



Full wwPDB NMR Structure Validation Report ⓘ

Nov 23, 2017 – 03:50 AM EST

PDB ID : 1PLS
Title : SOLUTION STRUCTURE OF A PLECKSTRIN HOMOLOGY DOMAIN
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Deposited on : unknown

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20030345
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

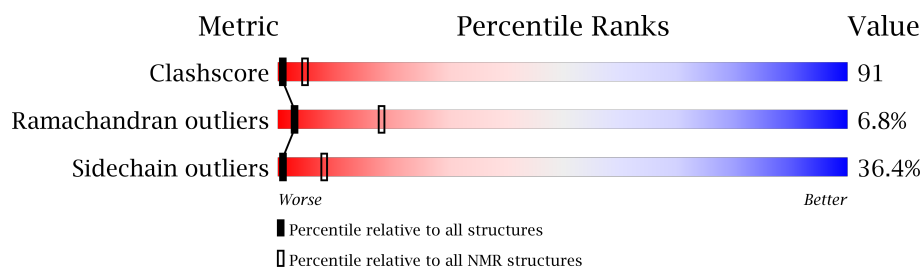
1 Overall quality at a glance

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 | 125131 | 11601 |
| Ramachandran outliers | 121729 | 10391 |
| Sidechain outliers | 121581 | 10367 |

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 | 113 |  |

2 Ensemble composition and analysis

This entry contains 25 models. Model 17 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:5-A:106 (102) | 0.56 | 17 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 2 single-model clusters were found.

| Cluster number | Models |
|-----------------------|-------------------------------------|
| 1 | 1, 2, 8, 10, 12, 15, 17, 18, 19, 22 |
| 2 | 5, 13, 21, 23 |
| 3 | 4, 9, 20 |
| 4 | 7, 24, 25 |
| 5 | 3, 6, 11 |
| Single-model clusters | 14; 16 |

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1876 atoms, of which 937 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PLECKSTRIN HOMOLOGY DOMAIN.

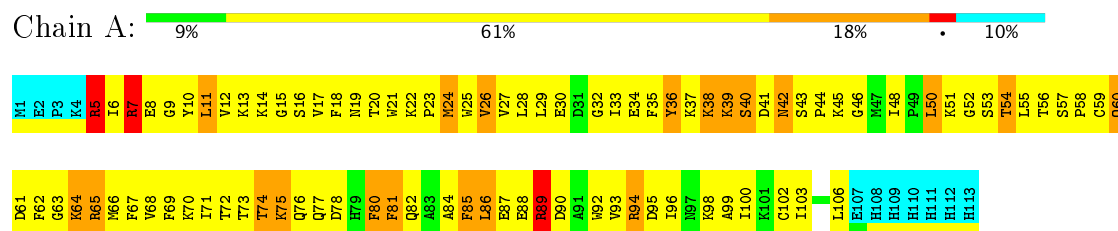
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 113 | Total | C | H | N | O | S | 0 |
| | | | 1876 | 605 | 937 | 166 | 162 | 6 | |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: PLECKSTRIN HOMOLOGY DOMAIN

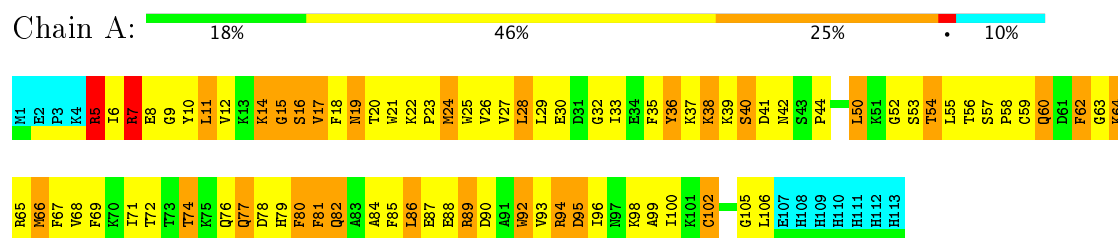


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

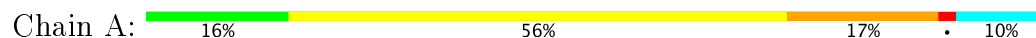
4.2.1 Score per residue for model 1

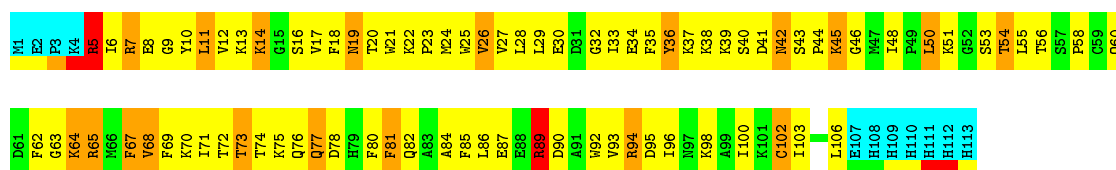
- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



4.2.2 Score per residue for model 2

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN

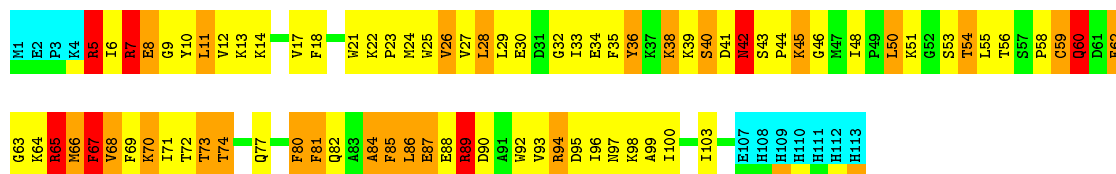




4.2.3 Score per residue for model 3

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN

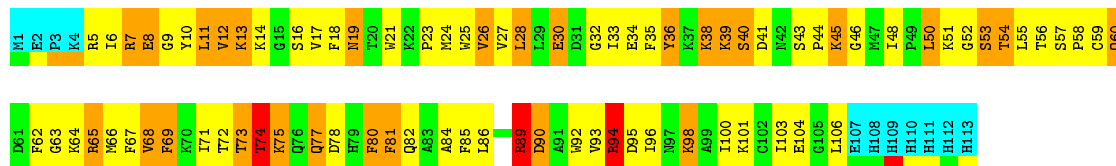
Chain A: 19% 43% 21% 6% 10%



4.2.4 Score per residue for model 4

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN

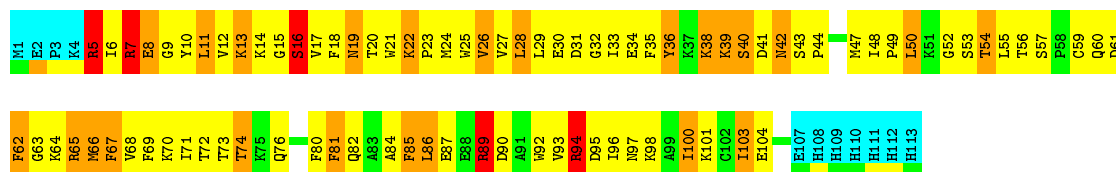
Chain A: 19% 44% 25% 10%



4.2.5 Score per residue for model 5

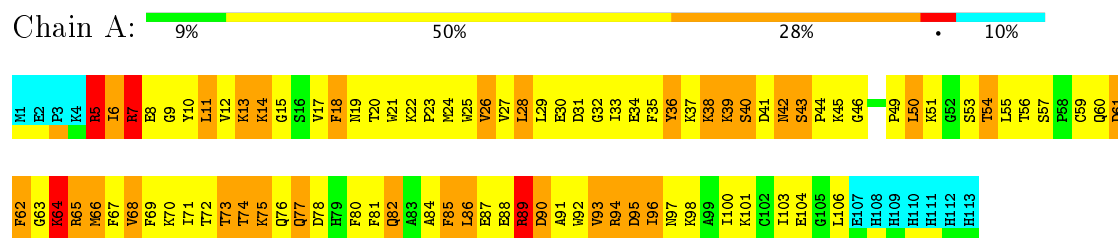
- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN

Chain A: 14% 50% 21% 10%



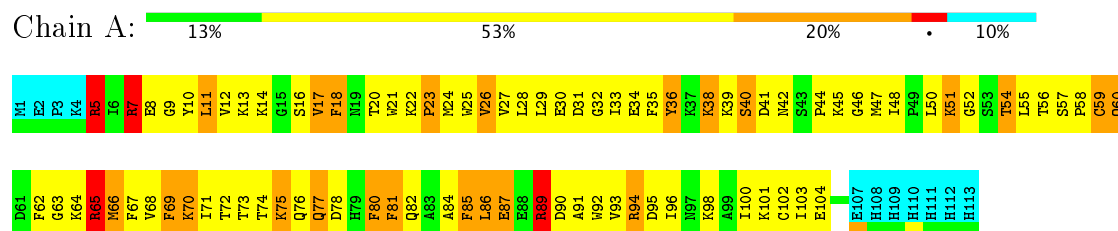
4.2.6 Score per residue for model 6

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



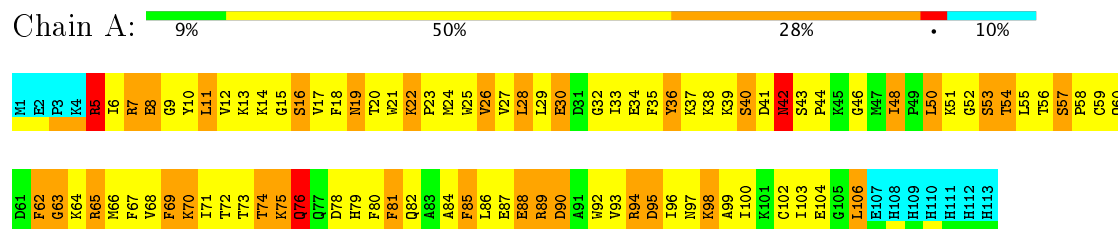
4.2.7 Score per residue for model 7

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



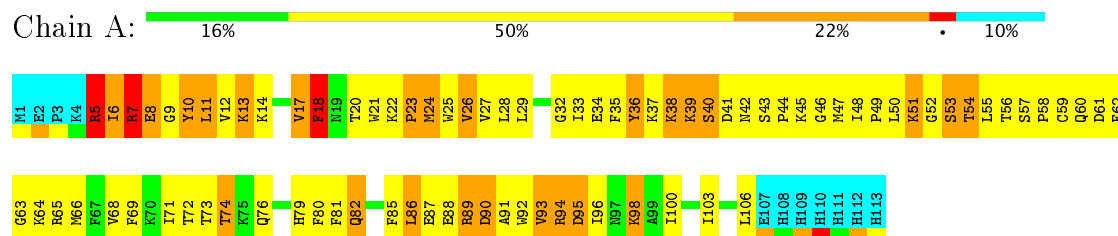
4.2.8 Score per residue for model 8

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



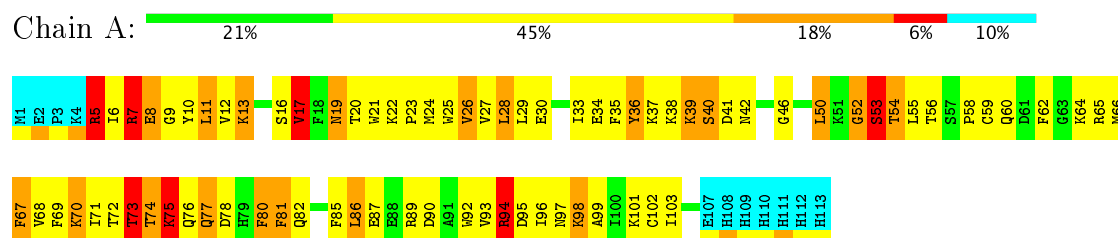
4.2.9 Score per residue for model 9

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



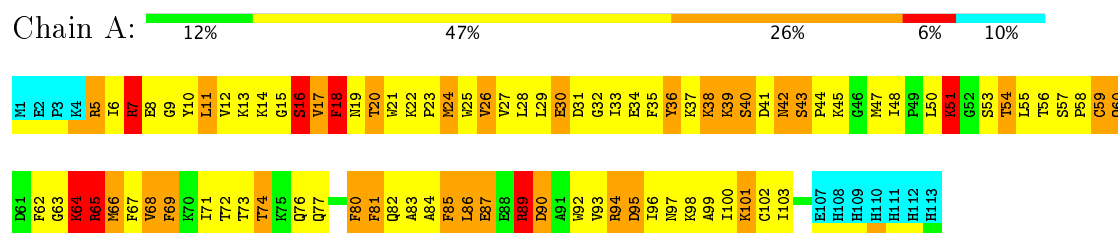
4.2.10 Score per residue for model 10

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



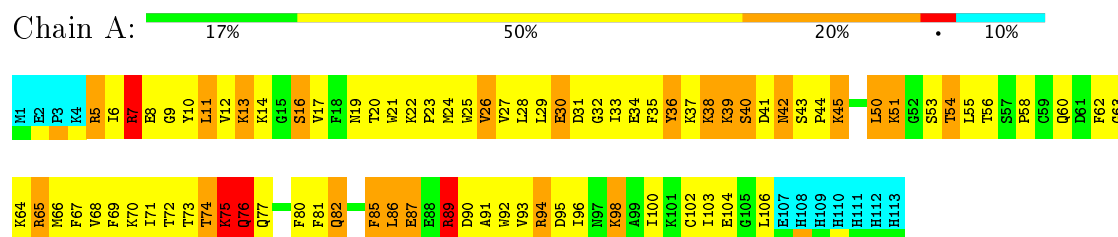
4.2.11 Score per residue for model 11

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



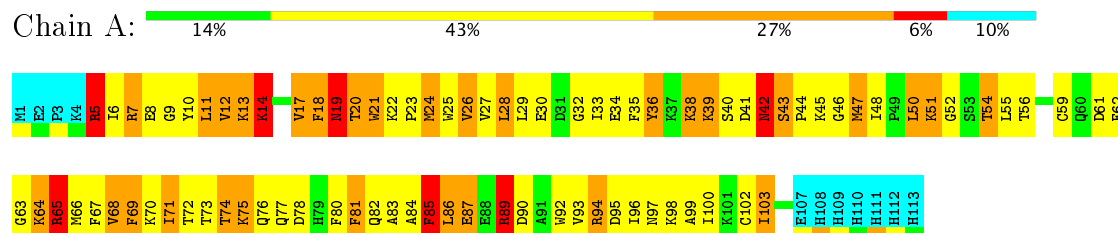
4.2.12 Score per residue for model 12

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



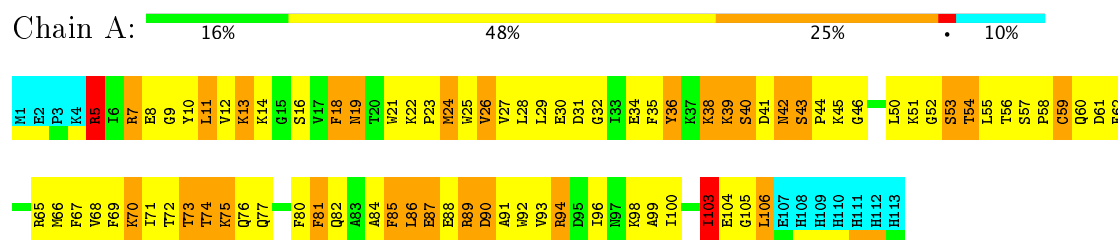
4.2.13 Score per residue for model 13

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



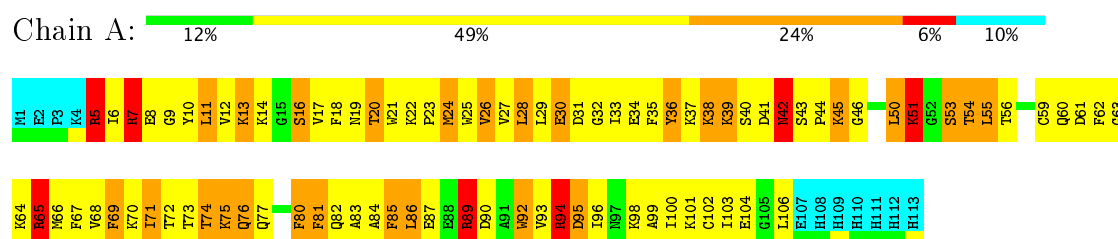
4.2.14 Score per residue for model 14

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



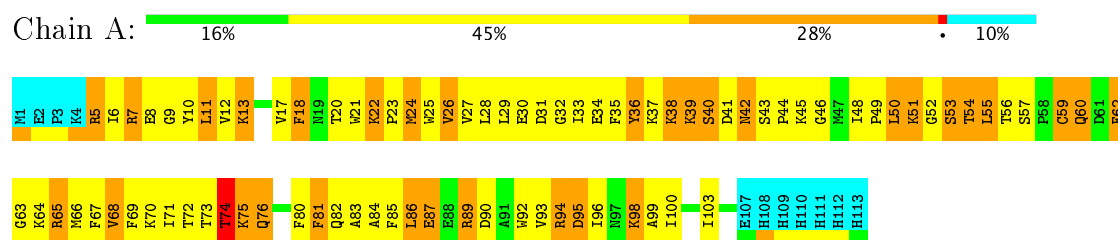
4.2.15 Score per residue for model 15

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



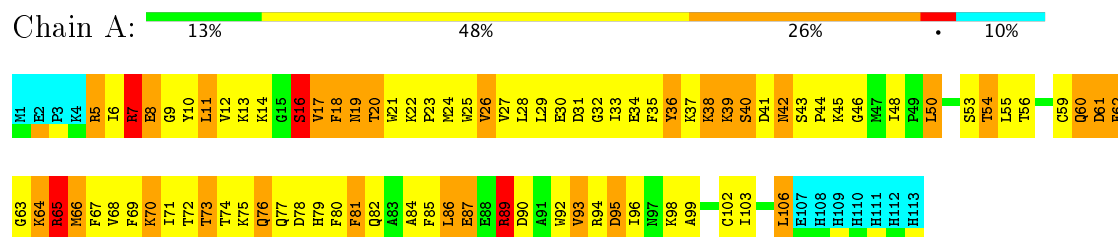
4.2.16 Score per residue for model 16

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



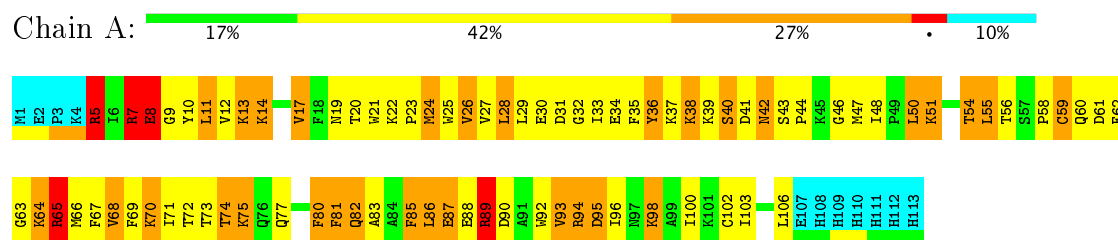
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



