



Full wwPDB NMR Structure Validation Report ⓘ

Feb 16, 2018 – 05:42 am GMT

PDB ID : 1IMO
Title : NMR STRUCTURE OF HUMAN DNA LIGASE IIIALPHA BRCT DOMAIN
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Deposited on : 2001-05-11

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20171227.v01 (using entries in the PDB archive December 27th 2017) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | trunk30686 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk30686 |

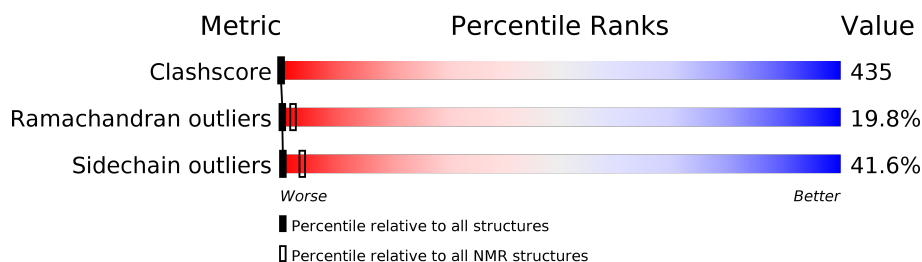
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 136279 | 12091 |
| Ramachandran outliers | 132675 | 10835 |
| Sidechain outliers | 132484 | 10811 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 88 | |

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1398 atoms, of which 697 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA LIGASE III.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 88 | Total | C | H | N | O | S | 0 |
| | | | 1398 | 446 | 697 | 124 | 127 | 4 | |

There are 2 discrepancies between the modelled and reference sequences:

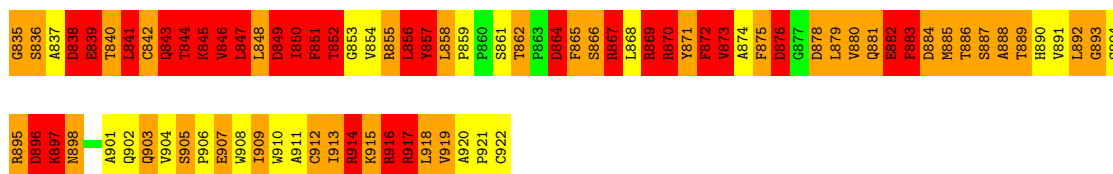
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | 835 | GLY | LYS | CLONING ARTIFACT | UNP P49916 |
| A | 836 | SER | ALA | CLONING ARTIFACT | UNP P49916 |

4 Residue-property plots

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

● Molecule 1: DNA LIGASE III

Chain A: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, simulated annealing, torsion angle dynamics*.

Of the 299 calculated structures, 1 were deposited, based on the following criterion: *structure with the least restraint violations, structure with the lowest energy, target function*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|--------------------|---------|
| DYANA | structure solution | 1.5 |
| DYANA | refinement | 1.5 |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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 (average) 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 | 15.59 | 145/718 (20.2%) | 15.90 | 174/976 (17.8%) |
| All | All | 15.59 | 145/718 (20.2%) | 15.90 | 174/976 (17.8%) |

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 | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 1 | 0 |
| All | All | 1 | 0 |

All bond outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | A | 867 | ARG | CZ-NH1 | -85.55 | 0.21 | 1.33 |
| 1 | A | 907 | GLU | CD-OE1 | -85.14 | 0.32 | 1.25 |
| 1 | A | 914 | ARG | CZ-NH1 | -74.16 | 0.36 | 1.33 |
| 1 | A | 907 | GLU | CD-OE2 | -67.83 | 0.51 | 1.25 |
| 1 | A | 839 | GLU | CD-OE2 | -65.45 | 0.53 | 1.25 |
| 1 | A | 839 | GLU | CD-OE1 | -64.91 | 0.54 | 1.25 |
| 1 | A | 836 | SER | CB-OG | -62.51 | 0.60 | 1.42 |
| 1 | A | 870 | ARG | CZ-NH1 | -60.43 | 0.54 | 1.33 |
| 1 | A | 882 | GLU | CD-OE2 | -60.37 | 0.59 | 1.25 |
| 1 | A | 835 | GLY | N-CA | -59.42 | 0.56 | 1.46 |
| 1 | A | 905 | SER | CB-OG | -59.42 | 0.65 | 1.42 |
| 1 | A | 855 | ARG | CZ-NH1 | -58.47 | 0.57 | 1.33 |
| 1 | A | 870 | ARG | CZ-NH2 | -58.34 | 0.57 | 1.33 |
| 1 | A | 882 | GLU | CD-OE1 | -56.95 | 0.63 | 1.25 |
| 1 | A | 916 | ARG | CG-CD | -53.64 | 0.17 | 1.51 |
| 1 | A | 871 | TYR | CG-CD2 | -51.11 | 0.72 | 1.39 |
| 1 | A | 871 | TYR | CE1-CZ | -50.65 | 0.72 | 1.38 |
| 1 | A | 857 | TYR | CG-CD2 | -50.23 | 0.73 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | A | 857 | TYR | CE1-CZ | -49.74 | 0.73 | 1.38 |
| 1 | A | 857 | TYR | CG-CD1 | -49.59 | 0.74 | 1.39 |
| 1 | A | 857 | TYR | CE2-CZ | -49.06 | 0.74 | 1.38 |
| 1 | A | 916 | ARG | NE-CZ | -48.87 | 0.69 | 1.33 |
| 1 | A | 870 | ARG | CD-NE | -48.48 | 0.64 | 1.46 |
| 1 | A | 883 | PHE | CG-CD2 | -47.02 | 0.68 | 1.38 |
| 1 | A | 871 | TYR | CG-CD1 | -45.38 | 0.80 | 1.39 |
| 1 | A | 872 | PHE | CG-CD1 | -45.16 | 0.71 | 1.38 |
| 1 | A | 871 | TYR | CE2-CZ | -44.92 | 0.80 | 1.38 |
| 1 | A | 916 | ARG | CZ-NH1 | -44.71 | 0.74 | 1.33 |
| 1 | A | 875 | PHE | CG-CD2 | -44.49 | 0.72 | 1.38 |
| 1 | A | 875 | PHE | CG-CD1 | -43.60 | 0.73 | 1.38 |
| 1 | A | 922 | CYS | CB-SG | -43.55 | 1.08 | 1.82 |
| 1 | A | 869 | ARG | CZ-NH1 | -42.99 | 0.77 | 1.33 |
| 1 | A | 883 | PHE | CG-CD1 | -42.94 | 0.74 | 1.38 |
| 1 | A | 895 | ARG | CZ-NH1 | -42.83 | 0.77 | 1.33 |
| 1 | A | 870 | ARG | NE-CZ | -42.52 | 0.77 | 1.33 |
| 1 | A | 838 | ASP | CB-CG | -41.92 | 0.63 | 1.51 |
| 1 | A | 847 | LEU | C-O | -41.84 | 0.43 | 1.23 |
| 1 | A | 849 | ASP | CG-OD1 | -41.29 | 0.30 | 1.25 |
| 1 | A | 872 | PHE | CG-CD2 | -40.64 | 0.77 | 1.38 |
| 1 | A | 838 | ASP | CG-OD1 | -40.21 | 0.32 | 1.25 |
| 1 | A | 838 | ASP | CG-OD2 | -39.67 | 0.34 | 1.25 |
| 1 | A | 917 | ARG | CG-CD | -38.02 | 0.56 | 1.51 |
| 1 | A | 865 | PHE | CG-CD2 | -37.44 | 0.82 | 1.38 |
| 1 | A | 835 | GLY | C-O | -37.08 | 0.64 | 1.23 |
| 1 | A | 846 | VAL | C-O | -36.66 | 0.53 | 1.23 |
| 1 | A | 883 | PHE | CE1-CZ | -36.41 | 0.68 | 1.37 |
| 1 | A | 851 | PHE | CG-CD2 | -36.14 | 0.84 | 1.38 |
| 1 | A | 851 | PHE | CG-CD1 | -36.05 | 0.84 | 1.38 |
| 1 | A | 865 | PHE | CG-CD1 | -36.03 | 0.84 | 1.38 |
| 1 | A | 914 | ARG | NE-CZ | -35.69 | 0.86 | 1.33 |
| 1 | A | 872 | PHE | CE2-CZ | -34.95 | 0.70 | 1.37 |
| 1 | A | 875 | PHE | CE1-CZ | -34.34 | 0.72 | 1.37 |
| 1 | A | 849 | ASP | CG-OD2 | -33.90 | 0.47 | 1.25 |
| 1 | A | 875 | PHE | CE2-CZ | -33.69 | 0.73 | 1.37 |
| 1 | A | 896 | ASP | CG-OD1 | -33.69 | 0.47 | 1.25 |
| 1 | A | 883 | PHE | CE2-CZ | -33.13 | 0.74 | 1.37 |
| 1 | A | 917 | ARG | NE-CZ | -32.97 | 0.90 | 1.33 |
| 1 | A | 881 | GLN | CD-NE2 | -31.63 | 0.53 | 1.32 |
| 1 | A | 896 | ASP | CG-OD2 | -31.54 | 0.52 | 1.25 |
| 1 | A | 878 | ASP | CG-OD2 | -31.43 | 0.53 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | A | 872 | PHE | CE1-CZ | -31.33 | 0.77 | 1.37 |
| 1 | A | 867 | ARG | NE-CZ | -30.77 | 0.93 | 1.33 |
| 1 | A | 922 | CYS | CA-CB | -30.64 | 0.86 | 1.53 |
| 1 | A | 864 | ASP | CG-OD1 | -30.34 | 0.55 | 1.25 |
| 1 | A | 893 | GLY | C-O | -29.54 | 0.76 | 1.23 |
| 1 | A | 849 | ASP | CB-CG | -29.43 | 0.90 | 1.51 |
| 1 | A | 907 | GLU | CG-CD | -29.09 | 1.08 | 1.51 |
| 1 | A | 865 | PHE | CE1-CZ | -28.79 | 0.82 | 1.37 |
| 1 | A | 844 | THR | C-O | -27.86 | 0.70 | 1.23 |
| 1 | A | 851 | PHE | CE1-CZ | -27.79 | 0.84 | 1.37 |
| 1 | A | 865 | PHE | CE2-CZ | -27.70 | 0.84 | 1.37 |
| 1 | A | 866 | SER | CB-OG | -27.69 | 1.06 | 1.42 |
| 1 | A | 851 | PHE | CE2-CZ | -27.67 | 0.84 | 1.37 |
| 1 | A | 842 | CYS | CB-SG | -27.09 | 1.36 | 1.82 |
| 1 | A | 876 | ASP | CG-OD1 | -26.73 | 0.63 | 1.25 |
| 1 | A | 914 | ARG | CZ-NH2 | -26.45 | 0.98 | 1.33 |
| 1 | A | 878 | ASP | CG-OD1 | -26.34 | 0.64 | 1.25 |
| 1 | A | 864 | ASP | CG-OD2 | -26.28 | 0.64 | 1.25 |
| 1 | A | 884 | ASP | CG-OD2 | -26.01 | 0.65 | 1.25 |
| 1 | A | 876 | ASP | CG-OD2 | -25.87 | 0.65 | 1.25 |
| 1 | A | 884 | ASP | CG-OD1 | -25.41 | 0.66 | 1.25 |
| 1 | A | 922 | CYS | CA-C | -24.78 | 0.88 | 1.52 |
| 1 | A | 917 | ARG | CZ-NH1 | -24.61 | 1.01 | 1.33 |
| 1 | A | 867 | ARG | CZ-NH2 | -24.36 | 1.01 | 1.33 |
| 1 | A | 914 | ARG | CG-CD | -24.16 | 0.91 | 1.51 |
| 1 | A | 847 | LEU | C-N | -23.75 | 0.79 | 1.34 |
| 1 | A | 895 | ARG | CZ-NH2 | -23.42 | 1.02 | 1.33 |
| 1 | A | 869 | ARG | NE-CZ | -22.60 | 1.03 | 1.33 |
| 1 | A | 881 | GLN | CD-OE1 | -22.33 | 0.74 | 1.24 |
| 1 | A | 846 | VAL | C-N | -22.17 | 0.83 | 1.34 |
| 1 | A | 846 | VAL | CB-CG2 | -22.17 | 1.06 | 1.52 |
| 1 | A | 855 | ARG | NE-CZ | -22.10 | 1.04 | 1.33 |
| 1 | A | 914 | ARG | CD-NE | -21.68 | 1.09 | 1.46 |
| 1 | A | 855 | ARG | CZ-NH2 | -20.45 | 1.06 | 1.33 |
| 1 | A | 835 | GLY | C-N | -20.17 | 0.87 | 1.34 |
| 1 | A | 922 | CYS | C-O | -20.15 | 0.85 | 1.23 |
| 1 | A | 840 | THR | CB-OG1 | -19.71 | 1.03 | 1.43 |
| 1 | A | 867 | ARG | CD-NE | -19.63 | 1.13 | 1.46 |
| 1 | A | 867 | ARG | CG-CD | -19.42 | 1.03 | 1.51 |
| 1 | A | 913 | ILE | CB-CG1 | -19.18 | 1.00 | 1.54 |
| 1 | A | 895 | ARG | CD-NE | -19.15 | 1.13 | 1.46 |
| 1 | A | 870 | ARG | CG-CD | -19.04 | 1.04 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | A | 916 | ARG | CZ-NH2 | -17.42 | 1.10 | 1.33 |
| 1 | A | 912 | CYS | CB-SG | -16.82 | 1.53 | 1.82 |
| 1 | A | 879 | LEU | CG-CD2 | -16.65 | 0.90 | 1.51 |
| 1 | A | 855 | ARG | CD-NE | -16.57 | 1.18 | 1.46 |
| 1 | A | 879 | LEU | CG-CD1 | -16.57 | 0.90 | 1.51 |
| 1 | A | 843 | GLN | CD-OE1 | -16.43 | 0.87 | 1.24 |
| 1 | A | 846 | VAL | CB-CG1 | -16.25 | 1.18 | 1.52 |
| 1 | A | 915 | LYS | CE-NZ | -16.15 | 1.08 | 1.49 |
| 1 | A | 895 | ARG | NE-CZ | -15.66 | 1.12 | 1.33 |
| 1 | A | 916 | ARG | CD-NE | -15.49 | 1.20 | 1.46 |
| 1 | A | 841 | LEU | CG-CD1 | -15.21 | 0.95 | 1.51 |
| 1 | A | 913 | ILE | CB-CG2 | -14.87 | 1.06 | 1.52 |
| 1 | A | 836 | SER | CA-CB | -14.54 | 1.31 | 1.52 |
| 1 | A | 917 | ARG | CZ-NH2 | -14.47 | 1.14 | 1.33 |
| 1 | A | 843 | GLN | CD-NE2 | -14.32 | 0.97 | 1.32 |
| 1 | A | 869 | ARG | CZ-NH2 | -14.23 | 1.14 | 1.33 |
| 1 | A | 835 | GLY | CA-C | -14.15 | 1.29 | 1.51 |
| 1 | A | 855 | ARG | CB-CG | -13.86 | 1.15 | 1.52 |
| 1 | A | 841 | LEU | CG-CD2 | -13.74 | 1.00 | 1.51 |
| 1 | A | 845 | LYS | CG-CD | -13.43 | 1.06 | 1.52 |
| 1 | A | 917 | ARG | CD-NE | -13.15 | 1.24 | 1.46 |
| 1 | A | 869 | ARG | CD-NE | -11.88 | 1.26 | 1.46 |
| 1 | A | 839 | GLU | CG-CD | -11.54 | 1.34 | 1.51 |
| 1 | A | 836 | SER | N-CA | -10.97 | 1.24 | 1.46 |
| 1 | A | 845 | LYS | CE-NZ | -10.74 | 1.22 | 1.49 |
| 1 | A | 844 | THR | C-N | -10.69 | 1.09 | 1.34 |
| 1 | A | 840 | THR | CB-CG2 | -10.42 | 1.18 | 1.52 |
| 1 | A | 841 | LEU | CB-CG | -10.05 | 1.23 | 1.52 |
| 1 | A | 896 | ASP | CB-CG | -9.88 | 1.30 | 1.51 |
| 1 | A | 869 | ARG | CG-CD | -9.79 | 1.27 | 1.51 |
| 1 | A | 856 | LEU | CG-CD2 | -9.47 | 1.16 | 1.51 |
| 1 | A | 893 | GLY | C-N | -8.20 | 1.15 | 1.34 |
| 1 | A | 907 | GLU | CB-CG | -8.15 | 1.36 | 1.52 |
| 1 | A | 898 | ASN | CG-OD1 | -8.11 | 1.06 | 1.24 |
| 1 | A | 903 | GLN | CD-NE2 | -7.80 | 1.13 | 1.32 |
| 1 | A | 852 | THR | CB-OG1 | -7.46 | 1.28 | 1.43 |
| 1 | A | 917 | ARG | CB-CG | -7.18 | 1.33 | 1.52 |
| 1 | A | 853 | GLY | C-O | -6.99 | 1.12 | 1.23 |
| 1 | A | 855 | ARG | CG-CD | -6.59 | 1.35 | 1.51 |
| 1 | A | 845 | LYS | CD-CE | -6.47 | 1.35 | 1.51 |
| 1 | A | 870 | ARG | CB-CG | -5.66 | 1.37 | 1.52 |
| 1 | A | 856 | LEU | CG-CD1 | -5.53 | 1.31 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 844 | THR | CB-OG1 | -5.46 | 1.32 | 1.43 |

