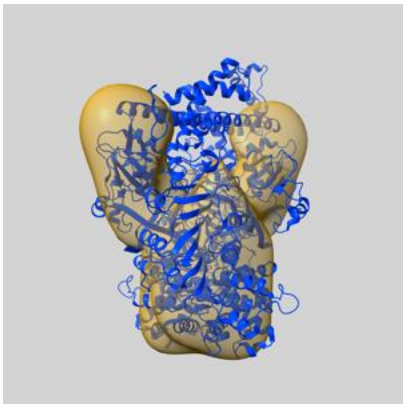
# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

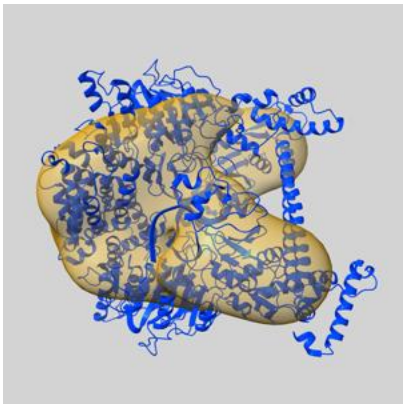
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1534 and PDB model 2Y7H. Per-residue inclusion information can be found in section 3 on page 6.

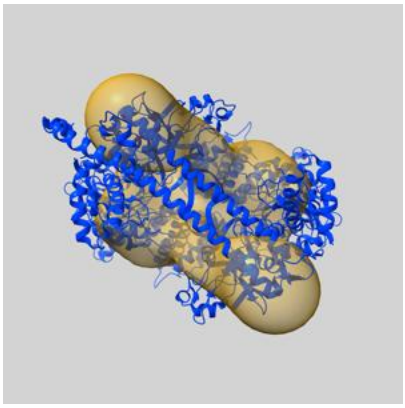
## 9.1 Map-model overlay



X



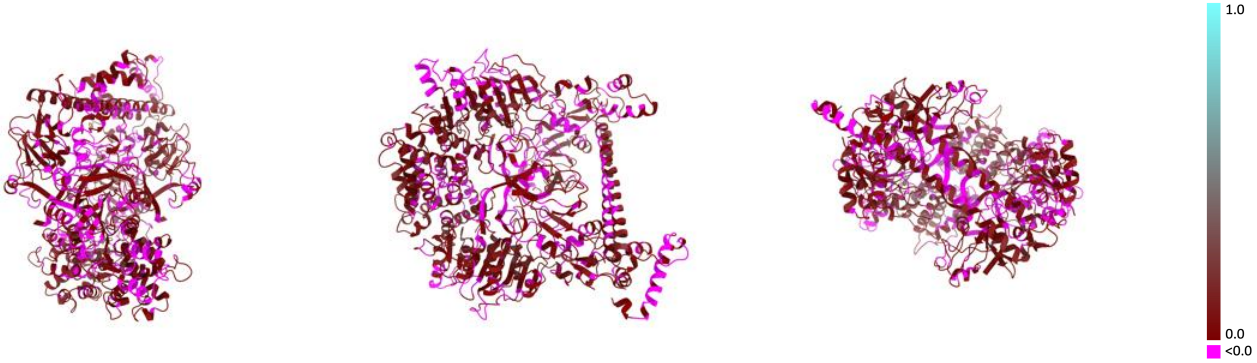
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.41 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

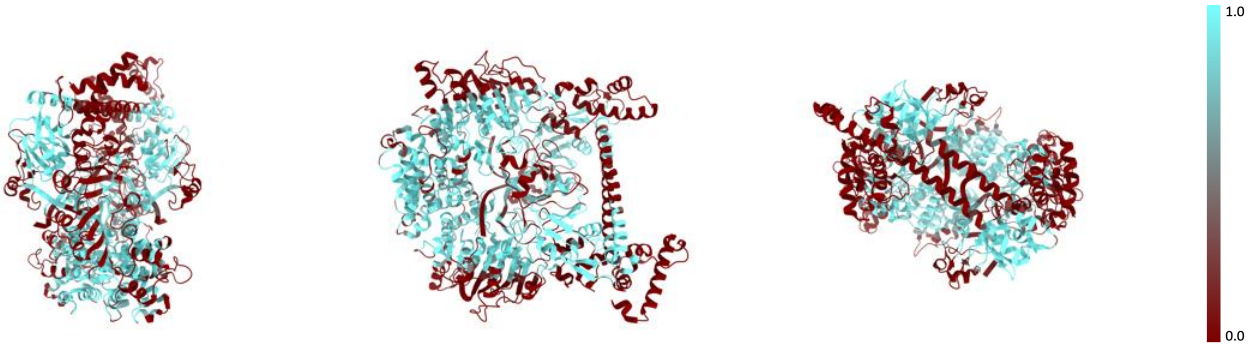
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