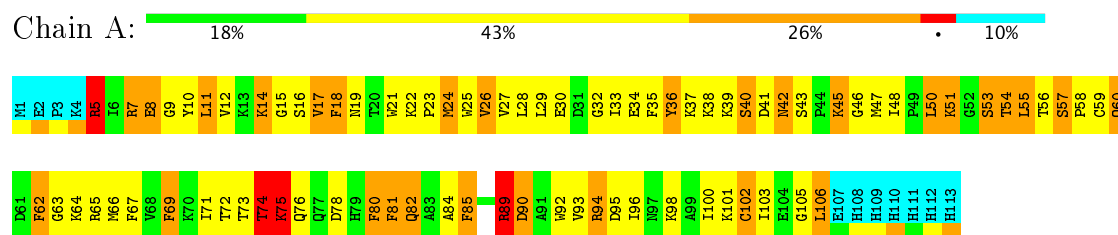
4.2.18 Score per residue for model 18

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



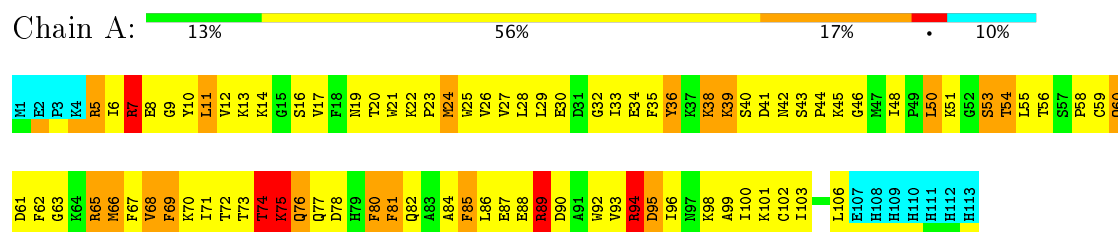
4.2.19 Score per residue for model 19

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



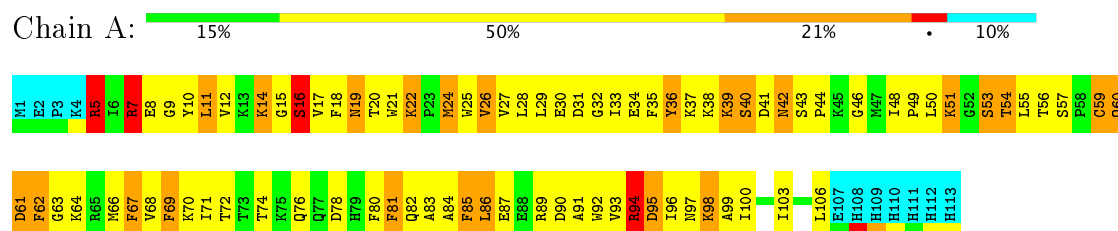
4.2.20 Score per residue for model 20

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



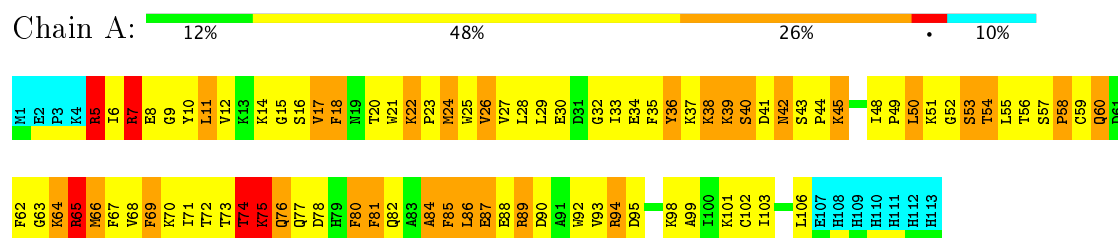
4.2.21 Score per residue for model 21

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



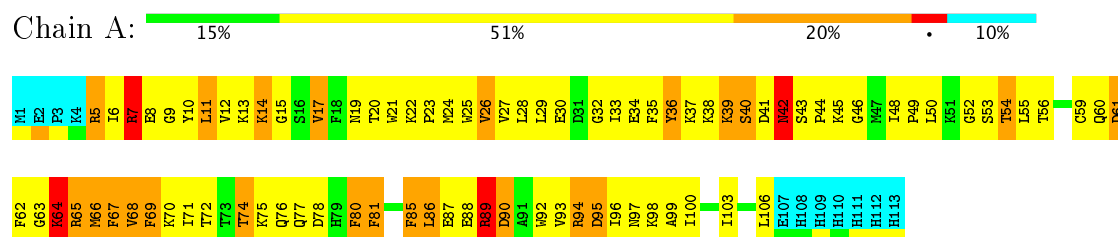
4.2.22 Score per residue for model 22

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



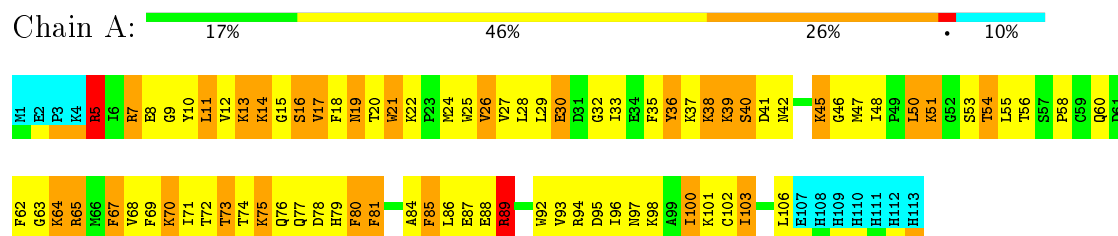
4.2.23 Score per residue for model 23

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



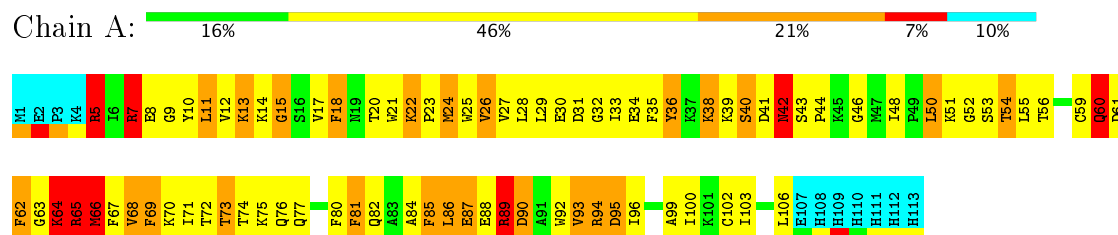
4.2.24 Score per residue for model 24

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



4.2.25 Score per residue for model 25

- Molecule 1: PLECKSTRIN HOMOLOGY DOMAIN



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 25 were deposited, based on the following criterion: ?.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| X-PLOR | refinement | |

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 ⓘ

There are no covalent bond-length or bond-angle outliers.

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 | 0.0±0.0 | 4.6±0.6 |
| All | All | 0 | 116 |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 5 | ARG | Sidechain | 24 |
| 1 | A | 94 | ARG | Sidechain | 24 |
| 1 | A | 65 | ARG | Sidechain | 23 |
| 1 | A | 89 | ARG | Sidechain | 23 |
| 1 | A | 7 | ARG | Sidechain | 22 |

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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 | 836 | 852 | 852 | 154±13 |
| All | All | 20900 | 21300 | 21300 | 3846 |