All angle outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 867 | ARG | NE-CZ-NH2 | 96.11 | 168.36 | 120.30 |
| 1 | A | 867 | ARG | NE-CZ-NH1 | -94.31 | 73.15 | 120.30 |
| 1 | A | 907 | GLU | OE1-CD-OE2 | -82.90 | 23.82 | 123.30 |
| 1 | A | 916 | ARG | NE-CZ-NH1 | -80.94 | 79.83 | 120.30 |
| 1 | A | 914 | ARG | NE-CZ-NH1 | -77.28 | 81.66 | 120.30 |
| 1 | A | 914 | ARG | NE-CZ-NH2 | 76.59 | 158.60 | 120.30 |
| 1 | A | 883 | PHE | CD1-CG-CD2 | -75.56 | 20.07 | 118.30 |
| 1 | A | 847 | LEU | O-C-N | -73.63 | 4.89 | 122.70 |
| 1 | A | 857 | TYR | CD1-CG-CD2 | -72.62 | 38.02 | 117.90 |
| 1 | A | 883 | PHE | CB-CG-CD1 | 71.00 | 170.50 | 120.80 |
| 1 | A | 883 | PHE | CB-CG-CD2 | 69.47 | 169.43 | 120.80 |
| 1 | A | 875 | PHE | CD1-CG-CD2 | -68.71 | 28.98 | 118.30 |
| 1 | A | 839 | GLU | OE1-CD-OE2 | -68.44 | 41.17 | 123.30 |
| 1 | A | 857 | TYR | CB-CG-CD1 | 66.90 | 161.14 | 121.00 |
| 1 | A | 857 | TYR | CB-CG-CD2 | 66.40 | 160.84 | 121.00 |
| 1 | A | 882 | GLU | OE1-CD-OE2 | -65.81 | 44.33 | 123.30 |
| 1 | A | 875 | PHE | CB-CG-CD1 | 64.06 | 165.64 | 120.80 |
| 1 | A | 871 | TYR | CD1-CG-CD2 | -63.91 | 47.59 | 117.90 |
| 1 | A | 875 | PHE | CB-CG-CD2 | 63.69 | 165.38 | 120.80 |
| 1 | A | 872 | PHE | CD1-CG-CD2 | -61.09 | 38.89 | 118.30 |
| 1 | A | 871 | TYR | CB-CG-CD1 | 60.75 | 157.45 | 121.00 |
| 1 | A | 872 | PHE | CB-CG-CD2 | 58.16 | 161.51 | 120.80 |
| 1 | A | 855 | ARG | NE-CZ-NH2 | 56.75 | 148.67 | 120.30 |
| 1 | A | 871 | TYR | CB-CG-CD2 | 56.59 | 154.95 | 121.00 |
| 1 | A | 883 | PHE | CE1-CZ-CE2 | -55.51 | 20.08 | 120.00 |
| 1 | A | 872 | PHE | CB-CG-CD1 | 55.42 | 159.60 | 120.80 |
| 1 | A | 896 | ASP | CB-CG-OD2 | 55.27 | 168.04 | 118.30 |
| 1 | A | 896 | ASP | CB-CG-OD1 | 53.89 | 166.80 | 118.30 |
| 1 | A | 896 | ASP | OD1-CG-OD2 | -51.65 | 25.16 | 123.30 |
| 1 | A | 857 | TYR | CE1-CZ-CE2 | -51.13 | 37.98 | 119.80 |
| 1 | A | 875 | PHE | CE1-CZ-CE2 | -50.55 | 29.01 | 120.00 |
| 1 | A | 857 | TYR | CG-CD1-CE1 | 49.79 | 161.13 | 121.30 |
| 1 | A | 857 | TYR | CG-CD2-CE2 | 49.44 | 160.85 | 121.30 |
| 1 | A | 864 | ASP | CB-CG-OD2 | 47.51 | 161.05 | 118.30 |
| 1 | A | 857 | TYR | CZ-CE2-CD2 | 45.88 | 161.10 | 119.80 |
| 1 | A | 857 | TYR | CD1-CE1-CZ | 45.69 | 160.92 | 119.80 |
| 1 | A | 883 | PHE | CG-CD1-CE1 | 45.18 | 170.50 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 871 | TYR | CG-CD1-CE1 | 45.14 | 157.41 | 121.30 |
| 1 | A | 871 | TYR | CE1-CZ-CE2 | -45.13 | 47.59 | 119.80 |
| 1 | A | 872 | PHE | CE1-CZ-CE2 | -45.01 | 38.99 | 120.00 |
| 1 | A | 883 | PHE | CG-CD2-CE2 | 44.21 | 169.44 | 120.80 |
| 1 | A | 864 | ASP | CB-CG-OD1 | 43.55 | 157.50 | 118.30 |
| 1 | A | 846 | VAL | O-C-N | -43.21 | 53.56 | 122.70 |
| 1 | A | 864 | ASP | OD1-CG-OD2 | -43.08 | 41.45 | 123.30 |
| 1 | A | 849 | ASP | CB-CG-OD2 | 42.88 | 156.89 | 118.30 |
| 1 | A | 878 | ASP | CB-CG-OD1 | 42.60 | 156.64 | 118.30 |
| 1 | A | 871 | TYR | CG-CD2-CE2 | 42.12 | 154.99 | 121.30 |
| 1 | A | 883 | PHE | CZ-CE2-CD2 | 41.95 | 170.44 | 120.10 |
| 1 | A | 871 | TYR | CZ-CE2-CD2 | 41.79 | 157.41 | 119.80 |
| 1 | A | 883 | PHE | CD1-CE1-CZ | 41.15 | 169.48 | 120.10 |
| 1 | A | 875 | PHE | CG-CD1-CE1 | 40.75 | 165.62 | 120.80 |
| 1 | A | 875 | PHE | CG-CD2-CE2 | 40.56 | 165.42 | 120.80 |
| 1 | A | 865 | PHE | CD1-CG-CD2 | -40.33 | 65.87 | 118.30 |
| 1 | A | 871 | TYR | CD1-CE1-CZ | 39.10 | 154.99 | 119.80 |
| 1 | A | 851 | PHE | CD1-CG-CD2 | -38.95 | 67.66 | 118.30 |
| 1 | A | 865 | PHE | CB-CG-CD1 | 38.25 | 147.57 | 120.80 |
| 1 | A | 875 | PHE | CZ-CE2-CD2 | 37.92 | 165.60 | 120.10 |
| 1 | A | 875 | PHE | CD1-CE1-CZ | 37.72 | 165.37 | 120.10 |
| 1 | A | 869 | ARG | NE-CZ-NH2 | 37.57 | 139.09 | 120.30 |
| 1 | A | 878 | ASP | OD1-CG-OD2 | -37.35 | 52.34 | 123.30 |
| 1 | A | 876 | ASP | CB-CG-OD2 | 37.26 | 151.84 | 118.30 |
| 1 | A | 872 | PHE | CG-CD2-CE2 | 37.03 | 161.53 | 120.80 |
| 1 | A | 865 | PHE | CB-CG-CD2 | 36.80 | 146.56 | 120.80 |
| 1 | A | 851 | PHE | CB-CG-CD1 | 36.44 | 146.31 | 120.80 |
| 1 | A | 878 | ASP | CB-CG-OD2 | 36.36 | 151.02 | 118.30 |
| 1 | A | 876 | ASP | CB-CG-OD1 | 36.21 | 150.89 | 118.30 |
| 1 | A | 851 | PHE | CB-CG-CD2 | 36.05 | 146.03 | 120.80 |
| 1 | A | 895 | ARG | NE-CZ-NH2 | 36.00 | 138.30 | 120.30 |
| 1 | A | 916 | ARG | NE-CZ-NH2 | 35.89 | 138.25 | 120.30 |
| 1 | A | 872 | PHE | CG-CD1-CE1 | 35.29 | 159.62 | 120.80 |
| 1 | A | 869 | ARG | NE-CZ-NH1 | -35.15 | 102.72 | 120.30 |
| 1 | A | 884 | ASP | CB-CG-OD1 | 34.98 | 149.78 | 118.30 |
| 1 | A | 876 | ASP | OD1-CG-OD2 | -34.75 | 57.27 | 123.30 |
| 1 | A | 872 | PHE | CD1-CE1-CZ | 34.44 | 161.43 | 120.10 |
| 1 | A | 884 | ASP | CB-CG-OD2 | 34.13 | 149.01 | 118.30 |
| 1 | A | 855 | ARG | NE-CZ-NH1 | -33.30 | 103.65 | 120.30 |
| 1 | A | 872 | PHE | CZ-CE2-CD2 | 32.87 | 159.54 | 120.10 |
| 1 | A | 884 | ASP | OD1-CG-OD2 | -32.68 | 61.20 | 123.30 |
| 1 | A | 849 | ASP | OD1-CG-OD2 | -32.64 | 61.29 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 867 | ARG | CD-NE-CZ | 32.36 | 168.90 | 123.60 |
| 1 | A | 870 | ARG | NE-CZ-NH2 | 31.03 | 135.81 | 120.30 |
| 1 | A | 865 | PHE | CE1-CZ-CE2 | -30.08 | 65.86 | 120.00 |
| 1 | A | 881 | GLN | OE1-CD-NE2 | -29.67 | 53.66 | 121.90 |
| 1 | A | 851 | PHE | CE1-CZ-CE2 | -29.05 | 67.71 | 120.00 |
| 1 | A | 847 | LEU | CA-C-N | 27.70 | 178.13 | 117.20 |
| 1 | A | 847 | LEU | CA-C-O | 27.08 | 176.98 | 120.10 |
| 1 | A | 917 | ARG | NE-CZ-NH1 | -27.02 | 106.79 | 120.30 |
| 1 | A | 907 | GLU | CG-CD-OE2 | 26.31 | 170.93 | 118.30 |
| 1 | A | 849 | ASP | CB-CG-OD1 | 26.14 | 141.82 | 118.30 |
| 1 | A | 914 | ARG | CD-NE-CZ | 25.74 | 159.64 | 123.60 |
| 1 | A | 870 | ARG | NH1-CZ-NH2 | -25.49 | 91.36 | 119.40 |
| 1 | A | 870 | ARG | NE-CZ-NH1 | 25.05 | 132.82 | 120.30 |
| 1 | A | 865 | PHE | CG-CD1-CE1 | 24.34 | 147.58 | 120.80 |
| 1 | A | 907 | GLU | CG-CD-OE1 | 23.48 | 165.25 | 118.30 |
| 1 | A | 865 | PHE | CG-CD2-CE2 | 23.42 | 146.56 | 120.80 |
| 1 | A | 851 | PHE | CG-CD1-CE1 | 23.22 | 146.34 | 120.80 |
| 1 | A | 851 | PHE | CG-CD2-CE2 | 22.95 | 146.04 | 120.80 |
| 1 | A | 865 | PHE | CZ-CE2-CD2 | 22.89 | 147.57 | 120.10 |
| 1 | A | 847 | LEU | C-N-CA | 22.61 | 178.23 | 121.70 |
| 1 | A | 916 | ARG | CG-CD-NE | -22.19 | 65.19 | 111.80 |
| 1 | A | 865 | PHE | CD1-CE1-CZ | 22.05 | 146.56 | 120.10 |
| 1 | A | 851 | PHE | CZ-CE2-CD2 | 21.80 | 146.25 | 120.10 |
| 1 | A | 851 | PHE | CD1-CE1-CZ | 21.58 | 146.00 | 120.10 |
| 1 | A | 916 | ARG | CB-CG-CD | 21.16 | 166.63 | 111.60 |
| 1 | A | 839 | GLU | CG-CD-OE1 | 20.66 | 159.61 | 118.30 |
| 1 | A | 916 | ARG | NH1-CZ-NH2 | 20.48 | 141.92 | 119.40 |
| 1 | A | 838 | ASP | CB-CG-OD2 | 20.47 | 136.72 | 118.30 |
| 1 | A | 839 | GLU | CG-CD-OE2 | 20.46 | 159.22 | 118.30 |
| 1 | A | 882 | GLU | CG-CD-OE1 | 20.14 | 158.58 | 118.30 |
| 1 | A | 882 | GLU | CG-CD-OE2 | 19.40 | 157.09 | 118.30 |
| 1 | A | 855 | ARG | CD-NE-CZ | 19.04 | 150.26 | 123.60 |
| 1 | A | 881 | GLN | CG-CD-OE1 | 18.99 | 159.58 | 121.60 |
| 1 | A | 835 | GLY | O-C-N | -18.57 | 92.98 | 122.70 |
| 1 | A | 846 | VAL | CA-C-N | 18.44 | 157.77 | 117.20 |
| 1 | A | 879 | LEU | CB-CG-CD2 | 18.36 | 142.21 | 111.00 |
| 1 | A | 879 | LEU | CB-CG-CD1 | 18.32 | 142.14 | 111.00 |
| 1 | A | 838 | ASP | OD1-CG-OD2 | -18.27 | 88.58 | 123.30 |
| 1 | A | 838 | ASP | CB-CG-OD1 | 18.22 | 134.69 | 118.30 |
| 1 | A | 838 | ASP | CA-CB-CG | 16.31 | 149.28 | 113.40 |
| 1 | A | 917 | ARG | CB-CG-CD | -16.03 | 69.92 | 111.60 |
| 1 | A | 879 | LEU | CD1-CG-CD2 | -15.85 | 62.95 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 857 | TYR | OH-CZ-CE2 | 15.18 | 161.09 | 120.10 |
| 1 | A | 914 | ARG | CG-CD-NE | 15.14 | 143.59 | 111.80 |
| 1 | A | 857 | TYR | CE1-CZ-OH | 15.12 | 160.93 | 120.10 |
| 1 | A | 846 | VAL | C-N-CA | 14.98 | 159.16 | 121.70 |
| 1 | A | 895 | ARG | NH1-CZ-NH2 | -14.24 | 103.73 | 119.40 |
| 1 | A | 871 | TYR | OH-CZ-CE2 | 13.81 | 157.40 | 120.10 |
| 1 | A | 844 | THR | O-C-N | -13.67 | 100.82 | 122.70 |
| 1 | A | 846 | VAL | CA-C-O | 13.60 | 148.67 | 120.10 |
| 1 | A | 871 | TYR | CE1-CZ-OH | 12.93 | 155.01 | 120.10 |
| 1 | A | 881 | GLN | CG-CD-NE2 | 12.52 | 146.76 | 116.70 |
| 1 | A | 869 | ARG | CD-NE-CZ | 12.41 | 140.97 | 123.60 |
| 1 | A | 895 | ARG | CD-NE-CZ | 12.16 | 140.63 | 123.60 |
| 1 | A | 922 | CYS | CA-C-O | 11.86 | 145.00 | 120.10 |
| 1 | A | 916 | ARG | CD-NE-CZ | 11.43 | 139.60 | 123.60 |
| 1 | A | 845 | LYS | CG-CD-CE | 11.41 | 146.12 | 111.90 |
| 1 | A | 870 | ARG | CD-NE-CZ | 10.83 | 138.76 | 123.60 |
| 1 | A | 835 | GLY | N-CA-C | 10.69 | 139.82 | 113.10 |
| 1 | A | 855 | ARG | NH1-CZ-NH2 | -10.66 | 107.68 | 119.40 |
| 1 | A | 844 | THR | CA-C-N | 10.65 | 140.63 | 117.20 |
| 1 | A | 913 | ILE | CG1-CB-CG2 | -10.52 | 88.26 | 111.40 |
| 1 | A | 893 | GLY | O-C-N | -10.51 | 105.89 | 122.70 |
| 1 | A | 917 | ARG | NH1-CZ-NH2 | 10.45 | 130.90 | 119.40 |
| 1 | A | 917 | ARG | CG-CD-NE | -10.40 | 89.95 | 111.80 |
| 1 | A | 843 | GLN | OE1-CD-NE2 | -10.38 | 98.02 | 121.90 |
| 1 | A | 835 | GLY | CA-C-N | 10.00 | 139.21 | 117.20 |
| 1 | A | 867 | ARG | CG-CD-NE | 9.82 | 132.42 | 111.80 |
| 1 | A | 922 | CYS | CA-CB-SG | 9.47 | 131.04 | 114.00 |
| 1 | A | 922 | CYS | CB-CA-C | -9.44 | 91.52 | 110.40 |
| 1 | A | 893 | GLY | CA-C-N | 9.42 | 137.93 | 117.20 |
| 1 | A | 845 | LYS | CB-CG-CD | 9.41 | 136.08 | 111.60 |
| 1 | A | 841 | LEU | CB-CG-CD2 | -9.24 | 95.28 | 111.00 |
| 1 | A | 846 | VAL | CA-CB-CG1 | 9.07 | 124.50 | 110.90 |
| 1 | A | 867 | ARG | CB-CG-CD | 8.98 | 134.95 | 111.60 |
| 1 | A | 905 | SER | CA-CB-OG | 8.97 | 135.42 | 111.20 |
| 1 | A | 844 | THR | C-N-CA | 8.83 | 143.77 | 121.70 |
| 1 | A | 913 | ILE | CA-CB-CG2 | 8.70 | 128.30 | 110.90 |
| 1 | A | 835 | GLY | C-N-CA | 8.18 | 142.15 | 121.70 |
| 1 | A | 893 | GLY | C-N-CA | 7.87 | 141.36 | 121.70 |
| 1 | A | 846 | VAL | CG1-CB-CG2 | -7.69 | 98.60 | 110.90 |
| 1 | A | 836 | SER | CA-CB-OG | 7.57 | 131.63 | 111.20 |
| 1 | A | 922 | CYS | N-CA-CB | 7.37 | 123.87 | 110.60 |
| 1 | A | 913 | ILE | CA-CB-CG1 | 6.85 | 124.02 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | A | 856 | LEU | CB-CG-CD1 | 6.67 | 122.34 | 111.00 |
| 1 | A | 855 | ARG | CA-CB-CG | 6.62 | 127.97 | 113.40 |
| 1 | A | 849 | ASP | CA-CB-CG | 6.47 | 127.64 | 113.40 |
| 1 | A | 869 | ARG | CG-CD-NE | 6.43 | 125.30 | 111.80 |
| 1 | A | 841 | LEU | CB-CG-CD1 | 6.37 | 121.83 | 111.00 |
| 1 | A | 840 | THR | CA-CB-CG2 | 6.25 | 121.16 | 112.40 |
| 1 | A | 885 | MET | CG-SD-CE | 6.21 | 110.14 | 100.20 |
| 1 | A | 843 | GLN | CG-CD-NE2 | 5.72 | 130.43 | 116.70 |
| 1 | A | 869 | ARG | CB-CG-CD | 5.64 | 126.26 | 111.60 |
| 1 | A | 922 | CYS | N-CA-C | 5.51 | 125.87 | 111.00 |
| 1 | A | 870 | ARG | CG-CD-NE | 5.34 | 123.02 | 111.80 |