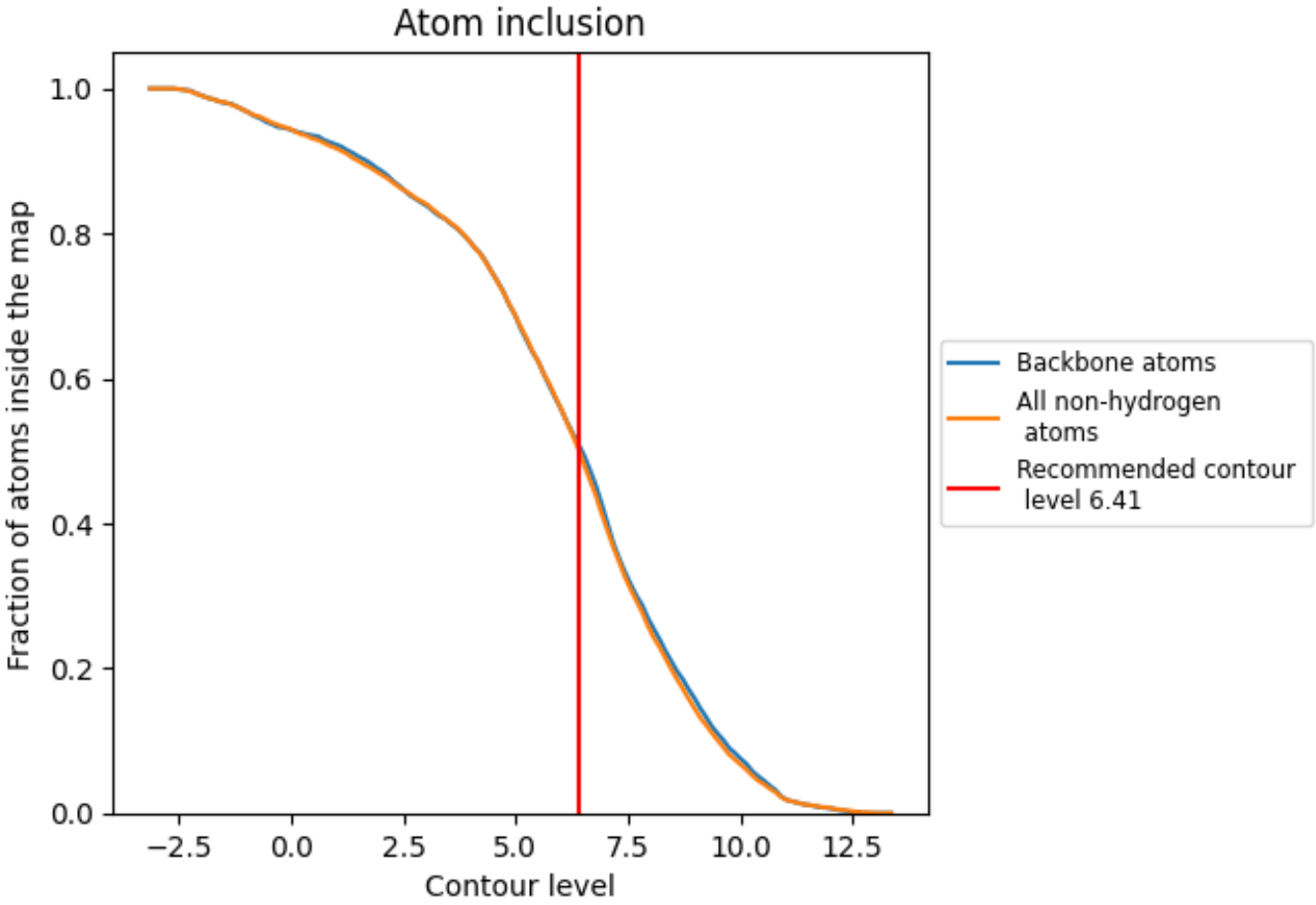
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.41).

## 9.4 Atom inclusion (i)




At the recommended contour level, 51% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (6.41) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5010 | 0.0340 |
| A | 0.4710 | 0.0330 |
| B | 0.5180 | 0.0400 |
| C | 0.5200 | 0.0350 |
| D | 0.4300 | -0.0030 |
| E | 0.4570 | -0.0010 |