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 91.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:50:LEU:HD12 | 1:A:103:ILE:HD13 | 1.05 | 1.27 | 5 | 1 |
| 1:A:11:LEU:HD23 | 1:A:81:PHE:CE2 | 1.01 | 1.91 | 12 | 4 |
| 1:A:32:GLY:N | 1:A:50:LEU:HD11 | 0.99 | 1.71 | 6 | 3 |
| 1:A:86:LEU:HD13 | 1:A:87:GLU:N | 0.97 | 1.74 | 6 | 1 |
| 1:A:11:LEU:HD21 | 1:A:92:TRP:CZ2 | 0.97 | 1.95 | 4 | 13 |
| 1:A:50:LEU:HD21 | 1:A:99:ALA:HB1 | 0.96 | 1.36 | 11 | 2 |
| 1:A:55:LEU:HD13 | 1:A:56:THR:N | 0.96 | 1.75 | 8 | 10 |
| 1:A:50:LEU:HD12 | 1:A:103:ILE:HG21 | 0.95 | 1.34 | 19 | 1 |
| 1:A:11:LEU:HD23 | 1:A:81:PHE:CZ | 0.95 | 1.96 | 7 | 6 |
| 1:A:28:LEU:HD23 | 1:A:92:TRP:CZ3 | 0.95 | 1.97 | 19 | 15 |
| 1:A:86:LEU:HD23 | 1:A:87:GLU:N | 0.95 | 1.76 | 25 | 18 |
| 1:A:28:LEU:HD22 | 1:A:96:ILE:CG1 | 0.95 | 1.90 | 4 | 12 |
| 1:A:96:ILE:O | 1:A:100:ILE:HD12 | 0.94 | 1.62 | 4 | 14 |
| 1:A:89:ARG:O | 1:A:93:VAL:HG13 | 0.94 | 1.63 | 3 | 12 |
| 1:A:8:GLU:CB | 1:A:27:VAL:HG12 | 0.94 | 1.93 | 17 | 25 |
| 1:A:7:ARG:CB | 1:A:28:LEU:HD21 | 0.93 | 1.94 | 3 | 13 |
| 1:A:56:THR:HG22 | 1:A:58:PRO:O | 0.93 | 1.64 | 7 | 13 |
| 1:A:12:VAL:HG23 | 1:A:22:LYS:C | 0.92 | 1.85 | 2 | 23 |
| 1:A:71:ILE:HD11 | 1:A:96:ILE:HG21 | 0.92 | 1.40 | 24 | 4 |
| 1:A:8:GLU:HB3 | 1:A:27:VAL:HG12 | 0.92 | 1.41 | 25 | 25 |
| 1:A:55:LEU:HD11 | 1:A:93:VAL:CG2 | 0.91 | 1.95 | 14 | 7 |
| 1:A:10:TYR:C | 1:A:11:LEU:HD13 | 0.91 | 1.86 | 5 | 22 |
| 1:A:28:LEU:HD22 | 1:A:96:ILE:HG13 | 0.90 | 1.44 | 8 | 13 |
| 1:A:50:LEU:O | 1:A:50:LEU:HD22 | 0.90 | 1.66 | 8 | 1 |
| 1:A:10:TYR:O | 1:A:11:LEU:HD13 | 0.89 | 1.68 | 13 | 16 |
| 1:A:11:LEU:HD21 | 1:A:92:TRP:CE2 | 0.89 | 2.03 | 20 | 22 |
| 1:A:11:LEU:HD21 | 1:A:92:TRP:NE1 | 0.88 | 1.84 | 25 | 3 |
| 1:A:55:LEU:O | 1:A:55:LEU:HD13 | 0.88 | 1.69 | 19 | 4 |
| 1:A:7:ARG:HB3 | 1:A:28:LEU:HD21 | 0.88 | 1.43 | 1 | 14 |
| 1:A:32:GLY:CA | 1:A:50:LEU:HD23 | 0.87 | 1.99 | 19 | 6 |
| 1:A:30:GLU:O | 1:A:103:ILE:HD13 | 0.87 | 1.68 | 22 | 6 |
| 1:A:50:LEU:HD12 | 1:A:103:ILE:CG2 | 0.86 | 1.99 | 19 | 1 |
| 1:A:32:GLY:HA2 | 1:A:50:LEU:HD23 | 0.85 | 1.47 | 15 | 6 |
| 1:A:59:CYS:SG | 1:A:68:VAL:HG22 | 0.84 | 2.11 | 16 | 3 |
| 1:A:50:LEU:HD13 | 1:A:51:LYS:N | 0.84 | 1.86 | 8 | 1 |
| 1:A:55:LEU:HD11 | 1:A:93:VAL:HG22 | 0.84 | 1.47 | 1 | 6 |
| 1:A:68:VAL:HG23 | 1:A:81:PHE:O | 0.83 | 1.72 | 14 | 8 |
| 1:A:50:LEU:HG | 1:A:103:ILE:HG21 | 0.83 | 1.51 | 12 | 1 |
| 1:A:31:ASP:C | 1:A:50:LEU:HD11 | 0.83 | 1.94 | 18 | 3 |
| 1:A:28:LEU:HD21 | 1:A:92:TRP:CZ3 | 0.82 | 2.09 | 14 | 4 |
| 1:A:11:LEU:HD13 | 1:A:11:LEU:N | 0.82 | 1.89 | 12 | 6 |
| 1:A:59:CYS:SG | 1:A:60:GLN:N | 0.82 | 2.52 | 11 | 13 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:50:LEU:HD11 | 1:A:103:ILE:CG1 | 0.81 | 2.05 | 14 | 1 |
| 1:A:26:VAL:HG13 | 1:A:92:TRP:CH2 | 0.81 | 2.11 | 13 | 5 |
| 1:A:28:LEU:HD23 | 1:A:92:TRP:CE3 | 0.81 | 2.10 | 7 | 5 |
| 1:A:28:LEU:HA | 1:A:33:ILE:HG23 | 0.81 | 1.52 | 16 | 15 |
| 1:A:28:LEU:HD13 | 1:A:96:ILE:CG1 | 0.80 | 2.06 | 18 | 4 |
| 1:A:50:LEU:HD23 | 1:A:103:ILE:HG13 | 0.80 | 1.53 | 25 | 2 |
| 1:A:33:ILE:HG21 | 1:A:48:ILE:HD12 | 0.80 | 1.50 | 5 | 3 |
| 1:A:12:VAL:HG13 | 1:A:82:GLN:HB2 | 0.80 | 1.52 | 25 | 1 |
| 1:A:55:LEU:HD22 | 1:A:56:THR:N | 0.80 | 1.92 | 19 | 7 |
| 1:A:47:MET:SD | 1:A:47:MET:N | 0.79 | 2.56 | 13 | 1 |
| 1:A:26:VAL:HG22 | 1:A:92:TRP:CH2 | 0.79 | 2.12 | 24 | 14 |
| 1:A:28:LEU:HD13 | 1:A:96:ILE:HG13 | 0.79 | 1.52 | 9 | 4 |
| 1:A:21:TRP:CH2 | 1:A:68:VAL:HG21 | 0.79 | 2.13 | 5 | 5 |
| 1:A:11:LEU:HD22 | 1:A:26:VAL:HG11 | 0.78 | 1.56 | 6 | 4 |
| 1:A:24:MET:SD | 1:A:25:TRP:O | 0.77 | 2.43 | 11 | 12 |
| 1:A:59:CYS:SG | 1:A:68:VAL:O | 0.77 | 2.43 | 23 | 1 |
| 1:A:71:ILE:CD1 | 1:A:96:ILE:HG21 | 0.77 | 2.09 | 24 | 4 |
| 1:A:59:CYS:SG | 1:A:70:LYS:CB | 0.77 | 2.72 | 25 | 3 |
| 1:A:48:ILE:HG22 | 1:A:73:THR:HG22 | 0.77 | 1.56 | 8 | 1 |
| 1:A:28:LEU:HD21 | 1:A:92:TRP:HZ3 | 0.77 | 1.40 | 18 | 3 |
| 1:A:11:LEU:HD12 | 1:A:83:ALA:HA | 0.77 | 1.56 | 11 | 2 |
| 1:A:50:LEU:HD13 | 1:A:100:ILE:HA | 0.77 | 1.56 | 16 | 5 |
| 1:A:55:LEU:HD23 | 1:A:56:THR:N | 0.77 | 1.95 | 1 | 4 |
| 1:A:55:LEU:HD13 | 1:A:55:LEU:O | 0.77 | 1.80 | 23 | 6 |
| 1:A:50:LEU:CD1 | 1:A:103:ILE:HG21 | 0.77 | 2.10 | 19 | 1 |
| 1:A:55:LEU:HD21 | 1:A:69:PHE:CD2 | 0.75 | 2.15 | 13 | 3 |
| 1:A:32:GLY:HA2 | 1:A:50:LEU:HD13 | 0.75 | 1.56 | 11 | 6 |
| 1:A:33:ILE:HD12 | 1:A:50:LEU:HB3 | 0.75 | 1.56 | 8 | 1 |
| 1:A:32:GLY:O | 1:A:33:ILE:HD13 | 0.75 | 1.80 | 19 | 1 |
| 1:A:55:LEU:HD21 | 1:A:93:VAL:HG23 | 0.75 | 1.56 | 22 | 5 |
| 1:A:59:CYS:SG | 1:A:63:GLY:N | 0.75 | 2.59 | 9 | 2 |
| 1:A:84:ALA:HB3 | 1:A:85:PHE:CE1 | 0.75 | 2.17 | 6 | 8 |
| 1:A:6:ILE:HG22 | 1:A:95:ASP:OD2 | 0.75 | 1.81 | 17 | 2 |
| 1:A:57:SER:HB2 | 1:A:93:VAL:HG21 | 0.75 | 1.56 | 21 | 1 |
| 1:A:28:LEU:O | 1:A:28:LEU:HD12 | 0.74 | 1.81 | 7 | 4 |
| 1:A:13:LYS:HB2 | 1:A:24:MET:SD | 0.74 | 2.22 | 9 | 10 |
| 1:A:103:ILE:HG22 | 1:A:104:GLU:N | 0.74 | 1.96 | 14 | 1 |
| 1:A:28:LEU:HD13 | 1:A:96:ILE:HG12 | 0.74 | 1.60 | 18 | 3 |
| 1:A:12:VAL:HG23 | 1:A:22:LYS:N | 0.74 | 1.98 | 21 | 18 |
| 1:A:28:LEU:HB2 | 1:A:33:ILE:HD12 | 0.74 | 1.60 | 25 | 4 |
| 1:A:50:LEU:HD23 | 1:A:100:ILE:HG12 | 0.74 | 1.59 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:59:CYS:SG | 1:A:70:LYS:HD3 | 0.74 | 2.22 | 15 | 3 |
| 1:A:50:LEU:HD12 | 1:A:103:ILE:CG1 | 0.74 | 2.13 | 20 | 2 |
| 1:A:59:CYS:SG | 1:A:69:PHE:C | 0.73 | 2.66 | 16 | 1 |
| 1:A:69:PHE:CE1 | 1:A:81:PHE:CD2 | 0.73 | 2.76 | 19 | 7 |
| 1:A:51:LYS:HB3 | 1:A:74:THR:HG21 | 0.73 | 1.60 | 18 | 4 |
| 1:A:57:SER:CB | 1:A:93:VAL:HG21 | 0.73 | 2.12 | 21 | 1 |
| 1:A:11:LEU:N | 1:A:11:LEU:HD13 | 0.73 | 1.95 | 19 | 12 |
| 1:A:50:LEU:CD1 | 1:A:103:ILE:HD13 | 0.73 | 2.12 | 5 | 1 |
| 1:A:50:LEU:HD21 | 1:A:103:ILE:HG13 | 0.72 | 1.60 | 8 | 2 |
| 1:A:59:CYS:SG | 1:A:70:LYS:CD | 0.72 | 2.77 | 15 | 3 |
| 1:A:17:VAL:HG23 | 1:A:18:PHE:CD2 | 0.72 | 2.19 | 21 | 1 |
| 1:A:69:PHE:CE2 | 1:A:81:PHE:CD1 | 0.72 | 2.77 | 9 | 7 |
| 1:A:60:GLN:HB2 | 1:A:68:VAL:HG21 | 0.72 | 1.61 | 25 | 2 |
| 1:A:55:LEU:HD11 | 1:A:93:VAL:HG21 | 0.72 | 1.61 | 22 | 4 |
| 1:A:50:LEU:HD23 | 1:A:103:ILE:CG1 | 0.72 | 2.15 | 25 | 5 |
| 1:A:13:LYS:CB | 1:A:24:MET:SD | 0.72 | 2.78 | 9 | 7 |
| 1:A:50:LEU:HD11 | 1:A:103:ILE:HG13 | 0.72 | 1.62 | 14 | 1 |
| 1:A:69:PHE:CE1 | 1:A:71:ILE:HD12 | 0.71 | 2.20 | 25 | 7 |
| 1:A:48:ILE:HG23 | 1:A:73:THR:HG22 | 0.71 | 1.59 | 3 | 12 |
| 1:A:69:PHE:CE2 | 1:A:81:PHE:CE2 | 0.71 | 2.79 | 5 | 6 |
| 1:A:28:LEU:HD22 | 1:A:96:ILE:HD11 | 0.71 | 1.62 | 10 | 2 |
| 1:A:55:LEU:CD1 | 1:A:93:VAL:HG22 | 0.71 | 2.16 | 1 | 6 |
| 1:A:86:LEU:HD22 | 1:A:86:LEU:O | 0.71 | 1.85 | 6 | 1 |
| 1:A:50:LEU:HD21 | 1:A:103:ILE:CG1 | 0.71 | 2.15 | 8 | 1 |
| 1:A:7:ARG:HB2 | 1:A:28:LEU:HD11 | 0.71 | 1.62 | 1 | 12 |
| 1:A:11:LEU:HD22 | 1:A:26:VAL:CG1 | 0.71 | 2.16 | 12 | 9 |
| 1:A:5:ARG:HG2 | 1:A:29:LEU:HD21 | 0.71 | 1.63 | 25 | 2 |
| 1:A:59:CYS:SG | 1:A:70:LYS:HB2 | 0.70 | 2.26 | 20 | 5 |
| 1:A:12:VAL:HG13 | 1:A:82:GLN:CB | 0.70 | 2.15 | 25 | 2 |
| 1:A:18:PHE:CZ | 1:A:20:THR:HG22 | 0.70 | 2.21 | 21 | 1 |
| 1:A:55:LEU:C | 1:A:55:LEU:HD13 | 0.70 | 2.07 | 23 | 10 |
| 1:A:50:LEU:HD21 | 1:A:103:ILE:HG12 | 0.70 | 1.64 | 12 | 1 |
| 1:A:7:ARG:HB2 | 1:A:28:LEU:HD21 | 0.70 | 1.64 | 6 | 12 |
| 1:A:33:ILE:CG2 | 1:A:48:ILE:HD12 | 0.70 | 2.17 | 5 | 2 |
| 1:A:69:PHE:CD1 | 1:A:81:PHE:CD1 | 0.70 | 2.79 | 11 | 4 |
| 1:A:69:PHE:CE2 | 1:A:81:PHE:CG | 0.70 | 2.80 | 9 | 4 |
| 1:A:71:ILE:HD11 | 1:A:96:ILE:CG2 | 0.70 | 2.16 | 24 | 1 |
| 1:A:28:LEU:HD11 | 1:A:95:ASP:OD1 | 0.70 | 1.87 | 19 | 5 |
| 1:A:69:PHE:CE2 | 1:A:81:PHE:CE1 | 0.69 | 2.80 | 16 | 4 |
| 1:A:55:LEU:HD13 | 1:A:55:LEU:C | 0.69 | 2.08 | 5 | 11 |
| 1:A:11:LEU:CD2 | 1:A:92:TRP:CE2 | 0.69 | 2.76 | 25 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:69:PHE:CE2 | 1:A:81:PHE:CD2 | 0.69 | 2.80 | 25 | 1 |
| 1:A:32:GLY:CA | 1:A:50:LEU:HD13 | 0.69 | 2.17 | 11 | 9 |
| 1:A:50:LEU:CG | 1:A:103:ILE:HG21 | 0.69 | 2.17 | 12 | 1 |
| 1:A:28:LEU:C | 1:A:28:LEU:HD12 | 0.69 | 2.08 | 23 | 2 |
| 1:A:32:GLY:CA | 1:A:50:LEU:HD11 | 0.69 | 2.17 | 17 | 3 |
| 1:A:13:LYS:HG3 | 1:A:24:MET:SD | 0.69 | 2.27 | 6 | 4 |
| 1:A:11:LEU:HD22 | 1:A:11:LEU:N | 0.69 | 2.03 | 5 | 11 |
| 1:A:5:ARG:CG | 1:A:29:LEU:HD21 | 0.68 | 2.19 | 25 | 8 |
| 1:A:89:ARG:O | 1:A:93:VAL:HG22 | 0.68 | 1.88 | 6 | 5 |
| 1:A:56:THR:O | 1:A:59:CYS:SG | 0.68 | 2.51 | 13 | 1 |
| 1:A:21:TRP:CH2 | 1:A:68:VAL:HG23 | 0.68 | 2.23 | 17 | 7 |
| 1:A:11:LEU:HD23 | 1:A:81:PHE:HE2 | 0.68 | 1.42 | 25 | 3 |
| 1:A:50:LEU:C | 1:A:50:LEU:HD13 | 0.68 | 2.08 | 8 | 1 |
| 1:A:24:MET:HE2 | 1:A:35:PHE:CD1 | 0.68 | 2.22 | 12 | 12 |
| 1:A:69:PHE:CZ | 1:A:81:PHE:CG | 0.68 | 2.81 | 9 | 2 |
| 1:A:59:CYS:SG | 1:A:68:VAL:HG13 | 0.68 | 2.28 | 9 | 1 |
| 1:A:24:MET:SD | 1:A:35:PHE:HB2 | 0.68 | 2.28 | 14 | 10 |
| 1:A:69:PHE:CE1 | 1:A:81:PHE:CD1 | 0.68 | 2.82 | 13 | 4 |
| 1:A:81:PHE:C | 1:A:81:PHE:CD1 | 0.67 | 2.68 | 20 | 12 |
| 1:A:11:LEU:HD21 | 1:A:92:TRP:CD2 | 0.67 | 2.24 | 9 | 3 |
| 1:A:28:LEU:HD12 | 1:A:28:LEU:C | 0.67 | 2.11 | 2 | 3 |
| 1:A:50:LEU:HD12 | 1:A:103:ILE:HG13 | 0.67 | 1.66 | 15 | 2 |
| 1:A:11:LEU:CB | 1:A:81:PHE:CE1 | 0.67 | 2.78 | 10 | 12 |
| 1:A:55:LEU:C | 1:A:55:LEU:HD22 | 0.66 | 2.10 | 19 | 1 |
| 1:A:28:LEU:HD22 | 1:A:96:ILE:CD1 | 0.66 | 2.20 | 10 | 3 |
| 1:A:50:LEU:O | 1:A:103:ILE:HG21 | 0.66 | 1.91 | 3 | 5 |
| 1:A:66:MET:SD | 1:A:86:LEU:HB2 | 0.66 | 2.31 | 7 | 1 |
| 1:A:28:LEU:CA | 1:A:33:ILE:HG23 | 0.66 | 2.21 | 1 | 9 |
| 1:A:86:LEU:C | 1:A:86:LEU:HD23 | 0.66 | 2.11 | 5 | 4 |
| 1:A:81:PHE:CD1 | 1:A:81:PHE:C | 0.66 | 2.69 | 4 | 12 |
| 1:A:28:LEU:HD12 | 1:A:28:LEU:O | 0.66 | 1.89 | 2 | 7 |
| 1:A:50:LEU:HD23 | 1:A:103:ILE:HG12 | 0.66 | 1.68 | 11 | 1 |
| 1:A:11:LEU:CD2 | 1:A:81:PHE:CZ | 0.66 | 2.79 | 9 | 4 |
| 1:A:21:TRP:CH2 | 1:A:68:VAL:CG2 | 0.65 | 2.78 | 8 | 10 |
| 1:A:86:LEU:C | 1:A:86:LEU:HD22 | 0.65 | 2.11 | 6 | 1 |
| 1:A:36:TYR:N | 1:A:36:TYR:CD1 | 0.65 | 2.65 | 23 | 13 |
| 1:A:69:PHE:CE1 | 1:A:71:ILE:CD1 | 0.65 | 2.80 | 9 | 7 |
| 1:A:36:TYR:CD1 | 1:A:36:TYR:N | 0.65 | 2.64 | 21 | 12 |
| 1:A:24:MET:CE | 1:A:35:PHE:CD1 | 0.65 | 2.80 | 23 | 25 |
| 1:A:24:MET:HE1 | 1:A:35:PHE:CD1 | 0.65 | 2.26 | 18 | 12 |
| 1:A:27:VAL:O | 1:A:27:VAL:HG23 | 0.65 | 1.92 | 19 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:69:PHE:CZ | 1:A:81:PHE:CD2 | 0.65 | 2.83 | 5 | 9 |
| 1:A:55:LEU:HD21 | 1:A:93:VAL:HG12 | 0.65 | 1.68 | 25 | 1 |
| 1:A:86:LEU:HD23 | 1:A:86:LEU:C | 0.64 | 2.13 | 16 | 10 |
| 1:A:12:VAL:HG23 | 1:A:22:LYS:O | 0.64 | 1.92 | 20 | 18 |
| 1:A:68:VAL:HG23 | 1:A:81:PHE:C | 0.64 | 2.11 | 14 | 2 |
| 1:A:21:TRP:NE1 | 1:A:62:PHE:CZ | 0.64 | 2.65 | 24 | 5 |
| 1:A:86:LEU:HD13 | 1:A:86:LEU:C | 0.64 | 2.12 | 6 | 1 |
| 1:A:28:LEU:HD11 | 1:A:92:TRP:CE3 | 0.64 | 2.26 | 9 | 1 |
| 1:A:21:TRP:CZ3 | 1:A:82:GLN:CG | 0.64 | 2.81 | 25 | 1 |
| 1:A:28:LEU:HD21 | 1:A:95:ASP:HB3 | 0.64 | 1.68 | 23 | 4 |
| 1:A:17:VAL:HG13 | 1:A:17:VAL:O | 0.64 | 1.92 | 19 | 2 |
| 1:A:28:LEU:CD2 | 1:A:92:TRP:CZ3 | 0.64 | 2.80 | 4 | 11 |
| 1:A:21:TRP:CZ2 | 1:A:80:PHE:CB | 0.64 | 2.80 | 8 | 2 |
| 1:A:69:PHE:CD2 | 1:A:93:VAL:HG12 | 0.64 | 2.28 | 5 | 1 |
| 1:A:21:TRP:NE1 | 1:A:62:PHE:CE1 | 0.64 | 2.66 | 12 | 12 |
| 1:A:86:LEU:HD13 | 1:A:87:GLU:CA | 0.64 | 2.22 | 6 | 1 |
| 1:A:69:PHE:CZ | 1:A:81:PHE:CE2 | 0.64 | 2.86 | 10 | 7 |
| 1:A:55:LEU:HD21 | 1:A:69:PHE:HD2 | 0.64 | 1.52 | 13 | 3 |
| 1:A:50:LEU:C | 1:A:50:LEU:HD22 | 0.63 | 2.13 | 8 | 1 |
| 1:A:50:LEU:HD13 | 1:A:103:ILE:HG13 | 0.63 | 1.69 | 17 | 1 |
| 1:A:5:ARG:HE | 1:A:27:VAL:HG21 | 0.63 | 1.52 | 24 | 1 |
| 1:A:69:PHE:CZ | 1:A:71:ILE:HD12 | 0.63 | 2.28 | 25 | 5 |
| 1:A:24:MET:SD | 1:A:36:TYR:O | 0.63 | 2.56 | 20 | 11 |
| 1:A:11:LEU:CD2 | 1:A:92:TRP:CZ2 | 0.63 | 2.79 | 13 | 4 |
| 1:A:69:PHE:CD1 | 1:A:69:PHE:C | 0.63 | 2.72 | 25 | 9 |
| 1:A:67:PHE:N | 1:A:67:PHE:CD1 | 0.63 | 2.66 | 25 | 5 |
| 1:A:11:LEU:N | 1:A:11:LEU:HD22 | 0.63 | 2.08 | 18 | 7 |
| 1:A:70:LYS:CD | 1:A:80:PHE:CZ | 0.63 | 2.82 | 2 | 2 |
| 1:A:89:ARG:HH11 | 1:A:93:VAL:HG11 | 0.63 | 1.54 | 3 | 1 |
| 1:A:86:LEU:CD1 | 1:A:87:GLU:N | 0.63 | 2.58 | 6 | 1 |
| 1:A:62:PHE:CD2 | 1:A:80:PHE:CD1 | 0.62 | 2.86 | 21 | 2 |
| 1:A:28:LEU:HD11 | 1:A:95:ASP:HB3 | 0.62 | 1.71 | 13 | 1 |
| 1:A:7:ARG:HB3 | 1:A:28:LEU:HD11 | 0.62 | 1.70 | 8 | 3 |
| 1:A:56:THR:CG2 | 1:A:59:CYS:SG | 0.62 | 2.87 | 13 | 1 |
| 1:A:6:ILE:HD11 | 1:A:30:GLU:HG3 | 0.62 | 1.72 | 17 | 2 |
| 1:A:53:SER:HB2 | 1:A:100:ILE:HG21 | 0.62 | 1.71 | 16 | 1 |
| 1:A:35:PHE:CE1 | 1:A:46:GLY:N | 0.62 | 2.68 | 18 | 3 |
| 1:A:9:GLY:O | 1:A:25:TRP:CE3 | 0.62 | 2.53 | 18 | 25 |
| 1:A:17:VAL:O | 1:A:17:VAL:HG13 | 0.62 | 1.93 | 12 | 1 |
| 1:A:70:LYS:CD | 1:A:80:PHE:CE2 | 0.62 | 2.82 | 5 | 2 |
| 1:A:56:THR:HB | 1:A:59:CYS:SG | 0.62 | 2.35 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:59:CYS:HG | 1:A:68:VAL:HG22 | 0.62 | 1.53 | 16 | 1 |
| 1:A:85:PHE:N | 1:A:85:PHE:CD1 | 0.62 | 2.68 | 25 | 5 |
| 1:A:33:ILE:HD11 | 1:A:50:LEU:HD11 | 0.62 | 1.70 | 24 | 3 |
| 1:A:35:PHE:CE1 | 1:A:46:GLY:CA | 0.62 | 2.83 | 2 | 15 |
| 1:A:69:PHE:CD2 | 1:A:81:PHE:CE1 | 0.62 | 2.88 | 3 | 4 |
| 1:A:86:LEU:HD23 | 1:A:87:GLU:H | 0.62 | 1.51 | 25 | 3 |
| 1:A:69:PHE:C | 1:A:69:PHE:CD1 | 0.61 | 2.72 | 20 | 16 |
| 1:A:99:ALA:O | 1:A:103:ILE:HG22 | 0.61 | 1.95 | 22 | 2 |
| 1:A:73:THR:O | 1:A:73:THR:HG23 | 0.61 | 1.94 | 22 | 1 |
| 1:A:7:ARG:HB2 | 1:A:28:LEU:HD12 | 0.61 | 1.73 | 9 | 1 |
| 1:A:51:LYS:CB | 1:A:74:THR:HG21 | 0.61 | 2.25 | 11 | 3 |
| 1:A:67:PHE:CD1 | 1:A:89:ARG:CD | 0.61 | 2.83 | 6 | 1 |
| 1:A:10:TYR:CD1 | 1:A:10:TYR:N | 0.61 | 2.68 | 3 | 8 |
| 1:A:30:GLU:O | 1:A:103:ILE:HD11 | 0.60 | 1.95 | 25 | 2 |
| 1:A:30:GLU:O | 1:A:50:LEU:HD22 | 0.60 | 1.96 | 4 | 4 |
| 1:A:50:LEU:HD23 | 1:A:100:ILE:CG1 | 0.60 | 2.25 | 6 | 2 |
| 1:A:8:GLU:HB2 | 1:A:27:VAL:HG12 | 0.60 | 1.73 | 4 | 17 |
| 1:A:14:LYS:CB | 1:A:21:TRP:CD1 | 0.60 | 2.85 | 24 | 2 |
| 1:A:13:LYS:HB3 | 1:A:24:MET:SD | 0.60 | 2.36 | 17 | 2 |
| 1:A:41:ASP:O | 1:A:42:ASN:CB | 0.60 | 2.50 | 9 | 7 |
| 1:A:11:LEU:HB3 | 1:A:81:PHE:CE1 | 0.60 | 2.32 | 20 | 11 |
| 1:A:67:PHE:CE1 | 1:A:86:LEU:N | 0.60 | 2.69 | 8 | 4 |
| 1:A:6:ILE:HD12 | 1:A:6:ILE:N | 0.60 | 2.10 | 20 | 1 |
| 1:A:11:LEU:CD2 | 1:A:26:VAL:CG1 | 0.60 | 2.79 | 12 | 12 |
| 1:A:84:ALA:O | 1:A:85:PHE:CD1 | 0.60 | 2.55 | 13 | 2 |
| 1:A:30:GLU:C | 1:A:50:LEU:HD22 | 0.60 | 2.17 | 1 | 4 |
| 1:A:56:THR:HG22 | 1:A:59:CYS:SG | 0.60 | 2.37 | 13 | 2 |
| 1:A:11:LEU:H | 1:A:11:LEU:HD22 | 0.60 | 1.56 | 5 | 4 |
| 1:A:5:ARG:HG3 | 1:A:29:LEU:HD21 | 0.59 | 1.74 | 8 | 3 |
| 1:A:17:VAL:HG13 | 1:A:18:PHE:N | 0.59 | 2.11 | 15 | 3 |
| 1:A:48:ILE:CG2 | 1:A:73:THR:HG22 | 0.59 | 2.26 | 8 | 3 |
| 1:A:59:CYS:SG | 1:A:70:LYS:HB3 | 0.59 | 2.37 | 25 | 2 |
| 1:A:55:LEU:CD2 | 1:A:93:VAL:HG23 | 0.59 | 2.27 | 22 | 1 |
| 1:A:14:LYS:HB2 | 1:A:21:TRP:CD1 | 0.59 | 2.33 | 24 | 3 |
| 1:A:28:LEU:HD12 | 1:A:95:ASP:HB3 | 0.59 | 1.74 | 10 | 2 |
| 1:A:21:TRP:HH2 | 1:A:68:VAL:HG23 | 0.59 | 1.57 | 10 | 7 |
| 1:A:11:LEU:N | 1:A:11:LEU:CD1 | 0.59 | 2.66 | 20 | 4 |
| 1:A:32:GLY:HA2 | 1:A:50:LEU:HD12 | 0.59 | 1.74 | 8 | 1 |
| 1:A:10:TYR:N | 1:A:10:TYR:CD1 | 0.59 | 2.70 | 20 | 14 |
| 1:A:29:LEU:HD11 | 1:A:34:GLU:HG2 | 0.59 | 1.74 | 18 | 6 |
| 1:A:55:LEU:HD11 | 1:A:93:VAL:HB | 0.59 | 1.73 | 18 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:TRP:CD1 | 1:A:62:PHE:CZ | 0.59 | 2.91 | 24 | 4 |
| 1:A:7:ARG:CB | 1:A:28:LEU:CD2 | 0.59 | 2.80 | 20 | 15 |
| 1:A:17:VAL:HG21 | 1:A:20:THR:OG1 | 0.59 | 1.98 | 1 | 1 |
| 1:A:48:ILE:N | 1:A:48:ILE:HD13 | 0.59 | 2.13 | 9 | 1 |
| 1:A:35:PHE:CE1 | 1:A:46:GLY:O | 0.59 | 2.56 | 15 | 12 |
| 1:A:66:MET:SD | 1:A:82:GLN:NE2 | 0.59 | 2.75 | 15 | 1 |
| 1:A:84:ALA:HB3 | 1:A:85:PHE:CZ | 0.58 | 2.33 | 7 | 4 |
| 1:A:50:LEU:HD12 | 1:A:99:ALA:O | 0.58 | 1.98 | 14 | 1 |
| 1:A:69:PHE:CE2 | 1:A:93:VAL:HG13 | 0.58 | 2.32 | 18 | 1 |
| 1:A:10:TYR:CG | 1:A:10:TYR:O | 0.58 | 2.56 | 6 | 5 |
| 1:A:55:LEU:CD1 | 1:A:93:VAL:CG2 | 0.58 | 2.79 | 22 | 4 |
| 1:A:14:LYS:CB | 1:A:80:PHE:CB | 0.58 | 2.80 | 6 | 2 |
| 1:A:20:THR:O | 1:A:21:TRP:CD1 | 0.58 | 2.57 | 25 | 12 |
| 1:A:35:PHE:CZ | 1:A:46:GLY:O | 0.58 | 2.56 | 4 | 10 |
| 1:A:10:TYR:O | 1:A:10:TYR:CG | 0.58 | 2.56 | 1 | 6 |
| 1:A:25:TRP:CD1 | 1:A:39:LYS:HA | 0.58 | 2.34 | 3 | 25 |
| 1:A:6:ILE:HD11 | 1:A:30:GLU:CB | 0.58 | 2.29 | 11 | 1 |
| 1:A:11:LEU:CD2 | 1:A:81:PHE:CE2 | 0.58 | 2.80 | 6 | 2 |
| 1:A:50:LEU:HB3 | 1:A:103:ILE:HG21 | 0.58 | 1.74 | 22 | 3 |
| 1:A:74:THR:O | 1:A:75:LYS:CB | 0.58 | 2.51 | 4 | 8 |
| 1:A:60:GLN:OE1 | 1:A:62:PHE:CZ | 0.58 | 2.57 | 7 | 1 |
| 1:A:67:PHE:CD1 | 1:A:67:PHE:N | 0.58 | 2.68 | 24 | 2 |
| 1:A:67:PHE:CD1 | 1:A:84:ALA:O | 0.58 | 2.57 | 22 | 1 |
| 1:A:11:LEU:HB2 | 1:A:81:PHE:CD2 | 0.58 | 2.33 | 13 | 6 |
| 1:A:81:PHE:CD1 | 1:A:81:PHE:O | 0.58 | 2.56 | 14 | 1 |
| 1:A:65:ARG:O | 1:A:67:PHE:CE2 | 0.58 | 2.57 | 19 | 2 |
| 1:A:71:ILE:CG2 | 1:A:72:THR:N | 0.57 | 2.67 | 22 | 24 |
| 1:A:12:VAL:HG23 | 1:A:23:PRO:N | 0.57 | 2.14 | 2 | 1 |
| 1:A:24:MET:HE3 | 1:A:35:PHE:CD1 | 0.57 | 2.34 | 19 | 11 |
| 1:A:27:VAL:HG22 | 1:A:34:GLU:O | 0.57 | 1.99 | 10 | 16 |
| 1:A:51:LYS:HB2 | 1:A:74:THR:HG21 | 0.57 | 1.76 | 3 | 3 |
| 1:A:54:THR:HG22 | 1:A:72:THR:CB | 0.57 | 2.29 | 7 | 7 |
| 1:A:63:GLY:O | 1:A:68:VAL:HG11 | 0.57 | 1.99 | 22 | 4 |
| 1:A:62:PHE:CD1 | 1:A:62:PHE:O | 0.57 | 2.57 | 12 | 1 |
| 1:A:84:ALA:HB1 | 1:A:85:PHE:CE1 | 0.57 | 2.34 | 5 | 1 |
| 1:A:17:VAL:O | 1:A:18:PHE:CD2 | 0.57 | 2.58 | 16 | 3 |
| 1:A:28:LEU:N | 1:A:28:LEU:HD23 | 0.57 | 2.14 | 10 | 2 |
| 1:A:50:LEU:HD23 | 1:A:51:LYS:N | 0.57 | 2.14 | 12 | 1 |