All chiral outliers are listed below.

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 1 | A | 922 | CYS | CA |

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 701 | 697 | 688 | 604 |
| All | All | 701 | 697 | 688 | 604 |

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 435.

All clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:885:MET:SD | 1:A:897:LYS:HB2 | 1.63 | 1.26 |
| 1:A:916:ARG:CG | 1:A:916:ARG:CZ | 1.55 | 1.76 |
| 1:A:846:VAL:C | 1:A:847:LEU:HD22 | 1.54 | 1.15 |
| 1:A:916:ARG:CD | 1:A:916:ARG:CZ | 1.51 | 1.78 |
| 1:A:850:ILE:CD1 | 1:A:913:ILE:HA | 1.49 | 1.35 |
| 1:A:850:ILE:HD12 | 1:A:913:ILE:CA | 1.43 | 1.39 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:871:TYR:CE2 | 1:A:871:TYR:CG | 1.43 | 2.07 |
| 1:A:872:PHE:CG | 1:A:872:PHE:CE1 | 1.42 | 2.07 |
| 1:A:871:TYR:CD1 | 1:A:871:TYR:CZ | 1.42 | 2.07 |
| 1:A:872:PHE:CD2 | 1:A:872:PHE:CZ | 1.42 | 2.07 |
| 1:A:883:PHE:CG | 1:A:883:PHE:CE2 | 1.42 | 2.06 |
| 1:A:883:PHE:CZ | 1:A:883:PHE:CD1 | 1.39 | 2.07 |
| 1:A:857:TYR:CG | 1:A:857:TYR:CE1 | 1.38 | 2.11 |
| 1:A:857:TYR:CD2 | 1:A:857:TYR:CZ | 1.37 | 2.11 |
| 1:A:857:TYR:CG | 1:A:857:TYR:CE2 | 1.37 | 2.10 |
| 1:A:857:TYR:CD1 | 1:A:857:TYR:CZ | 1.36 | 2.10 |
| 1:A:875:PHE:CZ | 1:A:875:PHE:CD2 | 1.36 | 2.11 |
| 1:A:875:PHE:CG | 1:A:875:PHE:CE2 | 1.36 | 2.10 |
| 1:A:875:PHE:CZ | 1:A:875:PHE:CD1 | 1.36 | 2.10 |
| 1:A:916:ARG:NH2 | 1:A:916:ARG:NE | 1.36 | 1.68 |
| 1:A:835:GLY:N | 1:A:835:GLY:C | 1.35 | 1.76 |
| 1:A:875:PHE:CG | 1:A:875:PHE:CE1 | 1.35 | 2.11 |
| 1:A:851:PHE:CG | 1:A:851:PHE:CE1 | 1.35 | 2.15 |
| 1:A:851:PHE:CZ | 1:A:851:PHE:CD2 | 1.35 | 2.15 |
| 1:A:846:VAL:O | 1:A:847:LEU:CD2 | 1.34 | 1.74 |
| 1:A:851:PHE:CG | 1:A:851:PHE:CE2 | 1.34 | 2.15 |
| 1:A:865:PHE:CD1 | 1:A:865:PHE:CZ | 1.34 | 2.13 |
| 1:A:851:PHE:CA | 1:A:918:LEU:HD11 | 1.34 | 1.51 |
| 1:A:865:PHE:CZ | 1:A:865:PHE:CD2 | 1.34 | 2.16 |
| 1:A:872:PHE:CG | 1:A:872:PHE:CE2 | 1.33 | 2.14 |
| 1:A:871:TYR:CG | 1:A:871:TYR:CE1 | 1.33 | 2.15 |
| 1:A:871:TYR:CD2 | 1:A:871:TYR:CZ | 1.33 | 2.15 |
| 1:A:872:PHE:CD1 | 1:A:872:PHE:CZ | 1.33 | 2.14 |
| 1:A:865:PHE:CG | 1:A:865:PHE:CE2 | 1.33 | 2.13 |
| 1:A:883:PHE:CG | 1:A:883:PHE:CE1 | 1.33 | 2.13 |
| 1:A:851:PHE:CZ | 1:A:851:PHE:CD1 | 1.32 | 2.15 |
| 1:A:871:TYR:OH | 1:A:913:ILE:HD11 | 1.32 | 1.14 |
| 1:A:854:VAL:HG11 | 1:A:908:TRP:CH2 | 1.32 | 1.58 |
| 1:A:865:PHE:CE1 | 1:A:865:PHE:CG | 1.31 | 2.16 |
| 1:A:914:ARG:CG | 1:A:914:ARG:NE | 1.31 | 1.90 |
| 1:A:854:VAL:CG2 | 1:A:918:LEU:HG | 1.31 | 1.56 |
| 1:A:896:ASP:CB | 1:A:896:ASP:OD1 | 1.31 | 1.77 |
| 1:A:883:PHE:CZ | 1:A:883:PHE:CD2 | 1.31 | 2.13 |
| 1:A:881:GLN:CG | 1:A:881:GLN:NE2 | 1.30 | 1.91 |
| 1:A:847:LEU:O | 1:A:848:LEU:CA | 1.30 | 1.80 |
| 1:A:836:SER:CA | 1:A:836:SER:OG | 1.30 | 1.77 |
| 1:A:885:MET:SD | 1:A:897:LYS:CB | 1.29 | 2.20 |
| 1:A:916:ARG:NH2 | 1:A:916:ARG:NH1 | 1.29 | 1.75 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:871:TYR:CB | 1:A:871:TYR:CD2 | 1.27 | 2.18 |
| 1:A:914:ARG:CD | 1:A:914:ARG:CB | 1.27 | 2.12 |
| 1:A:872:PHE:CD1 | 1:A:872:PHE:CB | 1.26 | 2.18 |
| 1:A:871:TYR:CE2 | 1:A:875:PHE:CZ | 1.25 | 2.23 |
| 1:A:896:ASP:CB | 1:A:896:ASP:OD2 | 1.25 | 1.82 |
| 1:A:883:PHE:CB | 1:A:883:PHE:CD2 | 1.24 | 2.17 |
| 1:A:846:VAL:C | 1:A:847:LEU:CD2 | 1.23 | 2.05 |
| 1:A:846:VAL:O | 1:A:847:LEU:CA | 1.23 | 1.86 |
| 1:A:839:GLU:CG | 1:A:839:GLU:OE2 | 1.22 | 1.85 |
| 1:A:850:ILE:HD12 | 1:A:913:ILE:C | 1.22 | 1.54 |
| 1:A:857:TYR:CD1 | 1:A:857:TYR:CB | 1.22 | 2.22 |
| 1:A:857:TYR:CD2 | 1:A:857:TYR:CB | 1.22 | 2.21 |
| 1:A:839:GLU:OE1 | 1:A:839:GLU:CG | 1.21 | 1.86 |
| 1:A:838:ASP:CA | 1:A:838:ASP:CG | 1.21 | 2.08 |
| 1:A:871:TYR:CE2 | 1:A:875:PHE:HZ | 1.20 | 1.51 |
| 1:A:875:PHE:CD2 | 1:A:875:PHE:CB | 1.20 | 2.21 |
| 1:A:875:PHE:CB | 1:A:875:PHE:CD1 | 1.20 | 2.22 |
| 1:A:879:LEU:CB | 1:A:879:LEU:CD2 | 1.20 | 2.19 |
| 1:A:878:ASP:CB | 1:A:878:ASP:OD2 | 1.19 | 1.89 |
| 1:A:851:PHE:CD1 | 1:A:851:PHE:CB | 1.19 | 2.26 |
| 1:A:879:LEU:CD1 | 1:A:879:LEU:CB | 1.19 | 2.19 |
| 1:A:865:PHE:CB | 1:A:865:PHE:CD2 | 1.19 | 2.24 |
| 1:A:851:PHE:HA | 1:A:918:LEU:CD1 | 1.18 | 1.66 |
| 1:A:865:PHE:CD1 | 1:A:865:PHE:CB | 1.18 | 2.26 |
| 1:A:885:MET:O | 1:A:888:ALA:N | 1.17 | 1.77 |
| 1:A:851:PHE:CD2 | 1:A:851:PHE:CB | 1.17 | 2.26 |
| 1:A:851:PHE:CZ | 1:A:909:ILE:CG1 | 1.16 | 2.29 |
| 1:A:850:ILE:CG1 | 1:A:913:ILE:HA | 1.16 | 1.43 |
| 1:A:847:LEU:O | 1:A:847:LEU:CA | 1.15 | 1.93 |
| 1:A:846:VAL:HG23 | 1:A:871:TYR:OH | 1.15 | 1.41 |
| 1:A:846:VAL:O | 1:A:846:VAL:CA | 1.13 | 1.97 |
| 1:A:850:ILE:CD1 | 1:A:913:ILE:CA | 1.12 | 2.12 |
| 1:A:871:TYR:CD2 | 1:A:875:PHE:CZ | 1.12 | 2.37 |
| 1:A:849:ASP:CA | 1:A:849:ASP:CG | 1.11 | 2.18 |
| 1:A:846:VAL:O | 1:A:847:LEU:HD22 | 1.11 | 0.97 |
| 1:A:871:TYR:OH | 1:A:871:TYR:CE1 | 1.11 | 2.03 |
| 1:A:871:TYR:CB | 1:A:871:TYR:CD1 | 1.11 | 2.26 |
| 1:A:856:LEU:HD12 | 1:A:856:LEU:O | 1.10 | 1.44 |
| 1:A:879:LEU:HG | 1:A:879:LEU:CD2 | 1.09 | 1.76 |
| 1:A:856:LEU:HD12 | 1:A:856:LEU:C | 1.09 | 1.62 |
| 1:A:854:VAL:HG21 | 1:A:918:LEU:CG | 1.09 | 1.76 |
| 1:A:856:LEU:N | 1:A:890:HIS:HB2 | 1.09 | 1.62 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:847:LEU:HD22 | 1:A:847:LEU:N | 1.09 | 1.56 |
| 1:A:858:LEU:CD2 | 1:A:868:LEU:HB3 | 1.09 | 1.75 |
| 1:A:847:LEU:HD13 | 1:A:871:TYR:CE1 | 1.09 | 1.81 |
| 1:A:878:ASP:CB | 1:A:878:ASP:OD1 | 1.08 | 2.02 |
| 1:A:879:LEU:HG | 1:A:879:LEU:CD1 | 1.08 | 1.76 |
| 1:A:856:LEU:CD2 | 1:A:892:LEU:HD12 | 1.07 | 1.78 |
| 1:A:871:TYR:OH | 1:A:913:ILE:CD1 | 1.07 | 2.00 |
| 1:A:846:VAL:C | 1:A:847:LEU:CA | 1.06 | 2.23 |
| 1:A:872:PHE:CD2 | 1:A:872:PHE:CB | 1.06 | 2.25 |
| 1:A:850:ILE:CG1 | 1:A:913:ILE:CA | 1.05 | 2.32 |
| 1:A:857:TYR:OH | 1:A:857:TYR:CE1 | 1.05 | 2.07 |
| 1:A:916:ARG:HG3 | 1:A:916:ARG:CZ | 1.05 | 1.78 |
| 1:A:856:LEU:HA | 1:A:890:HIS:CB | 1.05 | 1.80 |
| 1:A:864:ASP:CB | 1:A:864:ASP:OD1 | 1.05 | 2.02 |
| 1:A:847:LEU:C | 1:A:848:LEU:CA | 1.05 | 2.23 |
| 1:A:905:SER:CA | 1:A:905:SER:OG | 1.04 | 2.03 |
| 1:A:849:ASP:HB3 | 1:A:849:ASP:CG | 1.03 | 1.48 |
| 1:A:882:GLU:OE2 | 1:A:882:GLU:CG | 1.03 | 2.06 |
| 1:A:856:LEU:CA | 1:A:890:HIS:CB | 1.01 | 2.38 |
| 1:A:850:ILE:HD12 | 1:A:913:ILE:O | 1.01 | 1.52 |
| 1:A:848:LEU:HD22 | 1:A:916:ARG:HD2 | 1.01 | 1.25 |
| 1:A:880:VAL:HG21 | 1:A:888:ALA:CB | 1.01 | 1.85 |
| 1:A:905:SER:OG | 1:A:905:SER:HB3 | 1.00 | 1.28 |
| 1:A:849:ASP:HB2 | 1:A:849:ASP:CG | 1.00 | 1.48 |
| 1:A:855:ARG:C | 1:A:890:HIS:HB2 | 1.00 | 1.61 |