| 1:A:7:ARG:CB | 1:A:28:LEU:HD11 | 0.57 | 2.29 | 13 | 1 |
| 1:A:50:LEU:HD21 | 1:A:99:ALA:CB | 0.57 | 2.23 | 11 | 2 |
| 1:A:10:TYR:O | 1:A:10:TYR:CD2 | 0.57 | 2.57 | 4 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:36:TYR:CD2 | 1:A:40:SER:O | 0.57 | 2.57 | 16 | 8 |
| 1:A:12:VAL:CG1 | 1:A:82:GLN:CG | 0.57 | 2.81 | 8 | 1 |
| 1:A:50:LEU:HD22 | 1:A:103:ILE:HD12 | 0.57 | 1.74 | 9 | 1 |
| 1:A:78:ASP:OD1 | 1:A:80:PHE:CZ | 0.57 | 2.57 | 13 | 2 |
| 1:A:50:LEU:HD11 | 1:A:99:ALA:C | 0.57 | 2.19 | 20 | 3 |
| 1:A:12:VAL:CG1 | 1:A:82:GLN:CB | 0.57 | 2.82 | 25 | 1 |
| 1:A:11:LEU:HD22 | 1:A:11:LEU:H | 0.57 | 1.60 | 14 | 3 |
| 1:A:84:ALA:O | 1:A:85:PHE:CD2 | 0.57 | 2.57 | 14 | 1 |
| 1:A:62:PHE:O | 1:A:62:PHE:CD1 | 0.57 | 2.57 | 22 | 1 |
| 1:A:33:ILE:HD12 | 1:A:50:LEU:CD2 | 0.57 | 2.29 | 15 | 1 |
| 1:A:50:LEU:HD22 | 1:A:103:ILE:HG21 | 0.57 | 1.76 | 18 | 1 |
| 1:A:27:VAL:HG23 | 1:A:27:VAL:O | 0.57 | 2.00 | 24 | 3 |
| 1:A:6:ILE:HD11 | 1:A:30:GLU:HB3 | 0.57 | 1.77 | 13 | 4 |
| 1:A:67:PHE:CD1 | 1:A:89:ARG:HD2 | 0.57 | 2.35 | 6 | 1 |
| 1:A:28:LEU:HD22 | 1:A:96:ILE:HG12 | 0.57 | 1.74 | 4 | 4 |
| 1:A:85:PHE:CZ | 1:A:88:GLU:OE1 | 0.57 | 2.57 | 6 | 1 |
| 1:A:59:CYS:SG | 1:A:69:PHE:CA | 0.57 | 2.93 | 16 | 1 |
| 1:A:28:LEU:HD23 | 1:A:92:TRP:CH2 | 0.56 | 2.35 | 19 | 3 |
| 1:A:21:TRP:HH2 | 1:A:68:VAL:HG21 | 0.56 | 1.57 | 5 | 1 |
| 1:A:6:ILE:CD1 | 1:A:6:ILE:N | 0.56 | 2.68 | 20 | 1 |
| 1:A:77:GLN:O | 1:A:79:HIS:CD2 | 0.56 | 2.57 | 24 | 1 |
| 1:A:90:ASP:HA | 1:A:93:VAL:HG22 | 0.56 | 1.75 | 7 | 10 |
| 1:A:69:PHE:CD2 | 1:A:81:PHE:CD2 | 0.56 | 2.93 | 25 | 1 |
| 1:A:66:MET:O | 1:A:67:PHE:CB | 0.56 | 2.53 | 25 | 5 |
| 1:A:21:TRP:CZ2 | 1:A:62:PHE:CB | 0.56 | 2.88 | 7 | 1 |
| 1:A:60:GLN:HG3 | 1:A:62:PHE:CE2 | 0.56 | 2.36 | 16 | 1 |
| 1:A:11:LEU:HG | 1:A:81:PHE:CE2 | 0.56 | 2.35 | 11 | 8 |
| 1:A:66:MET:O | 1:A:67:PHE:CD2 | 0.56 | 2.59 | 8 | 2 |
| 1:A:33:ILE:N | 1:A:33:ILE:HD12 | 0.56 | 2.15 | 12 | 1 |
| 1:A:32:GLY:N | 1:A:50:LEU:HD23 | 0.56 | 2.15 | 13 | 2 |
| 1:A:103:ILE:CG2 | 1:A:104:GLU:N | 0.56 | 2.67 | 14 | 1 |
| 1:A:11:LEU:HD21 | 1:A:92:TRP:CH2 | 0.56 | 2.36 | 10 | 2 |
| 1:A:11:LEU:CD2 | 1:A:26:VAL:HG11 | 0.56 | 2.29 | 12 | 7 |
| 1:A:11:LEU:HB3 | 1:A:81:PHE:CD1 | 0.56 | 2.36 | 21 | 6 |
| 1:A:64:LYS:O | 1:A:64:LYS:CG | 0.56 | 2.54 | 21 | 5 |
| 1:A:26:VAL:CB | 1:A:35:PHE:HB3 | 0.56 | 2.31 | 8 | 24 |
| 1:A:63:GLY:HA2 | 1:A:68:VAL:HG13 | 0.56 | 1.76 | 20 | 3 |
| 1:A:60:GLN:O | 1:A:61:ASP:CB | 0.56 | 2.54 | 5 | 5 |
| 1:A:84:ALA:CB | 1:A:85:PHE:CE1 | 0.56 | 2.89 | 6 | 3 |
| 1:A:21:TRP:CZ2 | 1:A:80:PHE:HB3 | 0.56 | 2.35 | 24 | 2 |
| 1:A:17:VAL:HG22 | 1:A:18:PHE:N | 0.56 | 2.16 | 24 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:TRP:CZ2 | 1:A:80:PHE:HB2 | 0.56 | 2.35 | 8 | 4 |
| 1:A:62:PHE:CD1 | 1:A:62:PHE:N | 0.56 | 2.69 | 16 | 1 |
| 1:A:74:THR:O | 1:A:74:THR:OG1 | 0.55 | 2.24 | 10 | 1 |
| 1:A:10:TYR:CD2 | 1:A:10:TYR:O | 0.55 | 2.60 | 19 | 9 |
| 1:A:48:ILE:HG22 | 1:A:73:THR:CG2 | 0.55 | 2.29 | 8 | 1 |
| 1:A:11:LEU:HD22 | 1:A:26:VAL:HG13 | 0.55 | 1.78 | 20 | 1 |
| 1:A:11:LEU:CB | 1:A:81:PHE:CD1 | 0.55 | 2.90 | 19 | 8 |
| 1:A:5:ARG:CG | 1:A:29:LEU:CD2 | 0.55 | 2.84 | 25 | 7 |
| 1:A:6:ILE:HD11 | 1:A:30:GLU:CG | 0.55 | 2.31 | 8 | 2 |
| 1:A:35:PHE:CD1 | 1:A:35:PHE:O | 0.55 | 2.59 | 18 | 9 |
| 1:A:29:LEU:HD12 | 1:A:32:GLY:O | 0.55 | 2.02 | 7 | 6 |
| 1:A:69:PHE:CD2 | 1:A:81:PHE:CD1 | 0.55 | 2.95 | 24 | 2 |
| 1:A:66:MET:SD | 1:A:86:LEU:HD12 | 0.55 | 2.41 | 7 | 1 |
| 1:A:36:TYR:CG | 1:A:40:SER:O | 0.55 | 2.59 | 20 | 3 |
| 1:A:12:VAL:CG2 | 1:A:22:LYS:N | 0.55 | 2.69 | 8 | 12 |
| 1:A:41:ASP:O | 1:A:43:SER:N | 0.55 | 2.40 | 25 | 18 |
| 1:A:69:PHE:CE1 | 1:A:71:ILE:CG1 | 0.55 | 2.89 | 25 | 5 |
| 1:A:29:LEU:HD12 | 1:A:29:LEU:H | 0.55 | 1.60 | 5 | 1 |
| 1:A:32:GLY:N | 1:A:50:LEU:HD13 | 0.55 | 2.17 | 4 | 2 |
| 1:A:17:VAL:O | 1:A:18:PHE:CG | 0.55 | 2.60 | 8 | 2 |
| 1:A:14:LYS:CB | 1:A:20:THR:O | 0.55 | 2.55 | 21 | 1 |
| 1:A:11:LEU:HG | 1:A:81:PHE:CE1 | 0.55 | 2.37 | 7 | 11 |
| 1:A:50:LEU:HD21 | 1:A:99:ALA:C | 0.55 | 2.21 | 3 | 2 |
| 1:A:66:MET:C | 1:A:67:PHE:CG | 0.55 | 2.78 | 8 | 4 |
| 1:A:36:TYR:CD1 | 1:A:44:PRO:HA | 0.55 | 2.37 | 25 | 4 |
| 1:A:11:LEU:HD23 | 1:A:81:PHE:CE1 | 0.55 | 2.36 | 7 | 1 |
| 1:A:21:TRP:CZ2 | 1:A:62:PHE:HB3 | 0.55 | 2.36 | 7 | 1 |
| 1:A:78:ASP:HB2 | 1:A:80:PHE:CZ | 0.55 | 2.37 | 8 | 3 |
| 1:A:25:TRP:CB | 1:A:38:LYS:O | 0.55 | 2.55 | 25 | 15 |
| 1:A:67:PHE:CD1 | 1:A:86:LEU:N | 0.55 | 2.75 | 8 | 3 |
| 1:A:5:ARG:HD3 | 1:A:27:VAL:HG11 | 0.55 | 1.79 | 22 | 2 |
| 1:A:28:LEU:CD1 | 1:A:28:LEU:O | 0.55 | 2.54 | 24 | 3 |
| 1:A:28:LEU:O | 1:A:28:LEU:CD1 | 0.55 | 2.55 | 2 | 4 |
| 1:A:7:ARG:HB3 | 1:A:28:LEU:CD2 | 0.55 | 2.32 | 12 | 14 |
| 1:A:21:TRP:CH2 | 1:A:80:PHE:O | 0.55 | 2.60 | 16 | 1 |
| 1:A:21:TRP:CZ3 | 1:A:82:GLN:HG2 | 0.55 | 2.37 | 25 | 1 |
| 1:A:11:LEU:HD23 | 1:A:26:VAL:HG11 | 0.54 | 1.79 | 18 | 8 |
| 1:A:28:LEU:HD11 | 1:A:92:TRP:HE3 | 0.54 | 1.61 | 9 | 1 |
| 1:A:54:THR:O | 1:A:71:ILE:HG23 | 0.54 | 2.02 | 16 | 9 |
| 1:A:85:PHE:CD1 | 1:A:85:PHE:N | 0.54 | 2.75 | 8 | 6 |
| 1:A:30:GLU:O | 1:A:103:ILE:CD1 | 0.54 | 2.56 | 5 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:30:GLU:O | 1:A:103:ILE:CG1 | 0.54 | 2.55 | 18 | 5 |
| 1:A:6:ILE:HG21 | 1:A:95:ASP:OD1 | 0.54 | 2.01 | 9 | 2 |
| 1:A:86:LEU:O | 1:A:90:ASP:CB | 0.54 | 2.55 | 12 | 1 |
| 1:A:35:PHE:CZ | 1:A:46:GLY:C | 0.54 | 2.81 | 17 | 11 |
| 1:A:84:ALA:C | 1:A:85:PHE:CG | 0.54 | 2.81 | 7 | 7 |
| 1:A:32:GLY:N | 1:A:50:LEU:HD22 | 0.54 | 2.17 | 14 | 2 |
| 1:A:90:ASP:O | 1:A:94:ARG:CG | 0.54 | 2.56 | 18 | 8 |
| 1:A:62:PHE:CD1 | 1:A:62:PHE:C | 0.54 | 2.79 | 8 | 6 |
| 1:A:59:CYS:O | 1:A:60:GLN:CB | 0.54 | 2.56 | 17 | 1 |
| 1:A:28:LEU:CB | 1:A:33:ILE:HG23 | 0.54 | 2.33 | 25 | 2 |
| 1:A:94:ARG:O | 1:A:98:LYS:CB | 0.54 | 2.56 | 22 | 14 |
| 1:A:11:LEU:HB2 | 1:A:26:VAL:HG11 | 0.54 | 1.78 | 9 | 1 |
| 1:A:84:ALA:C | 1:A:85:PHE:CD1 | 0.54 | 2.80 | 19 | 5 |
| 1:A:6:ILE:HB | 1:A:28:LEU:HD12 | 0.54 | 1.79 | 15 | 3 |
| 1:A:74:THR:OG1 | 1:A:74:THR:O | 0.54 | 2.25 | 4 | 4 |
| 1:A:26:VAL:CG1 | 1:A:92:TRP:CH2 | 0.54 | 2.89 | 13 | 1 |
| 1:A:30:GLU:HA | 1:A:99:ALA:HB1 | 0.54 | 1.80 | 21 | 2 |
| 1:A:80:PHE:N | 1:A:80:PHE:CD1 | 0.54 | 2.75 | 11 | 7 |
| 1:A:50:LEU:HD13 | 1:A:100:ILE:CA | 0.54 | 2.32 | 16 | 2 |
| 1:A:26:VAL:HG22 | 1:A:92:TRP:CZ3 | 0.54 | 2.37 | 9 | 3 |
| 1:A:55:LEU:CD2 | 1:A:69:PHE:CD2 | 0.54 | 2.91 | 8 | 2 |
| 1:A:66:MET:C | 1:A:67:PHE:CD1 | 0.54 | 2.81 | 10 | 2 |
| 1:A:63:GLY:O | 1:A:68:VAL:CG1 | 0.54 | 2.56 | 17 | 2 |
| 1:A:73:THR:O | 1:A:73:THR:CG2 | 0.54 | 2.56 | 22 | 1 |
| 1:A:45:LYS:CD | 1:A:45:LYS:O | 0.54 | 2.56 | 6 | 1 |
| 1:A:65:ARG:O | 1:A:67:PHE:CD2 | 0.54 | 2.61 | 19 | 1 |
| 1:A:49:PRO:CD | 1:A:73:THR:OG1 | 0.54 | 2.56 | 22 | 1 |
| 1:A:13:LYS:CG | 1:A:80:PHE:O | 0.54 | 2.56 | 24 | 1 |
| 1:A:6:ILE:CG2 | 1:A:95:ASP:OD1 | 0.53 | 2.56 | 9 | 6 |
| 1:A:27:VAL:CG2 | 1:A:34:GLU:O | 0.53 | 2.56 | 5 | 21 |
| 1:A:78:ASP:O | 1:A:80:PHE:CE1 | 0.53 | 2.61 | 8 | 1 |
| 1:A:75:LYS:O | 1:A:76:GLN:CB | 0.53 | 2.56 | 24 | 5 |
| 1:A:11:LEU:CG | 1:A:81:PHE:CE1 | 0.53 | 2.91 | 7 | 11 |
| 1:A:66:MET:O | 1:A:67:PHE:CG | 0.53 | 2.61 | 8 | 4 |
| 1:A:14:LYS:HB3 | 1:A:80:PHE:CB | 0.53 | 2.33 | 9 | 2 |
| 1:A:14:LYS:CD | 1:A:62:PHE:CE2 | 0.53 | 2.91 | 7 | 1 |
| 1:A:96:ILE:O | 1:A:100:ILE:HD13 | 0.53 | 2.03 | 11 | 1 |
| 1:A:68:VAL:CG2 | 1:A:81:PHE:O | 0.53 | 2.56 | 25 | 3 |
| 1:A:30:GLU:O | 1:A:50:LEU:CD2 | 0.53 | 2.57 | 2 | 5 |
| 1:A:50:LEU:CD2 | 1:A:103:ILE:CG1 | 0.53 | 2.86 | 3 | 2 |
| 1:A:6:ILE:HD11 | 1:A:30:GLU:HB2 | 0.53 | 1.81 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:6:ILE:HB | 1:A:28:LEU:HD11 | 0.53 | 1.81 | 23 | 2 |
| 1:A:67:PHE:O | 1:A:82:GLN:CG | 0.53 | 2.57 | 1 | 4 |
| 1:A:55:LEU:HD21 | 1:A:93:VAL:HG21 | 0.53 | 1.81 | 1 | 2 |
| 1:A:35:PHE:CE1 | 1:A:46:GLY:HA3 | 0.53 | 2.38 | 23 | 11 |
| 1:A:55:LEU:HD21 | 1:A:69:PHE:CG | 0.53 | 2.39 | 9 | 3 |
| 1:A:21:TRP:CZ2 | 1:A:60:GLN:NE2 | 0.53 | 2.77 | 25 | 1 |
| 1:A:73:THR:O | 1:A:75:LYS:N | 0.53 | 2.41 | 20 | 10 |
| 1:A:78:ASP:CG | 1:A:80:PHE:CZ | 0.53 | 2.82 | 10 | 3 |
| 1:A:73:THR:OG1 | 1:A:77:GLN:CG | 0.53 | 2.56 | 24 | 1 |
| 1:A:68:VAL:CB | 1:A:81:PHE:O | 0.53 | 2.56 | 25 | 1 |
| 1:A:78:ASP:HB3 | 1:A:80:PHE:CZ | 0.53 | 2.39 | 1 | 2 |
| 1:A:89:ARG:NH1 | 1:A:93:VAL:HG11 | 0.53 | 2.18 | 2 | 2 |
| 1:A:32:GLY:C | 1:A:50:LEU:HD23 | 0.53 | 2.23 | 5 | 1 |
| 1:A:84:ALA:O | 1:A:85:PHE:CB | 0.53 | 2.57 | 13 | 2 |
| 1:A:62:PHE:C | 1:A:62:PHE:CD1 | 0.53 | 2.77 | 3 | 4 |
| 1:A:28:LEU:CD2 | 1:A:96:ILE:HD11 | 0.53 | 2.32 | 10 | 1 |
| 1:A:96:ILE:O | 1:A:100:ILE:CD1 | 0.53 | 2.57 | 12 | 3 |
| 1:A:35:PHE:C | 1:A:36:TYR:CD1 | 0.53 | 2.82 | 16 | 4 |
| 1:A:28:LEU:HD23 | 1:A:28:LEU:N | 0.53 | 2.17 | 14 | 1 |
| 1:A:60:GLN:CG | 1:A:62:PHE:CD2 | 0.53 | 2.92 | 16 | 1 |
| 1:A:69:PHE:CE1 | 1:A:71:ILE:HG13 | 0.53 | 2.39 | 24 | 11 |
| 1:A:65:ARG:O | 1:A:66:MET:CB | 0.53 | 2.57 | 5 | 1 |
| 1:A:29:LEU:CD1 | 1:A:32:GLY:O | 0.53 | 2.57 | 7 | 6 |
| 1:A:7:ARG:CG | 1:A:95:ASP:OD2 | 0.53 | 2.57 | 9 | 2 |
| 1:A:70:LYS:CG | 1:A:78:ASP:OD1 | 0.53 | 2.57 | 13 | 2 |
| 1:A:70:LYS:CG | 1:A:78:ASP:OD2 | 0.53 | 2.57 | 13 | 1 |
| 1:A:63:GLY:O | 1:A:64:LYS:CG | 0.53 | 2.57 | 16 | 2 |
| 1:A:67:PHE:CE1 | 1:A:86:LEU:HA | 0.53 | 2.39 | 17 | 1 |
| 1:A:28:LEU:CB | 1:A:96:ILE:CG1 | 0.53 | 2.87 | 5 | 1 |
| 1:A:50:LEU:CB | 1:A:103:ILE:HG21 | 0.53 | 2.34 | 6 | 3 |
| 1:A:17:VAL:CG2 | 1:A:20:THR:OG1 | 0.52 | 2.56 | 1 | 1 |
| 1:A:78:ASP:CB | 1:A:80:PHE:CZ | 0.52 | 2.92 | 23 | 3 |
| 1:A:56:THR:CB | 1:A:59:CYS:SG | 0.52 | 2.96 | 13 | 1 |
| 1:A:6:ILE:HD12 | 1:A:99:ALA:HB2 | 0.52 | 1.80 | 15 | 1 |
| 1:A:50:LEU:CD1 | 1:A:99:ALA:O | 0.52 | 2.57 | 15 | 2 |
| 1:A:45:LYS:O | 1:A:45:LYS:CE | 0.52 | 2.57 | 22 | 1 |
| 1:A:52:GLY:O | 1:A:74:THR:N | 0.52 | 2.42 | 5 | 4 |
| 1:A:26:VAL:HG23 | 1:A:35:PHE:HB3 | 0.52 | 1.82 | 20 | 19 |
| 1:A:63:GLY:O | 1:A:65:ARG:N | 0.52 | 2.43 | 11 | 10 |
| 1:A:21:TRP:CH2 | 1:A:80:PHE:CB | 0.52 | 2.93 | 3 | 4 |
| 1:A:11:LEU:HB2 | 1:A:81:PHE:CD1 | 0.52 | 2.40 | 19 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:72:THR:HG22 | 1:A:72:THR:O | 0.52 | 2.04 | 25 | 5 |
| 1:A:14:LYS:HG2 | 1:A:21:TRP:CD1 | 0.52 | 2.39 | 6 | 2 |
| 1:A:69:PHE:CD1 | 1:A:69:PHE:O | 0.52 | 2.63 | 19 | 4 |
| 1:A:90:ASP:O | 1:A:93:VAL:HG22 | 0.52 | 2.05 | 13 | 2 |
| 1:A:17:VAL:HG23 | 1:A:18:PHE:N | 0.52 | 2.18 | 1 | 2 |
| 1:A:93:VAL:O | 1:A:97:ASN:CB | 0.52 | 2.57 | 8 | 4 |
| 1:A:62:PHE:O | 1:A:68:VAL:CG1 | 0.52 | 2.57 | 4 | 3 |
| 1:A:55:LEU:O | 1:A:55:LEU:CD1 | 0.52 | 2.56 | 6 | 3 |
| 1:A:69:PHE:CZ | 1:A:81:PHE:CB | 0.52 | 2.93 | 9 | 2 |
| 1:A:33:ILE:CD1 | 1:A:50:LEU:HD11 | 0.52 | 2.34 | 24 | 3 |
| 1:A:28:LEU:CG | 1:A:28:LEU:O | 0.52 | 2.57 | 20 | 5 |
| 1:A:64:LYS:O | 1:A:65:ARG:CG | 0.52 | 2.57 | 18 | 2 |
| 1:A:14:LYS:HD3 | 1:A:21:TRP:CD1 | 0.52 | 2.39 | 24 | 1 |
| 1:A:15:GLY:O | 1:A:16:SER:CB | 0.52 | 2.56 | 1 | 5 |
| 1:A:67:PHE:CD1 | 1:A:85:PHE:C | 0.52 | 2.83 | 8 | 1 |
| 1:A:45:LYS:O | 1:A:45:LYS:CD | 0.52 | 2.58 | 19 | 4 |
| 1:A:49:PRO:CG | 1:A:73:THR:OG1 | 0.52 | 2.57 | 16 | 2 |
| 1:A:52:GLY:O | 1:A:74:THR:CA | 0.52 | 2.58 | 5 | 3 |
| 1:A:28:LEU:HB3 | 1:A:96:ILE:CG1 | 0.52 | 2.35 | 5 | 1 |
| 1:A:86:LEU:HD23 | 1:A:87:GLU:CA | 0.52 | 2.35 | 11 | 12 |
| 1:A:55:LEU:HD21 | 1:A:69:PHE:CE2 | 0.52 | 2.40 | 8 | 2 |
| 1:A:54:THR:HG22 | 1:A:72:THR:N | 0.52 | 2.19 | 14 | 13 |
| 1:A:18:PHE:O | 1:A:20:THR:N | 0.52 | 2.42 | 5 | 4 |
| 1:A:11:LEU:HG | 1:A:81:PHE:CZ | 0.52 | 2.40 | 12 | 2 |
| 1:A:53:SER:OG | 1:A:71:ILE:CG2 | 0.52 | 2.58 | 8 | 1 |
| 1:A:72:THR:O | 1:A:74:THR:N | 0.52 | 2.43 | 10 | 1 |
| 1:A:11:LEU:CB | 1:A:81:PHE:CD2 | 0.52 | 2.93 | 11 | 2 |
| 1:A:28:LEU:CD1 | 1:A:96:ILE:CG1 | 0.52 | 2.87 | 14 | 2 |
| 1:A:60:GLN:CB | 1:A:68:VAL:HG11 | 0.52 | 2.35 | 25 | 1 |
| 1:A:34:GLU:OE2 | 1:A:35:PHE:N | 0.51 | 2.43 | 14 | 1 |
| 1:A:6:ILE:HG22 | 1:A:95:ASP:OD1 | 0.51 | 2.04 | 8 | 3 |
| 1:A:50:LEU:O | 1:A:100:ILE:CG1 | 0.51 | 2.58 | 8 | 1 |
| 1:A:55:LEU:C | 1:A:55:LEU:CD2 | 0.51 | 2.79 | 16 | 1 |
| 1:A:14:LYS:CE | 1:A:62:PHE:CE2 | 0.51 | 2.93 | 18 | 1 |
| 1:A:50:LEU:HD22 | 1:A:103:ILE:HG13 | 0.51 | 1.82 | 21 | 1 |
| 1:A:54:THR:CG2 | 1:A:72:THR:HB | 0.51 | 2.36 | 7 | 14 |
| 1:A:28:LEU:CB | 1:A:96:ILE:HG12 | 0.51 | 2.35 | 5 | 9 |
| 1:A:62:PHE:CD2 | 1:A:80:PHE:CG | 0.51 | 2.98 | 21 | 2 |
| 1:A:50:LEU:HD23 | 1:A:103:ILE:HB | 0.51 | 1.82 | 23 | 3 |
| 1:A:50:LEU:CB | 1:A:103:ILE:HD12 | 0.51 | 2.34 | 24 | 1 |
| 1:A:13:LYS:CG | 1:A:24:MET:SD | 0.51 | 2.98 | 6 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:TRP:CH2 | 1:A:80:PHE:HB3 | 0.51 | 2.40 | 9 | 6 |
| 1:A:71:ILE:HG22 | 1:A:72:THR:N | 0.51 | 2.20 | 21 | 7 |
| 1:A:14:LYS:CB | 1:A:80:PHE:HB2 | 0.51 | 2.36 | 6 | 2 |
| 1:A:12:VAL:HG23 | 1:A:22:LYS:CA | 0.51 | 2.35 | 23 | 9 |
| 1:A:7:ARG:CB | 1:A:28:LEU:HD12 | 0.51 | 2.36 | 9 | 1 |
| 1:A:53:SER:OG | 1:A:54:THR:N | 0.51 | 2.43 | 20 | 2 |
| 1:A:36:TYR:CD2 | 1:A:44:PRO:HA | 0.51 | 2.40 | 23 | 18 |
| 1:A:73:THR:C | 1:A:74:THR:CG2 | 0.51 | 2.79 | 22 | 5 |
| 1:A:33:ILE:HD12 | 1:A:50:LEU:CB | 0.51 | 2.31 | 8 | 1 |
| 1:A:55:LEU:CD2 | 1:A:69:PHE:CE2 | 0.51 | 2.93 | 8 | 2 |
| 1:A:73:THR:O | 1:A:73:THR:OG1 | 0.51 | 2.28 | 10 | 1 |
| 1:A:31:ASP:C | 1:A:50:LEU:HD22 | 0.51 | 2.25 | 12 | 2 |
| 1:A:18:PHE:O | 1:A:20:THR:CG2 | 0.51 | 2.59 | 15 | 1 |
| 1:A:26:VAL:HB | 1:A:35:PHE:CB | 0.51 | 2.36 | 4 | 15 |
| 1:A:45:LYS:O | 1:A:45:LYS:CG | 0.51 | 2.58 | 6 | 1 |
| 1:A:55:LEU:CD1 | 1:A:55:LEU:C | 0.51 | 2.80 | 13 | 4 |
| 1:A:64:LYS:O | 1:A:65:ARG:CB | 0.51 | 2.59 | 15 | 2 |
| 1:A:65:ARG:O | 1:A:68:VAL:HG12 | 0.51 | 2.05 | 23 | 1 |
| 1:A:55:LEU:HD11 | 1:A:57:SER:OG | 0.51 | 2.06 | 6 | 2 |
| 1:A:50:LEU:CD2 | 1:A:103:ILE:HD12 | 0.51 | 2.36 | 9 | 1 |
| 1:A:73:THR:O | 1:A:74:THR:HG23 | 0.51 | 2.06 | 10 | 4 |
| 1:A:56:THR:HG21 | 1:A:70:LYS:HE3 | 0.51 | 1.81 | 24 | 2 |
| 1:A:27:VAL:CG2 | 1:A:27:VAL:O | 0.51 | 2.57 | 19 | 2 |
| 1:A:14:LYS:HG3 | 1:A:21:TRP:NE1 | 0.51 | 2.21 | 6 | 1 |
| 1:A:26:VAL:HA | 1:A:35:PHE:CB | 0.50 | 2.36 | 25 | 22 |
| 1:A:9:GLY:O | 1:A:25:TRP:CD2 | 0.50 | 2.64 | 20 | 18 |
| 1:A:12:VAL:CG1 | 1:A:82:GLN:HG2 | 0.50 | 2.36 | 8 | 3 |
| 1:A:15:GLY:O | 1:A:17:VAL:N | 0.50 | 2.44 | 11 | 2 |
| 1:A:67:PHE:CZ | 1:A:86:LEU:HB3 | 0.50 | 2.41 | 12 | 1 |
| 1:A:66:MET:SD | 1:A:84:ALA:O | 0.50 | 2.70 | 3 | 1 |
| 1:A:52:GLY:O | 1:A:53:SER:O | 0.50 | 2.30 | 10 | 1 |
| 1:A:25:TRP:CD1 | 1:A:38:LYS:O | 0.50 | 2.65 | 18 | 1 |
| 1:A:55:LEU:C | 1:A:55:LEU:CD1 | 0.50 | 2.80 | 21 | 8 |
| 1:A:7:ARG:HB2 | 1:A:28:LEU:CD2 | 0.50 | 2.35 | 6 | 8 |
| 1:A:35:PHE:CZ | 1:A:46:GLY:CA | 0.50 | 2.94 | 18 | 3 |
| 1:A:69:PHE:CE2 | 1:A:71:ILE:HG13 | 0.50 | 2.41 | 22 | 6 |
| 1:A:18:PHE:C | 1:A:20:THR:HG23 | 0.50 | 2.27 | 15 | 1 |
| 1:A:67:PHE:CE1 | 1:A:86:LEU:HB2 | 0.50 | 2.42 | 1 | 6 |
| 1:A:30:GLU:C | 1:A:50:LEU:CD2 | 0.50 | 2.80 | 23 | 3 |
| 1:A:32:GLY:CA | 1:A:50:LEU:HD12 | 0.50 | 2.36 | 8 | 1 |
| 1:A:80:PHE:CD1 | 1:A:80:PHE:N | 0.50 | 2.79 | 10 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:10:TYR:O | 1:A:11:LEU:HD12 | 0.50 | 2.06 | 9 | 1 |
| 1:A:25:TRP:CE2 | 1:A:39:LYS:HG2 | 0.50 | 2.41 | 25 | 3 |
| 1:A:70:LYS:O | 1:A:70:LYS:CG | 0.50 | 2.60 | 21 | 2 |
| 1:A:21:TRP:CE2 | 1:A:62:PHE:CE1 | 0.50 | 3.00 | 12 | 2 |
| 1:A:96:ILE:O | 1:A:100:ILE:CG1 | 0.50 | 2.60 | 12 | 2 |
| 1:A:17:VAL:CG1 | 1:A:20:THR:OG1 | 0.50 | 2.59 | 22 | 1 |
| 1:A:33:ILE:N | 1:A:33:ILE:HD13 | 0.50 | 2.21 | 24 | 1 |
| 1:A:25:TRP:CZ2 | 1:A:39:LYS:HD3 | 0.50 | 2.42 | 1 | 3 |
| 1:A:67:PHE:CD1 | 1:A:89:ARG:HG3 | 0.50 | 2.42 | 3 | 1 |
| 1:A:35:PHE:CZ | 1:A:46:GLY:HA3 | 0.50 | 2.42 | 20 | 7 |
| 1:A:11:LEU:CG | 1:A:81:PHE:CE2 | 0.50 | 2.95 | 11 | 6 |
| 1:A:14:LYS:HE3 | 1:A:62:PHE:CZ | 0.50 | 2.42 | 18 | 2 |
| 1:A:18:PHE:CE1 | 1:A:20:THR:CG2 | 0.50 | 2.95 | 5 | 1 |
| 1:A:78:ASP:HB3 | 1:A:80:PHE:CE2 | 0.50 | 2.41 | 22 | 1 |
| 1:A:70:LYS:HD2 | 1:A:80:PHE:CE2 | 0.50 | 2.41 | 5 | 1 |
| 1:A:99:ALA:O | 1:A:103:ILE:CG2 | 0.50 | 2.60 | 22 | 2 |
| 1:A:72:THR:CG2 | 1:A:75:LYS:HA | 0.49 | 2.37 | 16 | 5 |
| 1:A:63:GLY:CA | 1:A:68:VAL:CG1 | 0.49 | 2.90 | 5 | 1 |
| 1:A:34:GLU:O | 1:A:34:GLU:CG | 0.49 | 2.60 | 18 | 4 |
| 1:A:67:PHE:CE2 | 1:A:86:LEU:HB2 | 0.49 | 2.42 | 11 | 1 |
| 1:A:12:VAL:CG1 | 1:A:82:GLN:HB3 | 0.49 | 2.38 | 9 | 6 |
| 1:A:13:LYS:CG | 1:A:81:PHE:CB | 0.49 | 2.90 | 5 | 1 |
| 1:A:14:LYS:CD | 1:A:80:PHE:CD1 | 0.49 | 2.95 | 8 | 1 |
| 1:A:29:LEU:CD1 | 1:A:34:GLU:OE2 | 0.49 | 2.60 | 12 | 2 |
| 1:A:86:LEU:C | 1:A:86:LEU:CD2 | 0.49 | 2.80 | 5 | 6 |
| 1:A:63:GLY:O | 1:A:64:LYS:C | 0.49 | 2.50 | 23 | 13 |
| 1:A:53:SER:H | 1:A:100:ILE:HG21 | 0.49 | 1.67 | 2 | 1 |
| 1:A:6:ILE:CD1 | 1:A:30:GLU:N | 0.49 | 2.75 | 2 | 1 |
| 1:A:50:LEU:CD1 | 1:A:99:ALA:C | 0.49 | 2.81 | 16 | 3 |
| 1:A:29:LEU:N | 1:A:29:LEU:HD12 | 0.49 | 2.23 | 23 | 1 |
| 1:A:85:PHE:CE2 | 1:A:88:GLU:HB2 | 0.49 | 2.43 | 6 | 4 |
| 1:A:25:TRP:CE2 | 1:A:39:LYS:HA | 0.49 | 2.43 | 24 | 12 |
| 1:A:14:LYS:HB3 | 1:A:21:TRP:NE1 | 0.49 | 2.23 | 2 | 2 |
| 1:A:7:ARG:HB2 | 1:A:28:LEU:CD1 | 0.49 | 2.37 | 9 | 7 |
| 1:A:13:LYS:NZ | 1:A:35:PHE:CZ | 0.49 | 2.80 | 7 | 1 |
| 1:A:70:LYS:HG3 | 1:A:80:PHE:CE2 | 0.49 | 2.43 | 10 | 4 |
| 1:A:77:GLN:OE1 | 1:A:79:HIS:NE2 | 0.49 | 2.46 | 1 | 1 |
| 1:A:57:SER:CA | 1:A:58:PRO:O | 0.49 | 2.60 | 8 | 2 |
| 1:A:28:LEU:HD13 | 1:A:96:ILE:HA | 0.49 | 1.83 | 4 | 1 |
| 1:A:11:LEU:CD1 | 1:A:11:LEU:N | 0.49 | 2.64 | 12 | 4 |
| 1:A:84:ALA:C | 1:A:85:PHE:CD2 | 0.49 | 2.85 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:55:LEU:CD2 | 1:A:55:LEU:C | 0.49 | 2.81 | 15 | 2 |
| 1:A:16:SER:O | 1:A:17:VAL:CG1 | 0.49 | 2.60 | 17 | 1 |
| 1:A:35:PHE:O | 1:A:35:PHE:CD1 | 0.49 | 2.65 | 24 | 6 |
| 1:A:63:GLY:HA3 | 1:A:68:VAL:HG11 | 0.49 | 1.85 | 12 | 1 |
| 1:A:59:CYS:SG | 1:A:70:LYS:HG2 | 0.49 | 2.48 | 17 | 1 |
| 1:A:50:LEU:CD2 | 1:A:103:ILE:HG13 | 0.49 | 2.37 | 3 | 2 |
| 1:A:14:LYS:CG | 1:A:21:TRP:NE1 | 0.49 | 2.76 | 6 | 1 |
| 1:A:14:LYS:HG3 | 1:A:62:PHE:CE2 | 0.49 | 2.43 | 6 | 2 |
| 1:A:14:LYS:HB3 | 1:A:80:PHE:CD1 | 0.49 | 2.42 | 12 | 2 |
| 1:A:85:PHE:CD1 | 1:A:87:GLU:HB3 | 0.49 | 2.43 | 14 | 1 |
| 1:A:59:CYS:SG | 1:A:68:VAL:CG2 | 0.49 | 2.95 | 16 | 1 |
| 1:A:17:VAL:HG22 | 1:A:18:PHE:CD2 | 0.49 | 2.43 | 13 | 1 |
| 1:A:69:PHE:O | 1:A:69:PHE:CD1 | 0.49 | 2.65 | 21 | 1 |
| 1:A:48:ILE:HG22 | 1:A:53:SER:HB2 | 0.49 | 1.85 | 22 | 1 |
| 1:A:55:LEU:CD2 | 1:A:69:PHE:CD1 | 0.49 | 2.95 | 6 | 3 |
| 1:A:25:TRP:CZ2 | 1:A:39:LYS:HG2 | 0.49 | 2.43 | 25 | 2 |
| 1:A:55:LEU:HD21 | 1:A:69:PHE:CD1 | 0.49 | 2.42 | 5 | 1 |
| 1:A:14:LYS:HB3 | 1:A:80:PHE:CD2 | 0.49 | 2.43 | 6 | 2 |
| 1:A:84:ALA:CB | 1:A:85:PHE:CD1 | 0.49 | 2.96 | 6 | 2 |
| 1:A:106:LEU:HD13 | 1:A:106:LEU:C | 0.49 | 2.28 | 8 | 1 |
| 1:A:13:LYS:HD3 | 1:A:35:PHE:CZ | 0.49 | 2.43 | 9 | 1 |
| 1:A:13:LYS:O | 1:A:14:LYS:C | 0.49 | 2.50 | 13 | 1 |
| 1:A:50:LEU:HB3 | 1:A:103:ILE:HD12 | 0.49 | 1.83 | 24 | 1 |
| 1:A:14:LYS:HB3 | 1:A:21:TRP:CE2 | 0.49 | 2.42 | 24 | 1 |
| 1:A:10:TYR:HB3 | 1:A:25:TRP:CE3 | 0.49 | 2.42 | 6 | 2 |
| 1:A:11:LEU:CB | 1:A:81:PHE:CE2 | 0.49 | 2.96 | 13 | 5 |
| 1:A:7:ARG:HB3 | 1:A:28:LEU:CD1 | 0.49 | 2.37 | 13 | 4 |
| 1:A:28:LEU:CB | 1:A:33:ILE:HD12 | 0.49 | 2.37 | 16 | 3 |
| 1:A:67:PHE:CE2 | 1:A:85:PHE:HA | 0.48 | 2.43 | 1 | 3 |
| 1:A:25:TRP:CD2 | 1:A:39:LYS:HA | 0.48 | 2.43 | 12 | 6 |
| 1:A:13:LYS:HE3 | 1:A:81:PHE:CB | 0.48 | 2.38 | 10 | 2 |
| 1:A:21:TRP:CD1 | 1:A:62:PHE:CE1 | 0.48 | 3.01 | 22 | 4 |
| 1:A:13:LYS:HG3 | 1:A:81:PHE:CB | 0.48 | 2.38 | 13 | 1 |
| 1:A:36:TYR:CD2 | 1:A:44:PRO:CA | 0.48 | 2.96 | 18 | 3 |
| 1:A:41:ASP:OD1 | 1:A:43:SER:O | 0.48 | 2.31 | 3 | 2 |
| 1:A:8:GLU:CD | 1:A:8:GLU:N | 0.48 | 2.66 | 3 | 1 |
| 1:A:14:LYS:HG3 | 1:A:21:TRP:CD1 | 0.48 | 2.42 | 9 | 1 |
| 1:A:29:LEU:CD1 | 1:A:34:GLU:HG2 | 0.48 | 2.38 | 9 | 8 |
| 1:A:90:ASP:HA | 1:A:93:VAL:CG2 | 0.48 | 2.39 | 5 | 15 |
| 1:A:41:ASP:O | 1:A:41:ASP:OD1 | 0.48 | 2.31 | 3 | 4 |
| 1:A:28:LEU:CD1 | 1:A:95:ASP:OD1 | 0.48 | 2.61 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:25:TRP:CG | 1:A:39:LYS:HA | 0.48 | 2.43 | 4 | 10 |
| 1:A:50:LEU:HD23 | 1:A:103:ILE:CB | 0.48 | 2.38 | 23 | 3 |
| 1:A:7:ARG:HB2 | 1:A:28:LEU:CG | 0.48 | 2.38 | 9 | 5 |
| 1:A:19:ASN:N | 1:A:19:ASN:OD1 | 0.48 | 2.44 | 10 | 1 |
| 1:A:17:VAL:CG1 | 1:A:18:PHE:N | 0.48 | 2.76 | 15 | 1 |
| 1:A:8:GLU:N | 1:A:8:GLU:CD | 0.48 | 2.67 | 20 | 2 |
| 1:A:57:SER:HA | 1:A:58:PRO:C | 0.48 | 2.28 | 1 | 2 |
| 1:A:14:LYS:HB2 | 1:A:21:TRP:CE2 | 0.48 | 2.44 | 7 | 2 |
| 1:A:73:THR:CG2 | 1:A:79:HIS:NE2 | 0.48 | 2.77 | 9 | 1 |
| 1:A:16:SER:CB | 1:A:45:LYS:CE | 0.48 | 2.91 | 12 | 1 |
| 1:A:56:THR:HB | 1:A:59:CYS:HG | 0.48 | 1.68 | 13 | 1 |
| 1:A:50:LEU:HD12 | 1:A:103:ILE:HG12 | 0.48 | 1.85 | 20 | 1 |
| 1:A:14:LYS:HD2 | 1:A:62:PHE:CE2 | 0.48 | 2.43 | 20 | 1 |
| 1:A:68:VAL:O | 1:A:68:VAL:HG13 | 0.48 | 2.08 | 24 | 1 |
| 1:A:55:LEU:HD23 | 1:A:56:THR:H | 0.48 | 1.63 | 1 | 1 |
| 1:A:12:VAL:HG13 | 1:A:82:GLN:HB3 | 0.48 | 1.86 | 4 | 2 |
| 1:A:11:LEU:CG | 1:A:81:PHE:CZ | 0.48 | 2.97 | 12 | 2 |
| 1:A:18:PHE:CD1 | 1:A:19:ASN:O | 0.48 | 2.67 | 24 | 1 |
| 1:A:25:TRP:HB3 | 1:A:38:LYS:O | 0.48 | 2.09 | 6 | 22 |
| 1:A:11:LEU:CD2 | 1:A:81:PHE:CE1 | 0.48 | 2.96 | 7 | 1 |
| 1:A:11:LEU:HD21 | 1:A:92:TRP:CD1 | 0.48 | 2.43 | 25 | 2 |
| 1:A:73:THR:CG2 | 1:A:77:GLN:HB2 | 0.48 | 2.39 | 10 | 1 |
| 1:A:14:LYS:HA | 1:A:21:TRP:CD1 | 0.48 | 2.43 | 13 | 1 |
| 1:A:62:PHE:CE2 | 1:A:80:PHE:CD1 | 0.48 | 3.02 | 21 | 1 |
| 1:A:21:TRP:CZ2 | 1:A:80:PHE:O | 0.48 | 2.66 | 1 | 1 |
| 1:A:12:VAL:CA | 1:A:23:PRO:HA | 0.48 | 2.39 | 13 | 8 |
| 1:A:21:TRP:CZ3 | 1:A:82:GLN:HB2 | 0.48 | 2.43 | 25 | 4 |
| 1:A:16:SER:O | 1:A:17:VAL:O | 0.48 | 2.31 | 17 | 3 |
| 1:A:14:LYS:HD2 | 1:A:21:TRP:CD1 | 0.48 | 2.43 | 12 | 1 |
| 1:A:74:THR:O | 1:A:75:LYS:HB2 | 0.48 | 2.09 | 12 | 2 |
| 1:A:50:LEU:CD1 | 1:A:103:ILE:HG13 | 0.48 | 2.36 | 14 | 2 |
| 1:A:63:GLY:C | 1:A:68:VAL:HG11 | 0.48 | 2.28 | 22 | 1 |
| 1:A:54:THR:O | 1:A:71:ILE:HG12 | 0.48 | 2.09 | 8 | 13 |
| 1:A:70:LYS:HG3 | 1:A:80:PHE:CD2 | 0.48 | 2.44 | 22 | 1 |
| 1:A:68:VAL:HA | 1:A:81:PHE:O | 0.48 | 2.09 | 4 | 8 |
| 1:A:41:ASP:OD1 | 1:A:41:ASP:O | 0.48 | 2.32 | 16 | 3 |
| 1:A:51:LYS:HG3 | 1:A:103:ILE:HG22 | 0.48 | 1.86 | 13 | 1 |
| 1:A:60:GLN:HB2 | 1:A:68:VAL:CG2 | 0.48 | 2.38 | 25 | 2 |
| 1:A:89:ARG:CD | 1:A:90:ASP:OD1 | 0.48 | 2.62 | 17 | 1 |
| 1:A:78:ASP:HB2 | 1:A:80:PHE:CE2 | 0.48 | 2.43 | 19 | 1 |
| 1:A:48:ILE:HG23 | 1:A:49:PRO:HD2 | 0.48 | 1.84 | 23 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:41:ASP:OD2 | 1:A:43:SER:O | 0.48 | 2.32 | 5 | 10 |
| 1:A:29:LEU:CD1 | 1:A:34:GLU:CD | 0.48 | 2.82 | 16 | 1 |
| 1:A:40:SER:O | 1:A:42:ASN:ND2 | 0.47 | 2.47 | 1 | 1 |
| 1:A:40:SER:C | 1:A:42:ASN:N | 0.47 | 2.66 | 24 | 6 |
| 1:A:41:ASP:CG | 1:A:41:ASP:O | 0.47 | 2.53 | 14 | 7 |
| 1:A:28:LEU:HB2 | 1:A:33:ILE:CG1 | 0.47 | 2.38 | 7 | 1 |
| 1:A:5:ARG:HG2 | 1:A:29:LEU:CD2 | 0.47 | 2.38 | 13 | 2 |
| 1:A:83:ALA:O | 1:A:84:ALA:HB3 | 0.47 | 2.09 | 16 | 1 |
| 1:A:54:THR:OG1 | 1:A:72:THR:O | 0.47 | 2.32 | 15 | 10 |
| 1:A:54:THR:O | 1:A:71:ILE:HA | 0.47 | 2.10 | 8 | 18 |
| 1:A:41:ASP:O | 1:A:41:ASP:CG | 0.47 | 2.53 | 23 | 11 |
| 1:A:6:ILE:HD13 | 1:A:99:ALA:HB2 | 0.47 | 1.87 | 8 | 2 |
| 1:A:75:LYS:C | 1:A:76:GLN:CG | 0.47 | 2.82 | 15 | 3 |
| 1:A:55:LEU:CD2 | 1:A:93:VAL:HG12 | 0.47 | 2.39 | 25 | 1 |
| 1:A:28:LEU:HD21 | 1:A:95:ASP:CG | 0.47 | 2.29 | 2 | 1 |
| 1:A:60:GLN:HB3 | 1:A:62:PHE:CD1 | 0.47 | 2.44 | 3 | 1 |
| 1:A:55:LEU:CD1 | 1:A:57:SER:OG | 0.47 | 2.61 | 6 | 1 |
| 1:A:53:SER:O | 1:A:100:ILE:HG21 | 0.47 | 2.10 | 8 | 1 |
| 1:A:67:PHE:CD1 | 1:A:86:LEU:HA | 0.47 | 2.44 | 15 | 1 |
| 1:A:69:PHE:CD2 | 1:A:93:VAL:HG23 | 0.47 | 2.44 | 15 | 1 |
| 1:A:84:ALA:HB3 | 1:A:85:PHE:CD1 | 0.47 | 2.44 | 6 | 2 |
| 1:A:70:LYS:HD2 | 1:A:80:PHE:CZ | 0.47 | 2.44 | 2 | 2 |
| 1:A:28:LEU:C | 1:A:28:LEU:CD1 | 0.47 | 2.80 | 23 | 3 |
| 1:A:21:TRP:CH2 | 1:A:80:PHE:HB2 | 0.47 | 2.45 | 4 | 2 |
| 1:A:36:TYR:CE2 | 1:A:44:PRO:HB3 | 0.47 | 2.44 | 18 | 2 |
| 1:A:55:LEU:HD21 | 1:A:93:VAL:CG2 | 0.47 | 2.37 | 21 | 1 |
| 1:A:12:VAL:HA | 1:A:23:PRO:HA | 0.47 | 1.86 | 12 | 23 |
| 1:A:50:LEU:O | 1:A:103:ILE:CG2 | 0.47 | 2.63 | 17 | 3 |
| 1:A:7:ARG:HB3 | 1:A:28:LEU:CG | 0.47 | 2.40 | 13 | 4 |
| 1:A:50:LEU:C | 1:A:50:LEU:CD1 | 0.47 | 2.79 | 8 | 1 |
| 1:A:6:ILE:CD1 | 1:A:99:ALA:HB2 | 0.47 | 2.40 | 8 | 2 |
| 1:A:55:LEU:CD2 | 1:A:71:ILE:HG13 | 0.47 | 2.39 | 10 | 5 |
| 1:A:35:PHE:CD1 | 1:A:35:PHE:C | 0.47 | 2.88 | 18 | 1 |
| 1:A:56:THR:O | 1:A:58:PRO:O | 0.47 | 2.33 | 22 | 1 |
| 1:A:86:LEU:CD2 | 1:A:87:GLU:N | 0.47 | 2.70 | 3 | 11 |
| 1:A:5:ARG:HG3 | 1:A:29:LEU:CD2 | 0.47 | 2.39 | 7 | 5 |
| 1:A:59:CYS:HB2 | 1:A:70:LYS:CB | 0.47 | 2.40 | 20 | 5 |
| 1:A:18:PHE:O | 1:A:19:ASN:O | 0.47 | 2.33 | 4 | 1 |
| 1:A:86:LEU:CD1 | 1:A:89:ARG:NH2 | 0.47 | 2.78 | 4 | 1 |
| 1:A:69:PHE:CZ | 1:A:81:PHE:HB3 | 0.47 | 2.44 | 6 | 1 |
| 1:A:89:ARG:CD | 1:A:89:ARG:C | 0.47 | 2.83 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:48:ILE:HG23 | 1:A:79:HIS:NE2 | 0.47 | 2.25 | 8 | 1 |
| 1:A:55:LEU:HD22 | 1:A:55:LEU:C | 0.47 | 2.29 | 17 | 1 |
| 1:A:61:ASP:N | 1:A:61:ASP:OD1 | 0.47 | 2.47 | 21 | 1 |
| 1:A:70:LYS:HD3 | 1:A:80:PHE:CE2 | 0.47 | 2.44 | 16 | 2 |
| 1:A:53:SER:HB2 | 1:A:100:ILE:HD13 | 0.47 | 1.85 | 3 | 1 |
| 1:A:65:ARG:O | 1:A:66:MET:O | 0.47 | 2.33 | 20 | 4 |
| 1:A:90:ASP:HA | 1:A:93:VAL:HG23 | 0.47 | 1.86 | 17 | 3 |
| 1:A:81:PHE:O | 1:A:81:PHE:CD1 | 0.47 | 2.68 | 16 | 1 |
| 1:A:17:VAL:CG2 | 1:A:18:PHE:N | 0.47 | 2.78 | 24 | 1 |
| 1:A:28:LEU:CD2 | 1:A:96:ILE:HG13 | 0.47 | 2.39 | 2 | 2 |
| 1:A:63:GLY:HA2 | 1:A:68:VAL:CG1 | 0.47 | 2.40 | 4 | 2 |
| 1:A:28:LEU:CD2 | 1:A:96:ILE:CG1 | 0.47 | 2.93 | 23 | 2 |
| 1:A:67:PHE:CD1 | 1:A:89:ARG:HD3 | 0.47 | 2.45 | 6 | 1 |
| 1:A:48:ILE:CG2 | 1:A:79:HIS:CD2 | 0.47 | 2.98 | 8 | 1 |
| 1:A:78:ASP:HB2 | 1:A:80:PHE:CE1 | 0.47 | 2.44 | 8 | 2 |
| 1:A:14:LYS:CG | 1:A:20:THR:O | 0.47 | 2.63 | 9 | 2 |
| 1:A:78:ASP:OD1 | 1:A:78:ASP:O | 0.47 | 2.33 | 19 | 1 |
| 1:A:21:TRP:CZ3 | 1:A:82:GLN:CB | 0.47 | 2.97 | 25 | 1 |
| 1:A:14:LYS:HG2 | 1:A:62:PHE:CZ | 0.47 | 2.44 | 1 | 1 |
| 1:A:17:VAL:O | 1:A:17:VAL:CG1 | 0.47 | 2.63 | 19 | 2 |
| 1:A:50:LEU:HG | 1:A:100:ILE:HD12 | 0.47 | 1.86 | 11 | 1 |
| 1:A:28:LEU:CD1 | 1:A:96:ILE:HG13 | 0.47 | 2.39 | 14 | 2 |
| 1:A:67:PHE:HB3 | 1:A:89:ARG:CG | 0.46 | 2.40 | 2 | 3 |
| 1:A:14:LYS:HD2 | 1:A:80:PHE:CD1 | 0.46 | 2.45 | 8 | 2 |
| 1:A:13:LYS:CE | 1:A:81:PHE:HB3 | 0.46 | 2.41 | 15 | 2 |
| 1:A:60:GLN:CG | 1:A:62:PHE:CE2 | 0.46 | 2.98 | 16 | 1 |
| 1:A:69:PHE:CE2 | 1:A:93:VAL:CG1 | 0.46 | 2.98 | 18 | 1 |
| 1:A:89:ARG:CZ | 1:A:93:VAL:HG11 | 0.46 | 2.40 | 2 | 1 |
| 1:A:67:PHE:CG | 1:A:89:ARG:HG3 | 0.46 | 2.45 | 3 | 1 |
| 1:A:14:LYS:HE2 | 1:A:62:PHE:CE2 | 0.46 | 2.45 | 7 | 1 |
| 1:A:86:LEU:CD2 | 1:A:86:LEU:C | 0.46 | 2.80 | 10 | 3 |
| 1:A:33:ILE:HD12 | 1:A:50:LEU:CD1 | 0.46 | 2.40 | 21 | 1 |
| 1:A:18:PHE:CD1 | 1:A:18:PHE:C | 0.46 | 2.89 | 24 | 1 |
| 1:A:28:LEU:CB | 1:A:96:ILE:HG13 | 0.46 | 2.40 | 11 | 2 |
| 1:A:32:GLY:N | 1:A:50:LEU:CD1 | 0.46 | 2.67 | 17 | 1 |
| 1:A:73:THR:OG1 | 1:A:77:GLN:HG3 | 0.46 | 2.10 | 24 | 1 |
| 1:A:81:PHE:CD1 | 1:A:82:GLN:N | 0.46 | 2.84 | 2 | 7 |
| 1:A:26:VAL:CG2 | 1:A:35:PHE:HB3 | 0.46 | 2.40 | 19 | 17 |
| 1:A:19:ASN:OD1 | 1:A:19:ASN:N | 0.46 | 2.48 | 23 | 3 |
| 1:A:12:VAL:O | 1:A:81:PHE:HA | 0.46 | 2.10 | 5 | 7 |
| 1:A:69:PHE:CE2 | 1:A:71:ILE:CD1 | 0.46 | 2.99 | 7 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:51:LYS:O | 1:A:104:GLU:OE1 | 0.46 | 2.34 | 6 | 1 |
| 1:A:38:LYS:O | 1:A:40:SER:N | 0.46 | 2.49 | 6 | 7 |
| 1:A:75:LYS:O | 1:A:77:GLN:OE1 | 0.46 | 2.33 | 7 | 1 |
| 1:A:67:PHE:HB2 | 1:A:82:GLN:CG | 0.46 | 2.40 | 7 | 1 |
| 1:A:67:PHE:HB3 | 1:A:89:ARG:CB | 0.46 | 2.39 | 12 | 1 |
| 1:A:72:THR:O | 1:A:73:THR:O | 0.46 | 2.32 | 17 | 3 |
| 1:A:5:ARG:NH1 | 1:A:5:ARG:CB | 0.46 | 2.78 | 19 | 1 |
| 1:A:19:ASN:ND2 | 1:A:62:PHE:CZ | 0.46 | 2.83 | 24 | 1 |
| 1:A:72:THR:O | 1:A:73:THR:C | 0.46 | 2.54 | 15 | 11 |
| 1:A:93:VAL:O | 1:A:97:ASN:HB3 | 0.46 | 2.11 | 5 | 5 |
| 1:A:12:VAL:CG2 | 1:A:13:LYS:N | 0.46 | 2.78 | 4 | 1 |
| 1:A:13:LYS:NZ | 1:A:35:PHE:CE2 | 0.46 | 2.84 | 7 | 1 |
| 1:A:7:ARG:O | 1:A:8:GLU:OE1 | 0.46 | 2.33 | 9 | 1 |
| 1:A:29:LEU:O | 1:A:32:GLY:O | 0.46 | 2.34 | 20 | 1 |
| 1:A:69:PHE:CD2 | 1:A:81:PHE:CB | 0.46 | 2.99 | 25 | 1 |
| 1:A:85:PHE:CE1 | 1:A:88:GLU:CB | 0.46 | 2.98 | 25 | 1 |
| 1:A:33:ILE:CD1 | 1:A:96:ILE:HG23 | 0.46 | 2.41 | 1 | 1 |
| 1:A:90:ASP:O | 1:A:94:ARG:HG2 | 0.46 | 2.10 | 21 | 7 |
| 1:A:94:ARG:O | 1:A:98:LYS:HB2 | 0.46 | 2.11 | 5 | 15 |
| 1:A:33:ILE:CD1 | 1:A:100:ILE:HD11 | 0.46 | 2.40 | 6 | 1 |
| 1:A:49:PRO:O | 1:A:53:SER:OG | 0.46 | 2.33 | 21 | 3 |
| 1:A:40:SER:O | 1:A:42:ASN:N | 0.46 | 2.49 | 24 | 3 |
| 1:A:6:ILE:CG2 | 1:A:95:ASP:OD2 | 0.46 | 2.64 | 11 | 1 |
| 1:A:106:LEU:CD1 | 1:A:106:LEU:O | 0.46 | 2.63 | 8 | 1 |
| 1:A:12:VAL:CG2 | 1:A:22:LYS:C | 0.46 | 2.81 | 18 | 2 |
| 1:A:103:ILE:O | 1:A:104:GLU:C | 0.46 | 2.52 | 14 | 2 |
| 1:A:60:GLN:HA | 1:A:60:GLN:NE2 | 0.46 | 2.26 | 20 | 1 |
| 1:A:55:LEU:HD23 | 1:A:71:ILE:CG1 | 0.46 | 2.40 | 5 | 5 |
| 1:A:18:PHE:O | 1:A:20:THR:HG23 | 0.46 | 2.11 | 5 | 1 |
| 1:A:14:LYS:HD3 | 1:A:20:THR:N | 0.46 | 2.26 | 6 | 1 |
| 1:A:78:ASP:O | 1:A:78:ASP:OD1 | 0.46 | 2.33 | 7 | 1 |
| 1:A:21:TRP:CZ3 | 1:A:82:GLN:N | 0.46 | 2.84 | 17 | 1 |
| 1:A:67:PHE:HA | 1:A:89:ARG:CG | 0.46 | 2.41 | 24 | 1 |
| 1:A:38:LYS:O | 1:A:39:LYS:C | 0.45 | 2.54 | 7 | 17 |
| 1:A:11:LEU:O | 1:A:23:PRO:HA | 0.45 | 2.10 | 2 | 1 |
| 1:A:63:GLY:CA | 1:A:68:VAL:HG11 | 0.45 | 2.41 | 5 | 2 |
| 1:A:50:LEU:CD2 | 1:A:99:ALA:O | 0.45 | 2.63 | 3 | 1 |
| 1:A:50:LEU:HD21 | 1:A:99:ALA:O | 0.45 | 2.11 | 3 | 1 |
| 1:A:13:LYS:CG | 1:A:81:PHE:HB2 | 0.45 | 2.41 | 5 | 1 |
| 1:A:17:VAL:O | 1:A:18:PHE:O | 0.45 | 2.34 | 25 | 5 |
| 1:A:11:LEU:HB2 | 1:A:81:PHE:CE1 | 0.45 | 2.46 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:LYS:HE2 | 1:A:81:PHE:CB | 0.45 | 2.41 | 14 | 1 |
| 1:A:12:VAL:CG2 | 1:A:21:TRP:C | 0.45 | 2.85 | 24 | 1 |
| 1:A:72:THR:O | 1:A:72:THR:HG22 | 0.45 | 2.11 | 12 | 4 |
| 1:A:72:THR:HG22 | 1:A:75:LYS:CA | 0.45 | 2.41 | 10 | 5 |
| 1:A:67:PHE:CE2 | 1:A:86:LEU:N | 0.45 | 2.85 | 23 | 2 |
| 1:A:18:PHE:CD1 | 1:A:20:THR:CG2 | 0.45 | 3.00 | 5 | 1 |
| 1:A:50:LEU:CD1 | 1:A:100:ILE:HA | 0.45 | 2.41 | 20 | 4 |
| 1:A:89:ARG:HD3 | 1:A:90:ASP:OD1 | 0.45 | 2.11 | 17 | 1 |
| 1:A:13:LYS:HD2 | 1:A:81:PHE:CB | 0.45 | 2.41 | 18 | 1 |
| 1:A:14:LYS:O | 1:A:15:GLY:O | 0.45 | 2.35 | 25 | 1 |
| 1:A:62:PHE:C | 1:A:68:VAL:CG1 | 0.45 | 2.85 | 4 | 1 |
| 1:A:12:VAL:HG13 | 1:A:82:GLN:HG2 | 0.45 | 1.87 | 8 | 1 |
| 1:A:50:LEU:O | 1:A:100:ILE:HG13 | 0.45 | 2.12 | 8 | 1 |
| 1:A:5:ARG:O | 1:A:8:GLU:OE1 | 0.45 | 2.34 | 9 | 1 |
| 1:A:12:VAL:HG23 | 1:A:22:LYS:H | 0.45 | 1.69 | 13 | 1 |
| 1:A:70:LYS:HG3 | 1:A:78:ASP:OD2 | 0.45 | 2.12 | 13 | 1 |
| 1:A:60:GLN:O | 1:A:61:ASP:HB2 | 0.45 | 2.11 | 23 | 1 |
| 1:A:7:ARG:HG2 | 1:A:92:TRP:CE2 | 0.45 | 2.46 | 23 | 1 |
| 1:A:50:LEU:HA | 1:A:100:ILE:CG1 | 0.45 | 2.42 | 1 | 1 |
| 1:A:93:VAL:CG2 | 1:A:94:ARG:N | 0.45 | 2.79 | 4 | 6 |
| 1:A:52:GLY:O | 1:A:53:SER:C | 0.45 | 2.55 | 14 | 5 |
| 1:A:18:PHE:CD1 | 1:A:20:THR:HG23 | 0.45 | 2.46 | 5 | 1 |
| 1:A:84:ALA:HB1 | 1:A:85:PHE:CZ | 0.45 | 2.46 | 5 | 1 |
| 1:A:48:ILE:CG2 | 1:A:49:PRO:HD2 | 0.45 | 2.41 | 16 | 2 |
| 1:A:14:LYS:HG3 | 1:A:20:THR:O | 0.45 | 2.10 | 9 | 1 |
| 1:A:50:LEU:HD22 | 1:A:103:ILE:CD1 | 0.45 | 2.42 | 9 | 1 |
| 1:A:17:VAL:O | 1:A:18:PHE:C | 0.45 | 2.54 | 15 | 2 |
| 1:A:19:ASN:ND2 | 1:A:62:PHE:CE2 | 0.45 | 2.85 | 24 | 2 |
| 1:A:71:ILE:HG23 | 1:A:72:THR:N | 0.45 | 2.27 | 15 | 1 |
| 1:A:41:ASP:C | 1:A:43:SER:N | 0.45 | 2.70 | 19 | 18 |
| 1:A:32:GLY:HA2 | 1:A:50:LEU:CD1 | 0.45 | 2.41 | 24 | 2 |
| 1:A:5:ARG:HB2 | 1:A:29:LEU:CD2 | 0.45 | 2.42 | 19 | 1 |
| 1:A:66:MET:O | 1:A:67:PHE:CD1 | 0.45 | 2.70 | 19 | 1 |
| 1:A:28:LEU:CD2 | 1:A:95:ASP:HB3 | 0.45 | 2.42 | 25 | 3 |
| 1:A:14:LYS:HB3 | 1:A:21:TRP:CD1 | 0.45 | 2.47 | 21 | 1 |
| 1:A:63:GLY:O | 1:A:64:LYS:HG2 | 0.45 | 2.11 | 24 | 2 |
| 1:A:68:VAL:CA | 1:A:81:PHE:O | 0.45 | 2.64 | 25 | 1 |
| 1:A:25:TRP:NE1 | 1:A:39:LYS:HA | 0.45 | 2.26 | 11 | 7 |
| 1:A:54:THR:OG1 | 1:A:72:THR:HB | 0.45 | 2.12 | 12 | 11 |
| 1:A:57:SER:HA | 1:A:58:PRO:O | 0.45 | 2.11 | 8 | 2 |
| 1:A:67:PHE:CZ | 1:A:86:LEU:HB2 | 0.45 | 2.47 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:40:SER:O | 1:A:41:ASP:HB3 | 0.45 | 2.10 | 20 | 9 |
| 1:A:12:VAL:CG1 | 1:A:82:GLN:HG3 | 0.45 | 2.41 | 8 | 1 |
| 1:A:68:VAL:HB | 1:A:82:GLN:CG | 0.45 | 2.42 | 9 | 1 |
| 1:A:27:VAL:O | 1:A:29:LEU:CD1 | 0.45 | 2.65 | 23 | 2 |
| 1:A:19:ASN:C | 1:A:19:ASN:ND2 | 0.45 | 2.69 | 24 | 1 |
| 1:A:27:VAL:HG23 | 1:A:29:LEU:HD11 | 0.45 | 1.89 | 24 | 1 |
| 1:A:54:THR:HG22 | 1:A:72:THR:HB | 0.45 | 1.87 | 3 | 5 |
| 1:A:50:LEU:CD2 | 1:A:103:ILE:HB | 0.45 | 2.42 | 4 | 1 |
| 1:A:50:LEU:HB2 | 1:A:100:ILE:CG1 | 0.45 | 2.41 | 12 | 2 |
| 1:A:16:SER:C | 1:A:17:VAL:CG1 | 0.45 | 2.85 | 17 | 1 |
| 1:A:91:ALA:HA | 1:A:94:ARG:CG | 0.45 | 2.42 | 21 | 1 |
| 1:A:14:LYS:HG2 | 1:A:20:THR:O | 0.45 | 2.12 | 25 | 1 |
| 1:A:13:LYS:HE2 | 1:A:35:PHE:CE2 | 0.45 | 2.47 | 25 | 1 |
| 1:A:102:CYS:O | 1:A:106:LEU:HD23 | 0.45 | 2.11 | 2 | 2 |
| 1:A:41:ASP:O | 1:A:42:ASN:C | 0.45 | 2.55 | 22 | 17 |
| 1:A:21:TRP:CH2 | 1:A:81:PHE:CA | 0.45 | 2.99 | 17 | 2 |
| 1:A:17:VAL:CG1 | 1:A:17:VAL:O | 0.45 | 2.63 | 12 | 1 |
| 1:A:78:ASP:OD1 | 1:A:80:PHE:CE1 | 0.45 | 2.70 | 13 | 1 |
| 1:A:66:MET:CB | 1:A:82:GLN:OE1 | 0.45 | 2.65 | 22 | 1 |
| 1:A:91:ALA:HA | 1:A:94:ARG:CD | 0.44 | 2.42 | 9 | 3 |
| 1:A:28:LEU:CB | 1:A:33:ILE:CG1 | 0.44 | 2.95 | 7 | 2 |
| 1:A:89:ARG:HG3 | 1:A:90:ASP:N | 0.44 | 2.27 | 7 | 1 |
| 1:A:85:PHE:CD1 | 1:A:88:GLU:HB2 | 0.44 | 2.46 | 8 | 1 |
| 1:A:60:GLN:O | 1:A:62:PHE:N | 0.44 | 2.50 | 20 | 1 |
| 1:A:23:PRO:O | 1:A:24:MET:HB3 | 0.44 | 2.12 | 9 | 2 |
| 1:A:14:LYS:HD2 | 1:A:21:TRP:NE1 | 0.44 | 2.27 | 9 | 2 |
| 1:A:7:ARG:HB3 | 1:A:28:LEU:HD12 | 0.44 | 1.89 | 10 | 1 |
| 1:A:16:SER:HB2 | 1:A:45:LYS:CE | 0.44 | 2.41 | 12 | 1 |
| 1:A:16:SER:O | 1:A:17:VAL:C | 0.44 | 2.54 | 15 | 3 |
| 1:A:14:LYS:HG3 | 1:A:15:GLY:N | 0.44 | 2.27 | 24 | 1 |
| 1:A:33:ILE:CD1 | 1:A:50:LEU:CD1 | 0.44 | 2.95 | 2 | 1 |
| 1:A:14:LYS:HA | 1:A:20:THR:O | 0.44 | 2.12 | 21 | 3 |
| 1:A:14:LYS:HE3 | 1:A:80:PHE:CD2 | 0.44 | 2.47 | 6 | 1 |
| 1:A:54:THR:CG2 | 1:A:72:THR:CB | 0.44 | 2.96 | 14 | 3 |
| 1:A:106:LEU:CD1 | 1:A:106:LEU:C | 0.44 | 2.85 | 8 | 1 |
| 1:A:26:VAL:HB | 1:A:35:PHE:HB3 | 0.44 | 1.90 | 9 | 2 |
| 1:A:14:LYS:HB2 | 1:A:80:PHE:HB3 | 0.44 | 1.89 | 9 | 1 |
| 1:A:13:LYS:NZ | 1:A:79:HIS:HB3 | 0.44 | 2.28 | 17 | 1 |
| 1:A:49:PRO:HD2 | 1:A:73:THR:OG1 | 0.44 | 2.12 | 22 | 1 |
| 1:A:18:PHE:O | 1:A:19:ASN:C | 0.44 | 2.56 | 24 | 4 |
| 1:A:26:VAL:CB | 1:A:35:PHE:CB | 0.44 | 2.96 | 4 | 6 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:7:ARG:HG3 | 1:A:95:ASP:CB | 0.44 | 2.43 | 18 | 2 |
| 1:A:66:MET:HG3 | 1:A:67:PHE:CD1 | 0.44 | 2.47 | 7 | 1 |
| 1:A:28:LEU:CD1 | 1:A:95:ASP:HB3 | 0.44 | 2.43 | 10 | 1 |
| 1:A:50:LEU:O | 1:A:51:LYS:O | 0.44 | 2.35 | 15 | 1 |