| 1:A:858:LEU:HD21 | 1:A:868:LEU:CB | 0.99 | 1.87 |
| 1:A:905:SER:OG | 1:A:905:SER:HB2 | 0.99 | 1.28 |
| 1:A:857:TYR:OH | 1:A:857:TYR:CE2 | 0.99 | 2.08 |
| 1:A:882:GLU:OE1 | 1:A:882:GLU:CG | 0.99 | 2.10 |
| 1:A:884:ASP:OD2 | 1:A:884:ASP:CB | 0.99 | 2.10 |
| 1:A:836:SER:HB2 | 1:A:836:SER:OG | 0.99 | 1.26 |
| 1:A:879:LEU:HD23 | 1:A:879:LEU:CG | 0.99 | 1.53 |
| 1:A:849:ASP:CB | 1:A:849:ASP:CG | 0.99 | 0.90 |
| 1:A:876:ASP:CB | 1:A:876:ASP:OD1 | 0.98 | 2.09 |
| 1:A:876:ASP:CB | 1:A:876:ASP:OD2 | 0.98 | 2.12 |
| 1:A:884:ASP:CB | 1:A:884:ASP:OD1 | 0.98 | 2.12 |
| 1:A:836:SER:HB3 | 1:A:836:SER:OG | 0.98 | 1.26 |
| 1:A:856:LEU:CA | 1:A:890:HIS:HB2 | 0.98 | 1.89 |
| 1:A:905:SER:OG | 1:A:906:PRO:HD2 | 0.98 | 1.59 |
| 1:A:914:ARG:HG3 | 1:A:914:ARG:CD | 0.98 | 1.51 |
| 1:A:879:LEU:CG | 1:A:879:LEU:HD11 | 0.97 | 1.53 |
| 1:A:856:LEU:HD21 | 1:A:892:LEU:HD12 | 0.97 | 0.99 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:864:ASP:CB | 1:A:864:ASP:OD2 | 0.97 | 2.12 |
| 1:A:879:LEU:HD22 | 1:A:879:LEU:CG | 0.97 | 1.53 |
| 1:A:879:LEU:HD23 | 1:A:879:LEU:CD1 | 0.97 | 1.87 |
| 1:A:848:LEU:HD22 | 1:A:916:ARG:CD | 0.96 | 1.90 |
| 1:A:847:LEU:CA | 1:A:848:LEU:N | 0.96 | 2.29 |
| 1:A:879:LEU:CG | 1:A:879:LEU:HD12 | 0.96 | 1.53 |
| 1:A:846:VAL:CA | 1:A:847:LEU:N | 0.96 | 2.28 |
| 1:A:879:LEU:CG | 1:A:879:LEU:HD13 | 0.96 | 1.53 |
| 1:A:916:ARG:CB | 1:A:916:ARG:CZ | 0.96 | 2.42 |
| 1:A:879:LEU:CD2 | 1:A:879:LEU:HD12 | 0.96 | 1.87 |
| 1:A:855:ARG:HD2 | 1:A:889:THR:N | 0.96 | 1.75 |
| 1:A:854:VAL:HG11 | 1:A:908:TRP:HH2 | 0.96 | 0.89 |
| 1:A:914:ARG:HG2 | 1:A:914:ARG:CD | 0.95 | 1.51 |
| 1:A:905:SER:CB | 1:A:905:SER:OG | 0.94 | 0.65 |
| 1:A:881:GLN:CD | 1:A:881:GLN:OE1 | 0.94 | 0.74 |
| 1:A:879:LEU:HD21 | 1:A:879:LEU:CG | 0.94 | 1.53 |
| 1:A:881:GLN:CG | 1:A:881:GLN:OE1 | 0.94 | 2.15 |
| 1:A:851:PHE:HZ | 1:A:851:PHE:CE1 | 0.94 | 1.69 |
| 1:A:885:MET:O | 1:A:887:SER:N | 0.94 | 2.01 |
| 1:A:879:LEU:CD1 | 1:A:879:LEU:CD2 | 0.94 | 0.94 |
| 1:A:855:ARG:HG3 | 1:A:889:THR:N | 0.93 | 1.78 |
| 1:A:858:LEU:HD21 | 1:A:868:LEU:HB3 | 0.93 | 0.94 |
| 1:A:883:PHE:CB | 1:A:883:PHE:CD1 | 0.93 | 2.24 |
| 1:A:856:LEU:HD21 | 1:A:892:LEU:CD1 | 0.93 | 1.91 |
| 1:A:871:TYR:CE2 | 1:A:871:TYR:OH | 0.93 | 2.11 |
| 1:A:854:VAL:CG1 | 1:A:908:TRP:HH2 | 0.92 | 1.76 |
| 1:A:847:LEU:HD13 | 1:A:871:TYR:CD1 | 0.92 | 2.00 |
| 1:A:855:ARG:NE | 1:A:889:THR:CB | 0.92 | 2.01 |
| 1:A:845:LYS:O | 1:A:871:TYR:HE1 | 0.91 | 1.47 |
| 1:A:854:VAL:CG2 | 1:A:918:LEU:CG | 0.91 | 2.42 |
| 1:A:881:GLN:O | 1:A:884:ASP:N | 0.91 | 2.03 |
| 1:A:847:LEU:HD13 | 1:A:871:TYR:HE1 | 0.91 | 1.24 |
| 1:A:871:TYR:CE1 | 1:A:875:PHE:CZ | 0.91 | 2.51 |
| 1:A:914:ARG:CD | 1:A:914:ARG:CG | 0.91 | 0.91 |
| 1:A:847:LEU:CD2 | 1:A:847:LEU:N | 0.91 | 2.31 |
| 1:A:914:ARG:CG | 1:A:914:ARG:HD3 | 0.91 | 1.45 |
| 1:A:836:SER:CB | 1:A:836:SER:OG | 0.90 | 0.61 |
| 1:A:856:LEU:CD1 | 1:A:856:LEU:C | 0.90 | 2.28 |
| 1:A:914:ARG:HD2 | 1:A:914:ARG:CG | 0.90 | 1.45 |
| 1:A:879:LEU:CG | 1:A:879:LEU:CD1 | 0.90 | 0.90 |
| 1:A:879:LEU:CG | 1:A:879:LEU:CD2 | 0.90 | 0.90 |
| 1:A:854:VAL:HG12 | 1:A:872:PHE:HZ | 0.90 | 1.22 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:850:ILE:CD1 | 1:A:913:ILE:O | 0.90 | 2.20 |
| 1:A:855:ARG:CD | 1:A:889:THR:N | 0.90 | 2.35 |
| 1:A:854:VAL:CG1 | 1:A:908:TRP:CH2 | 0.89 | 2.52 |
| 1:A:855:ARG:H | 1:A:889:THR:CG2 | 0.89 | 1.78 |
| 1:A:871:TYR:CZ | 1:A:875:PHE:CZ | 0.89 | 2.59 |
| 1:A:856:LEU:HA | 1:A:890:HIS:C | 0.89 | 1.88 |
| 1:A:885:MET:HB2 | 1:A:898:ASN:CB | 0.89 | 1.96 |
| 1:A:871:TYR:CD1 | 1:A:875:PHE:CZ | 0.89 | 2.59 |
| 1:A:871:TYR:CZ | 1:A:913:ILE:CD1 | 0.88 | 2.56 |
| 1:A:846:VAL:CA | 1:A:847:LEU:HD22 | 0.88 | 1.99 |
| 1:A:889:THR:HG23 | 1:A:890:HIS:ND1 | 0.88 | 1.82 |
| 1:A:871:TYR:CD2 | 1:A:875:PHE:HZ | 0.88 | 1.78 |
| 1:A:851:PHE:CZ | 1:A:909:ILE:HA | 0.88 | 2.03 |
| 1:A:845:LYS:O | 1:A:871:TYR:CE1 | 0.88 | 2.26 |
| 1:A:851:PHE:CZ | 1:A:909:ILE:HG12 | 0.88 | 2.03 |
| 1:A:885:MET:CG | 1:A:898:ASN:HB2 | 0.87 | 1.98 |
| 1:A:846:VAL:C | 1:A:847:LEU:N | 0.87 | 0.83 |
| 1:A:847:LEU:CD1 | 1:A:871:TYR:CD1 | 0.87 | 2.57 |
| 1:A:841:LEU:HD11 | 1:A:845:LYS:CE | 0.86 | 2.01 |
| 1:A:884:ASP:CG | 1:A:884:ASP:OD1 | 0.86 | 0.66 |
| 1:A:895:ARG:O | 1:A:898:ASN:N | 0.86 | 2.09 |
| 1:A:855:ARG:H | 1:A:889:THR:HG21 | 0.85 | 1.26 |
| 1:A:876:ASP:OD2 | 1:A:876:ASP:CG | 0.85 | 0.65 |
| 1:A:851:PHE:CZ | 1:A:909:ILE:HG13 | 0.85 | 2.03 |
| 1:A:884:ASP:CG | 1:A:884:ASP:OD2 | 0.85 | 0.65 |
| 1:A:841:LEU:HD11 | 1:A:845:LYS:HE2 | 0.85 | 1.49 |
| 1:A:879:LEU:CD2 | 1:A:879:LEU:HD13 | 0.84 | 1.39 |
| 1:A:851:PHE:HZ | 1:A:851:PHE:CE2 | 0.84 | 1.70 |
| 1:A:864:ASP:CG | 1:A:864:ASP:OD2 | 0.84 | 0.64 |
| 1:A:878:ASP:CG | 1:A:878:ASP:OD1 | 0.84 | 0.64 |
| 1:A:851:PHE:CE1 | 1:A:909:ILE:HG13 | 0.84 | 2.08 |
| 1:A:851:PHE:CZ | 1:A:851:PHE:CE2 | 0.84 | 0.84 |
| 1:A:871:TYR:CZ | 1:A:913:ILE:HD11 | 0.84 | 2.06 |
| 1:A:838:ASP:O | 1:A:842:CYS:HB2 | 0.83 | 1.71 |
| 1:A:851:PHE:CD1 | 1:A:851:PHE:CG | 0.83 | 0.84 |
| 1:A:876:ASP:OD1 | 1:A:876:ASP:CG | 0.83 | 0.63 |
| 1:A:879:LEU:HD22 | 1:A:879:LEU:CD1 | 0.83 | 1.39 |
| 1:A:894:SER:O | 1:A:897:LYS:NZ | 0.83 | 2.11 |
| 1:A:870:ARG:O | 1:A:874:ALA:HB2 | 0.83 | 1.73 |
| 1:A:865:PHE:CD1 | 1:A:865:PHE:CG | 0.83 | 0.84 |
| 1:A:851:PHE:CZ | 1:A:851:PHE:CE1 | 0.83 | 0.84 |
| 1:A:865:PHE:CZ | 1:A:865:PHE:CE2 | 0.83 | 0.84 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:835:GLY:N | 1:A:835:GLY:HA2 | 0.83 | 1.22 |
| 1:A:851:PHE:C | 1:A:918:LEU:HD21 | 0.83 | 1.93 |
| 1:A:851:PHE:CD2 | 1:A:851:PHE:CG | 0.82 | 0.84 |
| 1:A:855:ARG:N | 1:A:889:THR:CG2 | 0.82 | 2.41 |
| 1:A:885:MET:CB | 1:A:898:ASN:HB2 | 0.82 | 2.04 |
| 1:A:835:GLY:N | 1:A:835:GLY:HA3 | 0.82 | 1.22 |
| 1:A:857:TYR:HB3 | 1:A:891:VAL:HG12 | 0.82 | 1.51 |
| 1:A:905:SER:CB | 1:A:906:PRO:HD2 | 0.82 | 2.03 |
| 1:A:855:ARG:HG3 | 1:A:889:THR:H | 0.82 | 1.29 |
| 1:A:851:PHE:HZ | 1:A:909:ILE:CB | 0.82 | 1.88 |
| 1:A:882:GLU:OE1 | 1:A:882:GLU:CD | 0.82 | 0.63 |
| 1:A:865:PHE:CE1 | 1:A:865:PHE:CZ | 0.82 | 0.82 |
| 1:A:846:VAL:O | 1:A:847:LEU:N | 0.81 | 0.67 |
| 1:A:857:TYR:H | 1:A:891:VAL:HA | 0.81 | 1.34 |
| 1:A:852:THR:N | 1:A:918:LEU:HD21 | 0.81 | 1.91 |
| 1:A:872:PHE:HZ | 1:A:872:PHE:CE2 | 0.81 | 1.61 |
| 1:A:838:ASP:CG | 1:A:838:ASP:HB2 | 0.81 | 1.24 |
| 1:A:865:PHE:CG | 1:A:865:PHE:CD2 | 0.80 | 0.82 |
| 1:A:838:ASP:CG | 1:A:838:ASP:HB3 | 0.80 | 1.24 |
| 1:A:883:PHE:HZ | 1:A:883:PHE:CE1 | 0.80 | 1.60 |
| 1:A:885:MET:CE | 1:A:897:LYS:HB2 | 0.80 | 2.06 |