| 1:A:5:ARG:CA | 1:A:29:LEU:HD23 | 0.44 | 2.43 | 19 | 1 |
| 1:A:33:ILE:CD1 | 1:A:50:LEU:CD2 | 0.44 | 2.96 | 20 | 1 |
| 1:A:50:LEU:HG | 1:A:100:ILE:CG1 | 0.44 | 2.41 | 25 | 5 |
| 1:A:73:THR:O | 1:A:74:THR:C | 0.44 | 2.56 | 6 | 4 |
| 1:A:65:ARG:O | 1:A:66:MET:C | 0.44 | 2.56 | 23 | 3 |
| 1:A:28:LEU:CD2 | 1:A:92:TRP:CE3 | 0.44 | 3.01 | 19 | 2 |
| 1:A:27:VAL:O | 1:A:29:LEU:HD12 | 0.44 | 2.12 | 17 | 2 |
| 1:A:16:SER:C | 1:A:17:VAL:HG12 | 0.44 | 2.32 | 17 | 1 |
| 1:A:10:TYR:HA | 1:A:24:MET:O | 0.44 | 2.13 | 19 | 5 |
| 1:A:53:SER:HB3 | 1:A:100:ILE:HD13 | 0.44 | 1.90 | 19 | 1 |
| 1:A:17:VAL:HG13 | 1:A:18:PHE:H | 0.44 | 1.72 | 22 | 1 |
| 1:A:70:LYS:O | 1:A:70:LYS:HG3 | 0.44 | 2.12 | 6 | 3 |
| 1:A:28:LEU:CB | 1:A:33:ILE:HG12 | 0.44 | 2.43 | 8 | 2 |
| 1:A:56:THR:CB | 1:A:70:LYS:O | 0.44 | 2.66 | 13 | 2 |
| 1:A:5:ARG:HB2 | 1:A:29:LEU:HD23 | 0.44 | 1.88 | 19 | 1 |
| 1:A:81:PHE:CZ | 1:A:92:TRP:HB3 | 0.44 | 2.48 | 24 | 1 |
| 1:A:50:LEU:HD23 | 1:A:103:ILE:CG2 | 0.44 | 2.42 | 4 | 2 |
| 1:A:73:THR:HG23 | 1:A:79:HIS:CD2 | 0.44 | 2.48 | 9 | 1 |
| 1:A:12:VAL:HB | 1:A:23:PRO:N | 0.44 | 2.27 | 13 | 1 |
| 1:A:50:LEU:CD1 | 1:A:103:ILE:CG1 | 0.44 | 2.90 | 14 | 1 |
| 1:A:73:THR:HG23 | 1:A:76:GLN:HB2 | 0.44 | 1.88 | 22 | 2 |
| 1:A:8:GLU:HB3 | 1:A:27:VAL:CG1 | 0.44 | 2.43 | 24 | 2 |
| 1:A:14:LYS:HD2 | 1:A:62:PHE:CZ | 0.44 | 2.48 | 22 | 1 |
| 1:A:55:LEU:CG | 1:A:93:VAL:HG23 | 0.44 | 2.43 | 22 | 1 |
| 1:A:13:LYS:HE2 | 1:A:35:PHE:CZ | 0.44 | 2.48 | 25 | 1 |
| 1:A:13:LYS:CE | 1:A:35:PHE:CE2 | 0.44 | 3.01 | 25 | 1 |
| 1:A:55:LEU:CD2 | 1:A:56:THR:N | 0.44 | 2.81 | 15 | 4 |
| 1:A:70:LYS:HB2 | 1:A:80:PHE:CD2 | 0.44 | 2.48 | 5 | 1 |
| 1:A:55:LEU:HG | 1:A:93:VAL:HG12 | 0.44 | 1.89 | 6 | 1 |
| 1:A:14:LYS:CD | 1:A:21:TRP:NE1 | 0.44 | 2.81 | 9 | 1 |
| 1:A:7:ARG:CB | 1:A:28:LEU:HG | 0.44 | 2.41 | 9 | 2 |
| 1:A:64:LYS:O | 1:A:64:LYS:HG3 | 0.44 | 2.11 | 23 | 1 |
| 1:A:11:LEU:HD23 | 1:A:26:VAL:CG1 | 0.44 | 2.43 | 24 | 1 |
| 1:A:13:LYS:NZ | 1:A:81:PHE:HB2 | 0.44 | 2.28 | 24 | 1 |
| 1:A:35:PHE:CE2 | 1:A:46:GLY:O | 0.44 | 2.70 | 18 | 4 |
| 1:A:55:LEU:CG | 1:A:93:VAL:HG12 | 0.44 | 2.42 | 6 | 1 |
| 1:A:14:LYS:HB3 | 1:A:80:PHE:CE1 | 0.44 | 2.48 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:56:THR:HB | 1:A:70:LYS:CG | 0.44 | 2.42 | 8 | 2 |
| 1:A:7:ARG:CB | 1:A:28:LEU:CG | 0.44 | 2.96 | 9 | 1 |
| 1:A:70:LYS:HG2 | 1:A:78:ASP:OD1 | 0.44 | 2.12 | 13 | 1 |
| 1:A:14:LYS:CE | 1:A:19:ASN:HB3 | 0.44 | 2.43 | 14 | 1 |
| 1:A:49:PRO:HG3 | 1:A:73:THR:OG1 | 0.44 | 2.13 | 16 | 1 |
| 1:A:70:LYS:CG | 1:A:70:LYS:O | 0.44 | 2.65 | 17 | 1 |
| 1:A:14:LYS:HE3 | 1:A:62:PHE:CE2 | 0.44 | 2.48 | 18 | 1 |
| 1:A:14:LYS:O | 1:A:15:GLY:C | 0.44 | 2.55 | 23 | 2 |
| 1:A:26:VAL:O | 1:A:92:TRP:CH2 | 0.44 | 2.71 | 24 | 1 |
| 1:A:11:LEU:CD2 | 1:A:11:LEU:N | 0.43 | 2.77 | 1 | 2 |
| 1:A:67:PHE:O | 1:A:82:GLN:HG2 | 0.43 | 2.13 | 2 | 3 |
| 1:A:36:TYR:CB | 1:A:41:ASP:HB3 | 0.43 | 2.43 | 3 | 1 |
| 1:A:100:ILE:HG22 | 1:A:101:LYS:N | 0.43 | 2.28 | 11 | 2 |
| 1:A:28:LEU:O | 1:A:28:LEU:CG | 0.43 | 2.66 | 2 | 4 |
| 1:A:14:LYS:HB3 | 1:A:80:PHE:HB2 | 0.43 | 1.90 | 6 | 2 |
| 1:A:15:GLY:O | 1:A:16:SER:HB2 | 0.43 | 2.13 | 8 | 1 |
| 1:A:65:ARG:O | 1:A:67:PHE:N | 0.43 | 2.51 | 11 | 1 |
| 1:A:7:ARG:C | 1:A:8:GLU:OE2 | 0.43 | 2.57 | 14 | 3 |
| 1:A:59:CYS:C | 1:A:60:GLN:CG | 0.43 | 2.86 | 17 | 1 |
| 1:A:45:LYS:HD3 | 1:A:45:LYS:O | 0.43 | 2.13 | 19 | 1 |
| 1:A:13:LYS:HG3 | 1:A:80:PHE:O | 0.43 | 2.13 | 25 | 1 |
| 1:A:59:CYS:O | 1:A:60:GLN:O | 0.43 | 2.37 | 3 | 1 |
| 1:A:28:LEU:HD12 | 1:A:95:ASP:CB | 0.43 | 2.43 | 10 | 1 |
| 1:A:92:TRP:CZ3 | 1:A:96:ILE:HD11 | 0.43 | 2.48 | 24 | 3 |
| 1:A:15:GLY:O | 1:A:16:SER:HB3 | 0.43 | 2.13 | 22 | 1 |
| 1:A:13:LYS:CE | 1:A:81:PHE:HB2 | 0.43 | 2.42 | 6 | 1 |
| 1:A:67:PHE:HA | 1:A:89:ARG:CB | 0.43 | 2.43 | 7 | 2 |
| 1:A:97:ASN:O | 1:A:98:LYS:C | 0.43 | 2.56 | 24 | 2 |
| 1:A:11:LEU:O | 1:A:24:MET:HG3 | 0.43 | 2.14 | 20 | 2 |
| 1:A:14:LYS:CE | 1:A:19:ASN:HB2 | 0.43 | 2.44 | 12 | 1 |
| 1:A:19:ASN:CG | 1:A:19:ASN:O | 0.43 | 2.57 | 12 | 1 |
| 1:A:12:VAL:HA | 1:A:22:LYS:O | 0.43 | 2.13 | 13 | 1 |
| 1:A:30:GLU:O | 1:A:103:ILE:HG12 | 0.43 | 2.14 | 18 | 1 |
| 1:A:11:LEU:O | 1:A:24:MET:HG2 | 0.43 | 2.13 | 4 | 8 |
| 1:A:65:ARG:O | 1:A:66:MET:HB2 | 0.43 | 2.13 | 19 | 3 |
| 1:A:50:LEU:O | 1:A:51:LYS:C | 0.43 | 2.56 | 11 | 5 |
| 1:A:7:ARG:CB | 1:A:28:LEU:CD1 | 0.43 | 2.97 | 9 | 1 |
| 1:A:6:ILE:HB | 1:A:28:LEU:O | 0.43 | 2.14 | 10 | 1 |
| 1:A:34:GLU:HG3 | 1:A:36:TYR:CZ | 0.43 | 2.49 | 14 | 1 |
| 1:A:74:THR:O | 1:A:75:LYS:HB3 | 0.43 | 2.11 | 16 | 1 |
| 1:A:50:LEU:HD23 | 1:A:103:ILE:HG21 | 0.43 | 1.90 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:14:LYS:HB3 | 1:A:80:PHE:CG | 0.43 | 2.47 | 6 | 1 |
| 1:A:63:GLY:HA3 | 1:A:68:VAL:CG1 | 0.43 | 2.44 | 12 | 1 |
| 1:A:70:LYS:CG | 1:A:78:ASP:CG | 0.43 | 2.87 | 13 | 1 |
| 1:A:18:PHE:CE1 | 1:A:19:ASN:O | 0.43 | 2.72 | 24 | 1 |
| 1:A:14:LYS:NZ | 1:A:19:ASN:HA | 0.43 | 2.29 | 1 | 1 |
| 1:A:14:LYS:C | 1:A:14:LYS:CD | 0.43 | 2.87 | 11 | 2 |
| 1:A:6:ILE:HD13 | 1:A:30:GLU:N | 0.43 | 2.29 | 2 | 1 |
| 1:A:77:GLN:O | 1:A:78:ASP:OD1 | 0.43 | 2.36 | 2 | 1 |
| 1:A:60:GLN:CG | 1:A:64:LYS:HA | 0.43 | 2.43 | 6 | 1 |
| 1:A:33:ILE:CD1 | 1:A:50:LEU:CB | 0.43 | 2.96 | 8 | 1 |
| 1:A:34:GLU:CG | 1:A:34:GLU:O | 0.43 | 2.67 | 12 | 2 |
| 1:A:35:PHE:CE1 | 1:A:46:GLY:C | 0.43 | 2.92 | 17 | 3 |
| 1:A:30:GLU:O | 1:A:103:ILE:CB | 0.43 | 2.67 | 18 | 1 |
| 1:A:5:ARG:CD | 1:A:27:VAL:HB | 0.43 | 2.44 | 19 | 1 |
| 1:A:19:ASN:HB2 | 1:A:62:PHE:CZ | 0.43 | 2.48 | 21 | 1 |
| 1:A:6:ILE:CD1 | 1:A:30:GLU:HB3 | 0.43 | 2.44 | 22 | 1 |
| 1:A:50:LEU:HG | 1:A:100:ILE:CD1 | 0.43 | 2.43 | 24 | 1 |
| 1:A:62:PHE:C | 1:A:68:VAL:HG11 | 0.43 | 2.34 | 4 | 1 |
| 1:A:30:GLU:O | 1:A:103:ILE:HB | 0.43 | 2.14 | 6 | 2 |
| 1:A:18:PHE:O | 1:A:19:ASN:OD1 | 0.43 | 2.37 | 6 | 1 |
| 1:A:86:LEU:O | 1:A:87:GLU:C | 0.43 | 2.57 | 21 | 3 |
| 1:A:64:LYS:CD | 1:A:64:LYS:O | 0.43 | 2.67 | 13 | 1 |
| 1:A:82:GLN:HG2 | 1:A:83:ALA:N | 0.43 | 2.29 | 21 | 2 |
| 1:A:29:LEU:HD11 | 1:A:34:GLU:OE2 | 0.43 | 2.13 | 22 | 1 |
| 1:A:85:PHE:O | 1:A:86:LEU:C | 0.43 | 2.57 | 23 | 1 |
| 1:A:105:GLY:O | 1:A:106:LEU:HD22 | 0.43 | 2.13 | 1 | 2 |
| 1:A:26:VAL:CG2 | 1:A:92:TRP:CZ3 | 0.43 | 3.02 | 13 | 1 |
| 1:A:50:LEU:HD12 | 1:A:99:ALA:C | 0.43 | 2.34 | 14 | 1 |
| 1:A:32:GLY:HA2 | 1:A:50:LEU:CG | 0.43 | 2.44 | 17 | 1 |
| 1:A:5:ARG:NE | 1:A:27:VAL:HG21 | 0.43 | 2.24 | 24 | 1 |
| 1:A:28:LEU:HB2 | 1:A:33:ILE:HG12 | 0.43 | 1.90 | 7 | 1 |
| 1:A:70:LYS:HB3 | 1:A:80:PHE:CD2 | 0.43 | 2.48 | 8 | 1 |
| 1:A:34:GLU:CD | 1:A:36:TYR:OH | 0.43 | 2.57 | 18 | 1 |
| 1:A:41:ASP:O | 1:A:42:ASN:HB2 | 0.42 | 2.13 | 1 | 2 |
| 1:A:41:ASP:O | 1:A:42:ASN:CG | 0.42 | 2.57 | 1 | 1 |
| 1:A:45:LYS:HG3 | 1:A:45:LYS:O | 0.42 | 2.14 | 6 | 6 |
| 1:A:33:ILE:O | 1:A:47:MET:HA | 0.42 | 2.14 | 5 | 5 |
| 1:A:31:ASP:OD1 | 1:A:31:ASP:C | 0.42 | 2.58 | 7 | 1 |
| 1:A:85:PHE:CE1 | 1:A:88:GLU:HB2 | 0.42 | 2.49 | 25 | 2 |
| 1:A:14:LYS:HB2 | 1:A:21:TRP:NE1 | 0.42 | 2.28 | 11 | 3 |
| 1:A:67:PHE:HB3 | 1:A:89:ARG:CD | 0.42 | 2.44 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:34:GLU:CG | 1:A:36:TYR:CZ | 0.42 | 3.02 | 14 | 1 |
| 1:A:32:GLY:HA2 | 1:A:50:LEU:HD11 | 0.42 | 1.89 | 17 | 1 |
| 1:A:28:LEU:HB2 | 1:A:33:ILE:CD1 | 0.42 | 2.42 | 23 | 1 |
| 1:A:7:ARG:C | 1:A:8:GLU:OE1 | 0.42 | 2.58 | 3 | 6 |
| 1:A:69:PHE:CE1 | 1:A:81:PHE:HB3 | 0.42 | 2.49 | 9 | 1 |
| 1:A:13:LYS:HE2 | 1:A:81:PHE:CD2 | 0.42 | 2.49 | 10 | 1 |
| 1:A:75:LYS:O | 1:A:76:GLN:HB2 | 0.42 | 2.15 | 12 | 1 |
| 1:A:94:ARG:HG3 | 1:A:95:ASP:N | 0.42 | 2.29 | 20 | 2 |
| 1:A:35:PHE:CD1 | 1:A:46:GLY:O | 0.42 | 2.72 | 25 | 2 |
| 1:A:74:THR:O | 1:A:75:LYS:CG | 0.42 | 2.67 | 19 | 1 |
| 1:A:25:TRP:CD1 | 1:A:39:LYS:O | 0.42 | 2.72 | 24 | 1 |
| 1:A:13:LYS:HG2 | 1:A:80:PHE:O | 0.42 | 2.15 | 24 | 1 |
| 1:A:90:ASP:O | 1:A:94:ARG:HB3 | 0.42 | 2.15 | 1 | 2 |
| 1:A:72:THR:HA | 1:A:77:GLN:O | 0.42 | 2.14 | 2 | 1 |
| 1:A:14:LYS:HB2 | 1:A:20:THR:O | 0.42 | 2.14 | 15 | 3 |
| 1:A:17:VAL:HG13 | 1:A:18:PHE:CD2 | 0.42 | 2.48 | 5 | 1 |
| 1:A:59:CYS:CA | 1:A:70:LYS:HD3 | 0.42 | 2.44 | 8 | 1 |
| 1:A:40:SER:O | 1:A:41:ASP:C | 0.42 | 2.57 | 9 | 2 |
| 1:A:89:ARG:HD3 | 1:A:90:ASP:N | 0.42 | 2.29 | 15 | 1 |
| 1:A:33:ILE:HD13 | 1:A:33:ILE:N | 0.42 | 2.30 | 25 | 1 |
| 1:A:36:TYR:CE1 | 1:A:44:PRO:HG3 | 0.42 | 2.48 | 25 | 1 |
| 1:A:14:LYS:HB2 | 1:A:80:PHE:CB | 0.42 | 2.45 | 6 | 1 |
| 1:A:52:GLY:C | 1:A:53:SER:OG | 0.42 | 2.57 | 10 | 1 |
| 1:A:50:LEU:HD23 | 1:A:99:ALA:O | 0.42 | 2.13 | 21 | 1 |
| 1:A:67:PHE:CE1 | 1:A:84:ALA:O | 0.42 | 2.73 | 22 | 1 |
| 1:A:87:GLU:O | 1:A:88:GLU:C | 0.42 | 2.57 | 22 | 1 |
| 1:A:21:TRP:CE2 | 1:A:62:PHE:HB3 | 0.42 | 2.49 | 7 | 1 |
| 1:A:12:VAL:HB | 1:A:23:PRO:CA | 0.42 | 2.44 | 13 | 1 |
| 1:A:93:VAL:O | 1:A:97:ASN:HB2 | 0.42 | 2.14 | 8 | 2 |
| 1:A:7:ARG:HB2 | 1:A:95:ASP:CG | 0.42 | 2.35 | 10 | 1 |
| 1:A:7:ARG:HB3 | 1:A:28:LEU:HD23 | 0.42 | 1.91 | 12 | 1 |
| 1:A:66:MET:O | 1:A:67:PHE:HB2 | 0.42 | 2.14 | 16 | 1 |
| 1:A:19:ASN:OD1 | 1:A:19:ASN:C | 0.42 | 2.58 | 20 | 1 |
| 1:A:28:LEU:HG | 1:A:28:LEU:O | 0.42 | 2.14 | 20 | 1 |
| 1:A:18:PHE:CZ | 1:A:20:THR:CG2 | 0.42 | 3.01 | 21 | 1 |
| 1:A:55:LEU:CG | 1:A:93:VAL:CG2 | 0.42 | 2.98 | 22 | 1 |
| 1:A:7:ARG:HG3 | 1:A:95:ASP:OD2 | 0.42 | 2.14 | 3 | 4 |
| 1:A:77:GLN:O | 1:A:78:ASP:C | 0.42 | 2.57 | 6 | 1 |
| 1:A:25:TRP:CG | 1:A:38:LYS:O | 0.42 | 2.73 | 11 | 1 |
| 1:A:48:ILE:HG21 | 1:A:71:ILE:HG21 | 0.42 | 1.91 | 21 | 1 |
| 1:A:90:ASP:O | 1:A:94:ARG:CB | 0.42 | 2.67 | 9 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:55:LEU:HD23 | 1:A:71:ILE:HG13 | 0.42 | 1.89 | 6 | 2 |
| 1:A:33:ILE:HD11 | 1:A:100:ILE:HD11 | 0.42 | 1.91 | 6 | 1 |
| 1:A:16:SER:O | 1:A:17:VAL:HB | 0.42 | 2.15 | 7 | 1 |
| 1:A:28:LEU:HD12 | 1:A:95:ASP:OD1 | 0.42 | 2.14 | 10 | 1 |
| 1:A:31:ASP:C | 1:A:31:ASP:OD1 | 0.42 | 2.58 | 11 | 3 |
| 1:A:56:THR:HB | 1:A:70:LYS:O | 0.42 | 2.15 | 23 | 3 |
| 1:A:83:ALA:CB | 1:A:89:ARG:HA | 0.42 | 2.45 | 15 | 1 |
| 1:A:86:LEU:CD1 | 1:A:89:ARG:HD2 | 0.42 | 2.45 | 24 | 1 |
| 1:A:26:VAL:HB | 1:A:35:PHE:HB2 | 0.42 | 1.92 | 4 | 1 |
| 1:A:18:PHE:C | 1:A:19:ASN:OD1 | 0.42 | 2.58 | 6 | 1 |
| 1:A:86:LEU:HD13 | 1:A:87:GLU:HA | 0.42 | 1.90 | 6 | 1 |
| 1:A:55:LEU:CD2 | 1:A:69:PHE:CG | 0.42 | 3.03 | 9 | 1 |
| 1:A:18:PHE:C | 1:A:20:THR:N | 0.42 | 2.71 | 15 | 1 |
| 1:A:17:VAL:O | 1:A:18:PHE:HB2 | 0.42 | 2.15 | 17 | 1 |
| 1:A:67:PHE:CE1 | 1:A:86:LEU:CA | 0.42 | 3.03 | 17 | 1 |
| 1:A:53:SER:OG | 1:A:71:ILE:HG23 | 0.42 | 2.15 | 1 | 1 |
| 1:A:63:GLY:HA2 | 1:A:68:VAL:HG11 | 0.42 | 1.92 | 2 | 1 |
| 1:A:65:ARG:C | 1:A:66:MET:CG | 0.42 | 2.88 | 5 | 1 |
| 1:A:51:LYS:O | 1:A:104:GLU:CD | 0.42 | 2.59 | 7 | 1 |
| 1:A:86:LEU:O | 1:A:89:ARG:HB3 | 0.42 | 2.15 | 9 | 1 |
| 1:A:28:LEU:N | 1:A:28:LEU:CD2 | 0.42 | 2.79 | 10 | 1 |
| 1:A:100:ILE:O | 1:A:103:ILE:HG22 | 0.42 | 2.14 | 12 | 1 |
| 1:A:29:LEU:O | 1:A:50:LEU:HD13 | 0.42 | 2.15 | 12 | 1 |
| 1:A:50:LEU:HG | 1:A:50:LEU:O | 0.42 | 2.14 | 14 | 1 |
| 1:A:59:CYS:O | 1:A:60:GLN:HB3 | 0.42 | 2.15 | 17 | 2 |
| 1:A:67:PHE:O | 1:A:82:GLN:HG3 | 0.42 | 2.15 | 22 | 1 |
| 1:A:11:LEU:CD2 | 1:A:26:VAL:HG13 | 0.42 | 2.43 | 24 | 1 |
| 1:A:90:ASP:CA | 1:A:93:VAL:HG22 | 0.41 | 2.44 | 7 | 2 |
| 1:A:91:ALA:O | 1:A:95:ASP:HB2 | 0.41 | 2.14 | 12 | 2 |
| 1:A:53:SER:CB | 1:A:100:ILE:HG21 | 0.41 | 2.42 | 16 | 1 |
| 1:A:45:LYS:HD2 | 1:A:45:LYS:O | 0.41 | 2.15 | 16 | 1 |
| 1:A:63:GLY:C | 1:A:65:ARG:N | 0.41 | 2.73 | 25 | 2 |
| 1:A:24:MET:CE | 1:A:45:LYS:HE3 | 0.41 | 2.45 | 17 | 1 |
| 1:A:90:ASP:OD1 | 1:A:93:VAL:CG2 | 0.41 | 2.68 | 2 | 1 |
| 1:A:28:LEU:HD21 | 1:A:95:ASP:CB | 0.41 | 2.45 | 2 | 1 |
| 1:A:73:THR:HG23 | 1:A:77:GLN:H | 0.41 | 1.75 | 4 | 1 |
| 1:A:21:TRP:CH2 | 1:A:80:PHE:C | 0.41 | 2.93 | 8 | 1 |
| 1:A:15:GLY:C | 1:A:16:SER:OG | 0.41 | 2.57 | 11 | 1 |
| 1:A:41:ASP:OD2 | 1:A:43:SER:HB3 | 0.41 | 2.14 | 11 | 1 |
| 1:A:67:PHE:O | 1:A:82:GLN:HA | 0.41 | 2.16 | 2 | 3 |
| 1:A:100:ILE:O | 1:A:104:GLU:HG3 | 0.41 | 2.15 | 12 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:TRP:O | 1:A:22:LYS:HG2 | 0.41 | 2.16 | 12 | 1 |
| 1:A:7:ARG:HB3 | 1:A:28:LEU:HG | 0.41 | 1.92 | 14 | 2 |
| 1:A:50:LEU:O | 1:A:103:ILE:HB | 0.41 | 2.15 | 16 | 1 |
| 1:A:60:GLN:HG2 | 1:A:62:PHE:CD2 | 0.41 | 2.51 | 16 | 1 |
| 1:A:5:ARG:CB | 1:A:29:LEU:HD23 | 0.41 | 2.46 | 19 | 1 |
| 1:A:75:LYS:O | 1:A:76:GLN:HB3 | 0.41 | 2.15 | 20 | 1 |
| 1:A:45:LYS:CD | 1:A:45:LYS:C | 0.41 | 2.89 | 22 | 1 |
| 1:A:50:LEU:C | 1:A:50:LEU:CD2 | 0.41 | 2.83 | 8 | 1 |
| 1:A:33:ILE:CG2 | 1:A:48:ILE:HG12 | 0.41 | 2.46 | 9 | 1 |
| 1:A:47:MET:C | 1:A:48:ILE:HD13 | 0.41 | 2.35 | 9 | 1 |
| 1:A:69:PHE:CZ | 1:A:71:ILE:CD1 | 0.41 | 3.04 | 9 | 1 |
| 1:A:96:ILE:O | 1:A:100:ILE:HG13 | 0.41 | 2.15 | 12 | 1 |
| 1:A:85:PHE:CE1 | 1:A:87:GLU:HB3 | 0.41 | 2.50 | 14 | 1 |
| 1:A:29:LEU:HD11 | 1:A:34:GLU:CG | 0.41 | 2.46 | 16 | 1 |
| 1:A:34:GLU:HG3 | 1:A:36:TYR:CE1 | 0.41 | 2.50 | 18 | 1 |
| 1:A:28:LEU:HA | 1:A:33:ILE:HD12 | 0.41 | 1.91 | 19 | 1 |
| 1:A:90:ASP:OD1 | 1:A:93:VAL:HG21 | 0.41 | 2.16 | 2 | 1 |
| 1:A:12:VAL:O | 1:A:81:PHE:HB2 | 0.41 | 2.16 | 5 | 4 |
| 1:A:29:LEU:HD12 | 1:A:33:ILE:HA | 0.41 | 1.93 | 5 | 1 |
| 1:A:55:LEU:HD11 | 1:A:57:SER:HB3 | 0.41 | 1.93 | 5 | 1 |
| 1:A:86:LEU:CD1 | 1:A:86:LEU:C | 0.41 | 2.81 | 6 | 1 |
| 1:A:34:GLU:CB | 1:A:47:MET:HG2 | 0.41 | 2.44 | 11 | 1 |
| 1:A:53:SER:HA | 1:A:74:THR:N | 0.41 | 2.30 | 15 | 1 |
| 1:A:55:LEU:C | 1:A:55:LEU:HD23 | 0.41 | 2.30 | 16 | 1 |
| 1:A:66:MET:O | 1:A:89:ARG:HD2 | 0.41 | 2.16 | 19 | 1 |
| 1:A:60:GLN:C | 1:A:61:ASP:OD1 | 0.41 | 2.59 | 21 | 1 |
| 1:A:27:VAL:HG23 | 1:A:34:GLU:HG2 | 0.41 | 1.93 | 22 | 1 |
| 1:A:45:LYS:O | 1:A:45:LYS:HG3 | 0.41 | 2.16 | 2 | 2 |
| 1:A:67:PHE:CE2 | 1:A:86:LEU:HA | 0.41 | 2.51 | 3 | 1 |
| 1:A:50:LEU:CD2 | 1:A:100:ILE:HA | 0.41 | 2.45 | 4 | 1 |
| 1:A:60:GLN:O | 1:A:61:ASP:HB3 | 0.41 | 2.15 | 5 | 1 |
| 1:A:38:LYS:C | 1:A:40:SER:N | 0.41 | 2.74 | 6 | 6 |
| 1:A:65:ARG:O | 1:A:66:MET:HB3 | 0.41 | 2.15 | 7 | 1 |
| 1:A:7:ARG:HG2 | 1:A:95:ASP:OD2 | 0.41 | 2.14 | 9 | 1 |
| 1:A:53:SER:HA | 1:A:73:THR:HA | 0.41 | 1.92 | 10 | 1 |
| 1:A:28:LEU:HD11 | 1:A:95:ASP:OD2 | 0.41 | 2.15 | 11 | 1 |
| 1:A:13:LYS:CE | 1:A:81:PHE:CB | 0.41 | 2.98 | 16 | 1 |
| 1:A:64:LYS:HG3 | 1:A:64:LYS:O | 0.41 | 2.16 | 2 | 1 |
| 1:A:21:TRP:CZ3 | 1:A:68:VAL:HG23 | 0.41 | 2.51 | 8 | 1 |
| 1:A:13:LYS:HE2 | 1:A:80:PHE:O | 0.41 | 2.16 | 9 | 1 |
| 1:A:51:LYS:O | 1:A:51:LYS:HG2 | 0.41 | 2.16 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:70:LYS:HG3 | 1:A:70:LYS:O | 0.41 | 2.16 | 17 | 1 |
| 1:A:29:LEU:HB2 | 1:A:32:GLY:O | 0.41 | 2.16 | 18 | 1 |
| 1:A:78:ASP:N | 1:A:78:ASP:OD1 | 0.41 | 2.52 | 24 | 1 |
| 1:A:56:THR:O | 1:A:69:PHE:HB2 | 0.41 | 2.16 | 3 | 2 |
| 1:A:69:PHE:HD2 | 1:A:93:VAL:HG12 | 0.41 | 1.72 | 5 | 1 |
| 1:A:21:TRP:CZ2 | 1:A:68:VAL:HG21 | 0.41 | 2.50 | 5 | 1 |
| 1:A:66:MET:O | 1:A:89:ARG:HD3 | 0.41 | 2.16 | 10 | 1 |
| 1:A:50:LEU:HA | 1:A:53:SER:OG | 0.41 | 2.16 | 14 | 1 |
| 1:A:102:CYS:SG | 1:A:106:LEU:HG | 0.41 | 2.55 | 17 | 1 |
| 1:A:86:LEU:HD12 | 1:A:89:ARG:CD | 0.41 | 2.46 | 24 | 1 |
| 1:A:93:VAL:HG23 | 1:A:94:ARG:N | 0.41 | 2.30 | 4 | 2 |
| 1:A:14:LYS:CD | 1:A:62:PHE:CD2 | 0.41 | 3.04 | 7 | 1 |
| 1:A:62:PHE:N | 1:A:62:PHE:CD1 | 0.41 | 2.88 | 8 | 1 |
| 1:A:28:LEU:HD21 | 1:A:92:TRP:CE3 | 0.41 | 2.50 | 9 | 1 |
| 1:A:73:THR:HG21 | 1:A:77:GLN:HB2 | 0.41 | 1.92 | 10 | 1 |
| 1:A:59:CYS:HG | 1:A:68:VAL:C | 0.41 | 2.20 | 16 | 1 |
| 1:A:14:LYS:HG3 | 1:A:14:LYS:O | 0.40 | 2.16 | 1 | 1 |
| 1:A:67:PHE:HB3 | 1:A:89:ARG:HB2 | 0.40 | 1.93 | 1 | 1 |
| 1:A:11:LEU:HB3 | 1:A:82:GLN:O | 0.40 | 2.16 | 12 | 2 |
| 1:A:59:CYS:HB2 | 1:A:70:LYS:HB2 | 0.40 | 1.93 | 7 | 1 |
| 1:A:14:LYS:CE | 1:A:19:ASN:HA | 0.40 | 2.47 | 8 | 1 |
| 1:A:14:LYS:HG3 | 1:A:62:PHE:CZ | 0.40 | 2.51 | 11 | 1 |
| 1:A:16:SER:HB3 | 1:A:45:LYS:HE2 | 0.40 | 1.93 | 12 | 1 |
| 1:A:13:LYS:O | 1:A:14:LYS:O | 0.40 | 2.39 | 13 | 1 |
| 1:A:64:LYS:O | 1:A:65:ARG:HG3 | 0.40 | 2.16 | 17 | 1 |
| 1:A:56:THR:CB | 1:A:70:LYS:HE3 | 0.40 | 2.46 | 18 | 1 |
| 1:A:32:GLY:C | 1:A:33:ILE:HD12 | 0.40 | 2.37 | 20 | 1 |
| 1:A:28:LEU:HB3 | 1:A:92:TRP:CZ3 | 0.40 | 2.51 | 20 | 1 |
| 1:A:51:LYS:O | 1:A:51:LYS:HG3 | 0.40 | 2.17 | 8 | 1 |
| 1:A:6:ILE:N | 1:A:28:LEU:O | 0.40 | 2.55 | 9 | 1 |
| 1:A:51:LYS:HB2 | 1:A:103:ILE:CG2 | 0.40 | 2.47 | 13 | 1 |
| 1:A:13:LYS:HG3 | 1:A:81:PHE:HB2 | 0.40 | 1.92 | 13 | 1 |
| 1:A:105:GLY:O | 1:A:106:LEU:C | 0.40 | 2.57 | 19 | 1 |
| 1:A:98:LYS:O | 1:A:102:CYS:HB3 | 0.40 | 2.16 | 19 | 1 |
| 1:A:66:MET:HB2 | 1:A:82:GLN:NE2 | 0.40 | 2.31 | 9 | 1 |
| 1:A:88:GLU:O | 1:A:91:ALA:HB3 | 0.40 | 2.14 | 9 | 1 |
| 1:A:34:GLU:C | 1:A:34:GLU:CD | 0.40 | 2.80 | 14 | 1 |
| 1:A:69:PHE:HE1 | 1:A:71:ILE:HD12 | 0.40 | 1.75 | 18 | 1 |
| 1:A:60:GLN:O | 1:A:61:ASP:C | 0.40 | 2.59 | 20 | 1 |
| 1:A:50:LEU:HB2 | 1:A:103:ILE:HG21 | 0.40 | 1.93 | 6 | 1 |
| 1:A:67:PHE:O | 1:A:82:GLN:HB2 | 0.40 | 2.16 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:16:SER:CB | 1:A:45:LYS:HE2 | 0.40 | 2.47 | 12 | 1 |
| 1:A:50:LEU:HD12 | 1:A:103:ILE:CB | 0.40 | 2.44 | 19 | 1 |
| 1:A:98:LYS:O | 1:A:102:CYS:HB2 | 0.40 | 2.16 | 22 | 1 |
| 1:A:20:THR:O | 1:A:21:TRP:HB2 | 0.40 | 2.15 | 24 | 1 |
| 1:A:28:LEU:HA | 1:A:33:ILE:CG2 | 0.40 | 2.40 | 1 | 1 |
| 1:A:5:ARG:HD3 | 1:A:27:VAL:CB | 0.40 | 2.46 | 1 | 1 |
| 1:A:30:GLU:O | 1:A:50:LEU:HD23 | 0.40 | 2.15 | 2 | 1 |
| 1:A:6:ILE:HB | 1:A:28:LEU:CD1 | 0.40 | 2.46 | 12 | 1 |
| 1:A:14:LYS:CB | 1:A:21:TRP:NE1 | 0.40 | 2.84 | 24 | 1 |
| 1:A:60:GLN:HB3 | 1:A:68:VAL:CG1 | 0.40 | 2.47 | 25 | 1 |

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 102/113 (90%) | 77±4 (75±4%) | 18±4 (18±4%) | 7±2 (7±2%) | 3 | 18 |
| All | All | 2550/2825 (90%) | 1915 (75%) | 461 (18%) | 174 (7%) | 3 | 18 |

All 33 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 42 | ASN | 18 |
| 1 | A | 17 | VAL | 14 |
| 1 | A | 5 | ARG | 12 |
| 1 | A | 66 | MET | 12 |
| 1 | A | 18 | PHE | 9 |
| 1 | A | 64 | LYS | 9 |
| 1 | A | 16 | SER | 9 |
| 1 | A | 75 | LYS | 9 |
| 1 | A | 60 | GLN | 8 |
| 1 | A | 19 | ASN | 8 |
| 1 | A | 84 | ALA | 7 |
| 1 | A | 65 | ARG | 7 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 76 | GLN | 6 |
| 1 | A | 73 | THR | 6 |
| 1 | A | 74 | THR | 6 |
| 1 | A | 15 | GLY | 4 |
| 1 | A | 61 | ASP | 4 |
| 1 | A | 53 | SER | 4 |
| 1 | A | 52 | GLY | 3 |
| 1 | A | 6 | ILE | 2 |
| 1 | A | 8 | GLU | 2 |
| 1 | A | 87 | GLU | 2 |
| 1 | A | 23 | PRO | 2 |
| 1 | A | 51 | LYS | 2 |
| 1 | A | 67 | PHE | 1 |
| 1 | A | 103 | ILE | 1 |
| 1 | A | 40 | SER | 1 |
| 1 | A | 63 | GLY | 1 |
| 1 | A | 24 | MET | 1 |
| 1 | A | 85 | PHE | 1 |
| 1 | A | 58 | PRO | 1 |
| 1 | A | 21 | TRP | 1 |
| 1 | A | 14 | LYS | 1 |