| 1:A:858:LEU:CD1 | 1:A:859:PRO:HD2 | 0.80 | 2.07 |
| 1:A:851:PHE:HZ | 1:A:909:ILE:CG2 | 0.80 | 1.90 |
| 1:A:847:LEU:CD1 | 1:A:871:TYR:HD1 | 0.80 | 1.87 |
| 1:A:851:PHE:CE1 | 1:A:909:ILE:CG1 | 0.79 | 2.65 |
| 1:A:854:VAL:HG21 | 1:A:918:LEU:HG | 0.79 | 0.85 |
| 1:A:855:ARG:CZ | 1:A:889:THR:CB | 0.79 | 2.53 |
| 1:A:848:LEU:HB2 | 1:A:850:ILE:HD11 | 0.79 | 1.51 |
| 1:A:854:VAL:HG12 | 1:A:872:PHE:CZ | 0.79 | 2.12 |
| 1:A:851:PHE:CE1 | 1:A:909:ILE:HA | 0.79 | 2.11 |
| 1:A:875:PHE:HZ | 1:A:875:PHE:CE2 | 0.79 | 1.65 |
| 1:A:855:ARG:CG | 1:A:889:THR:N | 0.79 | 2.39 |
| 1:A:850:ILE:HG13 | 1:A:913:ILE:HG13 | 0.79 | 1.53 |
| 1:A:851:PHE:CZ | 1:A:909:ILE:CB | 0.79 | 2.66 |
| 1:A:850:ILE:HG13 | 1:A:913:ILE:CB | 0.79 | 2.08 |
| 1:A:847:LEU:C | 1:A:848:LEU:N | 0.78 | 0.79 |
| 1:A:848:LEU:CB | 1:A:850:ILE:HD11 | 0.78 | 2.09 |
| 1:A:851:PHE:CZ | 1:A:909:ILE:CA | 0.77 | 2.67 |
| 1:A:914:ARG:HH11 | 1:A:914:ARG:CG | 0.77 | 1.88 |
| 1:A:919:VAL:HG23 | 1:A:920:ALA:N | 0.77 | 1.94 |
| 1:A:851:PHE:HZ | 1:A:909:ILE:CG1 | 0.77 | 1.93 |
| 1:A:851:PHE:HZ | 1:A:909:ILE:HG23 | 0.77 | 1.39 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:858:LEU:HD12 | 1:A:859:PRO:CD | 0.77 | 2.10 |
| 1:A:882:GLU:OE2 | 1:A:882:GLU:CD | 0.77 | 0.59 |
| 1:A:885:MET:HB2 | 1:A:898:ASN:CG | 0.77 | 2.00 |
| 1:A:865:PHE:HZ | 1:A:865:PHE:CE2 | 0.77 | 1.70 |
| 1:A:865:PHE:CE1 | 1:A:865:PHE:HZ | 0.76 | 1.68 |
| 1:A:871:TYR:CG | 1:A:871:TYR:CD1 | 0.76 | 0.80 |
| 1:A:871:TYR:CE2 | 1:A:871:TYR:CZ | 0.76 | 0.80 |
| 1:A:885:MET:HB2 | 1:A:898:ASN:HB2 | 0.76 | 1.56 |
| 1:A:885:MET:SD | 1:A:897:LYS:C | 0.76 | 2.65 |
| 1:A:881:GLN:OE1 | 1:A:881:GLN:NE2 | 0.75 | 0.61 |
| 1:A:875:PHE:HZ | 1:A:875:PHE:CE1 | 0.75 | 1.63 |
| 1:A:879:LEU:CD2 | 1:A:879:LEU:HD11 | 0.75 | 0.99 |
| 1:A:850:ILE:HG22 | 1:A:912:CYS:CB | 0.75 | 2.11 |
| 1:A:879:LEU:HD22 | 1:A:879:LEU:HD13 | 0.75 | 1.06 |
| 1:A:879:LEU:HD21 | 1:A:879:LEU:CD1 | 0.74 | 0.99 |
| 1:A:851:PHE:N | 1:A:918:LEU:HD11 | 0.74 | 1.98 |
| 1:A:851:PHE:HA | 1:A:918:LEU:HD11 | 0.74 | 0.77 |
| 1:A:864:ASP:CG | 1:A:864:ASP:OD1 | 0.74 | 0.55 |
| 1:A:871:TYR:CZ | 1:A:875:PHE:HZ | 0.73 | 2.01 |
| 1:A:850:ILE:HG22 | 1:A:912:CYS:HB3 | 0.73 | 1.61 |
| 1:A:838:ASP:CG | 1:A:838:ASP:CB | 0.72 | 0.63 |
| 1:A:855:ARG:HD2 | 1:A:889:THR:CA | 0.72 | 1.94 |
| 1:A:890:HIS:HA | 1:A:902:GLN:H | 0.72 | 1.44 |
| 1:A:856:LEU:CA | 1:A:890:HIS:HB3 | 0.72 | 2.14 |
| 1:A:895:ARG:C | 1:A:897:LYS:HE3 | 0.72 | 2.05 |
| 1:A:885:MET:SD | 1:A:898:ASN:HB2 | 0.72 | 2.25 |
| 1:A:889:THR:O | 1:A:901:ALA:HA | 0.72 | 1.83 |
| 1:A:846:VAL:C | 1:A:846:VAL:O | 0.72 | 0.53 |
| 1:A:851:PHE:CZ | 1:A:909:ILE:HG23 | 0.72 | 2.19 |
| 1:A:882:GLU:HA | 1:A:885:MET:CE | 0.72 | 2.15 |
| 1:A:885:MET:HA | 1:A:888:ALA:HB2 | 0.72 | 1.59 |
| 1:A:854:VAL:HG13 | 1:A:890:HIS:CD2 | 0.72 | 2.20 |
| 1:A:858:LEU:HD12 | 1:A:859:PRO:N | 0.71 | 2.00 |
| 1:A:871:TYR:CE2 | 1:A:875:PHE:CE1 | 0.71 | 2.78 |
| 1:A:885:MET:O | 1:A:886:THR:C | 0.71 | 2.28 |
| 1:A:850:ILE:HG13 | 1:A:913:ILE:CA | 0.71 | 2.15 |
| 1:A:835:GLY:N | 1:A:835:GLY:CA | 0.71 | 0.56 |
| 1:A:871:TYR:O | 1:A:874:ALA:HB3 | 0.71 | 1.86 |
| 1:A:880:VAL:HG21 | 1:A:888:ALA:HB2 | 0.71 | 1.62 |
| 1:A:857:TYR:HB3 | 1:A:891:VAL:HA | 0.71 | 1.61 |
| 1:A:872:PHE:CE1 | 1:A:872:PHE:CZ | 0.71 | 0.77 |
| 1:A:870:ARG:O | 1:A:874:ALA:CB | 0.71 | 2.38 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:871:TYR:CG | 1:A:875:PHE:CZ | 0.71 | 2.79 |
| 1:A:858:LEU:HD12 | 1:A:859:PRO:HD2 | 0.71 | 1.60 |
| 1:A:855:ARG:C | 1:A:890:HIS:CB | 0.70 | 2.50 |
| 1:A:878:ASP:CG | 1:A:878:ASP:OD2 | 0.70 | 0.53 |
| 1:A:859:PRO:CD | 1:A:892:LEU:HB3 | 0.70 | 2.16 |
| 1:A:895:ARG:CA | 1:A:897:LYS:HE3 | 0.70 | 2.16 |
| 1:A:894:SER:C | 1:A:897:LYS:NZ | 0.70 | 2.45 |
| 1:A:855:ARG:O | 1:A:889:THR:HG22 | 0.69 | 1.87 |
| 1:A:882:GLU:HA | 1:A:885:MET:HE1 | 0.69 | 1.63 |
| 1:A:908:TRP:O | 1:A:912:CYS:SG | 0.69 | 2.51 |
| 1:A:880:VAL:HG21 | 1:A:888:ALA:HB1 | 0.69 | 1.62 |
| 1:A:862:THR:CG2 | 1:A:868:LEU:HD12 | 0.69 | 2.18 |
| 1:A:895:ARG:HB3 | 1:A:903:GLN:NE2 | 0.69 | 2.02 |
| 1:A:872:PHE:CD2 | 1:A:872:PHE:CG | 0.69 | 0.77 |
| 1:A:871:TYR:HH | 1:A:913:ILE:HD11 | 0.69 | 1.45 |
| 1:A:850:ILE:O | 1:A:918:LEU:HD22 | 0.69 | 1.87 |
| 1:A:905:SER:CB | 1:A:906:PRO:CD | 0.69 | 2.70 |
| 1:A:839:GLU:OE1 | 1:A:839:GLU:CD | 0.68 | 0.54 |
| 1:A:850:ILE:HG13 | 1:A:913:ILE:CG1 | 0.68 | 2.19 |
| 1:A:856:LEU:HA | 1:A:890:HIS:HB3 | 0.68 | 1.61 |
| 1:A:846:VAL:O | 1:A:847:LEU:CG | 0.68 | 2.41 |
| 1:A:852:THR:O | 1:A:852:THR:CG2 | 0.68 | 2.41 |
| 1:A:856:LEU:HA | 1:A:890:HIS:CA | 0.68 | 2.17 |
| 1:A:875:PHE:O | 1:A:876:ASP:CB | 0.68 | 2.41 |
| 1:A:857:TYR:CE2 | 1:A:857:TYR:CZ | 0.68 | 0.74 |
| 1:A:854:VAL:HG23 | 1:A:918:LEU:CD2 | 0.67 | 2.19 |
| 1:A:856:LEU:CB | 1:A:890:HIS:HB3 | 0.67 | 2.19 |
| 1:A:839:GLU:CD | 1:A:839:GLU:OE2 | 0.67 | 0.53 |
| 1:A:895:ARG:O | 1:A:896:ASP:C | 0.67 | 2.33 |
| 1:A:851:PHE:HE1 | 1:A:909:ILE:HA | 0.67 | 1.48 |
| 1:A:871:TYR:CE1 | 1:A:871:TYR:CZ | 0.67 | 0.72 |
| 1:A:905:SER:OG | 1:A:906:PRO:CD | 0.67 | 2.41 |
| 1:A:850:ILE:CG1 | 1:A:913:ILE:HG13 | 0.67 | 2.20 |
| 1:A:871:TYR:CG | 1:A:871:TYR:CD2 | 0.67 | 0.72 |
| 1:A:875:PHE:CZ | 1:A:875:PHE:CE2 | 0.67 | 0.73 |
| 1:A:845:LYS:C | 1:A:847:LEU:CD2 | 0.66 | 2.63 |
| 1:A:851:PHE:CA | 1:A:918:LEU:CD1 | 0.66 | 2.46 |
| 1:A:884:ASP:OD2 | 1:A:884:ASP:OD1 | 0.66 | 0.67 |
| 1:A:846:VAL:O | 1:A:847:LEU:CB | 0.66 | 2.41 |
| 1:A:875:PHE:CZ | 1:A:875:PHE:CE1 | 0.66 | 0.72 |
| 1:A:883:PHE:CZ | 1:A:883:PHE:CE1 | 0.66 | 0.68 |
| 1:A:916:ARG:HH12 | 1:A:916:ARG:CZ | 0.66 | 1.39 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:850:ILE:O | 1:A:918:LEU:CD2 | 0.66 | 2.43 |
| 1:A:850:ILE:O | 1:A:918:LEU:HD13 | 0.66 | 1.89 |
| 1:A:883:PHE:CZ | 1:A:883:PHE:CE2 | 0.66 | 0.74 |
| 1:A:851:PHE:HD1 | 1:A:851:PHE:CG | 0.66 | 1.42 |
| 1:A:851:PHE:CZ | 1:A:851:PHE:HE2 | 0.66 | 1.43 |
| 1:A:872:PHE:CE2 | 1:A:872:PHE:CZ | 0.66 | 0.70 |
| 1:A:857:TYR:CD1 | 1:A:857:TYR:CG | 0.66 | 0.74 |
| 1:A:857:TYR:N | 1:A:891:VAL:HA | 0.66 | 2.06 |
| 1:A:851:PHE:CZ | 1:A:851:PHE:HE1 | 0.66 | 1.42 |
| 1:A:865:PHE:HE2 | 1:A:865:PHE:CZ | 0.65 | 1.42 |
| 1:A:850:ILE:O | 1:A:852:THR:N | 0.65 | 2.28 |
| 1:A:865:PHE:HD1 | 1:A:865:PHE:CG | 0.65 | 1.42 |
| 1:A:851:PHE:CG | 1:A:851:PHE:HD2 | 0.65 | 1.42 |
| 1:A:855:ARG:HD2 | 1:A:888:ALA:C | 0.65 | 2.12 |
| 1:A:865:PHE:HD2 | 1:A:865:PHE:CG | 0.65 | 1.41 |
| 1:A:865:PHE:HE1 | 1:A:865:PHE:CZ | 0.65 | 1.41 |
| 1:A:885:MET:SD | 1:A:897:LYS:CD | 0.65 | 2.85 |
| 1:A:850:ILE:O | 1:A:918:LEU:CD1 | 0.65 | 2.45 |
| 1:A:857:TYR:CE1 | 1:A:857:TYR:CZ | 0.64 | 0.73 |
| 1:A:855:ARG:CZ | 1:A:889:THR:OG1 | 0.64 | 2.46 |
| 1:A:857:TYR:CD2 | 1:A:857:TYR:CG | 0.64 | 0.73 |
| 1:A:871:TYR:CD2 | 1:A:875:PHE:CE1 | 0.64 | 2.86 |
| 1:A:845:LYS:O | 1:A:871:TYR:CZ | 0.64 | 2.51 |
| 1:A:841:LEU:CD1 | 1:A:845:LYS:CE | 0.64 | 2.76 |
| 1:A:858:LEU:HD11 | 1:A:862:THR:HG21 | 0.63 | 1.70 |
| 1:A:872:PHE:CD1 | 1:A:872:PHE:CG | 0.63 | 0.71 |
| 1:A:896:ASP:OD2 | 1:A:896:ASP:CG | 0.63 | 0.52 |
| 1:A:850:ILE:C | 1:A:852:THR:H | 0.63 | 1.97 |
| 1:A:850:ILE:HG13 | 1:A:913:ILE:HB | 0.62 | 1.70 |
| 1:A:875:PHE:CG | 1:A:875:PHE:CD2 | 0.62 | 0.72 |
| 1:A:895:ARG:N | 1:A:897:LYS:HE3 | 0.62 | 2.09 |
| 1:A:858:LEU:HD12 | 1:A:858:LEU:C | 0.62 | 2.15 |
| 1:A:855:ARG:NH1 | 1:A:889:THR:CB | 0.62 | 2.52 |
| 1:A:859:PRO:HD3 | 1:A:892:LEU:HB3 | 0.62 | 1.72 |
| 1:A:855:ARG:N | 1:A:889:THR:HG21 | 0.61 | 1.99 |
| 1:A:883:PHE:CG | 1:A:883:PHE:CD1 | 0.61 | 0.74 |
| 1:A:846:VAL:CG2 | 1:A:871:TYR:OH | 0.61 | 2.34 |
| 1:A:857:TYR:N | 1:A:890:HIS:O | 0.61 | 2.33 |
| 1:A:876:ASP:OD1 | 1:A:876:ASP:OD2 | 0.61 | 0.62 |
| 1:A:854:VAL:O | 1:A:872:PHE:CZ | 0.61 | 2.53 |
| 1:A:911:ALA:O | 1:A:915:LYS:CG | 0.61 | 2.49 |
| 1:A:857:TYR:H | 1:A:891:VAL:CA | 0.61 | 2.07 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:882:GLU:O | 1:A:885:MET:CE | 0.61 | 2.48 |
| 1:A:836:SER:N | 1:A:836:SER:OG | 0.61 | 2.32 |
| 1:A:881:GLN:CD | 1:A:881:GLN:HE22 | 0.60 | 1.22 |
| 1:A:846:VAL:HG23 | 1:A:871:TYR:CZ | 0.60 | 2.29 |
| 1:A:847:LEU:HD13 | 1:A:871:TYR:CZ | 0.60 | 2.31 |
| 1:A:885:MET:C | 1:A:898:ASN:ND2 | 0.60 | 2.54 |
| 1:A:895:ARG:HD3 | 1:A:903:GLN:NE2 | 0.60 | 2.12 |
| 1:A:916:ARG:NE | 1:A:916:ARG:CZ | 0.60 | 0.69 |
| 1:A:850:ILE:C | 1:A:918:LEU:CD1 | 0.60 | 2.70 |
| 1:A:881:GLN:CD | 1:A:881:GLN:HE21 | 0.60 | 1.22 |
| 1:A:891:VAL:HG13 | 1:A:901:ALA:CB | 0.60 | 2.27 |
| 1:A:841:LEU:CD1 | 1:A:845:LYS:HE3 | 0.59 | 2.27 |
| 1:A:875:PHE:CG | 1:A:875:PHE:CD1 | 0.59 | 0.73 |
| 1:A:896:ASP:O | 1:A:898:ASN:N | 0.59 | 2.35 |
| 1:A:850:ILE:CD1 | 1:A:913:ILE:HG13 | 0.59 | 2.27 |
| 1:A:916:ARG:NH1 | 1:A:916:ARG:CZ | 0.59 | 0.74 |
| 1:A:850:ILE:C | 1:A:918:LEU:HD13 | 0.59 | 2.18 |
| 1:A:857:TYR:HB3 | 1:A:891:VAL:CG1 | 0.59 | 2.27 |
| 1:A:857:TYR:CB | 1:A:891:VAL:HG12 | 0.58 | 2.27 |
| 1:A:855:ARG:NH1 | 1:A:889:THR:OG1 | 0.58 | 2.35 |
| 1:A:871:TYR:HE2 | 1:A:871:TYR:CZ | 0.58 | 1.34 |
| 1:A:896:ASP:OD1 | 1:A:896:ASP:CG | 0.58 | 0.47 |
| 1:A:848:LEU:CB | 1:A:850:ILE:CD1 | 0.58 | 2.81 |
| 1:A:871:TYR:CG | 1:A:871:TYR:HD1 | 0.58 | 1.34 |
| 1:A:891:VAL:HB | 1:A:897:LYS:NZ | 0.58 | 2.13 |
| 1:A:843:GLN:HB2 | 1:A:846:VAL:HG12 | 0.57 | 1.75 |
| 1:A:846:VAL:N | 1:A:847:LEU:HD22 | 0.57 | 2.15 |
| 1:A:856:LEU:HB2 | 1:A:890:HIS:HB3 | 0.57 | 1.76 |
| 1:A:865:PHE:HA | 1:A:868:LEU:HB2 | 0.57 | 1.76 |
| 1:A:851:PHE:HB3 | 1:A:854:VAL:HB | 0.57 | 1.77 |
| 1:A:840:THR:O | 1:A:846:VAL:HG11 | 0.57 | 1.99 |
| 1:A:881:GLN:CD | 1:A:881:GLN:NE2 | 0.57 | 0.53 |
| 1:A:844:THR:HG22 | 1:A:845:LYS:N | 0.56 | 2.15 |
| 1:A:856:LEU:CD1 | 1:A:856:LEU:O | 0.56 | 2.37 |
| 1:A:871:TYR:CZ | 1:A:913:ILE:HD12 | 0.56 | 2.33 |
| 1:A:875:PHE:O | 1:A:876:ASP:HB2 | 0.56 | 1.99 |
| 1:A:836:SER:N | 1:A:836:SER:HG | 0.56 | 1.98 |
| 1:A:845:LYS:C | 1:A:847:LEU:HD22 | 0.56 | 2.21 |
| 1:A:885:MET:O | 1:A:898:ASN:ND2 | 0.56 | 2.38 |
| 1:A:919:VAL:CG2 | 1:A:920:ALA:N | 0.56 | 2.67 |
| 1:A:847:LEU:N | 1:A:871:TYR:HH | 0.56 | 1.98 |
| 1:A:851:PHE:O | 1:A:854:VAL:HB | 0.56 | 2.00 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:881:GLN:O | 1:A:882:GLU:C | 0.56 | 2.43 |
| 1:A:844:THR:CG2 | 1:A:845:LYS:N | 0.55 | 2.64 |
| 1:A:871:TYR:CE2 | 1:A:913:ILE:CD1 | 0.55 | 2.90 |
| 1:A:872:PHE:O | 1:A:874:ALA:N | 0.55 | 2.39 |
| 1:A:852:THR:N | 1:A:918:LEU:CD2 | 0.55 | 2.69 |
| 1:A:885:MET:SD | 1:A:897:LYS:CA | 0.55 | 2.93 |
| 1:A:906:PRO:O | 1:A:910:TRP:CD1 | 0.55 | 2.60 |
| 1:A:854:VAL:HG23 | 1:A:918:LEU:CG | 0.55 | 2.30 |
| 1:A:908:TRP:CD1 | 1:A:921:PRO:HA | 0.55 | 2.37 |
| 1:A:851:PHE:HD1 | 1:A:908:TRP:CZ3 | 0.55 | 2.20 |
| 1:A:846:VAL:N | 1:A:847:LEU:CD2 | 0.55 | 2.70 |
| 1:A:894:SER:C | 1:A:897:LYS:HZ1 | 0.55 | 2.05 |
| 1:A:895:ARG:O | 1:A:897:LYS:HD2 | 0.54 | 2.03 |
| 1:A:858:LEU:HD13 | 1:A:892:LEU:HD13 | 0.54 | 1.80 |
| 1:A:880:VAL:HB | 1:A:884:ASP:O | 0.54 | 2.02 |
| 1:A:865:PHE:O | 1:A:866:SER:C | 0.54 | 2.45 |
| 1:A:854:VAL:CG2 | 1:A:918:LEU:CD2 | 0.54 | 2.83 |
| 1:A:872:PHE:HE1 | 1:A:872:PHE:CZ | 0.54 | 1.30 |
| 1:A:895:ARG:HD3 | 1:A:903:GLN:HE22 | 0.54 | 1.61 |
| 1:A:872:PHE:HD2 | 1:A:872:PHE:CG | 0.54 | 1.30 |
| 1:A:904:VAL:HG23 | 1:A:905:SER:N | 0.54 | 2.15 |
| 1:A:880:VAL:CG2 | 1:A:888:ALA:CB | 0.54 | 2.76 |
| 1:A:871:TYR:CG | 1:A:871:TYR:HD2 | 0.54 | 1.30 |
| 1:A:845:LYS:C | 1:A:847:LEU:HD21 | 0.53 | 2.24 |
| 1:A:870:ARG:CZ | 1:A:870:ARG:HH21 | 0.53 | 1.24 |
| 1:A:871:TYR:HE1 | 1:A:871:TYR:CZ | 0.53 | 1.30 |
| 1:A:862:THR:HG21 | 1:A:868:LEU:HD12 | 0.53 | 1.78 |
| 1:A:857:TYR:CG | 1:A:857:TYR:O | 0.53 | 2.61 |
| 1:A:851:PHE:O | 1:A:854:VAL:N | 0.53 | 2.29 |
| 1:A:857:TYR:HE2 | 1:A:857:TYR:CZ | 0.53 | 1.28 |
| 1:A:885:MET:HB2 | 1:A:898:ASN:ND2 | 0.53 | 2.18 |
| 1:A:887:SER:O | 1:A:888:ALA:O | 0.53 | 2.25 |
| 1:A:879:LEU:CA | 1:A:879:LEU:CD2 | 0.53 | 2.86 |
| 1:A:857:TYR:HD2 | 1:A:857:TYR:CG | 0.53 | 1.28 |
| 1:A:857:TYR:HE1 | 1:A:857:TYR:CZ | 0.53 | 1.28 |
| 1:A:914:ARG:HD2 | 1:A:914:ARG:CB | 0.53 | 2.02 |
| 1:A:878:ASP:OD2 | 1:A:878:ASP:OD1 | 0.53 | 0.53 |
| 1:A:880:VAL:CG1 | 1:A:884:ASP:O | 0.53 | 2.56 |
| 1:A:895:ARG:CA | 1:A:897:LYS:CE | 0.53 | 2.87 |
| 1:A:847:LEU:C | 1:A:847:LEU:O | 0.52 | 0.43 |
| 1:A:856:LEU:CB | 1:A:890:HIS:CB | 0.52 | 2.84 |
| 1:A:857:TYR:HD1 | 1:A:857:TYR:CG | 0.52 | 1.28 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:895:ARG:CB | 1:A:903:GLN:NE2 | 0.52 | 2.72 |
| 1:A:840:THR:O | 1:A:846:VAL:CG1 | 0.52 | 2.58 |
| 1:A:849:ASP:N | 1:A:849:ASP:CG | 0.52 | 2.63 |
| 1:A:885:MET:CE | 1:A:897:LYS:HD3 | 0.52 | 2.34 |
| 1:A:889:THR:CG2 | 1:A:890:HIS:N | 0.52 | 2.72 |
| 1:A:857:TYR:CB | 1:A:891:VAL:HA | 0.52 | 2.35 |
| 1:A:849:ASP:O | 1:A:916:ARG:O | 0.52 | 2.28 |
| 1:A:837:ALA:O | 1:A:841:LEU:N | 0.52 | 2.43 |
| 1:A:872:PHE:O | 1:A:873:VAL:C | 0.52 | 2.49 |
| 1:A:871:TYR:HE2 | 1:A:875:PHE:HZ | 0.52 | 1.27 |
| 1:A:911:ALA:O | 1:A:915:LYS:HG2 | 0.52 | 2.05 |
| 1:A:896:ASP:O | 1:A:897:LYS:C | 0.51 | 2.48 |
| 1:A:891:VAL:N | 1:A:902:GLN:O | 0.51 | 2.40 |
| 1:A:851:PHE:N | 1:A:918:LEU:CD1 | 0.51 | 2.70 |
| 1:A:883:PHE:CG | 1:A:883:PHE:CD2 | 0.51 | 0.68 |
| 1:A:845:LYS:O | 1:A:846:VAL:C | 0.51 | 2.48 |
| 1:A:850:ILE:C | 1:A:852:THR:N | 0.51 | 2.63 |
| 1:A:895:ARG:HB3 | 1:A:903:GLN:CG | 0.51 | 2.36 |
| 1:A:905:SER:CB | 1:A:905:SER:HG | 0.51 | 1.22 |
| 1:A:895:ARG:HA | 1:A:897:LYS:HZ2 | 0.51 | 1.64 |
| 1:A:854:VAL:HG11 | 1:A:908:TRP:CZ3 | 0.51 | 2.30 |
| 1:A:872:PHE:CZ | 1:A:872:PHE:HE2 | 0.51 | 1.26 |
| 1:A:916:ARG:HE | 1:A:916:ARG:CZ | 0.51 | 1.28 |
| 1:A:855:ARG:C | 1:A:889:THR:HG22 | 0.51 | 2.04 |
| 1:A:872:PHE:HD1 | 1:A:872:PHE:CG | 0.51 | 1.26 |
| 1:A:885:MET:CB | 1:A:898:ASN:CB | 0.51 | 2.72 |
| 1:A:851:PHE:CD1 | 1:A:908:TRP:CZ3 | 0.50 | 3.00 |
| 1:A:882:GLU:C | 1:A:884:ASP:H | 0.50 | 2.09 |
| 1:A:891:VAL:O | 1:A:902:GLN:O | 0.50 | 2.30 |
| 1:A:875:PHE:CG | 1:A:875:PHE:HD1 | 0.50 | 1.25 |
| 1:A:872:PHE:O | 1:A:875:PHE:N | 0.50 | 2.45 |
| 1:A:850:ILE:CD1 | 1:A:913:ILE:CG1 | 0.50 | 2.90 |
| 1:A:875:PHE:CZ | 1:A:875:PHE:HE2 | 0.50 | 1.25 |
| 1:A:881:GLN:O | 1:A:884:ASP:CA | 0.50 | 2.59 |
| 1:A:836:SER:O | 1:A:839:GLU:N | 0.50 | 2.44 |
| 1:A:851:PHE:HA | 1:A:918:LEU:CG | 0.50 | 2.34 |
| 1:A:871:TYR:CE2 | 1:A:913:ILE:HD12 | 0.49 | 2.41 |
| 1:A:867:ARG:O | 1:A:868:LEU:C | 0.49 | 2.49 |
| 1:A:895:ARG:HB3 | 1:A:903:GLN:HG3 | 0.49 | 1.82 |
| 1:A:875:PHE:O | 1:A:876:ASP:CG | 0.49 | 2.50 |
| 1:A:908:TRP:CE2 | 1:A:912:CYS:SG | 0.49 | 3.05 |
| 1:A:848:LEU:HB3 | 1:A:850:ILE:CD1 | 0.49 | 2.37 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:850:ILE:CD1 | 1:A:913:ILE:CB | 0.49 | 2.87 |
| 1:A:845:LYS:O | 1:A:847:LEU:HD13 | 0.49 | 2.07 |
| 1:A:852:THR:O | 1:A:852:THR:HG23 | 0.49 | 2.06 |
| 1:A:836:SER:O | 1:A:837:ALA:C | 0.49 | 2.49 |
| 1:A:836:SER:HG | 1:A:836:SER:CB | 0.48 | 1.19 |
| 1:A:845:LYS:O | 1:A:847:LEU:CD1 | 0.48 | 2.60 |
| 1:A:883:PHE:HE2 | 1:A:883:PHE:CZ | 0.48 | 1.24 |
| 1:A:836:SER:CA | 1:A:836:SER:HG | 0.48 | 1.92 |
| 1:A:851:PHE:CB | 1:A:854:VAL:HB | 0.48 | 2.39 |
| 1:A:845:LYS:HB3 | 1:A:847:LEU:HD11 | 0.48 | 1.83 |
| 1:A:880:VAL:CB | 1:A:884:ASP:O | 0.48 | 2.61 |
| 1:A:882:GLU:O | 1:A:885:MET:HE3 | 0.48 | 2.09 |
| 1:A:841:LEU:C | 1:A:843:GLN:N | 0.48 | 2.67 |
| 1:A:859:PRO:HD3 | 1:A:892:LEU:CB | 0.48 | 2.38 |
| 1:A:875:PHE:CZ | 1:A:875:PHE:HE1 | 0.48 | 1.24 |
| 1:A:883:PHE:CG | 1:A:883:PHE:HD1 | 0.47 | 1.23 |
| 1:A:845:LYS:O | 1:A:847:LEU:CD2 | 0.47 | 2.62 |
| 1:A:875:PHE:HD2 | 1:A:875:PHE:CG | 0.47 | 1.24 |
| 1:A:885:MET:HA | 1:A:888:ALA:CB | 0.47 | 2.37 |
| 1:A:880:VAL:HG12 | 1:A:884:ASP:O | 0.47 | 2.10 |
| 1:A:843:GLN:HB2 | 1:A:846:VAL:CG1 | 0.47 | 2.39 |
| 1:A:874:ALA:O | 1:A:875:PHE:C | 0.47 | 2.52 |
| 1:A:882:GLU:O | 1:A:885:MET:SD | 0.47 | 2.72 |
| 1:A:885:MET:C | 1:A:887:SER:N | 0.46 | 2.66 |
| 1:A:871:TYR:CD1 | 1:A:875:PHE:CE1 | 0.46 | 2.99 |
| 1:A:896:ASP:C | 1:A:898:ASN:N | 0.46 | 2.68 |
| 1:A:859:PRO:CD | 1:A:892:LEU:CB | 0.46 | 2.92 |
| 1:A:912:CYS:HA | 1:A:919:VAL:HG13 | 0.46 | 1.86 |
| 1:A:882:GLU:OE1 | 1:A:882:GLU:OE2 | 0.46 | 0.46 |
| 1:A:855:ARG:HG3 | 1:A:855:ARG:O | 0.46 | 2.11 |
| 1:A:856:LEU:CD1 | 1:A:857:TYR:N | 0.46 | 2.77 |
| 1:A:867:ARG:O | 1:A:871:TYR:N | 0.46 | 2.44 |
| 1:A:858:LEU:HD13 | 1:A:859:PRO:HD2 | 0.46 | 1.84 |
| 1:A:845:LYS:O | 1:A:847:LEU:HD22 | 0.46 | 2.10 |
| 1:A:851:PHE:CA | 1:A:854:VAL:HB | 0.46 | 2.40 |
| 1:A:871:TYR:CE1 | 1:A:875:PHE:CE1 | 0.46 | 2.95 |
| 1:A:885:MET:SD | 1:A:897:LYS:CG | 0.45 | 2.99 |
| 1:A:846:VAL:CA | 1:A:847:LEU:CD2 | 0.45 | 2.81 |
| 1:A:890:HIS:CG | 1:A:902:GLN:HB2 | 0.45 | 2.47 |
| 1:A:890:HIS:CD2 | 1:A:902:GLN:HB2 | 0.45 | 2.47 |
| 1:A:851:PHE:CE2 | 1:A:909:ILE:HG12 | 0.45 | 2.47 |
| 1:A:851:PHE:O | 1:A:852:THR:C | 0.45 | 2.55 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:891:VAL:HB | 1:A:897:LYS:HZ3 | 0.45 | 1.71 |
| 1:A:885:MET:SD | 1:A:898:ASN:N | 0.45 | 2.89 |
| 1:A:869:ARG:O | 1:A:873:VAL:HG12 | 0.44 | 2.12 |
| 1:A:914:ARG:HB3 | 1:A:914:ARG:HD2 | 0.44 | 1.83 |
| 1:A:889:THR:O | 1:A:901:ALA:CA | 0.44 | 2.59 |
| 1:A:883:PHE:CG | 1:A:883:PHE:HD2 | 0.44 | 1.20 |
| 1:A:867:ARG:O | 1:A:871:TYR:CB | 0.44 | 2.66 |
| 1:A:847:LEU:HA | 1:A:875:PHE:CE1 | 0.44 | 2.47 |
| 1:A:883:PHE:HE1 | 1:A:883:PHE:CZ | 0.44 | 1.20 |
| 1:A:840:THR:C | 1:A:842:CYS:N | 0.44 | 2.71 |
| 1:A:858:LEU:HD11 | 1:A:862:THR:CG2 | 0.44 | 2.41 |
| 1:A:850:ILE:CG2 | 1:A:912:CYS:CB | 0.44 | 2.90 |
| 1:A:885:MET:HG3 | 1:A:897:LYS:O | 0.44 | 2.13 |
| 1:A:858:LEU:CD2 | 1:A:868:LEU:CB | 0.43 | 2.70 |
| 1:A:881:GLN:HB2 | 1:A:884:ASP:HB2 | 0.43 | 1.90 |
| 1:A:845:LYS:C | 1:A:846:VAL:HG22 | 0.43 | 2.32 |
| 1:A:851:PHE:HB3 | 1:A:872:PHE:CZ | 0.43 | 2.47 |
| 1:A:880:VAL:CG2 | 1:A:888:ALA:HB2 | 0.43 | 2.39 |
| 1:A:895:ARG:HB3 | 1:A:903:GLN:CD | 0.43 | 2.32 |
| 1:A:864:ASP:OD1 | 1:A:864:ASP:OD2 | 0.43 | 0.43 |
| 1:A:880:VAL:CG2 | 1:A:888:ALA:HB1 | 0.43 | 2.40 |
| 1:A:892:LEU:HD11 | 1:A:909:ILE:CD1 | 0.43 | 2.43 |
| 1:A:855:ARG:O | 1:A:855:ARG:CG | 0.43 | 2.65 |
| 1:A:909:ILE:O | 1:A:913:ILE:HG22 | 0.43 | 2.14 |
| 1:A:871:TYR:HE2 | 1:A:913:ILE:HD12 | 0.43 | 1.71 |
| 1:A:869:ARG:O | 1:A:873:VAL:CG1 | 0.43 | 2.67 |
| 1:A:895:ARG:N | 1:A:897:LYS:CE | 0.43 | 2.80 |
| 1:A:885:MET:CB | 1:A:898:ASN:CG | 0.43 | 2.83 |
| 1:A:872:PHE:C | 1:A:874:ALA:N | 0.42 | 2.71 |
| 1:A:882:GLU:C | 1:A:884:ASP:N | 0.42 | 2.73 |
| 1:A:869:ARG:O | 1:A:870:ARG:C | 0.42 | 2.57 |
| 1:A:841:LEU:C | 1:A:843:GLN:H | 0.42 | 2.18 |
| 1:A:847:LEU:CD1 | 1:A:871:TYR:CG | 0.42 | 3.02 |
| 1:A:908:TRP:CD2 | 1:A:912:CYS:SG | 0.42 | 3.13 |
| 1:A:870:ARG:NH2 | 1:A:870:ARG:CZ | 0.42 | 0.57 |
| 1:A:851:PHE:CE2 | 1:A:909:ILE:CG1 | 0.42 | 2.91 |
| 1:A:854:VAL:HG13 | 1:A:890:HIS:CG | 0.41 | 2.50 |
| 1:A:917:ARG:O | 1:A:918:LEU:C | 0.41 | 2.57 |
| 1:A:851:PHE:CE1 | 1:A:909:ILE:CA | 0.41 | 2.95 |
| 1:A:859:PRO:HG2 | 1:A:862:THR:CB | 0.41 | 2.45 |
| 1:A:890:HIS:HA | 1:A:902:GLN:N | 0.41 | 2.22 |
| 1:A:851:PHE:CZ | 1:A:909:ILE:CG2 | 0.41 | 2.82 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|------------------|------------------|----------|-------------|
| 1:A:857:TYR:H | 1:A:890:HIS:C | 0.41 | 2.19 |
| 1:A:912:CYS:SG | 1:A:919:VAL:HG13 | 0.41 | 2.56 |
| 1:A:840:THR:C | 1:A:842:CYS:H | 0.41 | 2.19 |
| 1:A:882:GLU:CA | 1:A:885:MET:CE | 0.41 | 2.95 |
| 1:A:891:VAL:CG2 | 1:A:902:GLN:O | 0.41 | 2.68 |
| 1:A:852:THR:HG22 | 1:A:918:LEU:CD2 | 0.40 | 2.47 |
| 1:A:841:LEU:HD21 | 1:A:845:LYS:HA | 0.40 | 1.93 |
| 1:A:852:THR:O | 1:A:852:THR:HG22 | 0.40 | 2.15 |
| 1:A:868:LEU:HA | 1:A:868:LEU:HD23 | 0.40 | 1.67 |
| 1:A:885:MET:CA | 1:A:888:ALA:CB | 0.40 | 2.99 |

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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 | 86/88 (98%) | 43 (50%) | 26 (30%) | 17 (20%) | 0 | 2 |
| All | All | 86/88 (98%) | 43 (50%) | 26 (30%) | 17 (20%) | 0 | 2 |

All 17 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 886 | THR |
| 1 | A | 845 | LYS |
| 1 | A | 876 | ASP |
| 1 | A | 851 | PHE |
| 1 | A | 882 | GLU |
| 1 | A | 873 | VAL |
| 1 | A | 872 | PHE |
| 1 | A | 883 | PHE |
| 1 | A | 869 | ARG |
| 1 | A | 896 | ASP |
| 1 | A | 888 | ALA |
| 1 | A | 893 | GLY |
| 1 | A | 897 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 850 | ILE |
| 1 | A | 846 | VAL |
| 1 | A | 848 | LEU |
| 1 | A | 847 | LEU |

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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 | 77/77 (100%) | 45 (58%) | 32 (42%) | 0 | 4 |
| All | All | 77/77 (100%) | 45 (58%) | 32 (42%) | 0 | 4 |

All 32 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 845 | LYS |
| 1 | A | 914 | ARG |
| 1 | A | 919 | VAL |
| 1 | A | 880 | VAL |
| 1 | A | 839 | GLU |
| 1 | A | 918 | LEU |
| 1 | A | 847 | LEU |
| 1 | A | 896 | ASP |
| 1 | A | 889 | THR |
| 1 | A | 841 | LEU |
| 1 | A | 917 | ARG |
| 1 | A | 907 | GLU |
| 1 | A | 852 | THR |
| 1 | A | 861 | SER |
| 1 | A | 897 | LYS |
| 1 | A | 858 | LEU |
| 1 | A | 870 | ARG |
| 1 | A | 909 | ILE |
| 1 | A | 862 | THR |
| 1 | A | 887 | SER |
| 1 | A | 856 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 873 | VAL |
| 1 | A | 838 | ASP |
| 1 | A | 850 | ILE |
| 1 | A | 843 | GLN |
| 1 | A | 892 | LEU |
| 1 | A | 916 | ARG |
| 1 | A | 857 | TYR |
| 1 | A | 844 | THR |
| 1 | A | 849 | ASP |
| 1 | A | 864 | ASP |
| 1 | A | 867 | ARG |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | A | 5 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 893:GLY | C | 894:SER | N | 1.15 |
| 1 | A | 844:THR | C | 845:LYS | N | 1.09 |
| 1 | A | 835:GLY | C | 836:SER | N | 0.87 |
| 1 | A | 846:VAL | C | 847:LEU | N | 0.83 |
| 1 | A | 847:LEU | C | 848:LEU | N | 0.79 |

7 Chemical shift validation

No chemical shift data were provided