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 | 91/102 (89%) | 58±4 (64±5%) | 33±4 (36±5%) | 1 | 8 |
| All | All | 2275/2550 (89%) | 1446 (64%) | 829 (36%) | 1 | 8 |

All 76 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 54 | THR | 25 |
| 1 | A | 36 | TYR | 25 |
| 1 | A | 11 | LEU | 25 |
| 1 | A | 40 | SER | 24 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 85 | PHE | 24 |
| 1 | A | 74 | THR | 24 |
| 1 | A | 26 | VAL | 23 |
| 1 | A | 81 | PHE | 22 |
| 1 | A | 89 | ARG | 21 |
| 1 | A | 5 | ARG | 20 |
| 1 | A | 7 | ARG | 20 |
| 1 | A | 38 | LYS | 19 |
| 1 | A | 50 | LEU | 19 |
| 1 | A | 86 | LEU | 19 |
| 1 | A | 77 | GLN | 18 |
| 1 | A | 76 | GLN | 17 |
| 1 | A | 39 | LYS | 17 |
| 1 | A | 37 | LYS | 17 |
| 1 | A | 51 | LYS | 16 |
| 1 | A | 95 | ASP | 16 |
| 1 | A | 13 | LYS | 15 |
| 1 | A | 53 | SER | 15 |
| 1 | A | 106 | LEU | 14 |
| 1 | A | 45 | LYS | 14 |
| 1 | A | 102 | CYS | 14 |
| 1 | A | 75 | LYS | 14 |
| 1 | A | 87 | GLU | 13 |
| 1 | A | 14 | LYS | 13 |
| 1 | A | 80 | PHE | 13 |
| 1 | A | 69 | PHE | 12 |
| 1 | A | 62 | PHE | 12 |
| 1 | A | 24 | MET | 12 |
| 1 | A | 98 | LYS | 12 |
| 1 | A | 68 | VAL | 11 |
| 1 | A | 65 | ARG | 11 |
| 1 | A | 60 | GLN | 11 |
| 1 | A | 64 | LYS | 11 |
| 1 | A | 28 | LEU | 10 |
| 1 | A | 30 | GLU | 10 |
| 1 | A | 90 | ASP | 10 |
| 1 | A | 101 | LYS | 10 |
| 1 | A | 16 | SER | 9 |
| 1 | A | 57 | SER | 8 |
| 1 | A | 70 | LYS | 8 |
| 1 | A | 8 | GLU | 8 |
| 1 | A | 82 | GLN | 8 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 59 | CYS | 7 |
| 1 | A | 67 | PHE | 7 |
| 1 | A | 18 | PHE | 7 |
| 1 | A | 94 | ARG | 7 |
| 1 | A | 43 | SER | 7 |
| 1 | A | 19 | ASN | 7 |
| 1 | A | 42 | ASN | 6 |
| 1 | A | 66 | MET | 6 |
| 1 | A | 22 | LYS | 6 |
| 1 | A | 88 | GLU | 6 |
| 1 | A | 93 | VAL | 5 |
| 1 | A | 61 | ASP | 5 |
| 1 | A | 55 | LEU | 4 |
| 1 | A | 103 | ILE | 4 |
| 1 | A | 20 | THR | 4 |
| 1 | A | 73 | THR | 4 |
| 1 | A | 17 | VAL | 4 |
| 1 | A | 31 | ASP | 4 |
| 1 | A | 47 | MET | 3 |
| 1 | A | 10 | TYR | 2 |
| 1 | A | 104 | GLU | 2 |
| 1 | A | 71 | ILE | 2 |
| 1 | A | 92 | TRP | 2 |
| 1 | A | 100 | ILE | 2 |
| 1 | A | 12 | VAL | 2 |
| 1 | A | 96 | ILE | 1 |
| 1 | A | 78 | ASP | 1 |
| 1 | A | 48 | ILE | 1 |
| 1 | A | 21 | TRP | 1 |
| 1 | A | 97 | ASN | 1 |

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided