



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:49 PM BST

PDB ID : 1LUI
Title : NMR Structures of Itk SH2 domain, Pro287cis isoform, ensemble of 20 low energy structures
Authors : Mallis, R.J.; Brazin, K.N.; Fulton, B.F.; Andreotti, A.M.
Deposited on : 2002-05-22

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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

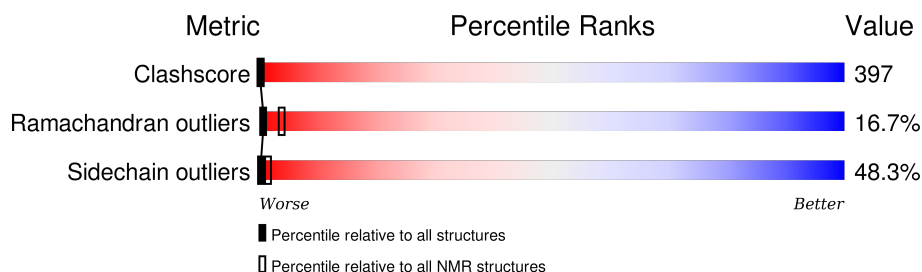
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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 | 114402 | 11133 |
| Ramachandran outliers | 111179 | 9975 |
| Sidechain outliers | 111093 | 9958 |

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 | 110 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:6-A:53, A:60-A:70, A:74-A:111 (97) | 0.35 | 11 |

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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1764 atoms, of which 877 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tyrosine-protein kinase ITK/TSK.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 110 | Total | C | H | N | O | S | 1 |
| | | | 1764 | 567 | 877 | 151 | 166 | 3 | |

There is a discrepancy between the modelled and reference sequences:

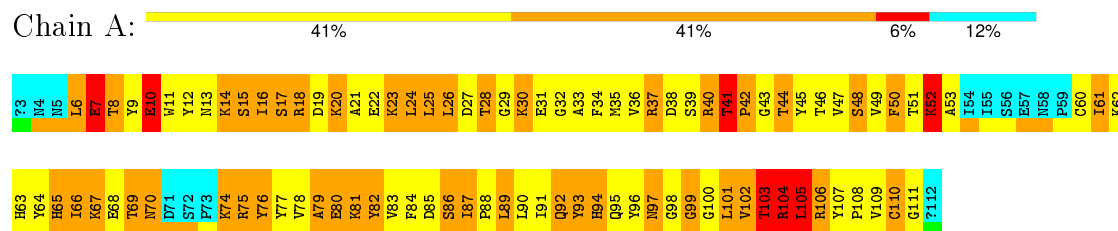
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | 111 | GLY | - | CLONING ARTIFACT | UNP Q03526 |

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: Tyrosine-protein kinase ITK/TSK

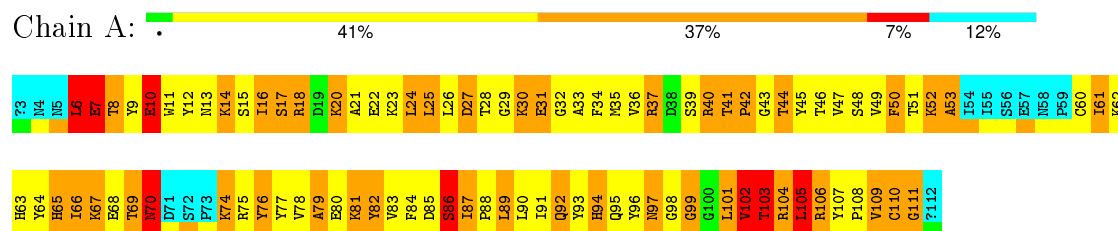


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

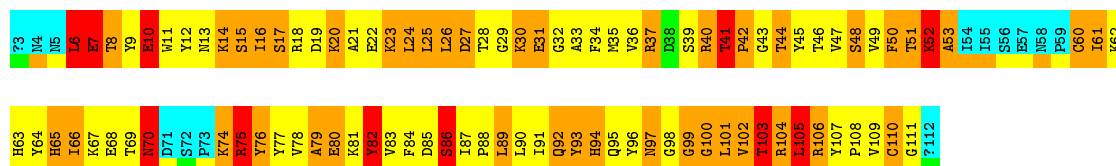
- Molecule 1: Tyrosine-protein kinase ITK/TSK



4.2.2 Score per residue for model 2

- Molecule 1: Tyrosine-protein kinase ITK/TSK

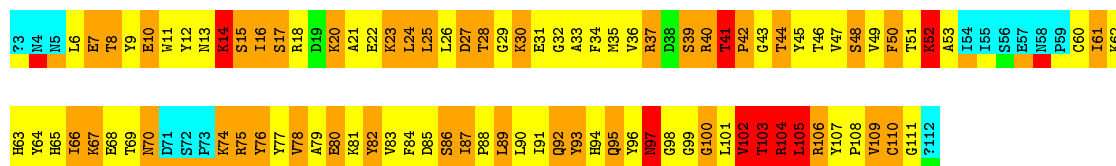




4.2.3 Score per residue for model 3

- Molecule 1: Tyrosine-protein kinase ITK/TSK

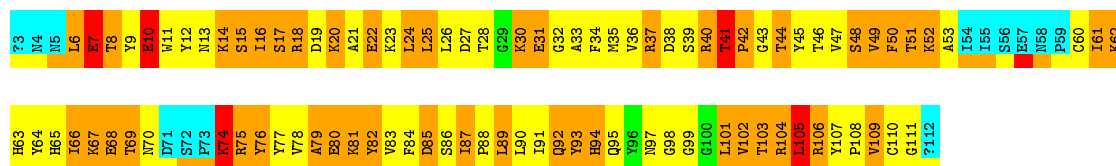
Chain A: .



4.2.4 Score per residue for model 4

- Molecule 1: Tyrosine-protein kinase ITK/TSK

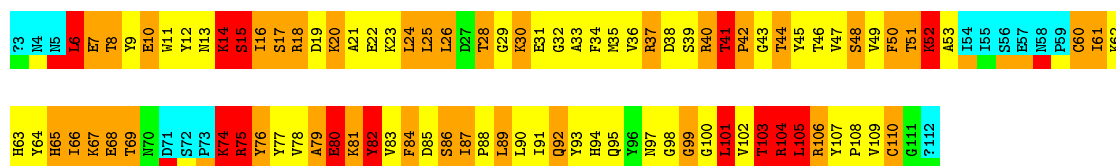
Chain A: .



4.2.5 Score per residue for model 5

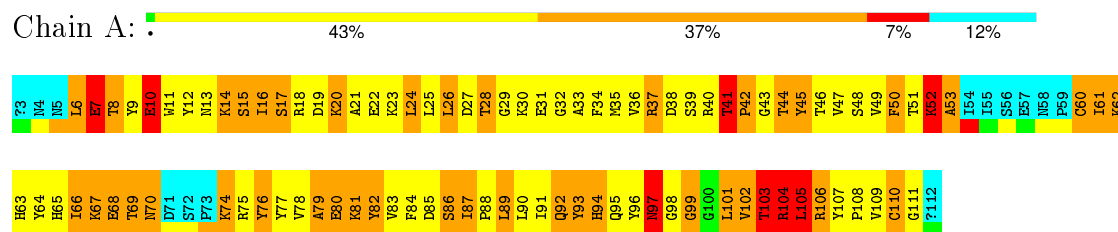
- Molecule 1: Tyrosine-protein kinase ITK/TSK

Chain A: .



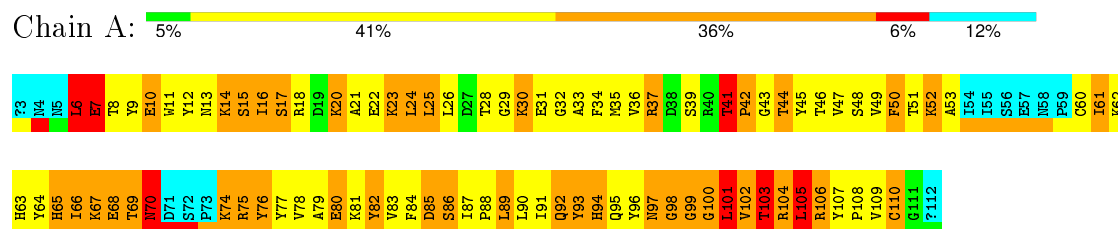
4.2.6 Score per residue for model 6

- Molecule 1: Tyrosine-protein kinase ITK/TSK



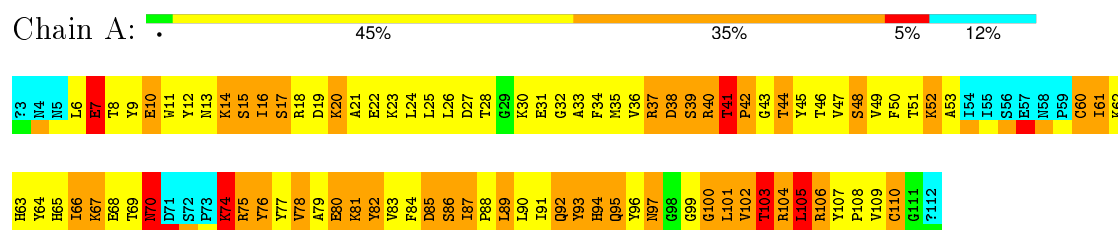
4.2.7 Score per residue for model 7

- Molecule 1: Tyrosine-protein kinase ITK/TSK



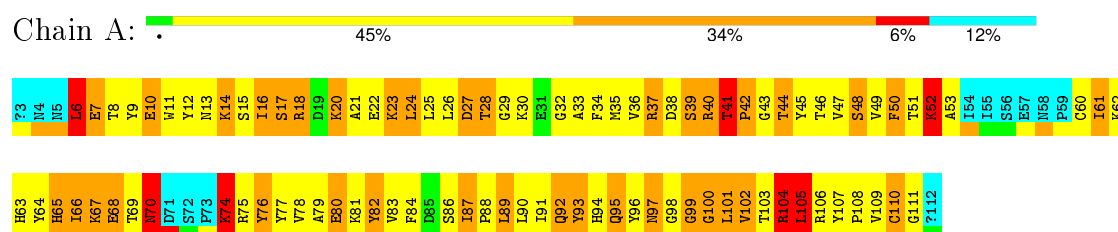
4.2.8 Score per residue for model 8

- Molecule 1: Tyrosine-protein kinase ITK/TSK



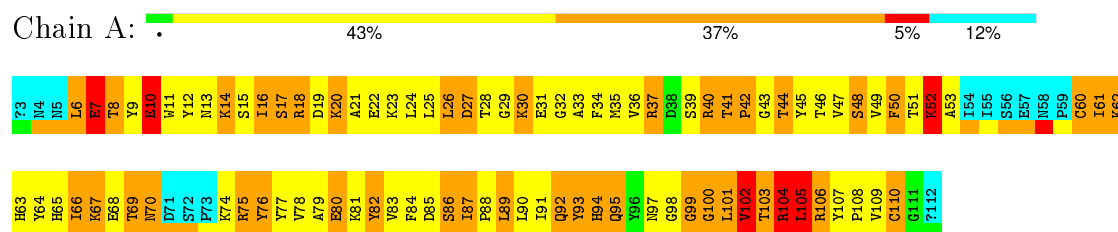
4.2.9 Score per residue for model 9

- Molecule 1: Tyrosine-protein kinase ITK/TSK



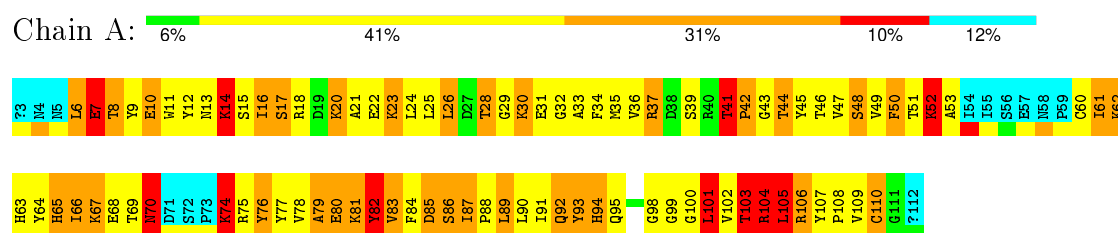
4.2.10 Score per residue for model 10

- Molecule 1: Tyrosine-protein kinase ITK/TSK



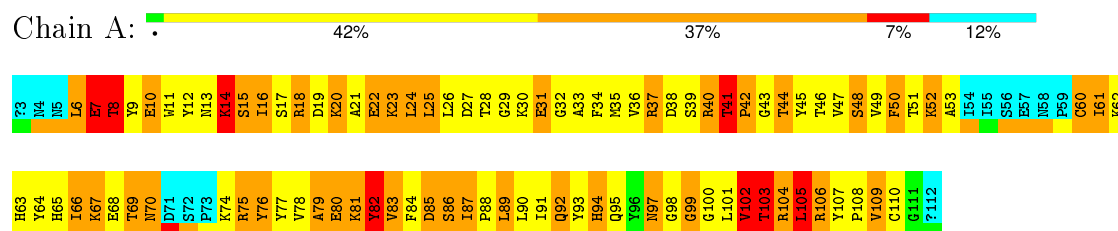
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Tyrosine-protein kinase ITK/TSK



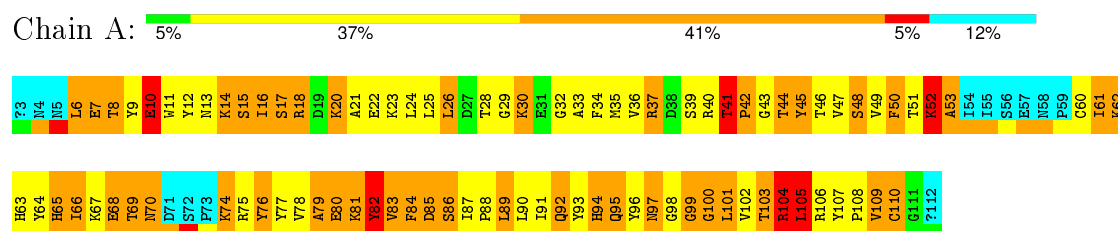
4.2.12 Score per residue for model 12

- Molecule 1: Tyrosine-protein kinase ITK/TSK



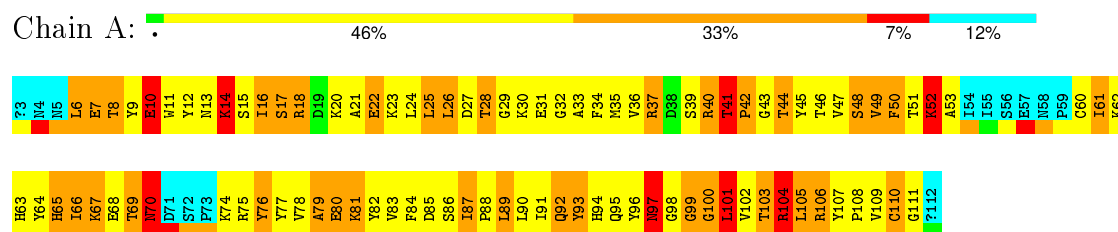
4.2.13 Score per residue for model 13

- Molecule 1: Tyrosine-protein kinase ITK/TSK



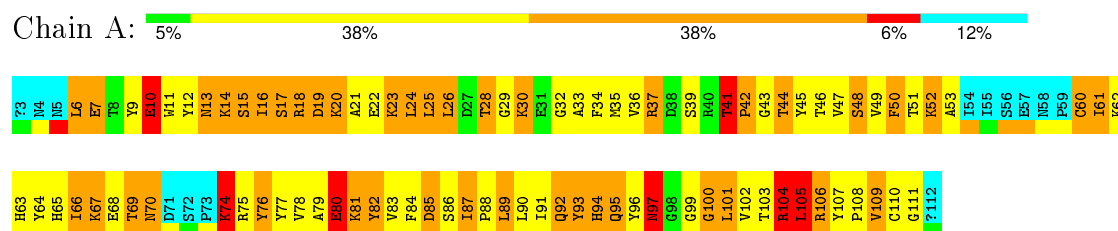
4.2.14 Score per residue for model 14

- Molecule 1: Tyrosine-protein kinase ITK/TSK



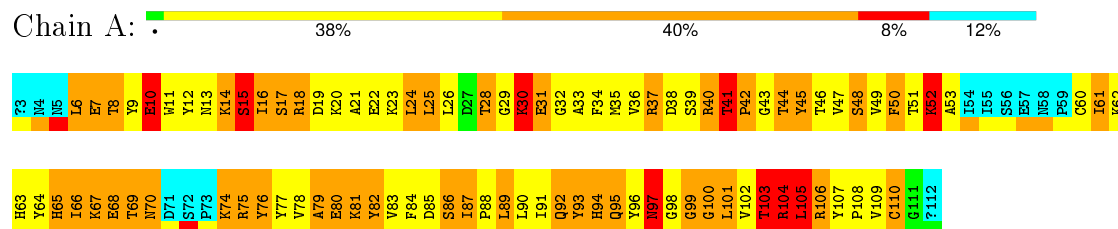
4.2.15 Score per residue for model 15

- Molecule 1: Tyrosine-protein kinase ITK/TSK



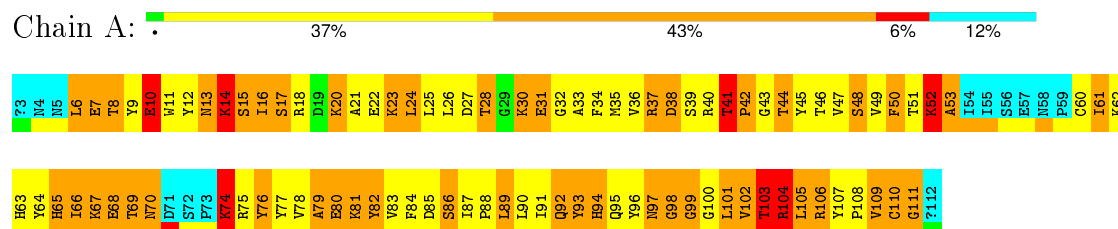
4.2.16 Score per residue for model 16

- Molecule 1: Tyrosine-protein kinase ITK/TSK



4.2.17 Score per residue for model 17

- Molecule 1: Tyrosine-protein kinase ITK/TSK



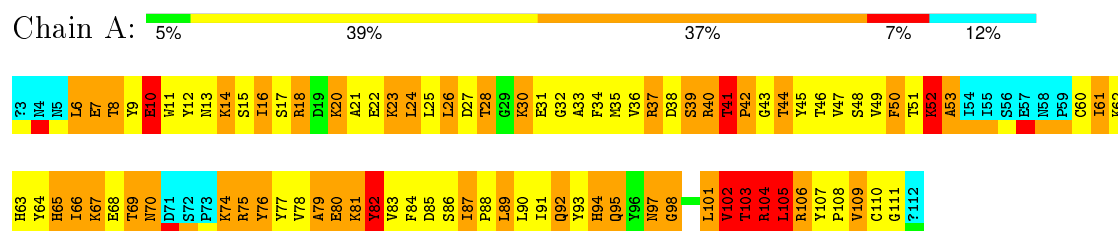
4.2.18 Score per residue for model 18

- Molecule 1: Tyrosine-protein kinase ITK/TSK



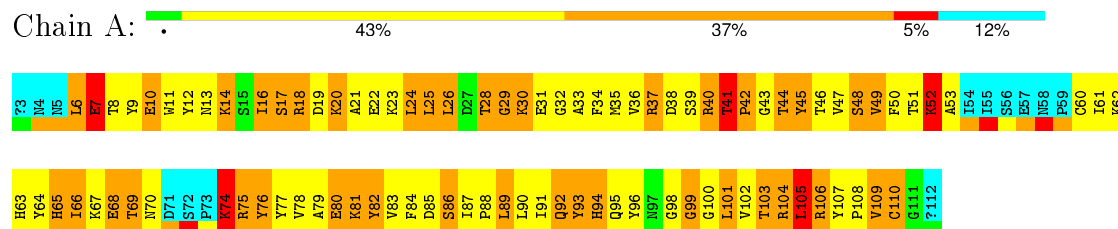
4.2.19 Score per residue for model 19

- Molecule 1: Tyrosine-protein kinase ITK/TSK



4.2.20 Score per residue for model 20

- Molecule 1: Tyrosine-protein kinase ITK/TSK



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry and simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| CNS | refinement | 1.0 |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| | |
|--|-----------------|
| Chemical shift file(s) | BMRB entry 5461 |
| Number of chemical shift lists | 2 |
| Total number of shifts | 2441 |
| Number of shifts mapped to atoms | 2315 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 126 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 81% |

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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 | 800 | 798 | 797 | 634±21 |
| All | All | 16000 | 15960 | 15940 | 12672 |

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 397.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:6:LEU:HD12 | 1:A:12:TYR:CD1 | 1.27 | 1.62 | 10 | 20 |
| 1:A:34:PHE:CG | 1:A:105:LEU:HD12 | 1.24 | 1.64 | 17 | 17 |
| 1:A:94:HIS:CB | 1:A:105:LEU:HD22 | 1.24 | 1.60 | 6 | 17 |
| 1:A:94:HIS:CD2 | 1:A:101:LEU:HD22 | 1.24 | 1.66 | 3 | 11 |
| 1:A:11:TRP:CG | 1:A:34:PHE:CE2 | 1.23 | 2.26 | 15 | 20 |
| 1:A:74:LYS:CG | 1:A:83:VAL:HG23 | 1.22 | 1.65 | 8 | 1 |
| 1:A:24:LEU:HD23 | 1:A:25:LEU:N | 1.21 | 1.48 | 20 | 3 |
| 1:A:24:LEU:HD11 | 1:A:35:MET:SD | 1.20 | 1.77 | 12 | 15 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:CG2 | 1.20 | 1.67 | 1 | 8 |
| 1:A:25:LEU:HD11 | 1:A:48:SER:OG | 1.19 | 1.37 | 16 | 9 |
| 1:A:6:LEU:O | 1:A:8:THR:HG22 | 1.19 | 1.36 | 5 | 5 |
| 1:A:41:THR:CG2 | 1:A:44:THR:HG23 | 1.19 | 1.66 | 2 | 15 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:50:PHE:CB | 1:A:61:ILE:HD13 | 1.18 | 1.69 | 8 | 11 |
| 1:A:34:PHE:CE1 | 1:A:47:VAL:HG13 | 1.17 | 1.75 | 13 | 20 |
| 1:A:33:ALA:HB3 | 1:A:50:PHE:CD1 | 1.16 | 1.74 | 8 | 17 |
| 1:A:34:PHE:CZ | 1:A:91:ILE:HD12 | 1.15 | 1.76 | 3 | 20 |
| 1:A:94:HIS:HB3 | 1:A:105:LEU:HD22 | 1.15 | 1.16 | 7 | 17 |
| 1:A:25:LEU:CD1 | 1:A:109:VAL:HG21 | 1.15 | 1.72 | 12 | 3 |
| 1:A:49:VAL:HG21 | 1:A:64:TYR:CZ | 1.14 | 1.75 | 15 | 3 |
| 1:A:50:PHE:CG | 1:A:61:ILE:HD13 | 1.14 | 1.77 | 2 | 10 |
| 1:A:67:LYS:O | 1:A:76:TYR:HA | 1.14 | 1.43 | 12 | 20 |
| 1:A:25:LEU:HD21 | 1:A:48:SER:OG | 1.13 | 1.42 | 12 | 3 |
| 1:A:65:HIS:O | 1:A:78:VAL:HG12 | 1.13 | 1.42 | 1 | 11 |
| 1:A:16:ILE:HD11 | 1:A:24:LEU:HD21 | 1.13 | 1.16 | 10 | 10 |
| 1:A:21:ALA:HA | 1:A:24:LEU:CD1 | 1.13 | 1.72 | 18 | 17 |
| 1:A:66:ILE:CG2 | 1:A:90:LEU:HD13 | 1.12 | 1.72 | 19 | 20 |
| 1:A:76:TYR:O | 1:A:83:VAL:HA | 1.12 | 1.41 | 3 | 19 |
| 1:A:91:ILE:O | 1:A:105:LEU:HD23 | 1.12 | 1.42 | 12 | 17 |
| 1:A:21:ALA:O | 1:A:24:LEU:HD13 | 1.12 | 1.43 | 18 | 6 |
| 1:A:74:LYS:HB3 | 1:A:83:VAL:HG23 | 1.12 | 1.21 | 15 | 9 |
| 1:A:6:LEU:HD11 | 1:A:45:TYR:CD2 | 1.11 | 1.78 | 2 | 11 |
| 1:A:45:TYR:O | 1:A:66:ILE:HG12 | 1.11 | 1.44 | 17 | 20 |
| 1:A:33:ALA:HB3 | 1:A:50:PHE:CD2 | 1.11 | 1.81 | 10 | 3 |
| 1:A:25:LEU:HD11 | 1:A:48:SER:CB | 1.10 | 1.75 | 2 | 14 |
| 1:A:25:LEU:HD13 | 1:A:61:ILE:CG2 | 1.10 | 1.75 | 2 | 11 |
| 1:A:64:TYR:CD2 | 1:A:101:LEU:HD23 | 1.10 | 1.81 | 12 | 2 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:CG1 | 1.09 | 1.77 | 4 | 7 |
| 1:A:24:LEU:HD13 | 1:A:25:LEU:N | 1.09 | 1.59 | 5 | 5 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:HD12 | 1.09 | 1.81 | 7 | 3 |
| 1:A:47:VAL:HG23 | 1:A:66:ILE:HD11 | 1.09 | 1.18 | 18 | 20 |
| 1:A:66:ILE:HG23 | 1:A:90:LEU:CD2 | 1.09 | 1.76 | 3 | 19 |
| 1:A:21:ALA:HA | 1:A:24:LEU:HD11 | 1.08 | 1.18 | 2 | 11 |
| 1:A:74:LYS:CB | 1:A:83:VAL:HG23 | 1.08 | 1.77 | 10 | 11 |
| 1:A:25:LEU:HD11 | 1:A:48:SER:HB3 | 1.08 | 1.18 | 2 | 6 |
| 1:A:102:VAL:HG23 | 1:A:103:THR:HG23 | 1.08 | 1.22 | 9 | 4 |
| 1:A:25:LEU:HD11 | 1:A:48:SER:HB2 | 1.07 | 1.24 | 20 | 6 |
| 1:A:77:TYR:HA | 1:A:90:LEU:HD11 | 1.07 | 1.22 | 8 | 20 |
| 1:A:25:LEU:HG | 1:A:109:VAL:HG11 | 1.07 | 1.25 | 8 | 6 |
| 1:A:84:PHE:CZ | 1:A:93:TYR:CD1 | 1.07 | 2.42 | 5 | 6 |
| 1:A:86:SER:O | 1:A:89:LEU:HD12 | 1.06 | 1.48 | 3 | 16 |
| 1:A:100:GLY:O | 1:A:101:LEU:HD23 | 1.06 | 1.47 | 2 | 1 |
| 1:A:66:ILE:N | 1:A:66:ILE:HD13 | 1.06 | 1.64 | 11 | 9 |
| 1:A:22:GLU:HA | 1:A:61:ILE:HG21 | 1.06 | 1.28 | 20 | 18 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:24:LEU:CD1 | 1:A:25:LEU:HD12 | 1.06 | 1.81 | 7 | 2 |
| 1:A:102:VAL:HG23 | 1:A:103:THR:HG22 | 1.06 | 1.23 | 3 | 11 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:HG21 | 1.05 | 1.23 | 3 | 8 |
| 1:A:86:SER:OG | 1:A:89:LEU:HD21 | 1.05 | 1.50 | 2 | 1 |
| 1:A:94:HIS:HB3 | 1:A:105:LEU:HD23 | 1.05 | 1.24 | 20 | 3 |
| 1:A:34:PHE:O | 1:A:109:VAL:N | 1.05 | 1.90 | 9 | 20 |
| 1:A:24:LEU:HD22 | 1:A:24:LEU:C | 1.05 | 1.72 | 18 | 3 |
| 1:A:33:ALA:HB1 | 1:A:109:VAL:CG2 | 1.05 | 1.82 | 9 | 3 |
| 1:A:21:ALA:CA | 1:A:24:LEU:HD12 | 1.04 | 1.81 | 4 | 5 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:HG11 | 1.04 | 1.30 | 11 | 7 |
| 1:A:41:THR:HG21 | 1:A:44:THR:HG23 | 1.04 | 1.22 | 2 | 8 |
| 1:A:28:THR:HG23 | 1:A:30:LYS:HD3 | 1.04 | 1.29 | 11 | 11 |
| 1:A:21:ALA:HA | 1:A:24:LEU:HD12 | 1.04 | 1.05 | 15 | 6 |
| 1:A:66:ILE:HD13 | 1:A:66:ILE:N | 1.04 | 1.67 | 5 | 8 |
| 1:A:81:LYS:CG | 1:A:82:TYR:CD2 | 1.03 | 2.41 | 14 | 2 |
| 1:A:26:LEU:HD12 | 1:A:61:ILE:HD11 | 1.03 | 1.19 | 1 | 3 |
| 1:A:25:LEU:HD23 | 1:A:109:VAL:HG21 | 1.03 | 1.30 | 4 | 5 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:HD3 | 1.03 | 1.25 | 13 | 4 |
| 1:A:25:LEU:CD2 | 1:A:109:VAL:HG21 | 1.03 | 1.83 | 4 | 6 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:CD | 1.03 | 1.84 | 8 | 14 |
| 1:A:26:LEU:CD1 | 1:A:61:ILE:HD11 | 1.03 | 1.83 | 20 | 6 |
| 1:A:66:ILE:HG22 | 1:A:90:LEU:HD13 | 1.03 | 1.29 | 8 | 20 |
| 1:A:16:ILE:HD11 | 1:A:24:LEU:CD2 | 1.02 | 1.83 | 8 | 10 |
| 1:A:47:VAL:CG2 | 1:A:66:ILE:HD11 | 1.02 | 1.84 | 3 | 12 |
| 1:A:26:LEU:HD11 | 1:A:61:ILE:CD1 | 1.02 | 1.83 | 17 | 1 |
| 1:A:94:HIS:NE2 | 1:A:101:LEU:HD21 | 1.02 | 1.68 | 4 | 8 |
| 1:A:28:THR:HG23 | 1:A:30:LYS:HG3 | 1.02 | 1.28 | 8 | 5 |
| 1:A:69:THR:HG23 | 1:A:75:ARG:O | 1.02 | 1.52 | 4 | 7 |
| 1:A:36:VAL:HG13 | 1:A:46:THR:O | 1.02 | 1.54 | 11 | 20 |
| 1:A:22:GLU:O | 1:A:26:LEU:HD12 | 1.02 | 1.52 | 4 | 4 |
| 1:A:21:ALA:O | 1:A:25:LEU:HD12 | 1.02 | 1.54 | 4 | 12 |
| 1:A:66:ILE:HG21 | 1:A:87:ILE:HD12 | 1.02 | 1.30 | 5 | 12 |
| 1:A:93:TYR:OH | 1:A:94:HIS:CE1 | 1.02 | 2.11 | 5 | 20 |
| 1:A:26:LEU:HD11 | 1:A:61:ILE:HD11 | 1.02 | 1.29 | 17 | 2 |
| 1:A:21:ALA:HA | 1:A:24:LEU:HD22 | 1.02 | 1.24 | 12 | 3 |
| 1:A:36:VAL:HG22 | 1:A:47:VAL:HG22 | 1.01 | 1.28 | 15 | 20 |
| 1:A:87:ILE:O | 1:A:91:ILE:HG12 | 1.01 | 1.55 | 4 | 20 |
| 1:A:34:PHE:CG | 1:A:105:LEU:CD1 | 1.01 | 2.42 | 20 | 20 |
| 1:A:34:PHE:CG | 1:A:105:LEU:HD13 | 1.01 | 1.90 | 4 | 3 |
| 1:A:16:ILE:HD11 | 1:A:24:LEU:HD13 | 1.01 | 1.28 | 12 | 3 |
| 1:A:64:TYR:OH | 1:A:102:VAL:HG13 | 1.01 | 1.54 | 20 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:24:LEU:HD13 | 1:A:35:MET:CE | 1.01 | 1.83 | 13 | 11 |
| 1:A:81:LYS:CG | 1:A:82:TYR:CD1 | 1.01 | 2.44 | 4 | 3 |
| 1:A:101:LEU:O | 1:A:102:VAL:HG22 | 1.01 | 1.55 | 17 | 1 |
| 1:A:16:ILE:HD12 | 1:A:35:MET:SD | 1.01 | 1.95 | 14 | 18 |
| 1:A:6:LEU:HD23 | 1:A:6:LEU:N | 1.00 | 1.71 | 14 | 3 |
| 1:A:21:ALA:CA | 1:A:24:LEU:HD22 | 1.00 | 1.85 | 16 | 3 |
| 1:A:77:TYR:CG | 1:A:83:VAL:HG12 | 1.00 | 1.91 | 1 | 15 |
| 1:A:34:PHE:O | 1:A:108:PRO:HA | 1.00 | 1.57 | 9 | 20 |
| 1:A:24:LEU:HD21 | 1:A:35:MET:HE3 | 1.00 | 1.29 | 5 | 9 |
| 1:A:66:ILE:HG23 | 1:A:90:LEU:HD22 | 0.99 | 1.32 | 8 | 18 |
| 1:A:41:THR:HG22 | 1:A:44:THR:HG22 | 0.99 | 1.33 | 4 | 4 |
| 1:A:24:LEU:HD13 | 1:A:35:MET:HE1 | 0.99 | 1.30 | 17 | 6 |
| 1:A:84:PHE:CE1 | 1:A:93:TYR:CD2 | 0.99 | 2.50 | 17 | 9 |
| 1:A:34:PHE:CD1 | 1:A:105:LEU:CD1 | 0.98 | 2.46 | 17 | 20 |
| 1:A:25:LEU:O | 1:A:28:THR:HG22 | 0.98 | 1.55 | 19 | 15 |
| 1:A:25:LEU:HD23 | 1:A:50:PHE:HD1 | 0.98 | 1.17 | 8 | 2 |
| 1:A:33:ALA:HB1 | 1:A:109:VAL:HG21 | 0.98 | 1.36 | 9 | 2 |
| 1:A:33:ALA:HB3 | 1:A:50:PHE:HD1 | 0.98 | 1.18 | 18 | 16 |
| 1:A:21:ALA:O | 1:A:24:LEU:CD1 | 0.98 | 2.11 | 4 | 17 |
| 1:A:11:TRP:CH2 | 1:A:87:ILE:HG22 | 0.98 | 1.94 | 13 | 20 |
| 1:A:24:LEU:HD22 | 1:A:25:LEU:N | 0.98 | 1.72 | 18 | 2 |
| 1:A:50:PHE:HB3 | 1:A:61:ILE:HG23 | 0.98 | 1.35 | 5 | 17 |
| 1:A:74:LYS:HB3 | 1:A:83:VAL:HG22 | 0.98 | 1.32 | 12 | 3 |
| 1:A:101:LEU:HD13 | 1:A:101:LEU:N | 0.98 | 1.74 | 20 | 6 |
| 1:A:25:LEU:HD13 | 1:A:61:ILE:HG23 | 0.98 | 1.36 | 9 | 6 |
| 1:A:25:LEU:CG | 1:A:109:VAL:HG11 | 0.97 | 1.87 | 8 | 4 |
| 1:A:26:LEU:HD12 | 1:A:61:ILE:CD1 | 0.97 | 1.88 | 20 | 4 |
| 1:A:25:LEU:HB2 | 1:A:61:ILE:HD12 | 0.97 | 1.36 | 13 | 6 |
| 1:A:84:PHE:CZ | 1:A:93:TYR:CE1 | 0.97 | 2.53 | 5 | 3 |
| 1:A:25:LEU:HD11 | 1:A:109:VAL:HG21 | 0.97 | 1.35 | 12 | 1 |
| 1:A:6:LEU:HD22 | 1:A:88:PRO:HD3 | 0.96 | 1.38 | 4 | 14 |
| 1:A:30:LYS:NZ | 1:A:109:VAL:HG12 | 0.96 | 1.75 | 6 | 2 |
| 1:A:66:ILE:CG2 | 1:A:90:LEU:HD22 | 0.96 | 1.90 | 3 | 17 |
| 1:A:50:PHE:CB | 1:A:61:ILE:HG23 | 0.96 | 1.90 | 14 | 10 |
| 1:A:94:HIS:NE2 | 1:A:101:LEU:HD11 | 0.96 | 1.74 | 8 | 4 |
| 1:A:21:ALA:O | 1:A:24:LEU:HD23 | 0.96 | 1.59 | 16 | 3 |
| 1:A:84:PHE:CZ | 1:A:93:TYR:CG | 0.96 | 2.53 | 1 | 20 |
| 1:A:81:LYS:HD3 | 1:A:82:TYR:CE1 | 0.96 | 1.94 | 12 | 4 |
| 1:A:34:PHE:CD2 | 1:A:105:LEU:HD12 | 0.96 | 1.96 | 20 | 4 |
| 1:A:11:TRP:CE3 | 1:A:36:VAL:CG2 | 0.96 | 2.48 | 18 | 20 |
| 1:A:21:ALA:CA | 1:A:24:LEU:HD11 | 0.96 | 1.91 | 2 | 11 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:77:TYR:CA | 1:A:90:LEU:HD11 | 0.96 | 1.91 | 3 | 20 |
| 1:A:93:TYR:CE2 | 1:A:94:HIS:CE1 | 0.96 | 2.54 | 19 | 15 |
| 1:A:32:GLY:N | 1:A:51:THR:OG1 | 0.95 | 1.99 | 18 | 17 |
| 1:A:26:LEU:HG | 1:A:61:ILE:HD11 | 0.95 | 1.34 | 14 | 5 |
| 1:A:50:PHE:HB2 | 1:A:61:ILE:HD13 | 0.95 | 1.32 | 20 | 15 |
| 1:A:53:ALA:HB3 | 1:A:60:CYS:SG | 0.95 | 2.01 | 19 | 1 |
| 1:A:24:LEU:C | 1:A:24:LEU:HD22 | 0.95 | 1.82 | 4 | 3 |
| 1:A:26:LEU:CG | 1:A:61:ILE:HD11 | 0.95 | 1.91 | 14 | 4 |
| 1:A:84:PHE:CE1 | 1:A:93:TYR:CD1 | 0.95 | 2.53 | 1 | 4 |
| 1:A:94:HIS:CB | 1:A:105:LEU:CD2 | 0.95 | 2.45 | 17 | 19 |
| 1:A:44:THR:CB | 1:A:66:ILE:O | 0.95 | 2.15 | 5 | 18 |
| 1:A:6:LEU:HD12 | 1:A:12:TYR:CE1 | 0.95 | 1.96 | 19 | 17 |
| 1:A:34:PHE:CE2 | 1:A:91:ILE:HG21 | 0.95 | 1.97 | 14 | 20 |
| 1:A:102:VAL:HG13 | 1:A:103:THR:HG22 | 0.95 | 1.36 | 4 | 3 |
| 1:A:47:VAL:HG23 | 1:A:66:ILE:CD1 | 0.94 | 1.91 | 18 | 20 |
| 1:A:24:LEU:HD21 | 1:A:35:MET:CE | 0.94 | 1.91 | 5 | 8 |
| 1:A:86:SER:CB | 1:A:89:LEU:HD11 | 0.94 | 1.93 | 5 | 15 |
| 1:A:82:TYR:CD2 | 1:A:93:TYR:CE1 | 0.94 | 2.56 | 2 | 9 |
| 1:A:84:PHE:CE2 | 1:A:93:TYR:CE1 | 0.94 | 2.55 | 4 | 1 |
| 1:A:25:LEU:HD12 | 1:A:50:PHE:CD1 | 0.94 | 1.96 | 19 | 2 |
| 1:A:69:THR:N | 1:A:75:ARG:O | 0.94 | 2.00 | 4 | 20 |
| 1:A:34:PHE:CE2 | 1:A:91:ILE:CG2 | 0.94 | 2.51 | 15 | 20 |
| 1:A:16:ILE:HG22 | 1:A:37:ARG:HB2 | 0.94 | 1.38 | 9 | 20 |
| 1:A:30:LYS:HB2 | 1:A:33:ALA:HB2 | 0.94 | 1.40 | 9 | 11 |
| 1:A:93:TYR:CE2 | 1:A:94:HIS:ND1 | 0.94 | 2.36 | 19 | 16 |
| 1:A:90:LEU:O | 1:A:93:TYR:CD1 | 0.94 | 2.21 | 1 | 6 |
| 1:A:100:GLY:C | 1:A:101:LEU:HD12 | 0.93 | 1.83 | 12 | 2 |
| 1:A:24:LEU:HD11 | 1:A:25:LEU:HD23 | 0.93 | 1.36 | 5 | 1 |
| 1:A:86:SER:N | 1:A:89:LEU:HD11 | 0.93 | 1.79 | 3 | 16 |
| 1:A:84:PHE:CE2 | 1:A:93:TYR:CD2 | 0.93 | 2.56 | 7 | 5 |
| 1:A:77:TYR:CB | 1:A:83:VAL:HG12 | 0.93 | 1.94 | 1 | 15 |
| 1:A:11:TRP:HB3 | 1:A:108:PRO:HB3 | 0.93 | 1.40 | 7 | 20 |
| 1:A:34:PHE:CD1 | 1:A:47:VAL:HG13 | 0.92 | 1.98 | 20 | 20 |
| 1:A:84:PHE:CE1 | 1:A:93:TYR:CE1 | 0.92 | 2.58 | 19 | 5 |
| 1:A:94:HIS:CB | 1:A:105:LEU:HD23 | 0.92 | 1.94 | 20 | 3 |
| 1:A:41:THR:CG2 | 1:A:42:PRO:HD2 | 0.92 | 1.94 | 3 | 20 |
| 1:A:84:PHE:CZ | 1:A:93:TYR:CD2 | 0.92 | 2.57 | 2 | 19 |
| 1:A:9:TYR:CZ | 1:A:88:PRO:HB3 | 0.92 | 2.00 | 4 | 20 |
| 1:A:24:LEU:HD11 | 1:A:35:MET:CE | 0.92 | 1.93 | 1 | 8 |
| 1:A:19:ASP:O | 1:A:23:LYS:CE | 0.92 | 2.18 | 2 | 1 |
| 1:A:50:PHE:HB3 | 1:A:61:ILE:HD13 | 0.92 | 1.40 | 9 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:64:TYR:HB3 | 1:A:78:VAL:HG21 | 0.92 | 1.41 | 8 | 4 |
| 1:A:94:HIS:CD2 | 1:A:101:LEU:HD21 | 0.92 | 2.00 | 4 | 5 |
| 1:A:6:LEU:HD13 | 1:A:11:TRP:CH2 | 0.92 | 1.99 | 11 | 10 |
| 1:A:21:ALA:O | 1:A:24:LEU:CD2 | 0.92 | 2.18 | 16 | 3 |
| 1:A:82:TYR:CD1 | 1:A:93:TYR:CZ | 0.91 | 2.57 | 9 | 14 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:HD13 | 0.91 | 2.00 | 1 | 2 |
| 1:A:93:TYR:CZ | 1:A:94:HIS:CE1 | 0.91 | 2.59 | 19 | 20 |
| 1:A:35:MET:HB3 | 1:A:48:SER:HB3 | 0.91 | 1.41 | 19 | 13 |
| 1:A:81:LYS:HG2 | 1:A:82:TYR:CD2 | 0.91 | 1.99 | 14 | 2 |
| 1:A:78:VAL:HG12 | 1:A:79:ALA:N | 0.91 | 1.77 | 9 | 4 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:HG12 | 0.91 | 1.40 | 4 | 4 |
| 1:A:16:ILE:CD1 | 1:A:24:LEU:HD21 | 0.91 | 1.95 | 19 | 10 |
| 1:A:77:TYR:CE2 | 1:A:80:GLU:HA | 0.91 | 2.00 | 8 | 20 |
| 1:A:66:ILE:HG23 | 1:A:90:LEU:HD13 | 0.91 | 1.42 | 5 | 4 |
| 1:A:11:TRP:CB | 1:A:34:PHE:CE2 | 0.91 | 2.54 | 20 | 20 |
| 1:A:66:ILE:HG13 | 1:A:87:ILE:CG1 | 0.91 | 1.96 | 2 | 18 |
| 1:A:91:ILE:HG23 | 1:A:105:LEU:HG | 0.91 | 1.38 | 10 | 17 |
| 1:A:82:TYR:CG | 1:A:93:TYR:CE1 | 0.91 | 2.58 | 7 | 10 |
| 1:A:33:ALA:CB | 1:A:50:PHE:CE1 | 0.91 | 2.54 | 20 | 14 |
| 1:A:86:SER:CB | 1:A:89:LEU:HD21 | 0.91 | 1.96 | 17 | 4 |
| 1:A:81:LYS:HB3 | 1:A:82:TYR:CD1 | 0.91 | 2.01 | 10 | 12 |
| 1:A:45:TYR:CD1 | 1:A:87:ILE:HD13 | 0.90 | 2.01 | 2 | 5 |
| 1:A:79:ALA:O | 1:A:81:LYS:N | 0.90 | 2.04 | 8 | 20 |
| 1:A:11:TRP:CH2 | 1:A:87:ILE:CG2 | 0.90 | 2.54 | 2 | 20 |
| 1:A:102:VAL:HG23 | 1:A:103:THR:CG2 | 0.90 | 1.95 | 19 | 10 |
| 1:A:24:LEU:HD21 | 1:A:109:VAL:HG13 | 0.90 | 1.39 | 15 | 2 |
| 1:A:81:LYS:HG2 | 1:A:82:TYR:CD1 | 0.90 | 2.01 | 4 | 2 |
| 1:A:94:HIS:CD2 | 1:A:99:GLY:CA | 0.90 | 2.54 | 17 | 7 |
| 1:A:86:SER:HB3 | 1:A:89:LEU:HD21 | 0.90 | 1.40 | 6 | 2 |
| 1:A:30:LYS:HD3 | 1:A:107:TYR:CD2 | 0.90 | 2.02 | 12 | 4 |
| 1:A:81:LYS:HG2 | 1:A:82:TYR:N | 0.90 | 1.78 | 13 | 4 |
| 1:A:82:TYR:CD1 | 1:A:93:TYR:CE1 | 0.90 | 2.60 | 20 | 11 |
| 1:A:94:HIS:HB2 | 1:A:105:LEU:CD2 | 0.90 | 1.96 | 19 | 17 |
| 1:A:28:THR:HG23 | 1:A:30:LYS:CG | 0.90 | 1.97 | 20 | 3 |
| 1:A:6:LEU:HD21 | 1:A:45:TYR:CE2 | 0.90 | 2.00 | 17 | 2 |
| 1:A:86:SER:HB2 | 1:A:89:LEU:HD11 | 0.90 | 1.41 | 13 | 9 |
| 1:A:82:TYR:CD2 | 1:A:93:TYR:OH | 0.90 | 2.23 | 14 | 1 |
| 1:A:86:SER:HB2 | 1:A:89:LEU:HD21 | 0.89 | 1.42 | 17 | 1 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:CD1 | 0.89 | 2.55 | 10 | 7 |
| 1:A:21:ALA:HA | 1:A:24:LEU:CD2 | 0.89 | 1.98 | 16 | 14 |
| 1:A:78:VAL:O | 1:A:78:VAL:HG23 | 0.89 | 1.67 | 5 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:24:LEU:CD2 | 1:A:24:LEU:C | 0.89 | 2.41 | 18 | 5 |
| 1:A:21:ALA:HA | 1:A:24:LEU:CG | 0.89 | 1.97 | 9 | 11 |
| 1:A:25:LEU:HD13 | 1:A:109:VAL:HG21 | 0.89 | 1.39 | 18 | 1 |
| 1:A:94:HIS:HB2 | 1:A:105:LEU:HD22 | 0.89 | 1.41 | 6 | 13 |
| 1:A:9:TYR:CG | 1:A:11:TRP:CZ2 | 0.89 | 2.61 | 3 | 20 |
| 1:A:11:TRP:CD2 | 1:A:34:PHE:CE2 | 0.89 | 2.61 | 15 | 20 |
| 1:A:81:LYS:CD | 1:A:82:TYR:CD1 | 0.89 | 2.56 | 12 | 4 |
| 1:A:25:LEU:HD22 | 1:A:109:VAL:HG21 | 0.89 | 1.45 | 5 | 1 |
| 1:A:66:ILE:HG22 | 1:A:76:TYR:HB3 | 0.88 | 1.43 | 19 | 6 |
| 1:A:41:THR:CG2 | 1:A:44:THR:HG22 | 0.88 | 1.98 | 1 | 11 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:HD23 | 0.88 | 2.03 | 12 | 4 |
| 1:A:77:TYR:HB3 | 1:A:83:VAL:HG12 | 0.88 | 1.44 | 15 | 16 |
| 1:A:24:LEU:HD22 | 1:A:35:MET:CE | 0.88 | 1.99 | 6 | 1 |
| 1:A:21:ALA:HA | 1:A:24:LEU:HD21 | 0.88 | 1.41 | 7 | 11 |
| 1:A:44:THR:HG23 | 1:A:65:HIS:NE2 | 0.88 | 1.84 | 4 | 2 |
| 1:A:25:LEU:HG | 1:A:109:VAL:HG21 | 0.88 | 1.45 | 7 | 3 |
| 1:A:25:LEU:HD22 | 1:A:109:VAL:CG2 | 0.88 | 1.99 | 5 | 1 |
| 1:A:41:THR:OG1 | 1:A:42:PRO:CD | 0.88 | 2.22 | 10 | 18 |
| 1:A:24:LEU:HD21 | 1:A:109:VAL:CG1 | 0.88 | 1.97 | 15 | 2 |
| 1:A:34:PHE:CZ | 1:A:91:ILE:CD1 | 0.87 | 2.58 | 19 | 20 |
| 1:A:24:LEU:CD1 | 1:A:35:MET:CE | 0.87 | 2.52 | 2 | 15 |
| 1:A:87:ILE:HG23 | 1:A:91:ILE:CG1 | 0.87 | 1.97 | 13 | 14 |
| 1:A:22:GLU:C | 1:A:26:LEU:HD12 | 0.87 | 1.88 | 4 | 4 |
| 1:A:41:THR:HG23 | 1:A:42:PRO:HD2 | 0.87 | 1.47 | 15 | 20 |
| 1:A:11:TRP:CG | 1:A:34:PHE:HE2 | 0.87 | 1.86 | 11 | 20 |
| 1:A:25:LEU:HD13 | 1:A:61:ILE:HG21 | 0.87 | 1.44 | 2 | 5 |
| 1:A:101:LEU:CD1 | 1:A:101:LEU:N | 0.87 | 2.35 | 20 | 7 |
| 1:A:24:LEU:HG | 1:A:35:MET:HE1 | 0.87 | 1.42 | 4 | 7 |
| 1:A:24:LEU:HD13 | 1:A:25:LEU:H | 0.87 | 1.25 | 1 | 5 |
| 1:A:82:TYR:CD1 | 1:A:93:TYR:OH | 0.87 | 2.27 | 6 | 15 |
| 1:A:11:TRP:O | 1:A:35:MET:CG | 0.87 | 2.22 | 14 | 14 |
| 1:A:28:THR:CG2 | 1:A:109:VAL:HG21 | 0.87 | 1.99 | 17 | 6 |
| 1:A:50:PHE:CD2 | 1:A:61:ILE:CD1 | 0.87 | 2.58 | 7 | 11 |
| 1:A:76:TYR:O | 1:A:83:VAL:CA | 0.87 | 2.22 | 3 | 16 |
| 1:A:50:PHE:CG | 1:A:61:ILE:CD1 | 0.87 | 2.58 | 10 | 12 |
| 1:A:49:VAL:HG21 | 1:A:64:TYR:CE2 | 0.87 | 2.05 | 15 | 3 |
| 1:A:69:THR:HG21 | 1:A:83:VAL:HG11 | 0.87 | 1.47 | 4 | 8 |
| 1:A:76:TYR:N | 1:A:76:TYR:CD1 | 0.87 | 2.38 | 6 | 7 |
| 1:A:10:GLU:CG | 1:A:108:PRO:O | 0.87 | 2.22 | 14 | 11 |
| 1:A:41:THR:CG2 | 1:A:44:THR:CG2 | 0.86 | 2.53 | 3 | 20 |
| 1:A:30:LYS:HE2 | 1:A:109:VAL:HG23 | 0.86 | 1.42 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:25:LEU:HD23 | 1:A:50:PHE:CD1 | 0.86 | 2.05 | 8 | 2 |
| 1:A:50:PHE:CD1 | 1:A:61:ILE:CD1 | 0.86 | 2.57 | 11 | 2 |
| 1:A:36:VAL:HA | 1:A:46:THR:O | 0.86 | 1.70 | 8 | 20 |
| 1:A:82:TYR:HD1 | 1:A:93:TYR:HH | 0.86 | 0.96 | 4 | 2 |
| 1:A:11:TRP:CB | 1:A:34:PHE:CD2 | 0.86 | 2.58 | 4 | 20 |
| 1:A:6:LEU:CD1 | 1:A:12:TYR:CD1 | 0.86 | 2.58 | 11 | 15 |
| 1:A:34:PHE:HE1 | 1:A:47:VAL:HG13 | 0.86 | 1.28 | 7 | 20 |
| 1:A:24:LEU:HD13 | 1:A:35:MET:HE3 | 0.86 | 1.47 | 13 | 8 |
| 1:A:78:VAL:HG23 | 1:A:78:VAL:O | 0.86 | 1.70 | 6 | 6 |
| 1:A:94:HIS:O | 1:A:104:ARG:HB2 | 0.86 | 1.70 | 17 | 16 |
| 1:A:81:LYS:HD3 | 1:A:82:TYR:CD1 | 0.86 | 2.03 | 12 | 4 |
| 1:A:12:TYR:OH | 1:A:14:LYS:CG | 0.86 | 2.24 | 20 | 1 |
| 1:A:9:TYR:CB | 1:A:11:TRP:CE2 | 0.86 | 2.59 | 8 | 20 |
| 1:A:32:GLY:CA | 1:A:103:THR:HG21 | 0.86 | 2.01 | 16 | 8 |
| 1:A:66:ILE:CG2 | 1:A:90:LEU:CD1 | 0.85 | 2.53 | 4 | 20 |
| 1:A:86:SER:N | 1:A:89:LEU:CD1 | 0.85 | 2.38 | 3 | 20 |
| 1:A:41:THR:HG23 | 1:A:42:PRO:CD | 0.85 | 2.01 | 2 | 20 |
| 1:A:84:PHE:CD2 | 1:A:90:LEU:HA | 0.85 | 2.05 | 3 | 6 |
| 1:A:94:HIS:HB3 | 1:A:105:LEU:CD2 | 0.85 | 2.01 | 20 | 6 |
| 1:A:6:LEU:CB | 1:A:12:TYR:CD1 | 0.85 | 2.59 | 12 | 2 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:HE2 | 0.85 | 1.85 | 6 | 10 |
| 1:A:36:VAL:CG1 | 1:A:46:THR:O | 0.85 | 2.24 | 19 | 20 |
| 1:A:11:TRP:HB3 | 1:A:108:PRO:CB | 0.85 | 2.02 | 7 | 20 |
| 1:A:87:ILE:O | 1:A:91:ILE:N | 0.85 | 2.10 | 17 | 20 |
| 1:A:67:LYS:N | 1:A:77:TYR:O | 0.85 | 2.10 | 15 | 20 |
| 1:A:74:LYS:CB | 1:A:83:VAL:CG2 | 0.85 | 2.55 | 19 | 13 |
| 1:A:24:LEU:CD1 | 1:A:35:MET:SD | 0.85 | 2.65 | 12 | 13 |
| 1:A:94:HIS:CD2 | 1:A:101:LEU:CD2 | 0.85 | 2.60 | 7 | 12 |
| 1:A:30:LYS:CE | 1:A:109:VAL:CG1 | 0.85 | 2.54 | 12 | 3 |
| 1:A:88:PRO:O | 1:A:92:GLN:CD | 0.85 | 2.14 | 17 | 7 |
| 1:A:21:ALA:CA | 1:A:24:LEU:CD1 | 0.85 | 2.54 | 18 | 17 |
| 1:A:34:PHE:CD1 | 1:A:105:LEU:HD13 | 0.84 | 2.06 | 14 | 3 |
| 1:A:49:VAL:CG2 | 1:A:64:TYR:CE1 | 0.84 | 2.59 | 15 | 13 |
| 1:A:61:ILE:N | 1:A:61:ILE:HD12 | 0.84 | 1.85 | 18 | 1 |
| 1:A:34:PHE:CD1 | 1:A:105:LEU:HD12 | 0.84 | 2.04 | 17 | 16 |
| 1:A:66:ILE:CD1 | 1:A:66:ILE:N | 0.84 | 2.39 | 11 | 8 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:CG | 0.84 | 2.39 | 12 | 4 |
| 1:A:49:VAL:CG2 | 1:A:64:TYR:CZ | 0.84 | 2.60 | 10 | 3 |
| 1:A:16:ILE:HG22 | 1:A:37:ARG:CB | 0.84 | 2.01 | 15 | 14 |
| 1:A:44:THR:OG1 | 1:A:65:HIS:CD2 | 0.84 | 2.30 | 3 | 7 |
| 1:A:20:LYS:O | 1:A:24:LEU:HG | 0.84 | 1.72 | 7 | 11 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:82:TYR:CB | 1:A:93:TYR:CZ | 0.84 | 2.60 | 14 | 1 |
| 1:A:24:LEU:HD12 | 1:A:25:LEU:HD12 | 0.84 | 1.48 | 7 | 2 |
| 1:A:24:LEU:HD23 | 1:A:111:GLY:CA | 0.84 | 2.02 | 1 | 3 |
| 1:A:82:TYR:CD1 | 1:A:82:TYR:N | 0.84 | 2.46 | 2 | 8 |
| 1:A:33:ALA:HB1 | 1:A:109:VAL:HG23 | 0.84 | 1.45 | 14 | 2 |
| 1:A:64:TYR:CD2 | 1:A:101:LEU:CD2 | 0.84 | 2.61 | 6 | 2 |
| 1:A:101:LEU:N | 1:A:101:LEU:HD13 | 0.84 | 1.87 | 7 | 1 |
| 1:A:49:VAL:HG23 | 1:A:102:VAL:HG11 | 0.84 | 1.49 | 4 | 4 |
| 1:A:81:LYS:CG | 1:A:82:TYR:CE1 | 0.84 | 2.61 | 4 | 2 |
| 1:A:74:LYS:HB3 | 1:A:83:VAL:CG2 | 0.84 | 2.02 | 12 | 8 |
| 1:A:25:LEU:O | 1:A:50:PHE:CZ | 0.84 | 2.30 | 19 | 14 |
| 1:A:21:ALA:C | 1:A:25:LEU:HD12 | 0.84 | 1.92 | 4 | 10 |
| 1:A:94:HIS:CD2 | 1:A:99:GLY:HA3 | 0.84 | 2.08 | 5 | 10 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:HD2 | 0.84 | 1.47 | 3 | 6 |
| 1:A:9:TYR:HB3 | 1:A:11:TRP:CE2 | 0.83 | 2.08 | 11 | 20 |
| 1:A:33:ALA:CB | 1:A:50:PHE:CD2 | 0.83 | 2.61 | 10 | 3 |
| 1:A:34:PHE:CE1 | 1:A:47:VAL:CG1 | 0.83 | 2.61 | 9 | 20 |
| 1:A:35:MET:HB3 | 1:A:48:SER:HB2 | 0.83 | 1.50 | 20 | 9 |
| 1:A:33:ALA:HB3 | 1:A:50:PHE:CE1 | 0.83 | 2.06 | 20 | 8 |
| 1:A:74:LYS:CB | 1:A:83:VAL:HG22 | 0.83 | 2.03 | 13 | 2 |
| 1:A:11:TRP:O | 1:A:35:MET:HG3 | 0.83 | 1.73 | 4 | 19 |
| 1:A:49:VAL:HG23 | 1:A:102:VAL:CG1 | 0.83 | 2.03 | 4 | 6 |
| 1:A:33:ALA:CB | 1:A:50:PHE:CD1 | 0.83 | 2.60 | 8 | 17 |
| 1:A:16:ILE:HD11 | 1:A:24:LEU:CD1 | 0.83 | 2.02 | 20 | 5 |
| 1:A:91:ILE:HG23 | 1:A:105:LEU:HD12 | 0.83 | 1.47 | 4 | 3 |
| 1:A:93:TYR:CZ | 1:A:94:HIS:NE2 | 0.83 | 2.46 | 5 | 1 |
| 1:A:6:LEU:N | 1:A:6:LEU:CD2 | 0.83 | 2.40 | 14 | 1 |
| 1:A:74:LYS:HB2 | 1:A:83:VAL:HG23 | 0.83 | 1.50 | 10 | 4 |
| 1:A:30:LYS:CD | 1:A:109:VAL:HG22 | 0.83 | 2.03 | 9 | 2 |
| 1:A:68:GLU:HA | 1:A:75:ARG:O | 0.83 | 1.74 | 3 | 18 |
| 1:A:20:LYS:O | 1:A:23:LYS:HG3 | 0.83 | 1.74 | 7 | 10 |
| 1:A:50:PHE:CB | 1:A:61:ILE:HG13 | 0.83 | 2.03 | 12 | 2 |
| 1:A:44:THR:HG1 | 1:A:65:HIS:CD2 | 0.83 | 1.92 | 3 | 6 |
| 1:A:82:TYR:CE1 | 1:A:93:TYR:OH | 0.83 | 2.30 | 3 | 4 |
| 1:A:32:GLY:HA3 | 1:A:103:THR:HG21 | 0.83 | 1.50 | 16 | 4 |
| 1:A:50:PHE:HB2 | 1:A:61:ILE:HA | 0.83 | 1.49 | 18 | 16 |
| 1:A:22:GLU:HA | 1:A:61:ILE:HD12 | 0.83 | 1.49 | 3 | 2 |
| 1:A:25:LEU:CD1 | 1:A:109:VAL:HG11 | 0.83 | 2.03 | 8 | 1 |
| 1:A:26:LEU:CD1 | 1:A:61:ILE:CD1 | 0.83 | 2.57 | 17 | 5 |
| 1:A:11:TRP:CE3 | 1:A:36:VAL:HG23 | 0.82 | 2.09 | 9 | 20 |
| 1:A:74:LYS:C | 1:A:83:VAL:HG23 | 0.82 | 1.95 | 11 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:77:TYR:HB2 | 1:A:82:TYR:O | 0.82 | 1.74 | 8 | 7 |
| 1:A:10:GLU:O | 1:A:110:CYS:CB | 0.82 | 2.27 | 20 | 7 |
| 1:A:81:LYS:CG | 1:A:82:TYR:CE2 | 0.82 | 2.62 | 19 | 2 |
| 1:A:21:ALA:O | 1:A:24:LEU:HD12 | 0.82 | 1.72 | 19 | 11 |
| 1:A:34:PHE:CD1 | 1:A:105:LEU:HD11 | 0.82 | 2.10 | 16 | 19 |
| 1:A:67:LYS:O | 1:A:76:TYR:CA | 0.82 | 2.27 | 19 | 20 |
| 1:A:17:SER:CB | 1:A:20:LYS:CD | 0.82 | 2.57 | 9 | 16 |
| 1:A:81:LYS:NZ | 1:A:94:HIS:CE1 | 0.82 | 2.47 | 2 | 3 |
| 1:A:30:LYS:HG2 | 1:A:107:TYR:CD2 | 0.82 | 2.09 | 16 | 13 |
| 1:A:77:TYR:CB | 1:A:82:TYR:O | 0.82 | 2.27 | 8 | 8 |
| 1:A:64:TYR:CD2 | 1:A:101:LEU:HD13 | 0.82 | 2.08 | 1 | 2 |
| 1:A:25:LEU:CD1 | 1:A:48:SER:OG | 0.82 | 2.27 | 4 | 11 |
| 1:A:77:TYR:HB3 | 1:A:83:VAL:CB | 0.82 | 2.05 | 12 | 4 |
| 1:A:84:PHE:HB3 | 1:A:89:LEU:HD12 | 0.82 | 1.48 | 6 | 4 |
| 1:A:24:LEU:CD1 | 1:A:25:LEU:HD23 | 0.82 | 2.04 | 5 | 1 |
| 1:A:34:PHE:CZ | 1:A:36:VAL:HG23 | 0.82 | 2.10 | 9 | 20 |
| 1:A:35:MET:HB3 | 1:A:48:SER:CB | 0.82 | 2.05 | 20 | 15 |
| 1:A:6:LEU:HD12 | 1:A:12:TYR:HD1 | 0.82 | 1.31 | 1 | 10 |
| 1:A:28:THR:HG23 | 1:A:30:LYS:CD | 0.82 | 2.05 | 10 | 8 |
| 1:A:13:ASN:N | 1:A:36:VAL:O | 0.82 | 2.12 | 17 | 20 |
| 1:A:34:PHE:CD2 | 1:A:105:LEU:CD1 | 0.82 | 2.62 | 20 | 3 |
| 1:A:24:LEU:O | 1:A:24:LEU:HD22 | 0.82 | 1.75 | 3 | 3 |
| 1:A:25:LEU:HD11 | 1:A:109:VAL:CG2 | 0.82 | 2.04 | 12 | 1 |
| 1:A:67:LYS:CG | 1:A:77:TYR:CE1 | 0.81 | 2.63 | 17 | 19 |
| 1:A:24:LEU:HD11 | 1:A:35:MET:HE3 | 0.81 | 1.49 | 1 | 3 |
| 1:A:76:TYR:CD1 | 1:A:76:TYR:N | 0.81 | 2.44 | 17 | 13 |
| 1:A:9:TYR:CZ | 1:A:88:PRO:HG3 | 0.81 | 2.09 | 15 | 9 |
| 1:A:39:SER:CB | 1:A:65:HIS:NE2 | 0.81 | 2.43 | 17 | 12 |
| 1:A:100:GLY:O | 1:A:101:LEU:HD12 | 0.81 | 1.75 | 3 | 3 |
| 1:A:62:LYS:HG2 | 1:A:64:TYR:CE1 | 0.81 | 2.10 | 11 | 13 |
| 1:A:66:ILE:N | 1:A:66:ILE:CD1 | 0.81 | 2.41 | 16 | 9 |
| 1:A:30:LYS:HE3 | 1:A:107:TYR:CE2 | 0.81 | 2.09 | 17 | 6 |
| 1:A:44:THR:CG2 | 1:A:65:HIS:NE2 | 0.81 | 2.43 | 4 | 2 |
| 1:A:66:ILE:HG23 | 1:A:90:LEU:CD1 | 0.81 | 2.05 | 19 | 7 |
| 1:A:95:GLN:CG | 1:A:105:LEU:CB | 0.81 | 2.59 | 17 | 5 |
| 1:A:85:ASP:C | 1:A:89:LEU:HD11 | 0.81 | 1.95 | 1 | 5 |
| 1:A:66:ILE:HG22 | 1:A:90:LEU:CD1 | 0.81 | 2.06 | 8 | 14 |
| 1:A:99:GLY:O | 1:A:101:LEU:HD13 | 0.81 | 1.75 | 5 | 6 |
| 1:A:65:HIS:O | 1:A:78:VAL:HG22 | 0.81 | 1.74 | 9 | 2 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:CE | 0.81 | 2.06 | 4 | 5 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:CE | 0.81 | 2.43 | 8 | 14 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:ALA:HB1 | 1:A:109:VAL:CG1 | 0.81 | 2.05 | 10 | 5 |
| 1:A:76:TYR:N | 1:A:76:TYR:HD1 | 0.81 | 1.71 | 6 | 8 |
| 1:A:67:LYS:CG | 1:A:77:TYR:CZ | 0.81 | 2.64 | 5 | 14 |
| 1:A:82:TYR:CD1 | 1:A:93:TYR:CE2 | 0.81 | 2.68 | 4 | 3 |
| 1:A:22:GLU:HG3 | 1:A:63:HIS:HE2 | 0.81 | 1.36 | 11 | 2 |
| 1:A:41:THR:OG1 | 1:A:42:PRO:HD2 | 0.80 | 1.77 | 7 | 20 |
| 1:A:94:HIS:CD2 | 1:A:99:GLY:O | 0.80 | 2.34 | 16 | 4 |
| 1:A:90:LEU:O | 1:A:93:TYR:CE1 | 0.80 | 2.34 | 19 | 6 |
| 1:A:24:LEU:CD2 | 1:A:35:MET:HE3 | 0.80 | 2.04 | 16 | 8 |
| 1:A:81:LYS:HB3 | 1:A:82:TYR:CE1 | 0.80 | 2.11 | 6 | 12 |
| 1:A:11:TRP:CD1 | 1:A:34:PHE:CE2 | 0.80 | 2.69 | 6 | 20 |
| 1:A:45:TYR:CG | 1:A:87:ILE:HG12 | 0.80 | 2.11 | 6 | 14 |
| 1:A:44:THR:OG1 | 1:A:45:TYR:N | 0.80 | 2.11 | 2 | 14 |
| 1:A:16:ILE:CG2 | 1:A:37:ARG:HB2 | 0.80 | 2.06 | 9 | 8 |
| 1:A:25:LEU:O | 1:A:50:PHE:CE1 | 0.80 | 2.34 | 8 | 11 |
| 1:A:24:LEU:CG | 1:A:35:MET:HE1 | 0.80 | 2.05 | 1 | 6 |
| 1:A:47:VAL:N | 1:A:64:TYR:O | 0.80 | 2.14 | 19 | 20 |
| 1:A:93:TYR:CZ | 1:A:94:HIS:ND1 | 0.80 | 2.49 | 1 | 15 |
| 1:A:82:TYR:CG | 1:A:93:TYR:CZ | 0.80 | 2.70 | 14 | 13 |
| 1:A:67:LYS:HB3 | 1:A:77:TYR:CE1 | 0.80 | 2.12 | 8 | 20 |
| 1:A:78:VAL:O | 1:A:79:ALA:CB | 0.80 | 2.29 | 17 | 12 |
| 1:A:30:LYS:CE | 1:A:109:VAL:HG12 | 0.80 | 2.06 | 6 | 3 |
| 1:A:65:HIS:C | 1:A:78:VAL:HG22 | 0.80 | 1.97 | 3 | 1 |
| 1:A:74:LYS:HG2 | 1:A:83:VAL:HG23 | 0.80 | 1.50 | 8 | 1 |
| 1:A:24:LEU:CD2 | 1:A:35:MET:CE | 0.80 | 2.60 | 6 | 8 |
| 1:A:49:VAL:HG21 | 1:A:64:TYR:CE1 | 0.80 | 2.10 | 15 | 11 |
| 1:A:81:LYS:HD2 | 1:A:82:TYR:CE2 | 0.80 | 2.11 | 19 | 1 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:HG3 | 0.80 | 1.91 | 14 | 7 |
| 1:A:94:HIS:NE2 | 1:A:101:LEU:CD2 | 0.80 | 2.45 | 11 | 10 |
| 1:A:24:LEU:HD23 | 1:A:25:LEU:H | 0.80 | 1.37 | 16 | 2 |
| 1:A:6:LEU:O | 1:A:12:TYR:CE2 | 0.79 | 2.35 | 10 | 2 |
| 1:A:87:ILE:HG23 | 1:A:91:ILE:HG12 | 0.79 | 1.53 | 13 | 10 |
| 1:A:74:LYS:HE2 | 1:A:83:VAL:HG23 | 0.79 | 1.52 | 14 | 1 |
| 1:A:33:ALA:HB3 | 1:A:50:PHE:HD2 | 0.79 | 1.38 | 11 | 3 |
| 1:A:11:TRP:O | 1:A:35:MET:CA | 0.79 | 2.31 | 9 | 19 |
| 1:A:69:THR:HG23 | 1:A:74:LYS:O | 0.79 | 1.76 | 11 | 3 |
| 1:A:34:PHE:HE2 | 1:A:91:ILE:HG21 | 0.79 | 1.32 | 15 | 20 |
| 1:A:9:TYR:HB3 | 1:A:11:TRP:NE1 | 0.79 | 1.93 | 8 | 20 |
| 1:A:30:LYS:HE3 | 1:A:107:TYR:CD2 | 0.79 | 2.12 | 6 | 4 |
| 1:A:50:PHE:CD2 | 1:A:61:ILE:HD13 | 0.79 | 2.12 | 14 | 7 |
| 1:A:81:LYS:HG3 | 1:A:82:TYR:CD1 | 0.79 | 2.10 | 13 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:14:LYS:CG | 1:A:15:SER:N | 0.79 | 2.45 | 19 | 5 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:HB2 | 0.79 | 1.92 | 9 | 1 |
| 1:A:34:PHE:CZ | 1:A:36:VAL:CG2 | 0.79 | 2.66 | 7 | 20 |
| 1:A:84:PHE:CD1 | 1:A:90:LEU:HA | 0.79 | 2.12 | 15 | 13 |
| 1:A:10:GLU:O | 1:A:109:VAL:C | 0.79 | 2.20 | 9 | 20 |
| 1:A:10:GLU:O | 1:A:110:CYS:N | 0.79 | 2.16 | 13 | 9 |
| 1:A:11:TRP:HB3 | 1:A:34:PHE:CD2 | 0.79 | 2.12 | 4 | 20 |
| 1:A:30:LYS:NZ | 1:A:107:TYR:CE2 | 0.79 | 2.51 | 4 | 9 |
| 1:A:28:THR:CG2 | 1:A:30:LYS:HE2 | 0.79 | 2.08 | 6 | 2 |
| 1:A:94:HIS:NE2 | 1:A:101:LEU:HD13 | 0.79 | 1.93 | 3 | 4 |
| 1:A:68:GLU:OE1 | 1:A:68:GLU:N | 0.79 | 2.16 | 7 | 2 |
| 1:A:9:TYR:CE2 | 1:A:88:PRO:HG3 | 0.79 | 2.13 | 16 | 5 |
| 1:A:79:ALA:CB | 1:A:81:LYS:HE2 | 0.79 | 2.06 | 11 | 1 |
| 1:A:81:LYS:CD | 1:A:82:TYR:CD2 | 0.79 | 2.66 | 14 | 2 |
| 1:A:34:PHE:O | 1:A:108:PRO:CA | 0.79 | 2.30 | 9 | 15 |
| 1:A:68:GLU:CD | 1:A:76:TYR:CE1 | 0.79 | 2.56 | 19 | 12 |
| 1:A:35:MET:N | 1:A:48:SER:O | 0.78 | 2.16 | 17 | 20 |
| 1:A:11:TRP:CZ3 | 1:A:36:VAL:HG21 | 0.78 | 2.12 | 12 | 20 |
| 1:A:68:GLU:HG2 | 1:A:76:TYR:CD1 | 0.78 | 2.13 | 5 | 13 |
| 1:A:81:LYS:HG3 | 1:A:82:TYR:CE1 | 0.78 | 2.13 | 13 | 2 |
| 1:A:30:LYS:CG | 1:A:107:TYR:CD2 | 0.78 | 2.66 | 15 | 5 |
| 1:A:6:LEU:CB | 1:A:12:TYR:CG | 0.78 | 2.66 | 12 | 3 |
| 1:A:35:MET:HB3 | 1:A:48:SER:OG | 0.78 | 1.78 | 4 | 7 |
| 1:A:81:LYS:HD3 | 1:A:82:TYR:CD2 | 0.78 | 2.13 | 14 | 1 |
| 1:A:25:LEU:CD1 | 1:A:48:SER:CB | 0.78 | 2.60 | 20 | 9 |
| 1:A:32:GLY:CA | 1:A:103:THR:CG2 | 0.78 | 2.61 | 5 | 9 |
| 1:A:35:MET:HE2 | 1:A:109:VAL:O | 0.78 | 1.78 | 10 | 11 |
| 1:A:49:VAL:HG21 | 1:A:102:VAL:HG13 | 0.78 | 1.52 | 9 | 3 |
| 1:A:82:TYR:O | 1:A:84:PHE:CE2 | 0.78 | 2.37 | 2 | 4 |
| 1:A:35:MET:O | 1:A:48:SER:N | 0.78 | 2.16 | 7 | 20 |
| 1:A:25:LEU:HG | 1:A:109:VAL:CG1 | 0.78 | 2.09 | 8 | 3 |
| 1:A:40:ARG:O | 1:A:41:THR:HG22 | 0.78 | 1.77 | 1 | 2 |
| 1:A:24:LEU:C | 1:A:24:LEU:HD23 | 0.78 | 1.99 | 20 | 1 |
| 1:A:39:SER:HB2 | 1:A:65:HIS:CE1 | 0.78 | 2.13 | 9 | 8 |
| 1:A:101:LEU:HD13 | 1:A:101:LEU:H | 0.78 | 1.38 | 7 | 2 |
| 1:A:90:LEU:O | 1:A:94:HIS:CD2 | 0.78 | 2.37 | 14 | 1 |
| 1:A:25:LEU:O | 1:A:50:PHE:CE2 | 0.78 | 2.37 | 11 | 3 |
| 1:A:39:SER:CB | 1:A:65:HIS:CE1 | 0.78 | 2.65 | 4 | 12 |
| 1:A:77:TYR:CD2 | 1:A:80:GLU:HA | 0.78 | 2.13 | 9 | 12 |
| 1:A:50:PHE:CG | 1:A:61:ILE:HD12 | 0.78 | 2.13 | 4 | 6 |
| 1:A:6:LEU:HB3 | 1:A:12:TYR:CG | 0.78 | 2.14 | 12 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:36:VAL:CA | 1:A:46:THR:O | 0.78 | 2.32 | 8 | 20 |
| 1:A:93:TYR:O | 1:A:97:ASN:ND2 | 0.78 | 2.16 | 3 | 3 |
| 1:A:34:PHE:CE2 | 1:A:91:ILE:HG23 | 0.78 | 2.14 | 19 | 20 |
| 1:A:33:ALA:O | 1:A:49:VAL:HA | 0.78 | 1.79 | 8 | 20 |
| 1:A:9:TYR:CE1 | 1:A:88:PRO:HB3 | 0.78 | 2.14 | 12 | 12 |
| 1:A:21:ALA:C | 1:A:24:LEU:HD13 | 0.78 | 2.00 | 18 | 1 |
| 1:A:35:MET:CB | 1:A:48:SER:OG | 0.78 | 2.32 | 16 | 5 |
| 1:A:24:LEU:HD23 | 1:A:24:LEU:C | 0.78 | 1.98 | 12 | 1 |
| 1:A:68:GLU:CD | 1:A:76:TYR:CE2 | 0.78 | 2.58 | 3 | 1 |
| 1:A:41:THR:O | 1:A:43:GLY:N | 0.77 | 2.17 | 4 | 20 |
| 1:A:50:PHE:CA | 1:A:60:CYS:O | 0.77 | 2.32 | 1 | 15 |
| 1:A:39:SER:HB2 | 1:A:65:HIS:NE2 | 0.77 | 1.94 | 5 | 11 |
| 1:A:44:THR:OG1 | 1:A:66:ILE:O | 0.77 | 2.02 | 7 | 20 |
| 1:A:9:TYR:CE2 | 1:A:88:PRO:HB3 | 0.77 | 2.14 | 9 | 6 |
| 1:A:28:THR:CG2 | 1:A:30:LYS:CE | 0.77 | 2.62 | 9 | 3 |
| 1:A:79:ALA:CB | 1:A:81:LYS:HD2 | 0.77 | 2.09 | 8 | 9 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:CB | 0.77 | 2.67 | 20 | 4 |
| 1:A:87:ILE:HG22 | 1:A:91:ILE:HG12 | 0.77 | 1.55 | 19 | 10 |
| 1:A:18:ARG:O | 1:A:63:HIS:CE1 | 0.77 | 2.37 | 18 | 10 |
| 1:A:87:ILE:HG22 | 1:A:91:ILE:CG1 | 0.77 | 2.08 | 19 | 14 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:HG22 | 0.77 | 1.53 | 1 | 1 |
| 1:A:13:ASN:HB3 | 1:A:16:ILE:HB | 0.77 | 1.56 | 19 | 13 |
| 1:A:76:TYR:O | 1:A:84:PHE:N | 0.77 | 2.17 | 19 | 20 |
| 1:A:34:PHE:CB | 1:A:105:LEU:HD12 | 0.77 | 2.09 | 7 | 16 |
| 1:A:25:LEU:CD1 | 1:A:109:VAL:CG1 | 0.77 | 2.62 | 8 | 1 |
| 1:A:25:LEU:CD2 | 1:A:109:VAL:CG2 | 0.77 | 2.62 | 10 | 6 |
| 1:A:34:PHE:CE1 | 1:A:105:LEU:HD11 | 0.77 | 2.14 | 20 | 19 |
| 1:A:101:LEU:N | 1:A:101:LEU:CD1 | 0.77 | 2.47 | 11 | 4 |
| 1:A:86:SER:OG | 1:A:88:PRO:HG2 | 0.77 | 1.79 | 6 | 2 |
| 1:A:35:MET:HG2 | 1:A:48:SER:OG | 0.77 | 1.79 | 9 | 2 |
| 1:A:24:LEU:CG | 1:A:35:MET:CE | 0.77 | 2.62 | 4 | 9 |
| 1:A:93:TYR:CD1 | 1:A:97:ASN:OD1 | 0.77 | 2.37 | 14 | 1 |
| 1:A:25:LEU:HB3 | 1:A:50:PHE:CD2 | 0.77 | 2.15 | 10 | 3 |
| 1:A:50:PHE:HA | 1:A:60:CYS:O | 0.77 | 1.79 | 16 | 17 |
| 1:A:17:SER:CB | 1:A:20:LYS:CE | 0.77 | 2.62 | 5 | 6 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:HE2 | 0.77 | 1.53 | 11 | 3 |
| 1:A:68:GLU:OE2 | 1:A:76:TYR:CZ | 0.77 | 2.38 | 18 | 9 |
| 1:A:11:TRP:CZ3 | 1:A:87:ILE:HG21 | 0.77 | 2.15 | 4 | 20 |
| 1:A:11:TRP:CB | 1:A:108:PRO:HB3 | 0.77 | 2.10 | 4 | 20 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:HG | 0.77 | 2.15 | 3 | 10 |
| 1:A:87:ILE:N | 1:A:88:PRO:HD2 | 0.77 | 1.94 | 4 | 16 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:GLU:CD | 1:A:76:TYR:CD1 | 0.77 | 2.58 | 17 | 5 |
| 1:A:68:GLU:HG3 | 1:A:76:TYR:CE1 | 0.77 | 2.15 | 13 | 6 |
| 1:A:20:LYS:O | 1:A:24:LEU:CD2 | 0.77 | 2.33 | 2 | 2 |
| 1:A:22:GLU:OE1 | 1:A:63:HIS:CE1 | 0.77 | 2.38 | 12 | 3 |
| 1:A:17:SER:HB2 | 1:A:20:LYS:CE | 0.76 | 2.11 | 19 | 15 |
| 1:A:30:LYS:CE | 1:A:109:VAL:HG23 | 0.76 | 2.11 | 19 | 1 |
| 1:A:34:PHE:CE2 | 1:A:105:LEU:HD12 | 0.76 | 2.15 | 20 | 3 |
| 1:A:79:ALA:O | 1:A:81:LYS:HG3 | 0.76 | 1.80 | 3 | 12 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:SD | 0.76 | 2.58 | 13 | 10 |
| 1:A:102:VAL:CG2 | 1:A:103:THR:HG23 | 0.76 | 2.09 | 9 | 1 |
| 1:A:64:TYR:HD2 | 1:A:78:VAL:HG11 | 0.76 | 1.41 | 3 | 3 |
| 1:A:50:PHE:CB | 1:A:61:ILE:HA | 0.76 | 2.09 | 18 | 17 |
| 1:A:20:LYS:C | 1:A:24:LEU:CD2 | 0.76 | 2.53 | 2 | 2 |
| 1:A:25:LEU:CD2 | 1:A:109:VAL:HG11 | 0.76 | 2.10 | 1 | 4 |
| 1:A:11:TRP:O | 1:A:36:VAL:N | 0.76 | 2.18 | 9 | 20 |
| 1:A:33:ALA:N | 1:A:50:PHE:O | 0.76 | 2.19 | 5 | 20 |
| 1:A:104:ARG:O | 1:A:106:ARG:N | 0.76 | 2.18 | 12 | 18 |
| 1:A:68:GLU:OE2 | 1:A:76:TYR:CG | 0.76 | 2.39 | 16 | 4 |
| 1:A:21:ALA:N | 1:A:24:LEU:HD21 | 0.76 | 1.94 | 2 | 3 |
| 1:A:50:PHE:CD2 | 1:A:61:ILE:HD12 | 0.76 | 2.16 | 4 | 4 |
| 1:A:35:MET:HE3 | 1:A:109:VAL:HG13 | 0.76 | 1.57 | 8 | 4 |
| 1:A:16:ILE:CD1 | 1:A:35:MET:SD | 0.76 | 2.74 | 14 | 16 |
| 1:A:68:GLU:OE2 | 1:A:76:TYR:CD1 | 0.76 | 2.39 | 17 | 4 |
| 1:A:94:HIS:NE2 | 1:A:101:LEU:CD1 | 0.76 | 2.49 | 17 | 6 |
| 1:A:44:THR:HB | 1:A:66:ILE:O | 0.76 | 1.81 | 18 | 18 |
| 1:A:50:PHE:HB2 | 1:A:61:ILE:CA | 0.76 | 2.11 | 18 | 13 |
| 1:A:34:PHE:HB2 | 1:A:105:LEU:HD12 | 0.76 | 1.58 | 18 | 16 |
| 1:A:78:VAL:O | 1:A:79:ALA:HB2 | 0.76 | 1.80 | 11 | 12 |
| 1:A:45:TYR:O | 1:A:65:HIS:ND1 | 0.76 | 2.19 | 7 | 13 |
| 1:A:25:LEU:CD1 | 1:A:109:VAL:CG2 | 0.76 | 2.60 | 12 | 3 |
| 1:A:74:LYS:HG3 | 1:A:83:VAL:HG23 | 0.76 | 1.57 | 8 | 1 |
| 1:A:24:LEU:CD1 | 1:A:35:MET:HE3 | 0.76 | 2.11 | 14 | 8 |
| 1:A:79:ALA:CB | 1:A:81:LYS:CD | 0.76 | 2.63 | 8 | 5 |
| 1:A:88:PRO:O | 1:A:92:GLN:N | 0.75 | 2.19 | 6 | 16 |
| 1:A:81:LYS:CD | 1:A:82:TYR:CE2 | 0.75 | 2.69 | 14 | 2 |
| 1:A:39:SER:OG | 1:A:65:HIS:CE1 | 0.75 | 2.39 | 10 | 4 |
| 1:A:50:PHE:CB | 1:A:61:ILE:CD1 | 0.75 | 2.63 | 3 | 12 |
| 1:A:74:LYS:CE | 1:A:83:VAL:O | 0.75 | 2.35 | 14 | 2 |
| 1:A:81:LYS:NZ | 1:A:82:TYR:O | 0.75 | 2.20 | 19 | 1 |
| 1:A:12:TYR:OH | 1:A:14:LYS:CD | 0.75 | 2.33 | 20 | 1 |
| 1:A:11:TRP:O | 1:A:35:MET:HA | 0.75 | 1.81 | 16 | 19 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:82:TYR:O | 1:A:84:PHE:CE1 | 0.75 | 2.39 | 19 | 5 |
| 1:A:23:LYS:H | 1:A:23:LYS:HE2 | 0.75 | 1.41 | 2 | 1 |
| 1:A:86:SER:CB | 1:A:89:LEU:CD2 | 0.75 | 2.65 | 17 | 3 |
| 1:A:24:LEU:HD12 | 1:A:25:LEU:N | 0.75 | 1.95 | 13 | 9 |
| 1:A:6:LEU:HD13 | 1:A:11:TRP:CZ3 | 0.75 | 2.17 | 3 | 10 |
| 1:A:30:LYS:HZ3 | 1:A:107:TYR:HE2 | 0.75 | 1.24 | 16 | 4 |
| 1:A:50:PHE:HD2 | 1:A:61:ILE:HD13 | 0.75 | 1.39 | 14 | 1 |
| 1:A:32:GLY:CA | 1:A:51:THR:OG1 | 0.75 | 2.34 | 16 | 17 |
| 1:A:7:GLU:N | 1:A:12:TYR:CD2 | 0.75 | 2.55 | 12 | 6 |
| 1:A:6:LEU:O | 1:A:8:THR:N | 0.75 | 2.18 | 13 | 14 |
| 1:A:30:LYS:CD | 1:A:109:VAL:HG13 | 0.75 | 2.11 | 12 | 1 |
| 1:A:87:ILE:CG2 | 1:A:91:ILE:CG1 | 0.75 | 2.63 | 18 | 20 |
| 1:A:86:SER:CB | 1:A:89:LEU:CD1 | 0.75 | 2.65 | 5 | 12 |
| 1:A:28:THR:OG1 | 1:A:30:LYS:CE | 0.75 | 2.35 | 12 | 8 |
| 1:A:24:LEU:HD22 | 1:A:24:LEU:O | 0.75 | 1.82 | 5 | 2 |
| 1:A:11:TRP:CD1 | 1:A:108:PRO:HB3 | 0.75 | 2.16 | 17 | 20 |
| 1:A:94:HIS:NE2 | 1:A:99:GLY:HA3 | 0.75 | 1.97 | 5 | 9 |
| 1:A:25:LEU:CD2 | 1:A:109:VAL:CG1 | 0.75 | 2.64 | 1 | 3 |
| 1:A:21:ALA:O | 1:A:24:LEU:HD22 | 0.75 | 1.81 | 20 | 2 |
| 1:A:20:LYS:O | 1:A:23:LYS:CG | 0.74 | 2.35 | 16 | 9 |
| 1:A:90:LEU:O | 1:A:93:TYR:CD2 | 0.74 | 2.40 | 14 | 10 |
| 1:A:78:VAL:CG1 | 1:A:79:ALA:N | 0.74 | 2.49 | 9 | 3 |
| 1:A:66:ILE:CG2 | 1:A:87:ILE:HD12 | 0.74 | 2.12 | 3 | 5 |
| 1:A:13:ASN:HD22 | 1:A:24:LEU:HD11 | 0.74 | 1.41 | 20 | 1 |
| 1:A:16:ILE:O | 1:A:37:ARG:NH1 | 0.74 | 2.21 | 20 | 4 |
| 1:A:47:VAL:CG2 | 1:A:66:ILE:CD1 | 0.74 | 2.65 | 18 | 11 |
| 1:A:67:LYS:O | 1:A:77:TYR:N | 0.74 | 2.21 | 3 | 20 |
| 1:A:65:HIS:O | 1:A:78:VAL:CG2 | 0.74 | 2.36 | 9 | 2 |
| 1:A:50:PHE:HB2 | 1:A:60:CYS:O | 0.74 | 1.82 | 7 | 17 |
| 1:A:88:PRO:O | 1:A:92:GLN:NE2 | 0.74 | 2.20 | 17 | 3 |
| 1:A:95:GLN:CG | 1:A:105:LEU:HB3 | 0.74 | 2.12 | 2 | 12 |
| 1:A:6:LEU:HB3 | 1:A:9:TYR:CE2 | 0.74 | 2.18 | 13 | 13 |
| 1:A:77:TYR:CD1 | 1:A:83:VAL:HG12 | 0.74 | 2.17 | 6 | 13 |
| 1:A:30:LYS:HE2 | 1:A:109:VAL:CG2 | 0.74 | 2.11 | 19 | 1 |
| 1:A:22:GLU:CD | 1:A:63:HIS:CE1 | 0.74 | 2.61 | 4 | 3 |
| 1:A:10:GLU:OE2 | 1:A:107:TYR:CZ | 0.74 | 2.41 | 5 | 1 |
| 1:A:77:TYR:N | 1:A:90:LEU:CD1 | 0.74 | 2.50 | 3 | 15 |
| 1:A:11:TRP:CZ3 | 1:A:36:VAL:CG2 | 0.74 | 2.71 | 17 | 20 |
| 1:A:36:VAL:CG2 | 1:A:47:VAL:HG22 | 0.74 | 2.09 | 15 | 19 |
| 1:A:82:TYR:N | 1:A:82:TYR:CD1 | 0.74 | 2.55 | 5 | 8 |
| 1:A:22:GLU:O | 1:A:26:LEU:HD13 | 0.74 | 1.83 | 17 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:24:LEU:HD22 | 1:A:35:MET:HE1 | 0.74 | 1.57 | 6 | 2 |
| 1:A:18:ARG:O | 1:A:63:HIS:NE2 | 0.74 | 2.20 | 4 | 12 |
| 1:A:25:LEU:HD23 | 1:A:109:VAL:CG2 | 0.74 | 2.13 | 4 | 5 |
| 1:A:28:THR:OG1 | 1:A:30:LYS:HE3 | 0.73 | 1.83 | 14 | 5 |
| 1:A:66:ILE:O | 1:A:68:GLU:OE1 | 0.73 | 2.06 | 7 | 2 |
| 1:A:81:LYS:CG | 1:A:82:TYR:N | 0.73 | 2.51 | 13 | 2 |
| 1:A:103:THR:O | 1:A:104:ARG:O | 0.73 | 2.06 | 13 | 16 |
| 1:A:64:TYR:CD2 | 1:A:101:LEU:HG | 0.73 | 2.18 | 14 | 10 |
| 1:A:10:GLU:OE1 | 1:A:107:TYR:CE1 | 0.73 | 2.41 | 6 | 2 |
| 1:A:25:LEU:HD13 | 1:A:48:SER:OG | 0.73 | 1.83 | 7 | 1 |
| 1:A:84:PHE:CE2 | 1:A:93:TYR:CD1 | 0.73 | 2.76 | 5 | 3 |
| 1:A:21:ALA:C | 1:A:24:LEU:HD22 | 0.73 | 2.04 | 20 | 3 |
| 1:A:47:VAL:O | 1:A:64:TYR:N | 0.73 | 2.18 | 19 | 20 |
| 1:A:91:ILE:CG2 | 1:A:105:LEU:HG | 0.73 | 2.13 | 17 | 13 |
| 1:A:30:LYS:CG | 1:A:107:TYR:CE2 | 0.73 | 2.70 | 15 | 3 |
| 1:A:68:GLU:OE2 | 1:A:76:TYR:CE2 | 0.73 | 2.40 | 3 | 1 |
| 1:A:45:TYR:HB2 | 1:A:87:ILE:CG1 | 0.73 | 2.14 | 3 | 15 |
| 1:A:102:VAL:O | 1:A:103:THR:HG22 | 0.73 | 1.83 | 2 | 6 |
| 1:A:26:LEU:CD1 | 1:A:61:ILE:CG1 | 0.73 | 2.67 | 1 | 2 |
| 1:A:25:LEU:CD1 | 1:A:61:ILE:CG2 | 0.73 | 2.66 | 11 | 8 |
| 1:A:81:LYS:HZ1 | 1:A:100:GLY:N | 0.73 | 1.82 | 3 | 2 |
| 1:A:81:LYS:HD2 | 1:A:82:TYR:CD2 | 0.73 | 2.19 | 19 | 1 |
| 1:A:62:LYS:HB3 | 1:A:64:TYR:CE1 | 0.73 | 2.18 | 20 | 11 |
| 1:A:11:TRP:CZ3 | 1:A:87:ILE:CG2 | 0.73 | 2.71 | 4 | 20 |
| 1:A:41:THR:CB | 1:A:42:PRO:CD | 0.73 | 2.67 | 18 | 20 |
| 1:A:101:LEU:O | 1:A:103:THR:N | 0.73 | 2.21 | 7 | 10 |
| 1:A:53:ALA:CB | 1:A:60:CYS:SG | 0.73 | 2.76 | 19 | 1 |
| 1:A:86:SER:O | 1:A:89:LEU:CD1 | 0.73 | 2.36 | 20 | 6 |
| 1:A:30:LYS:HZ1 | 1:A:109:VAL:HG12 | 0.73 | 1.41 | 6 | 1 |
| 1:A:61:ILE:HD12 | 1:A:61:ILE:N | 0.73 | 1.99 | 12 | 1 |
| 1:A:21:ALA:HB3 | 1:A:63:HIS:HE1 | 0.73 | 1.43 | 2 | 3 |
| 1:A:62:LYS:NZ | 1:A:64:TYR:OH | 0.73 | 2.19 | 6 | 4 |
| 1:A:24:LEU:HD23 | 1:A:111:GLY:N | 0.73 | 1.99 | 4 | 2 |
| 1:A:26:LEU:CD2 | 1:A:61:ILE:HD11 | 0.73 | 2.14 | 10 | 3 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:HB3 | 0.73 | 2.19 | 20 | 6 |
| 1:A:81:LYS:HD2 | 1:A:82:TYR:CE1 | 0.73 | 2.19 | 2 | 2 |
| 1:A:103:THR:OG1 | 1:A:106:ARG:CD | 0.73 | 2.37 | 13 | 1 |
| 1:A:37:ARG:NH1 | 1:A:46:THR:HG21 | 0.73 | 1.99 | 12 | 1 |
| 1:A:37:ARG:O | 1:A:46:THR:N | 0.73 | 2.22 | 8 | 20 |
| 1:A:25:LEU:HB3 | 1:A:50:PHE:CD1 | 0.73 | 2.18 | 13 | 11 |
| 1:A:94:HIS:O | 1:A:104:ARG:CB | 0.73 | 2.36 | 17 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:94:HIS:HB3 | 1:A:105:LEU:CG | 0.73 | 2.14 | 4 | 2 |
| 1:A:77:TYR:HA | 1:A:90:LEU:CD1 | 0.72 | 2.13 | 9 | 20 |
| 1:A:22:GLU:CD | 1:A:63:HIS:NE2 | 0.72 | 2.42 | 4 | 4 |
| 1:A:10:GLU:O | 1:A:110:CYS:CA | 0.72 | 2.37 | 11 | 7 |
| 1:A:41:THR:HG22 | 1:A:44:THR:HG23 | 0.72 | 1.59 | 18 | 11 |
| 1:A:67:LYS:CB | 1:A:77:TYR:O | 0.72 | 2.37 | 6 | 8 |
| 1:A:74:LYS:HB2 | 1:A:84:PHE:CA | 0.72 | 2.15 | 6 | 1 |
| 1:A:6:LEU:HD12 | 1:A:12:TYR:CG | 0.72 | 2.19 | 6 | 2 |
| 1:A:67:LYS:HG2 | 1:A:77:TYR:CE1 | 0.72 | 2.19 | 4 | 7 |
| 1:A:50:PHE:CB | 1:A:60:CYS:O | 0.72 | 2.38 | 1 | 14 |
| 1:A:25:LEU:HD12 | 1:A:50:PHE:HD1 | 0.72 | 1.40 | 19 | 1 |
| 1:A:81:LYS:HG3 | 1:A:82:TYR:CE2 | 0.72 | 2.18 | 19 | 2 |
| 1:A:50:PHE:CD1 | 1:A:61:ILE:HD13 | 0.72 | 2.19 | 10 | 3 |
| 1:A:67:LYS:HG2 | 1:A:77:TYR:CZ | 0.72 | 2.20 | 8 | 19 |
| 1:A:9:TYR:CE1 | 1:A:88:PRO:HG3 | 0.72 | 2.19 | 14 | 3 |
| 1:A:102:VAL:C | 1:A:103:THR:HG22 | 0.72 | 2.03 | 2 | 9 |
| 1:A:12:TYR:OH | 1:A:14:LYS:HG3 | 0.72 | 1.83 | 20 | 2 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:CD2 | 0.72 | 2.71 | 6 | 4 |
| 1:A:93:TYR:OH | 1:A:94:HIS:NE2 | 0.72 | 2.22 | 5 | 1 |
| 1:A:77:TYR:CE2 | 1:A:80:GLU:CA | 0.72 | 2.73 | 9 | 20 |
| 1:A:17:SER:CB | 1:A:20:LYS:HD3 | 0.72 | 2.15 | 16 | 13 |
| 1:A:45:TYR:O | 1:A:66:ILE:CG1 | 0.72 | 2.37 | 2 | 11 |
| 1:A:62:LYS:CE | 1:A:64:TYR:CZ | 0.72 | 2.72 | 16 | 1 |
| 1:A:91:ILE:HA | 1:A:105:LEU:HD21 | 0.72 | 1.61 | 5 | 12 |
| 1:A:31:GLU:O | 1:A:106:ARG:CG | 0.72 | 2.37 | 7 | 5 |
| 1:A:99:GLY:O | 1:A:101:LEU:N | 0.72 | 2.23 | 3 | 2 |
| 1:A:95:GLN:HG3 | 1:A:105:LEU:CB | 0.72 | 2.14 | 17 | 3 |
| 1:A:22:GLU:O | 1:A:26:LEU:CD1 | 0.72 | 2.38 | 11 | 5 |
| 1:A:76:TYR:CD2 | 1:A:86:SER:HA | 0.72 | 2.20 | 3 | 4 |
| 1:A:28:THR:CG2 | 1:A:109:VAL:CG2 | 0.72 | 2.67 | 17 | 5 |
| 1:A:64:TYR:HE2 | 1:A:101:LEU:HD22 | 0.72 | 1.45 | 2 | 3 |
| 1:A:28:THR:HG21 | 1:A:30:LYS:HE2 | 0.72 | 1.62 | 6 | 2 |
| 1:A:64:TYR:CZ | 1:A:101:LEU:HB3 | 0.72 | 2.19 | 7 | 6 |
| 1:A:37:ARG:NH1 | 1:A:46:THR:OG1 | 0.72 | 2.23 | 17 | 5 |
| 1:A:9:TYR:CZ | 1:A:88:PRO:CG | 0.72 | 2.73 | 15 | 9 |
| 1:A:6:LEU:HD22 | 1:A:88:PRO:CD | 0.72 | 2.13 | 4 | 6 |
| 1:A:45:TYR:CD1 | 1:A:87:ILE:CD1 | 0.72 | 2.72 | 7 | 16 |
| 1:A:25:LEU:CB | 1:A:61:ILE:HD12 | 0.72 | 2.13 | 2 | 3 |
| 1:A:84:PHE:CE1 | 1:A:93:TYR:CE2 | 0.72 | 2.78 | 14 | 3 |
| 1:A:11:TRP:O | 1:A:13:ASN:ND2 | 0.71 | 2.22 | 7 | 2 |
| 1:A:7:GLU:HA | 1:A:12:TYR:CD2 | 0.71 | 2.20 | 18 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:32:GLY:N | 1:A:51:THR:HB | 0.71 | 2.00 | 2 | 3 |
| 1:A:66:ILE:HD12 | 1:A:87:ILE:HG13 | 0.71 | 1.61 | 20 | 2 |
| 1:A:25:LEU:CD1 | 1:A:61:ILE:HG21 | 0.71 | 2.14 | 2 | 6 |
| 1:A:68:GLU:OE2 | 1:A:76:TYR:CE1 | 0.71 | 2.43 | 15 | 10 |
| 1:A:21:ALA:CA | 1:A:24:LEU:HD21 | 0.71 | 2.14 | 2 | 5 |
| 1:A:40:ARG:O | 1:A:41:THR:O | 0.71 | 2.09 | 9 | 12 |
| 1:A:26:LEU:HA | 1:A:50:PHE:CE2 | 0.71 | 2.20 | 3 | 5 |
| 1:A:24:LEU:HD12 | 1:A:25:LEU:HD22 | 0.71 | 1.61 | 19 | 1 |
| 1:A:68:GLU:CD | 1:A:68:GLU:N | 0.71 | 2.44 | 7 | 1 |
| 1:A:74:LYS:CE | 1:A:83:VAL:HG23 | 0.71 | 2.15 | 14 | 1 |
| 1:A:86:SER:CA | 1:A:89:LEU:CD1 | 0.71 | 2.68 | 5 | 15 |
| 1:A:81:LYS:CD | 1:A:82:TYR:CE1 | 0.71 | 2.73 | 4 | 2 |
| 1:A:64:TYR:HH | 1:A:102:VAL:HG13 | 0.71 | 1.44 | 20 | 1 |
| 1:A:82:TYR:HB2 | 1:A:93:TYR:CZ | 0.71 | 2.20 | 14 | 1 |
| 1:A:28:THR:HG23 | 1:A:30:LYS:HD2 | 0.71 | 1.62 | 10 | 2 |
| 1:A:64:TYR:CZ | 1:A:101:LEU:CD1 | 0.71 | 2.74 | 10 | 1 |
| 1:A:67:LYS:HG3 | 1:A:77:TYR:CE1 | 0.71 | 2.21 | 2 | 13 |
| 1:A:81:LYS:HG2 | 1:A:82:TYR:CG | 0.71 | 2.21 | 19 | 2 |
| 1:A:17:SER:HB2 | 1:A:20:LYS:CD | 0.71 | 2.16 | 9 | 15 |
| 1:A:6:LEU:HB3 | 1:A:9:TYR:CD2 | 0.71 | 2.21 | 7 | 13 |
| 1:A:35:MET:CG | 1:A:48:SER:OG | 0.71 | 2.39 | 17 | 2 |
| 1:A:28:THR:HG21 | 1:A:30:LYS:HD2 | 0.71 | 1.63 | 14 | 3 |
| 1:A:88:PRO:O | 1:A:92:GLN:OE1 | 0.71 | 2.08 | 19 | 5 |
| 1:A:91:ILE:HG22 | 1:A:95:GLN:CD | 0.71 | 2.06 | 3 | 4 |
| 1:A:6:LEU:HB3 | 1:A:12:TYR:CD1 | 0.71 | 2.19 | 12 | 2 |
| 1:A:24:LEU:HD13 | 1:A:35:MET:SD | 0.71 | 2.25 | 9 | 4 |
| 1:A:84:PHE:CB | 1:A:89:LEU:HD12 | 0.71 | 2.15 | 1 | 4 |
| 1:A:28:THR:HG23 | 1:A:30:LYS:HG2 | 0.71 | 1.61 | 20 | 1 |
| 1:A:37:ARG:HD3 | 1:A:46:THR:CG2 | 0.71 | 2.15 | 10 | 19 |
| 1:A:11:TRP:CE3 | 1:A:36:VAL:HG21 | 0.71 | 2.21 | 3 | 18 |
| 1:A:49:VAL:O | 1:A:62:LYS:N | 0.71 | 2.24 | 18 | 12 |
| 1:A:104:ARG:O | 1:A:104:ARG:CD | 0.71 | 2.39 | 5 | 3 |
| 1:A:9:TYR:CG | 1:A:11:TRP:CE2 | 0.71 | 2.79 | 19 | 18 |
| 1:A:16:ILE:HD13 | 1:A:21:ALA:HB2 | 0.71 | 1.63 | 14 | 13 |
| 1:A:94:HIS:CG | 1:A:101:LEU:HD22 | 0.71 | 2.19 | 17 | 4 |
| 1:A:66:ILE:HG21 | 1:A:87:ILE:CD1 | 0.71 | 2.13 | 19 | 4 |
| 1:A:28:THR:OG1 | 1:A:30:LYS:NZ | 0.71 | 2.24 | 3 | 7 |
| 1:A:94:HIS:O | 1:A:104:ARG:CG | 0.71 | 2.39 | 17 | 1 |
| 1:A:84:PHE:CD1 | 1:A:84:PHE:N | 0.71 | 2.57 | 5 | 2 |
| 1:A:6:LEU:HA | 1:A:9:TYR:CE1 | 0.71 | 2.21 | 14 | 1 |
| 1:A:32:GLY:CA | 1:A:103:THR:OG1 | 0.70 | 2.39 | 10 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:35:MET:O | 1:A:47:VAL:HA | 0.70 | 1.86 | 10 | 19 |
| 1:A:18:ARG:HA | 1:A:63:HIS:CE1 | 0.70 | 2.22 | 20 | 6 |
| 1:A:98:GLY:O | 1:A:100:GLY:N | 0.70 | 2.24 | 9 | 7 |
| 1:A:91:ILE:O | 1:A:95:GLN:CG | 0.70 | 2.38 | 13 | 5 |
| 1:A:75:ARG:CG | 1:A:85:ASP:HA | 0.70 | 2.16 | 2 | 7 |
| 1:A:94:HIS:HB2 | 1:A:105:LEU:HD23 | 0.70 | 1.62 | 17 | 2 |
| 1:A:81:LYS:NZ | 1:A:99:GLY:O | 0.70 | 2.24 | 5 | 3 |
| 1:A:25:LEU:HD23 | 1:A:109:VAL:HG11 | 0.70 | 1.61 | 1 | 4 |
| 1:A:95:GLN:CA | 1:A:105:LEU:HB2 | 0.70 | 2.16 | 17 | 20 |
| 1:A:25:LEU:HD11 | 1:A:48:SER:HG | 0.70 | 1.42 | 9 | 1 |
| 1:A:64:TYR:CD2 | 1:A:78:VAL:HG11 | 0.70 | 2.21 | 3 | 3 |
| 1:A:81:LYS:O | 1:A:81:LYS:NZ | 0.70 | 2.24 | 19 | 1 |
| 1:A:77:TYR:HB2 | 1:A:81:LYS:O | 0.70 | 1.86 | 12 | 4 |
| 1:A:103:THR:O | 1:A:104:ARG:CG | 0.70 | 2.39 | 20 | 6 |
| 1:A:6:LEU:HD11 | 1:A:45:TYR:CE2 | 0.70 | 2.21 | 2 | 3 |
| 1:A:49:VAL:HB | 1:A:102:VAL:CG1 | 0.70 | 2.16 | 13 | 1 |
| 1:A:14:LYS:HG3 | 1:A:15:SER:N | 0.70 | 2.01 | 19 | 5 |
| 1:A:66:ILE:HG13 | 1:A:87:ILE:CD1 | 0.70 | 2.17 | 15 | 17 |
| 1:A:77:TYR:HB3 | 1:A:83:VAL:CA | 0.70 | 2.16 | 12 | 11 |
| 1:A:39:SER:HB3 | 1:A:65:HIS:NE2 | 0.70 | 2.00 | 9 | 10 |
| 1:A:14:LYS:O | 1:A:16:ILE:N | 0.70 | 2.24 | 13 | 14 |
| 1:A:84:PHE:N | 1:A:84:PHE:CD1 | 0.70 | 2.56 | 13 | 3 |
| 1:A:16:ILE:CD1 | 1:A:24:LEU:CD2 | 0.70 | 2.66 | 9 | 2 |
| 1:A:6:LEU:O | 1:A:9:TYR:CD2 | 0.70 | 2.44 | 12 | 2 |
| 1:A:97:ASN:O | 1:A:104:ARG:CG | 0.70 | 2.38 | 5 | 1 |
| 1:A:91:ILE:O | 1:A:95:GLN:HG3 | 0.70 | 1.87 | 3 | 5 |
| 1:A:14:LYS:HG2 | 1:A:38:ASP:CB | 0.70 | 2.16 | 20 | 1 |
| 1:A:37:ARG:HG2 | 1:A:37:ARG:O | 0.70 | 1.86 | 17 | 12 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:CG | 0.70 | 2.16 | 3 | 11 |
| 1:A:25:LEU:CD2 | 1:A:48:SER:OG | 0.70 | 2.34 | 12 | 3 |
| 1:A:64:TYR:HE2 | 1:A:101:LEU:HD12 | 0.70 | 1.44 | 7 | 1 |
| 1:A:32:GLY:HA2 | 1:A:103:THR:CG2 | 0.70 | 2.17 | 5 | 9 |
| 1:A:33:ALA:CB | 1:A:50:PHE:CE2 | 0.70 | 2.73 | 10 | 2 |
| 1:A:9:TYR:OH | 1:A:88:PRO:HB3 | 0.70 | 1.86 | 14 | 15 |
| 1:A:67:LYS:HB3 | 1:A:77:TYR:CD1 | 0.70 | 2.22 | 16 | 20 |
| 1:A:51:THR:N | 1:A:60:CYS:O | 0.70 | 2.24 | 17 | 11 |
| 1:A:93:TYR:O | 1:A:97:ASN:CB | 0.70 | 2.40 | 19 | 4 |
| 1:A:30:LYS:CD | 1:A:109:VAL:CG1 | 0.70 | 2.69 | 12 | 2 |
| 1:A:34:PHE:HE1 | 1:A:47:VAL:CG1 | 0.70 | 1.96 | 4 | 20 |
| 1:A:36:VAL:HG22 | 1:A:47:VAL:CG2 | 0.70 | 2.13 | 15 | 19 |
| 1:A:87:ILE:HG23 | 1:A:91:ILE:HD11 | 0.70 | 1.64 | 4 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:45:TYR:CD1 | 1:A:87:ILE:HG12 | 0.70 | 2.21 | 5 | 6 |
| 1:A:74:LYS:CE | 1:A:83:VAL:HB | 0.70 | 2.17 | 7 | 1 |
| 1:A:110:CYS:SG | 1:A:110:CYS:O | 0.70 | 2.50 | 8 | 4 |
| 1:A:41:THR:CB | 1:A:42:PRO:HD2 | 0.70 | 2.17 | 15 | 20 |
| 1:A:18:ARG:HB2 | 1:A:63:HIS:CD2 | 0.70 | 2.22 | 18 | 8 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:HG2 | 0.70 | 1.63 | 11 | 4 |
| 1:A:13:ASN:OD1 | 1:A:35:MET:HE1 | 0.70 | 1.87 | 7 | 2 |
| 1:A:31:GLU:O | 1:A:106:ARG:CD | 0.70 | 2.39 | 16 | 6 |
| 1:A:24:LEU:HG | 1:A:35:MET:CE | 0.70 | 2.17 | 15 | 4 |
| 1:A:17:SER:HB3 | 1:A:20:LYS:CE | 0.70 | 2.17 | 2 | 4 |
| 1:A:70:ASN:O | 1:A:74:LYS:CD | 0.70 | 2.39 | 20 | 1 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:HA | 0.70 | 2.21 | 16 | 3 |
| 1:A:49:VAL:HG22 | 1:A:62:LYS:HB3 | 0.70 | 1.60 | 9 | 8 |
| 1:A:24:LEU:CD1 | 1:A:25:LEU:HD22 | 0.70 | 2.17 | 19 | 1 |
| 1:A:19:ASP:O | 1:A:23:LYS:HE3 | 0.70 | 1.87 | 2 | 1 |
| 1:A:94:HIS:O | 1:A:104:ARG:CD | 0.70 | 2.39 | 17 | 3 |
| 1:A:102:VAL:O | 1:A:103:THR:CG2 | 0.70 | 2.40 | 10 | 4 |
| 1:A:110:CYS:O | 1:A:110:CYS:SG | 0.70 | 2.50 | 19 | 15 |
| 1:A:98:GLY:HA2 | 1:A:104:ARG:CG | 0.70 | 2.16 | 3 | 7 |
| 1:A:81:LYS:NZ | 1:A:93:TYR:OH | 0.70 | 2.23 | 8 | 2 |
| 1:A:91:ILE:HG23 | 1:A:105:LEU:CD1 | 0.70 | 2.17 | 4 | 3 |
| 1:A:64:TYR:OH | 1:A:101:LEU:HD12 | 0.69 | 1.86 | 10 | 1 |
| 1:A:103:THR:OG1 | 1:A:106:ARG:CG | 0.69 | 2.39 | 13 | 4 |
| 1:A:30:LYS:HG3 | 1:A:107:TYR:CD2 | 0.69 | 2.22 | 15 | 2 |
| 1:A:74:LYS:CA | 1:A:83:VAL:HG23 | 0.69 | 2.17 | 1 | 5 |
| 1:A:31:GLU:O | 1:A:106:ARG:CB | 0.69 | 2.40 | 4 | 4 |
| 1:A:75:ARG:N | 1:A:84:PHE:O | 0.69 | 2.25 | 5 | 5 |
| 1:A:69:THR:CG2 | 1:A:75:ARG:O | 0.69 | 2.40 | 12 | 9 |
| 1:A:97:ASN:O | 1:A:104:ARG:CD | 0.69 | 2.40 | 16 | 4 |
| 1:A:11:TRP:CD1 | 1:A:34:PHE:HE2 | 0.69 | 2.06 | 6 | 20 |
| 1:A:21:ALA:CA | 1:A:24:LEU:CG | 0.69 | 2.70 | 9 | 11 |
| 1:A:9:TYR:CD2 | 1:A:11:TRP:CZ2 | 0.69 | 2.80 | 11 | 19 |
| 1:A:25:LEU:HD13 | 1:A:61:ILE:HG22 | 0.69 | 1.64 | 11 | 5 |
| 1:A:10:GLU:HG2 | 1:A:108:PRO:CB | 0.69 | 2.17 | 4 | 13 |
| 1:A:74:LYS:HE2 | 1:A:83:VAL:O | 0.69 | 1.87 | 14 | 2 |
| 1:A:34:PHE:CE1 | 1:A:105:LEU:CD1 | 0.69 | 2.74 | 20 | 4 |
| 1:A:75:ARG:HG3 | 1:A:76:TYR:CD1 | 0.69 | 2.22 | 3 | 4 |
| 1:A:52:LYS:CD | 1:A:52:LYS:O | 0.69 | 2.40 | 14 | 1 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:CG | 0.69 | 2.75 | 15 | 10 |
| 1:A:49:VAL:CG2 | 1:A:102:VAL:CG1 | 0.69 | 2.69 | 13 | 7 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:HG23 | 0.69 | 1.64 | 8 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:69:THR:O | 1:A:75:ARG:CD | 0.69 | 2.39 | 17 | 1 |
| 1:A:87:ILE:CG2 | 1:A:91:ILE:HG12 | 0.69 | 2.17 | 7 | 19 |
| 1:A:25:LEU:HB3 | 1:A:50:PHE:CG | 0.69 | 2.21 | 9 | 7 |
| 1:A:45:TYR:CD2 | 1:A:87:ILE:HD13 | 0.69 | 2.23 | 17 | 1 |
| 1:A:74:LYS:HB2 | 1:A:83:VAL:CG2 | 0.69 | 2.18 | 3 | 7 |
| 1:A:32:GLY:HA2 | 1:A:51:THR:OG1 | 0.69 | 1.86 | 14 | 14 |
| 1:A:33:ALA:HA | 1:A:107:TYR:O | 0.69 | 1.88 | 6 | 16 |
| 1:A:30:LYS:HE2 | 1:A:109:VAL:CG1 | 0.69 | 2.18 | 6 | 1 |
| 1:A:50:PHE:HB3 | 1:A:61:ILE:CG2 | 0.69 | 2.17 | 14 | 3 |
| 1:A:75:ARG:CZ | 1:A:85:ASP:OD1 | 0.69 | 2.40 | 1 | 1 |
| 1:A:37:ARG:O | 1:A:37:ARG:HG2 | 0.69 | 1.88 | 16 | 8 |
| 1:A:94:HIS:O | 1:A:104:ARG:HB3 | 0.69 | 1.87 | 7 | 1 |
| 1:A:95:GLN:CG | 1:A:105:LEU:HB2 | 0.69 | 2.17 | 17 | 2 |
| 1:A:106:ARG:CZ | 1:A:106:ARG:O | 0.69 | 2.41 | 15 | 2 |
| 1:A:22:GLU:CD | 1:A:63:HIS:HE2 | 0.69 | 1.91 | 5 | 2 |
| 1:A:82:TYR:HB2 | 1:A:84:PHE:CZ | 0.69 | 2.22 | 2 | 13 |
| 1:A:17:SER:CB | 1:A:20:LYS:NZ | 0.69 | 2.56 | 2 | 5 |
| 1:A:30:LYS:HD2 | 1:A:109:VAL:CG2 | 0.69 | 2.18 | 14 | 2 |
| 1:A:39:SER:HB3 | 1:A:65:HIS:CE1 | 0.69 | 2.23 | 14 | 7 |
| 1:A:106:ARG:O | 1:A:106:ARG:NH2 | 0.69 | 2.26 | 17 | 1 |
| 1:A:24:LEU:HD21 | 1:A:35:MET:SD | 0.69 | 2.27 | 16 | 3 |
| 1:A:22:GLU:OE1 | 1:A:22:GLU:N | 0.69 | 2.26 | 4 | 2 |
| 1:A:25:LEU:CD1 | 1:A:48:SER:HB3 | 0.69 | 2.17 | 20 | 3 |
| 1:A:85:ASP:O | 1:A:86:SER:HB2 | 0.69 | 1.87 | 3 | 1 |
| 1:A:96:TYR:O | 1:A:98:GLY:N | 0.69 | 2.26 | 1 | 2 |
| 1:A:13:ASN:HB3 | 1:A:16:ILE:CB | 0.69 | 2.18 | 10 | 13 |
| 1:A:13:ASN:HB3 | 1:A:16:ILE:CG1 | 0.69 | 2.18 | 6 | 15 |
| 1:A:81:LYS:CB | 1:A:82:TYR:CD1 | 0.69 | 2.76 | 3 | 13 |
| 1:A:65:HIS:C | 1:A:78:VAL:HG12 | 0.69 | 2.07 | 13 | 5 |
| 1:A:66:ILE:CD1 | 1:A:87:ILE:HG13 | 0.69 | 2.18 | 20 | 2 |
| 1:A:70:ASN:HA | 1:A:75:ARG:HG2 | 0.69 | 1.65 | 6 | 1 |
| 1:A:91:ILE:HG22 | 1:A:95:GLN:NE2 | 0.69 | 2.02 | 4 | 4 |
| 1:A:25:LEU:CG | 1:A:109:VAL:HG21 | 0.69 | 2.18 | 7 | 6 |
| 1:A:76:TYR:N | 1:A:84:PHE:O | 0.69 | 2.25 | 12 | 14 |
| 1:A:94:HIS:HB3 | 1:A:105:LEU:HG | 0.69 | 1.63 | 4 | 1 |
| 1:A:75:ARG:HG3 | 1:A:76:TYR:CE1 | 0.69 | 2.22 | 5 | 3 |
| 1:A:98:GLY:HA3 | 1:A:104:ARG:CB | 0.69 | 2.18 | 20 | 1 |
| 1:A:11:TRP:CG | 1:A:34:PHE:CD2 | 0.68 | 2.80 | 15 | 19 |
| 1:A:39:SER:OG | 1:A:65:HIS:NE2 | 0.68 | 2.26 | 7 | 2 |
| 1:A:81:LYS:HZ1 | 1:A:99:GLY:HA2 | 0.68 | 1.47 | 8 | 2 |
| 1:A:21:ALA:CB | 1:A:48:SER:OG | 0.68 | 2.41 | 18 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:50:PHE:HB2 | 1:A:61:ILE:CD1 | 0.68 | 2.18 | 9 | 14 |
| 1:A:6:LEU:HD13 | 1:A:11:TRP:HH2 | 0.68 | 1.43 | 11 | 8 |
| 1:A:30:LYS:CE | 1:A:107:TYR:CE2 | 0.68 | 2.76 | 4 | 7 |
| 1:A:81:LYS:HZ1 | 1:A:99:GLY:CA | 0.68 | 2.01 | 8 | 2 |
| 1:A:82:TYR:HD1 | 1:A:82:TYR:N | 0.68 | 1.87 | 2 | 3 |
| 1:A:101:LEU:O | 1:A:102:VAL:CG2 | 0.68 | 2.40 | 17 | 1 |
| 1:A:51:THR:O | 1:A:52:LYS:C | 0.68 | 2.30 | 4 | 20 |
| 1:A:62:LYS:HD3 | 1:A:102:VAL:HG12 | 0.68 | 1.65 | 17 | 2 |
| 1:A:77:TYR:HB3 | 1:A:83:VAL:CG1 | 0.68 | 2.19 | 10 | 16 |
| 1:A:78:VAL:HG23 | 1:A:79:ALA:H | 0.68 | 1.48 | 7 | 4 |
| 1:A:79:ALA:O | 1:A:80:GLU:C | 0.68 | 2.31 | 8 | 19 |
| 1:A:10:GLU:O | 1:A:110:CYS:HB3 | 0.68 | 1.87 | 19 | 6 |
| 1:A:51:THR:HG22 | 1:A:51:THR:O | 0.68 | 1.87 | 16 | 4 |
| 1:A:23:LYS:CE | 1:A:23:LYS:H | 0.68 | 2.01 | 2 | 1 |
| 1:A:66:ILE:HG13 | 1:A:87:ILE:HG13 | 0.68 | 1.66 | 10 | 18 |
| 1:A:76:TYR:O | 1:A:90:LEU:HD12 | 0.68 | 1.88 | 12 | 16 |
| 1:A:30:LYS:C | 1:A:52:LYS:CE | 0.68 | 2.62 | 11 | 1 |
| 1:A:17:SER:HB3 | 1:A:20:LYS:CD | 0.68 | 2.18 | 4 | 14 |
| 1:A:28:THR:OG1 | 1:A:30:LYS:HE2 | 0.68 | 1.88 | 19 | 4 |
| 1:A:65:HIS:C | 1:A:78:VAL:CG2 | 0.68 | 2.62 | 3 | 2 |
| 1:A:82:TYR:CD1 | 1:A:93:TYR:HE2 | 0.68 | 2.07 | 4 | 3 |
| 1:A:106:ARG:NE | 1:A:106:ARG:O | 0.68 | 2.27 | 15 | 1 |
| 1:A:67:LYS:C | 1:A:68:GLU:OE1 | 0.68 | 2.32 | 9 | 6 |
| 1:A:30:LYS:HD3 | 1:A:107:TYR:CE2 | 0.68 | 2.24 | 12 | 4 |
| 1:A:74:LYS:HE3 | 1:A:74:LYS:N | 0.68 | 2.02 | 8 | 1 |
| 1:A:86:SER:O | 1:A:89:LEU:HG | 0.68 | 1.89 | 2 | 4 |
| 1:A:22:GLU:OE1 | 1:A:63:HIS:NE2 | 0.68 | 2.27 | 12 | 1 |
| 1:A:106:ARG:O | 1:A:106:ARG:NH1 | 0.68 | 2.27 | 16 | 1 |
| 1:A:98:GLY:HA2 | 1:A:104:ARG:CB | 0.68 | 2.18 | 3 | 5 |
| 1:A:91:ILE:HA | 1:A:105:LEU:CD2 | 0.68 | 2.19 | 12 | 15 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:HG3 | 0.68 | 1.66 | 15 | 7 |
| 1:A:94:HIS:NE2 | 1:A:99:GLY:O | 0.68 | 2.26 | 16 | 4 |
| 1:A:45:TYR:CD1 | 1:A:87:ILE:HD11 | 0.68 | 2.23 | 8 | 7 |
| 1:A:39:SER:O | 1:A:41:THR:N | 0.68 | 2.27 | 5 | 2 |
| 1:A:21:ALA:HB3 | 1:A:63:HIS:CE1 | 0.68 | 2.23 | 7 | 2 |
| 1:A:81:LYS:HZ1 | 1:A:94:HIS:CE1 | 0.68 | 2.05 | 2 | 2 |
| 1:A:77:TYR:HB3 | 1:A:83:VAL:HA | 0.68 | 1.66 | 14 | 20 |
| 1:A:76:TYR:C | 1:A:90:LEU:CD1 | 0.68 | 2.62 | 3 | 16 |
| 1:A:25:LEU:CD1 | 1:A:50:PHE:CD1 | 0.68 | 2.76 | 19 | 1 |
| 1:A:95:GLN:N | 1:A:105:LEU:HB2 | 0.68 | 2.04 | 15 | 20 |
| 1:A:25:LEU:HB2 | 1:A:61:ILE:CD1 | 0.68 | 2.18 | 9 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:96:TYR:O | 1:A:104:ARG:NH1 | 0.68 | 2.27 | 20 | 2 |
| 1:A:88:PRO:O | 1:A:92:GLN:CG | 0.68 | 2.41 | 17 | 6 |
| 1:A:102:VAL:CG2 | 1:A:103:THR:HG22 | 0.68 | 2.12 | 12 | 1 |
| 1:A:68:GLU:HG2 | 1:A:76:TYR:CD2 | 0.68 | 2.24 | 3 | 1 |
| 1:A:24:LEU:HD11 | 1:A:35:MET:HE1 | 0.68 | 1.64 | 20 | 1 |
| 1:A:79:ALA:CB | 1:A:81:LYS:HG3 | 0.68 | 2.19 | 17 | 8 |
| 1:A:11:TRP:CZ3 | 1:A:12:TYR:HB2 | 0.68 | 2.24 | 6 | 8 |
| 1:A:32:GLY:HA3 | 1:A:106:ARG:HB2 | 0.68 | 1.64 | 20 | 7 |
| 1:A:6:LEU:HD11 | 1:A:45:TYR:CG | 0.68 | 2.24 | 17 | 2 |
| 1:A:30:LYS:HG2 | 1:A:107:TYR:CE2 | 0.68 | 2.23 | 16 | 5 |
| 1:A:61:ILE:N | 1:A:61:ILE:CD1 | 0.68 | 2.57 | 18 | 1 |
| 1:A:86:SER:HB2 | 1:A:89:LEU:CD2 | 0.68 | 2.19 | 17 | 1 |
| 1:A:62:LYS:HE2 | 1:A:64:TYR:CZ | 0.68 | 2.23 | 16 | 1 |
| 1:A:25:LEU:HD23 | 1:A:109:VAL:CG1 | 0.67 | 2.19 | 1 | 3 |
| 1:A:33:ALA:HB1 | 1:A:109:VAL:HG11 | 0.67 | 1.63 | 10 | 3 |
| 1:A:50:PHE:HD2 | 1:A:61:ILE:CD1 | 0.67 | 2.00 | 19 | 3 |
| 1:A:30:LYS:HE3 | 1:A:109:VAL:CG1 | 0.67 | 2.20 | 12 | 1 |
| 1:A:95:GLN:NE2 | 1:A:105:LEU:O | 0.67 | 2.26 | 14 | 1 |
| 1:A:41:THR:HG22 | 1:A:44:THR:CG2 | 0.67 | 2.20 | 3 | 10 |
| 1:A:33:ALA:HB1 | 1:A:109:VAL:HG13 | 0.67 | 1.64 | 6 | 4 |
| 1:A:13:ASN:OD1 | 1:A:35:MET:HG3 | 0.67 | 1.89 | 11 | 2 |
| 1:A:20:LYS:C | 1:A:24:LEU:HD21 | 0.67 | 2.10 | 2 | 1 |
| 1:A:82:TYR:CG | 1:A:93:TYR:CE2 | 0.67 | 2.83 | 4 | 3 |
| 1:A:98:GLY:CA | 1:A:104:ARG:CB | 0.67 | 2.72 | 20 | 2 |
| 1:A:49:VAL:HG11 | 1:A:64:TYR:CD2 | 0.67 | 2.24 | 20 | 1 |
| 1:A:95:GLN:O | 1:A:104:ARG:NH1 | 0.67 | 2.27 | 10 | 5 |
| 1:A:37:ARG:N | 1:A:46:THR:O | 0.67 | 2.27 | 9 | 20 |
| 1:A:7:GLU:OE1 | 1:A:14:LYS:NZ | 0.67 | 2.27 | 14 | 3 |
| 1:A:41:THR:HG21 | 1:A:44:THR:CG2 | 0.67 | 2.17 | 9 | 15 |
| 1:A:17:SER:HA | 1:A:37:ARG:NH1 | 0.67 | 2.05 | 16 | 10 |
| 1:A:30:LYS:HD2 | 1:A:109:VAL:HG22 | 0.67 | 1.65 | 9 | 2 |
| 1:A:13:ASN:O | 1:A:16:ILE:HB | 0.67 | 1.88 | 7 | 10 |
| 1:A:35:MET:CE | 1:A:109:VAL:O | 0.67 | 2.42 | 10 | 4 |
| 1:A:93:TYR:O | 1:A:97:ASN:HB2 | 0.67 | 1.88 | 2 | 13 |
| 1:A:81:LYS:HZ3 | 1:A:82:TYR:HE1 | 0.67 | 1.31 | 17 | 4 |
| 1:A:13:ASN:CG | 1:A:35:MET:CE | 0.67 | 2.63 | 7 | 5 |
| 1:A:30:LYS:CD | 1:A:107:TYR:CE2 | 0.67 | 2.77 | 12 | 5 |
| 1:A:74:LYS:CB | 1:A:84:PHE:C | 0.67 | 2.63 | 6 | 1 |
| 1:A:87:ILE:O | 1:A:91:ILE:CG1 | 0.67 | 2.43 | 12 | 20 |
| 1:A:41:THR:CG2 | 1:A:42:PRO:CD | 0.67 | 2.70 | 18 | 20 |
| 1:A:10:GLU:O | 1:A:109:VAL:O | 0.67 | 2.11 | 6 | 13 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:69:THR:CG2 | 1:A:74:LYS:O | 0.67 | 2.43 | 11 | 1 |
| 1:A:32:GLY:HA3 | 1:A:103:THR:CG2 | 0.67 | 2.19 | 6 | 5 |
| 1:A:78:VAL:O | 1:A:78:VAL:CG2 | 0.67 | 2.40 | 5 | 4 |
| 1:A:84:PHE:CE2 | 1:A:90:LEU:HA | 0.67 | 2.24 | 4 | 5 |
| 1:A:45:TYR:O | 1:A:66:ILE:N | 0.67 | 2.27 | 3 | 10 |
| 1:A:84:PHE:HD2 | 1:A:90:LEU:HD12 | 0.67 | 1.50 | 4 | 5 |
| 1:A:91:ILE:HG23 | 1:A:105:LEU:CD2 | 0.67 | 2.20 | 12 | 11 |
| 1:A:51:THR:O | 1:A:60:CYS:SG | 0.67 | 2.52 | 19 | 1 |
| 1:A:86:SER:OG | 1:A:88:PRO:HD2 | 0.67 | 1.90 | 1 | 6 |
| 1:A:81:LYS:NZ | 1:A:99:GLY:CA | 0.67 | 2.58 | 8 | 5 |
| 1:A:6:LEU:O | 1:A:12:TYR:CD2 | 0.67 | 2.48 | 20 | 2 |
| 1:A:91:ILE:CG2 | 1:A:95:GLN:NE2 | 0.67 | 2.58 | 4 | 3 |
| 1:A:93:TYR:CE2 | 1:A:94:HIS:CD2 | 0.67 | 2.83 | 5 | 2 |
| 1:A:34:PHE:CD1 | 1:A:35:MET:N | 0.67 | 2.63 | 2 | 18 |
| 1:A:85:ASP:N | 1:A:89:LEU:CD1 | 0.67 | 2.58 | 1 | 2 |
| 1:A:47:VAL:HG12 | 1:A:49:VAL:CG1 | 0.67 | 2.20 | 14 | 4 |
| 1:A:81:LYS:NZ | 1:A:100:GLY:N | 0.67 | 2.43 | 3 | 1 |
| 1:A:41:THR:OG1 | 1:A:42:PRO:HD3 | 0.66 | 1.90 | 18 | 17 |
| 1:A:37:ARG:HD3 | 1:A:46:THR:HG21 | 0.66 | 1.68 | 4 | 18 |
| 1:A:104:ARG:O | 1:A:105:LEU:C | 0.66 | 2.33 | 5 | 10 |
| 1:A:11:TRP:HB2 | 1:A:34:PHE:CE2 | 0.66 | 2.22 | 20 | 13 |
| 1:A:6:LEU:HB2 | 1:A:12:TYR:CD2 | 0.66 | 2.26 | 11 | 3 |
| 1:A:84:PHE:HE1 | 1:A:93:TYR:CE1 | 0.66 | 2.07 | 12 | 3 |
| 1:A:94:HIS:NE2 | 1:A:99:GLY:CA | 0.66 | 2.58 | 5 | 6 |
| 1:A:86:SER:OG | 1:A:89:LEU:CD2 | 0.66 | 2.39 | 2 | 1 |
| 1:A:10:GLU:OE1 | 1:A:107:TYR:CZ | 0.66 | 2.48 | 4 | 1 |
| 1:A:81:LYS:HZ1 | 1:A:101:LEU:HD11 | 0.66 | 1.49 | 12 | 1 |
| 1:A:95:GLN:NE2 | 1:A:105:LEU:HB3 | 0.66 | 2.04 | 20 | 2 |
| 1:A:12:TYR:CE1 | 1:A:14:LYS:HG3 | 0.66 | 2.25 | 20 | 1 |
| 1:A:13:ASN:HB3 | 1:A:16:ILE:HG13 | 0.66 | 1.65 | 13 | 13 |
| 1:A:20:LYS:HA | 1:A:23:LYS:HG2 | 0.66 | 1.66 | 1 | 10 |
| 1:A:103:THR:O | 1:A:104:ARG:HG2 | 0.66 | 1.90 | 7 | 3 |
| 1:A:6:LEU:CB | 1:A:9:TYR:CD2 | 0.66 | 2.78 | 2 | 10 |
| 1:A:22:GLU:HB2 | 1:A:23:LYS:CE | 0.66 | 2.20 | 2 | 1 |
| 1:A:100:GLY:C | 1:A:101:LEU:CD1 | 0.66 | 2.64 | 17 | 3 |
| 1:A:84:PHE:CD2 | 1:A:90:LEU:HD12 | 0.66 | 2.24 | 4 | 2 |
| 1:A:39:SER:OG | 1:A:40:ARG:N | 0.66 | 2.27 | 1 | 6 |
| 1:A:24:LEU:CD1 | 1:A:25:LEU:N | 0.66 | 2.51 | 5 | 5 |
| 1:A:30:LYS:CE | 1:A:109:VAL:HG13 | 0.66 | 2.20 | 12 | 1 |
| 1:A:97:ASN:O | 1:A:104:ARG:CB | 0.66 | 2.43 | 5 | 2 |
| 1:A:31:GLU:OE2 | 1:A:106:ARG:NH2 | 0.66 | 2.29 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:62:LYS:HE2 | 1:A:64:TYR:CE1 | 0.66 | 2.25 | 10 | 2 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:HD22 | 0.66 | 2.26 | 1 | 3 |
| 1:A:81:LYS:CE | 1:A:94:HIS:CE1 | 0.66 | 2.78 | 2 | 2 |
| 1:A:70:ASN:HA | 1:A:75:ARG:CG | 0.66 | 2.21 | 6 | 1 |
| 1:A:34:PHE:O | 1:A:109:VAL:HG22 | 0.66 | 1.90 | 4 | 2 |
| 1:A:24:LEU:C | 1:A:24:LEU:CD2 | 0.66 | 2.58 | 4 | 3 |
| 1:A:79:ALA:CB | 1:A:81:LYS:CE | 0.66 | 2.74 | 4 | 1 |
| 1:A:20:LYS:N | 1:A:20:LYS:CD | 0.66 | 2.58 | 16 | 2 |
| 1:A:6:LEU:O | 1:A:7:GLU:CD | 0.66 | 2.34 | 10 | 1 |
| 1:A:44:THR:HB | 1:A:68:GLU:OE1 | 0.66 | 1.91 | 7 | 5 |
| 1:A:69:THR:OG1 | 1:A:70:ASN:N | 0.66 | 2.27 | 19 | 3 |
| 1:A:64:TYR:HB3 | 1:A:78:VAL:CG2 | 0.66 | 2.20 | 8 | 1 |
| 1:A:64:TYR:CZ | 1:A:101:LEU:HA | 0.66 | 2.26 | 17 | 3 |
| 1:A:75:ARG:CG | 1:A:84:PHE:O | 0.66 | 2.44 | 20 | 4 |
| 1:A:29:GLY:O | 1:A:30:LYS:O | 0.66 | 2.13 | 15 | 3 |
| 1:A:18:ARG:NH1 | 1:A:19:ASP:OD2 | 0.66 | 2.29 | 10 | 1 |
| 1:A:66:ILE:CG2 | 1:A:90:LEU:CD2 | 0.66 | 2.73 | 8 | 14 |
| 1:A:76:TYR:HD1 | 1:A:76:TYR:N | 0.66 | 1.85 | 17 | 12 |
| 1:A:86:SER:C | 1:A:89:LEU:HD12 | 0.66 | 2.09 | 18 | 14 |
| 1:A:21:ALA:O | 1:A:25:LEU:N | 0.66 | 2.28 | 12 | 11 |
| 1:A:6:LEU:C | 1:A:12:TYR:CD2 | 0.66 | 2.69 | 20 | 3 |
| 1:A:26:LEU:CD1 | 1:A:61:ILE:HD12 | 0.66 | 2.21 | 17 | 1 |
| 1:A:66:ILE:HA | 1:A:78:VAL:CG1 | 0.66 | 2.20 | 6 | 2 |
| 1:A:30:LYS:HD2 | 1:A:109:VAL:CG1 | 0.66 | 2.19 | 12 | 1 |
| 1:A:93:TYR:CD1 | 1:A:97:ASN:ND2 | 0.66 | 2.64 | 3 | 1 |
| 1:A:67:LYS:O | 1:A:68:GLU:OE1 | 0.66 | 2.13 | 20 | 2 |
| 1:A:28:THR:CG2 | 1:A:30:LYS:HD3 | 0.66 | 2.21 | 10 | 7 |
| 1:A:10:GLU:HG2 | 1:A:108:PRO:HB2 | 0.66 | 1.68 | 17 | 13 |
| 1:A:79:ALA:CB | 1:A:81:LYS:HD3 | 0.66 | 2.13 | 13 | 3 |
| 1:A:75:ARG:NH2 | 1:A:85:ASP:HB2 | 0.66 | 2.05 | 13 | 1 |
| 1:A:6:LEU:C | 1:A:7:GLU:HG2 | 0.66 | 2.10 | 10 | 3 |
| 1:A:99:GLY:O | 1:A:100:GLY:C | 0.66 | 2.35 | 8 | 8 |
| 1:A:9:TYR:OH | 1:A:88:PRO:CG | 0.66 | 2.43 | 3 | 9 |
| 1:A:47:VAL:HB | 1:A:64:TYR:O | 0.66 | 1.90 | 15 | 20 |
| 1:A:6:LEU:O | 1:A:8:THR:CG2 | 0.66 | 2.31 | 14 | 2 |
| 1:A:64:TYR:CE1 | 1:A:101:LEU:HB3 | 0.66 | 2.26 | 7 | 1 |
| 1:A:75:ARG:CZ | 1:A:85:ASP:HB2 | 0.66 | 2.21 | 7 | 3 |
| 1:A:91:ILE:O | 1:A:95:GLN:N | 0.65 | 2.29 | 10 | 13 |
| 1:A:47:VAL:HG12 | 1:A:49:VAL:HG13 | 0.65 | 1.68 | 12 | 15 |
| 1:A:77:TYR:CD2 | 1:A:80:GLU:N | 0.65 | 2.64 | 14 | 18 |
| 1:A:65:HIS:C | 1:A:66:ILE:HD13 | 0.65 | 2.11 | 11 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:34:PHE:CD2 | 1:A:105:LEU:HG | 0.65 | 2.25 | 2 | 11 |
| 1:A:7:GLU:O | 1:A:8:THR:HB | 0.65 | 1.89 | 14 | 2 |
| 1:A:17:SER:CB | 1:A:20:LYS:HE2 | 0.65 | 2.20 | 5 | 2 |
| 1:A:74:LYS:HE3 | 1:A:74:LYS:H | 0.65 | 1.50 | 8 | 1 |
| 1:A:24:LEU:CD1 | 1:A:35:MET:HE1 | 0.65 | 2.21 | 20 | 3 |
| 1:A:79:ALA:C | 1:A:81:LYS:N | 0.65 | 2.48 | 3 | 20 |
| 1:A:22:GLU:CG | 1:A:63:HIS:NE2 | 0.65 | 2.59 | 14 | 4 |
| 1:A:69:THR:HG22 | 1:A:75:ARG:O | 0.65 | 1.91 | 5 | 8 |
| 1:A:93:TYR:O | 1:A:97:ASN:CG | 0.65 | 2.34 | 14 | 2 |
| 1:A:24:LEU:CD2 | 1:A:25:LEU:N | 0.65 | 2.44 | 20 | 3 |
| 1:A:77:TYR:CA | 1:A:90:LEU:CD1 | 0.65 | 2.70 | 3 | 17 |
| 1:A:91:ILE:HG22 | 1:A:95:GLN:CG | 0.65 | 2.20 | 9 | 7 |
| 1:A:26:LEU:CD1 | 1:A:61:ILE:HG13 | 0.65 | 2.22 | 1 | 1 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:HE1 | 0.65 | 2.07 | 19 | 5 |
| 1:A:68:GLU:HG3 | 1:A:76:TYR:CD1 | 0.65 | 2.26 | 7 | 6 |
| 1:A:53:ALA:CA | 1:A:60:CYS:SG | 0.65 | 2.84 | 19 | 1 |
| 1:A:53:ALA:N | 1:A:60:CYS:SG | 0.65 | 2.69 | 19 | 1 |
| 1:A:11:TRP:CE3 | 1:A:12:TYR:N | 0.65 | 2.65 | 6 | 12 |
| 1:A:13:ASN:CG | 1:A:35:MET:SD | 0.65 | 2.75 | 3 | 6 |
| 1:A:86:SER:HB2 | 1:A:89:LEU:CD1 | 0.65 | 2.21 | 12 | 3 |
| 1:A:28:THR:CG2 | 1:A:30:LYS:HE3 | 0.65 | 2.21 | 14 | 2 |
| 1:A:69:THR:O | 1:A:70:ASN:C | 0.65 | 2.34 | 8 | 8 |
| 1:A:74:LYS:C | 1:A:83:VAL:CG2 | 0.65 | 2.65 | 13 | 4 |
| 1:A:19:ASP:OD1 | 1:A:20:LYS:NZ | 0.65 | 2.30 | 10 | 1 |
| 1:A:11:TRP:CA | 1:A:35:MET:HA | 0.65 | 2.21 | 20 | 15 |
| 1:A:7:GLU:HB3 | 1:A:14:LYS:CD | 0.65 | 2.21 | 1 | 5 |
| 1:A:74:LYS:CE | 1:A:74:LYS:N | 0.65 | 2.59 | 8 | 1 |
| 1:A:81:LYS:HE2 | 1:A:94:HIS:CE1 | 0.65 | 2.25 | 2 | 1 |
| 1:A:24:LEU:CB | 1:A:111:GLY:C | 0.65 | 2.65 | 6 | 1 |
| 1:A:22:GLU:HG2 | 1:A:63:HIS:NE2 | 0.65 | 2.06 | 14 | 1 |
| 1:A:64:TYR:OH | 1:A:101:LEU:CD1 | 0.65 | 2.45 | 10 | 1 |
| 1:A:30:LYS:C | 1:A:52:LYS:HE3 | 0.65 | 2.12 | 11 | 1 |
| 1:A:23:LYS:HG2 | 1:A:24:LEU:N | 0.65 | 2.07 | 15 | 4 |
| 1:A:92:GLN:NE2 | 1:A:95:GLN:OE1 | 0.65 | 2.29 | 3 | 1 |
| 1:A:20:LYS:HB3 | 1:A:23:LYS:CE | 0.65 | 2.22 | 3 | 2 |
| 1:A:6:LEU:HB2 | 1:A:12:TYR:CD1 | 0.65 | 2.27 | 12 | 2 |
| 1:A:87:ILE:N | 1:A:88:PRO:CD | 0.65 | 2.60 | 20 | 18 |
| 1:A:6:LEU:HB3 | 1:A:9:TYR:CD1 | 0.65 | 2.27 | 9 | 2 |
| 1:A:86:SER:OG | 1:A:89:LEU:HD11 | 0.65 | 1.92 | 12 | 5 |
| 1:A:22:GLU:HB2 | 1:A:23:LYS:NZ | 0.65 | 2.07 | 2 | 1 |
| 1:A:94:HIS:CD2 | 1:A:101:LEU:HD13 | 0.65 | 2.27 | 17 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:86:SER:HB3 | 1:A:89:LEU:CD2 | 0.65 | 2.21 | 6 | 3 |
| 1:A:94:HIS:HB2 | 1:A:105:LEU:HG | 0.65 | 1.69 | 14 | 1 |
| 1:A:62:LYS:CE | 1:A:64:TYR:CE1 | 0.64 | 2.80 | 10 | 2 |
| 1:A:77:TYR:CE2 | 1:A:80:GLU:N | 0.64 | 2.65 | 14 | 17 |
| 1:A:20:LYS:O | 1:A:23:LYS:HG2 | 0.64 | 1.92 | 16 | 16 |
| 1:A:60:CYS:C | 1:A:61:ILE:HD12 | 0.64 | 2.12 | 12 | 2 |
| 1:A:51:THR:O | 1:A:53:ALA:N | 0.64 | 2.30 | 4 | 3 |
| 1:A:25:LEU:HD21 | 1:A:35:MET:CB | 0.64 | 2.21 | 5 | 1 |
| 1:A:62:LYS:HB2 | 1:A:102:VAL:CG1 | 0.64 | 2.22 | 8 | 4 |
| 1:A:67:LYS:CE | 1:A:67:LYS:HA | 0.64 | 2.22 | 18 | 3 |
| 1:A:98:GLY:O | 1:A:99:GLY:O | 0.64 | 2.15 | 20 | 3 |
| 1:A:25:LEU:O | 1:A:28:THR:HG23 | 0.64 | 1.92 | 5 | 1 |
| 1:A:30:LYS:O | 1:A:52:LYS:CE | 0.64 | 2.46 | 11 | 1 |
| 1:A:21:ALA:CA | 1:A:24:LEU:CD2 | 0.64 | 2.70 | 16 | 7 |
| 1:A:21:ALA:O | 1:A:25:LEU:CD1 | 0.64 | 2.45 | 3 | 4 |
| 1:A:30:LYS:HG3 | 1:A:107:TYR:CE2 | 0.64 | 2.27 | 15 | 1 |
| 1:A:34:PHE:HZ | 1:A:91:ILE:CD1 | 0.64 | 2.05 | 9 | 20 |
| 1:A:43:GLY:O | 1:A:68:GLU:OE2 | 0.64 | 2.16 | 18 | 5 |
| 1:A:12:TYR:CZ | 1:A:14:LYS:HG3 | 0.64 | 2.27 | 20 | 2 |
| 1:A:66:ILE:CG1 | 1:A:87:ILE:CG1 | 0.64 | 2.74 | 17 | 3 |
| 1:A:6:LEU:HD22 | 1:A:87:ILE:HB | 0.64 | 1.67 | 6 | 2 |
| 1:A:20:LYS:HA | 1:A:23:LYS:CG | 0.64 | 2.23 | 7 | 9 |
| 1:A:74:LYS:HD3 | 1:A:74:LYS:N | 0.64 | 2.08 | 7 | 3 |
| 1:A:98:GLY:O | 1:A:99:GLY:C | 0.64 | 2.35 | 7 | 8 |
| 1:A:14:LYS:CG | 1:A:38:ASP:HB2 | 0.64 | 2.22 | 20 | 1 |
| 1:A:82:TYR:CB | 1:A:84:PHE:CZ | 0.64 | 2.81 | 7 | 8 |
| 1:A:22:GLU:HG3 | 1:A:63:HIS:NE2 | 0.64 | 2.07 | 11 | 5 |
| 1:A:20:LYS:O | 1:A:24:LEU:CG | 0.64 | 2.45 | 2 | 5 |
| 1:A:28:THR:CG2 | 1:A:30:LYS:HG3 | 0.64 | 2.22 | 20 | 3 |
| 1:A:81:LYS:NZ | 1:A:99:GLY:HA3 | 0.64 | 2.08 | 12 | 2 |
| 1:A:21:ALA:CA | 1:A:24:LEU:HD13 | 0.64 | 2.21 | 18 | 1 |
| 1:A:7:GLU:CB | 1:A:14:LYS:HD3 | 0.64 | 2.21 | 1 | 3 |
| 1:A:103:THR:OG1 | 1:A:106:ARG:HG3 | 0.64 | 1.91 | 13 | 3 |
| 1:A:30:LYS:CE | 1:A:109:VAL:HG22 | 0.64 | 2.23 | 14 | 1 |
| 1:A:82:TYR:CE1 | 1:A:93:TYR:CE1 | 0.64 | 2.86 | 18 | 8 |
| 1:A:100:GLY:O | 1:A:101:LEU:O | 0.64 | 2.16 | 8 | 7 |
| 1:A:30:LYS:CE | 1:A:107:TYR:HE2 | 0.64 | 2.05 | 19 | 4 |
| 1:A:66:ILE:O | 1:A:68:GLU:OE2 | 0.64 | 2.16 | 7 | 1 |
| 1:A:69:THR:HG23 | 1:A:83:VAL:HG11 | 0.64 | 1.67 | 17 | 2 |
| 1:A:25:LEU:HD11 | 1:A:35:MET:HB2 | 0.64 | 1.70 | 8 | 1 |
| 1:A:45:TYR:HD2 | 1:A:87:ILE:HD13 | 0.64 | 1.51 | 17 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:86:SER:CB | 1:A:89:LEU:CG | 0.64 | 2.76 | 17 | 1 |
| 1:A:13:ASN:HD21 | 1:A:35:MET:HE2 | 0.64 | 1.53 | 18 | 5 |
| 1:A:66:ILE:CG1 | 1:A:87:ILE:HG13 | 0.64 | 2.23 | 17 | 6 |
| 1:A:31:GLU:CG | 1:A:106:ARG:HD3 | 0.64 | 2.23 | 12 | 1 |
| 1:A:81:LYS:HD3 | 1:A:82:TYR:CE2 | 0.64 | 2.26 | 14 | 1 |
| 1:A:49:VAL:HG23 | 1:A:49:VAL:O | 0.64 | 1.93 | 13 | 7 |
| 1:A:17:SER:N | 1:A:20:LYS:HE3 | 0.64 | 2.08 | 3 | 4 |
| 1:A:93:TYR:HH | 1:A:94:HIS:CE1 | 0.64 | 2.09 | 19 | 2 |
| 1:A:50:PHE:CG | 1:A:61:ILE:HG13 | 0.64 | 2.28 | 12 | 2 |
| 1:A:30:LYS:CE | 1:A:107:TYR:CD2 | 0.64 | 2.81 | 4 | 2 |
| 1:A:18:ARG:CD | 1:A:18:ARG:C | 0.64 | 2.67 | 14 | 1 |
| 1:A:93:TYR:OH | 1:A:94:HIS:HE1 | 0.64 | 1.76 | 8 | 4 |
| 1:A:6:LEU:HB2 | 1:A:12:TYR:CG | 0.63 | 2.28 | 11 | 5 |
| 1:A:91:ILE:HG23 | 1:A:105:LEU:CG | 0.63 | 2.23 | 9 | 14 |
| 1:A:91:ILE:O | 1:A:105:LEU:CD2 | 0.63 | 2.46 | 17 | 5 |
| 1:A:97:ASN:ND2 | 1:A:98:GLY:N | 0.63 | 2.46 | 3 | 1 |
| 1:A:74:LYS:HE3 | 1:A:83:VAL:O | 0.63 | 1.92 | 7 | 2 |
| 1:A:35:MET:HE3 | 1:A:109:VAL:CG1 | 0.63 | 2.22 | 15 | 5 |
| 1:A:70:ASN:CA | 1:A:75:ARG:HG2 | 0.63 | 2.23 | 6 | 1 |
| 1:A:28:THR:CG2 | 1:A:30:LYS:CD | 0.63 | 2.76 | 14 | 4 |
| 1:A:12:TYR:CE2 | 1:A:14:LYS:HG3 | 0.63 | 2.28 | 18 | 2 |
| 1:A:44:THR:CG2 | 1:A:66:ILE:O | 0.63 | 2.46 | 14 | 3 |
| 1:A:84:PHE:CE2 | 1:A:93:TYR:CG | 0.63 | 2.86 | 5 | 2 |
| 1:A:64:TYR:CZ | 1:A:101:LEU:HD12 | 0.63 | 2.28 | 10 | 1 |
| 1:A:67:LYS:CB | 1:A:77:TYR:CE1 | 0.63 | 2.81 | 12 | 20 |
| 1:A:16:ILE:HG23 | 1:A:17:SER:N | 0.63 | 2.09 | 11 | 20 |
| 1:A:74:LYS:HB2 | 1:A:83:VAL:HB | 0.63 | 1.68 | 7 | 3 |
| 1:A:30:LYS:CD | 1:A:107:TYR:CD2 | 0.63 | 2.80 | 8 | 3 |
| 1:A:101:LEU:C | 1:A:103:THR:H | 0.63 | 1.96 | 17 | 1 |
| 1:A:30:LYS:CD | 1:A:109:VAL:CG2 | 0.63 | 2.75 | 14 | 1 |
| 1:A:93:TYR:CE2 | 1:A:94:HIS:NE2 | 0.63 | 2.66 | 14 | 2 |
| 1:A:10:GLU:O | 1:A:110:CYS:HB2 | 0.63 | 1.93 | 8 | 6 |
| 1:A:6:LEU:O | 1:A:7:GLU:C | 0.63 | 2.36 | 14 | 8 |
| 1:A:25:LEU:CB | 1:A:61:ILE:CD1 | 0.63 | 2.75 | 15 | 4 |
| 1:A:50:PHE:HB2 | 1:A:61:ILE:CG1 | 0.63 | 2.23 | 12 | 5 |
| 1:A:28:THR:CB | 1:A:109:VAL:CG2 | 0.63 | 2.77 | 17 | 1 |
| 1:A:86:SER:OG | 1:A:88:PRO:CG | 0.63 | 2.47 | 1 | 2 |
| 1:A:95:GLN:HG2 | 1:A:105:LEU:HB3 | 0.63 | 1.68 | 17 | 11 |
| 1:A:45:TYR:N | 1:A:45:TYR:CD1 | 0.63 | 2.67 | 20 | 10 |
| 1:A:10:GLU:CG | 1:A:108:PRO:C | 0.63 | 2.67 | 4 | 9 |
| 1:A:101:LEU:N | 1:A:101:LEU:HD12 | 0.63 | 2.09 | 6 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:7:GLU:HA | 1:A:12:TYR:CE2 | 0.63 | 2.29 | 20 | 1 |
| 1:A:82:TYR:CG | 1:A:93:TYR:OH | 0.63 | 2.51 | 14 | 1 |
| 1:A:7:GLU:HB3 | 1:A:14:LYS:CE | 0.63 | 2.23 | 11 | 3 |
| 1:A:23:LYS:HG3 | 1:A:24:LEU:N | 0.63 | 2.09 | 19 | 9 |
| 1:A:66:ILE:O | 1:A:68:GLU:CD | 0.63 | 2.37 | 7 | 1 |
| 1:A:96:TYR:O | 1:A:97:ASN:O | 0.63 | 2.17 | 17 | 6 |
| 1:A:76:TYR:C | 1:A:90:LEU:HD12 | 0.63 | 2.14 | 17 | 10 |
| 1:A:94:HIS:CG | 1:A:105:LEU:HD23 | 0.63 | 2.28 | 20 | 1 |
| 1:A:69:THR:O | 1:A:69:THR:HG23 | 0.63 | 1.94 | 11 | 1 |
| 1:A:81:LYS:O | 1:A:82:TYR:C | 0.63 | 2.36 | 5 | 5 |
| 1:A:25:LEU:HD11 | 1:A:35:MET:HB3 | 0.63 | 1.70 | 7 | 1 |
| 1:A:18:ARG:O | 1:A:22:GLU:HG2 | 0.63 | 1.93 | 4 | 2 |
| 1:A:100:GLY:C | 1:A:101:LEU:HD13 | 0.63 | 2.14 | 20 | 1 |
| 1:A:9:TYR:HB3 | 1:A:11:TRP:CD1 | 0.63 | 2.29 | 19 | 14 |
| 1:A:34:PHE:HA | 1:A:48:SER:O | 0.63 | 1.93 | 4 | 12 |
| 1:A:37:ARG:CZ | 1:A:46:THR:HG21 | 0.63 | 2.23 | 12 | 1 |
| 1:A:9:TYR:OH | 1:A:88:PRO:CB | 0.62 | 2.46 | 14 | 10 |
| 1:A:9:TYR:CZ | 1:A:88:PRO:CB | 0.62 | 2.81 | 14 | 11 |
| 1:A:94:HIS:NE2 | 1:A:101:LEU:HD22 | 0.62 | 2.07 | 9 | 5 |
| 1:A:39:SER:O | 1:A:40:ARG:C | 0.62 | 2.37 | 9 | 2 |
| 1:A:6:LEU:O | 1:A:8:THR:OG1 | 0.62 | 2.10 | 9 | 3 |
| 1:A:74:LYS:HB2 | 1:A:83:VAL:HG21 | 0.62 | 1.71 | 20 | 2 |
| 1:A:74:LYS:HE3 | 1:A:83:VAL:CA | 0.62 | 2.23 | 7 | 1 |
| 1:A:93:TYR:CZ | 1:A:94:HIS:CD2 | 0.62 | 2.87 | 5 | 1 |
| 1:A:69:THR:CG2 | 1:A:83:VAL:HG11 | 0.62 | 2.25 | 9 | 9 |
| 1:A:25:LEU:HG | 1:A:109:VAL:CG2 | 0.62 | 2.24 | 7 | 1 |
| 1:A:32:GLY:CA | 1:A:103:THR:HG23 | 0.62 | 2.23 | 5 | 4 |
| 1:A:75:ARG:NH2 | 1:A:85:ASP:CB | 0.62 | 2.63 | 13 | 2 |
| 1:A:34:PHE:CE1 | 1:A:36:VAL:HG23 | 0.62 | 2.29 | 15 | 18 |
| 1:A:11:TRP:CE3 | 1:A:36:VAL:HB | 0.62 | 2.29 | 18 | 20 |
| 1:A:26:LEU:HG | 1:A:61:ILE:CD1 | 0.62 | 2.24 | 7 | 5 |
| 1:A:77:TYR:N | 1:A:90:LEU:HD11 | 0.62 | 2.08 | 16 | 11 |
| 1:A:61:ILE:N | 1:A:61:ILE:HD13 | 0.62 | 2.09 | 4 | 3 |
| 1:A:66:ILE:CG2 | 1:A:76:TYR:HB3 | 0.62 | 2.22 | 19 | 5 |
| 1:A:38:ASP:OD1 | 1:A:39:SER:N | 0.62 | 2.31 | 12 | 4 |
| 1:A:65:HIS:O | 1:A:78:VAL:CG1 | 0.62 | 2.36 | 1 | 3 |
| 1:A:18:ARG:O | 1:A:22:GLU:OE1 | 0.62 | 2.18 | 12 | 1 |
| 1:A:11:TRP:O | 1:A:35:MET:HG2 | 0.62 | 1.93 | 16 | 4 |
| 1:A:32:GLY:HA3 | 1:A:103:THR:OG1 | 0.62 | 1.93 | 9 | 3 |
| 1:A:49:VAL:CG2 | 1:A:62:LYS:HB3 | 0.62 | 2.24 | 9 | 12 |
| 1:A:69:THR:OG1 | 1:A:74:LYS:O | 0.62 | 2.17 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:94:HIS:O | 1:A:105:LEU:N | 0.62 | 2.32 | 4 | 6 |
| 1:A:81:LYS:HZ1 | 1:A:101:LEU:CD1 | 0.62 | 2.07 | 12 | 1 |
| 1:A:30:LYS:NZ | 1:A:109:VAL:HG23 | 0.62 | 2.08 | 3 | 1 |
| 1:A:102:VAL:O | 1:A:103:THR:HG23 | 0.62 | 1.94 | 10 | 1 |
| 1:A:97:ASN:OD1 | 1:A:97:ASN:N | 0.62 | 2.32 | 19 | 1 |
| 1:A:34:PHE:CD2 | 1:A:95:GLN:NE2 | 0.62 | 2.68 | 20 | 1 |
| 1:A:17:SER:CB | 1:A:20:LYS:HD2 | 0.62 | 2.24 | 2 | 11 |
| 1:A:28:THR:HG21 | 1:A:30:LYS:CD | 0.62 | 2.24 | 14 | 3 |
| 1:A:20:LYS:O | 1:A:23:LYS:CD | 0.62 | 2.47 | 7 | 1 |
| 1:A:13:ASN:CG | 1:A:35:MET:HE1 | 0.62 | 2.15 | 7 | 2 |
| 1:A:92:GLN:HA | 1:A:92:GLN:NE2 | 0.62 | 2.08 | 4 | 7 |
| 1:A:94:HIS:CE1 | 1:A:101:LEU:HD11 | 0.62 | 2.29 | 8 | 1 |
| 1:A:44:THR:HG21 | 1:A:66:ILE:O | 0.62 | 1.95 | 14 | 3 |
| 1:A:25:LEU:HD22 | 1:A:50:PHE:HD1 | 0.62 | 1.55 | 17 | 3 |
| 1:A:77:TYR:CD2 | 1:A:80:GLU:CA | 0.62 | 2.82 | 9 | 13 |
| 1:A:34:PHE:N | 1:A:107:TYR:O | 0.62 | 2.30 | 20 | 18 |
| 1:A:60:CYS:C | 1:A:61:ILE:HD13 | 0.62 | 2.15 | 19 | 6 |
| 1:A:75:ARG:HB3 | 1:A:76:TYR:CD1 | 0.62 | 2.30 | 17 | 8 |
| 1:A:35:MET:HB3 | 1:A:109:VAL:O | 0.62 | 1.95 | 9 | 1 |
| 1:A:20:LYS:HA | 1:A:23:LYS:CD | 0.62 | 2.25 | 17 | 2 |
| 1:A:53:ALA:N | 1:A:60:CYS:HG | 0.62 | 1.91 | 19 | 1 |
| 1:A:103:THR:C | 1:A:104:ARG:CG | 0.62 | 2.67 | 7 | 3 |
| 1:A:22:GLU:CG | 1:A:61:ILE:HB | 0.62 | 2.25 | 2 | 5 |
| 1:A:93:TYR:O | 1:A:97:ASN:CA | 0.62 | 2.48 | 4 | 1 |
| 1:A:35:MET:HB2 | 1:A:48:SER:OG | 0.62 | 1.95 | 12 | 2 |
| 1:A:93:TYR:HA | 1:A:97:ASN:ND2 | 0.62 | 2.09 | 1 | 1 |
| 1:A:37:ARG:HG2 | 1:A:46:THR:CB | 0.62 | 2.25 | 19 | 18 |
| 1:A:31:GLU:N | 1:A:52:LYS:HE3 | 0.62 | 2.10 | 11 | 1 |
| 1:A:45:TYR:O | 1:A:66:ILE:CD1 | 0.62 | 2.47 | 13 | 9 |
| 1:A:67:LYS:HB3 | 1:A:77:TYR:O | 0.62 | 1.94 | 9 | 6 |
| 1:A:6:LEU:HA | 1:A:9:TYR:CE2 | 0.62 | 2.29 | 2 | 8 |
| 1:A:28:THR:CB | 1:A:30:LYS:HD2 | 0.62 | 2.25 | 4 | 1 |
| 1:A:81:LYS:NZ | 1:A:82:TYR:HE1 | 0.62 | 1.93 | 18 | 12 |
| 1:A:44:THR:HB | 1:A:68:GLU:CD | 0.62 | 2.15 | 17 | 4 |
| 1:A:79:ALA:O | 1:A:81:LYS:HB3 | 0.62 | 1.95 | 14 | 6 |
| 1:A:105:LEU:CD2 | 1:A:105:LEU:N | 0.62 | 2.61 | 14 | 3 |
| 1:A:21:ALA:O | 1:A:25:LEU:HD22 | 0.62 | 1.95 | 12 | 1 |
| 1:A:95:GLN:OE1 | 1:A:105:LEU:O | 0.62 | 2.18 | 20 | 1 |
| 1:A:11:TRP:CE3 | 1:A:36:VAL:CB | 0.61 | 2.83 | 18 | 20 |
| 1:A:34:PHE:CD2 | 1:A:108:PRO:HB3 | 0.61 | 2.30 | 6 | 16 |
| 1:A:22:GLU:CD | 1:A:61:ILE:HB | 0.61 | 2.15 | 4 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:95:GLN:HG2 | 1:A:105:LEU:CB | 0.61 | 2.25 | 9 | 8 |
| 1:A:24:LEU:CG | 1:A:35:MET:HE3 | 0.61 | 2.25 | 18 | 3 |
| 1:A:78:VAL:CG2 | 1:A:78:VAL:O | 0.61 | 2.44 | 6 | 2 |
| 1:A:74:LYS:HG2 | 1:A:85:ASP:CB | 0.61 | 2.24 | 6 | 1 |
| 1:A:74:LYS:HB2 | 1:A:84:PHE:C | 0.61 | 2.15 | 6 | 1 |
| 1:A:16:ILE:HA | 1:A:20:LYS:NZ | 0.61 | 2.10 | 20 | 3 |
| 1:A:62:LYS:CD | 1:A:64:TYR:CE1 | 0.61 | 2.83 | 16 | 1 |
| 1:A:45:TYR:C | 1:A:65:HIS:CE1 | 0.61 | 2.73 | 9 | 12 |
| 1:A:49:VAL:HG21 | 1:A:102:VAL:CG1 | 0.61 | 2.24 | 9 | 2 |
| 1:A:74:LYS:HB2 | 1:A:83:VAL:CB | 0.61 | 2.25 | 8 | 3 |
| 1:A:82:TYR:O | 1:A:83:VAL:HG13 | 0.61 | 1.93 | 8 | 1 |
| 1:A:98:GLY:N | 1:A:104:ARG:HD3 | 0.61 | 2.10 | 2 | 1 |
| 1:A:47:VAL:HB | 1:A:64:TYR:HB2 | 0.61 | 1.71 | 15 | 7 |
| 1:A:11:TRP:HE3 | 1:A:36:VAL:CG2 | 0.61 | 2.08 | 4 | 17 |
| 1:A:41:THR:HG23 | 1:A:42:PRO:N | 0.61 | 2.10 | 9 | 20 |
| 1:A:10:GLU:HG2 | 1:A:108:PRO:O | 0.61 | 1.94 | 9 | 11 |
| 1:A:88:PRO:O | 1:A:92:GLN:HG2 | 0.61 | 1.95 | 17 | 9 |
| 1:A:82:TYR:CD2 | 1:A:93:TYR:CE2 | 0.61 | 2.88 | 19 | 2 |
| 1:A:51:THR:OG1 | 1:A:51:THR:O | 0.61 | 2.16 | 2 | 2 |
| 1:A:18:ARG:CZ | 1:A:19:ASP:OD2 | 0.61 | 2.48 | 10 | 1 |
| 1:A:34:PHE:CE1 | 1:A:36:VAL:CG2 | 0.61 | 2.83 | 19 | 17 |
| 1:A:84:PHE:CD2 | 1:A:90:LEU:CA | 0.61 | 2.83 | 3 | 6 |
| 1:A:96:TYR:O | 1:A:97:ASN:C | 0.61 | 2.38 | 6 | 6 |
| 1:A:11:TRP:CD1 | 1:A:95:GLN:NE2 | 0.61 | 2.69 | 5 | 2 |
| 1:A:11:TRP:CB | 1:A:108:PRO:CB | 0.61 | 2.75 | 7 | 14 |
| 1:A:91:ILE:C | 1:A:105:LEU:HD23 | 0.61 | 2.12 | 12 | 10 |
| 1:A:45:TYR:HB2 | 1:A:87:ILE:HG12 | 0.61 | 1.70 | 18 | 10 |
| 1:A:61:ILE:CD1 | 1:A:61:ILE:N | 0.61 | 2.63 | 12 | 2 |
| 1:A:9:TYR:CD1 | 1:A:11:TRP:CZ2 | 0.61 | 2.89 | 15 | 10 |
| 1:A:28:THR:CG2 | 1:A:29:GLY:N | 0.61 | 2.63 | 6 | 10 |
| 1:A:21:ALA:O | 1:A:24:LEU:CG | 0.61 | 2.49 | 7 | 11 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:HE3 | 0.61 | 2.10 | 9 | 1 |
| 1:A:12:TYR:OH | 1:A:14:LYS:CE | 0.61 | 2.49 | 20 | 1 |
| 1:A:95:GLN:HA | 1:A:105:LEU:HB2 | 0.61 | 1.73 | 5 | 19 |
| 1:A:45:TYR:HB2 | 1:A:87:ILE:HG13 | 0.61 | 1.72 | 19 | 14 |
| 1:A:45:TYR:C | 1:A:65:HIS:HD1 | 0.61 | 1.98 | 11 | 11 |
| 1:A:103:THR:O | 1:A:104:ARG:HG3 | 0.61 | 1.96 | 20 | 12 |
| 1:A:10:GLU:CD | 1:A:108:PRO:O | 0.61 | 2.39 | 6 | 11 |
| 1:A:110:CYS:O | 1:A:111:GLY:O | 0.61 | 2.18 | 17 | 2 |
| 1:A:22:GLU:HG3 | 1:A:63:HIS:CE1 | 0.61 | 2.30 | 5 | 3 |
| 1:A:74:LYS:HE2 | 1:A:83:VAL:CG2 | 0.61 | 2.25 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:81:LYS:NZ | 1:A:82:TYR:CE1 | 0.61 | 2.69 | 18 | 10 |
| 1:A:94:HIS:O | 1:A:104:ARG:C | 0.61 | 2.39 | 9 | 7 |
| 1:A:81:LYS:CB | 1:A:81:LYS:NZ | 0.61 | 2.63 | 11 | 1 |
| 1:A:31:GLU:O | 1:A:106:ARG:HB3 | 0.61 | 1.96 | 4 | 4 |
| 1:A:13:ASN:HD21 | 1:A:35:MET:HE3 | 0.61 | 1.53 | 9 | 1 |
| 1:A:62:LYS:NZ | 1:A:64:TYR:CZ | 0.61 | 2.60 | 7 | 4 |
| 1:A:86:SER:N | 1:A:89:LEU:HD13 | 0.61 | 2.11 | 5 | 3 |
| 1:A:74:LYS:HB3 | 1:A:83:VAL:O | 0.61 | 1.95 | 12 | 4 |
| 1:A:82:TYR:HB2 | 1:A:93:TYR:OH | 0.61 | 1.96 | 14 | 1 |
| 1:A:20:LYS:H | 1:A:20:LYS:CD | 0.61 | 2.09 | 16 | 2 |
| 1:A:34:PHE:CD1 | 1:A:47:VAL:CG1 | 0.61 | 2.82 | 8 | 20 |
| 1:A:9:TYR:O | 1:A:11:TRP:N | 0.61 | 2.34 | 5 | 18 |
| 1:A:66:ILE:H | 1:A:66:ILE:HD13 | 0.61 | 1.55 | 12 | 8 |
| 1:A:11:TRP:CH2 | 1:A:87:ILE:HG21 | 0.61 | 2.29 | 2 | 6 |
| 1:A:98:GLY:HA2 | 1:A:104:ARG:CD | 0.61 | 2.26 | 9 | 6 |
| 1:A:32:GLY:HA3 | 1:A:106:ARG:CB | 0.61 | 2.26 | 20 | 14 |
| 1:A:74:LYS:O | 1:A:75:ARG:HG3 | 0.61 | 1.95 | 9 | 2 |
| 1:A:23:LYS:CE | 1:A:23:LYS:N | 0.61 | 2.64 | 2 | 1 |
| 1:A:21:ALA:O | 1:A:25:LEU:HB2 | 0.60 | 1.96 | 20 | 6 |
| 1:A:91:ILE:O | 1:A:95:GLN:HG2 | 0.60 | 1.96 | 18 | 5 |
| 1:A:100:GLY:O | 1:A:101:LEU:CD2 | 0.60 | 2.40 | 2 | 1 |
| 1:A:10:GLU:OE2 | 1:A:108:PRO:O | 0.60 | 2.19 | 16 | 3 |
| 1:A:84:PHE:CZ | 1:A:93:TYR:CZ | 0.60 | 2.89 | 5 | 3 |
| 1:A:103:THR:CG2 | 1:A:106:ARG:HG3 | 0.60 | 2.26 | 13 | 1 |
| 1:A:30:LYS:NZ | 1:A:109:VAL:CG1 | 0.60 | 2.64 | 12 | 1 |
| 1:A:93:TYR:O | 1:A:97:ASN:OD1 | 0.60 | 2.18 | 14 | 1 |
| 1:A:31:GLU:CG | 1:A:31:GLU:O | 0.60 | 2.49 | 1 | 2 |
| 1:A:66:ILE:CG1 | 1:A:87:ILE:CD1 | 0.60 | 2.80 | 14 | 9 |
| 1:A:35:MET:HG2 | 1:A:36:VAL:N | 0.60 | 2.11 | 14 | 10 |
| 1:A:69:THR:O | 1:A:75:ARG:HA | 0.60 | 1.95 | 9 | 12 |
| 1:A:95:GLN:NE2 | 1:A:108:PRO:HD3 | 0.60 | 2.11 | 20 | 3 |
| 1:A:64:TYR:CB | 1:A:78:VAL:HG21 | 0.60 | 2.21 | 8 | 1 |
| 1:A:10:GLU:CG | 1:A:108:PRO:HB2 | 0.60 | 2.25 | 4 | 3 |
| 1:A:68:GLU:CA | 1:A:75:ARG:O | 0.60 | 2.46 | 3 | 12 |
| 1:A:95:GLN:HG2 | 1:A:105:LEU:O | 0.60 | 1.97 | 19 | 5 |
| 1:A:103:THR:C | 1:A:104:ARG:HG3 | 0.60 | 2.17 | 11 | 12 |
| 1:A:22:GLU:OE2 | 1:A:61:ILE:O | 0.60 | 2.19 | 15 | 2 |
| 1:A:28:THR:HG21 | 1:A:30:LYS:CE | 0.60 | 2.24 | 9 | 2 |
| 1:A:102:VAL:CG2 | 1:A:103:THR:CG2 | 0.60 | 2.77 | 12 | 3 |
| 1:A:50:PHE:CB | 1:A:61:ILE:CG1 | 0.60 | 2.79 | 12 | 2 |
| 1:A:18:ARG:HG2 | 1:A:19:ASP:N | 0.60 | 2.10 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:76:TYR:CE2 | 1:A:86:SER:HA | 0.60 | 2.30 | 5 | 3 |
| 1:A:94:HIS:O | 1:A:104:ARG:HD2 | 0.60 | 1.96 | 1 | 5 |
| 1:A:77:TYR:CG | 1:A:83:VAL:CG1 | 0.60 | 2.80 | 11 | 5 |
| 1:A:66:ILE:CG1 | 1:A:87:ILE:HD11 | 0.60 | 2.26 | 2 | 4 |
| 1:A:78:VAL:HG23 | 1:A:81:LYS:HE3 | 0.60 | 1.73 | 2 | 1 |
| 1:A:17:SER:HB2 | 1:A:20:LYS:HD3 | 0.60 | 1.72 | 4 | 3 |
| 1:A:86:SER:OG | 1:A:88:PRO:CD | 0.60 | 2.49 | 1 | 2 |
| 1:A:35:MET:HB2 | 1:A:109:VAL:HG23 | 0.60 | 1.73 | 4 | 3 |
| 1:A:50:PHE:CB | 1:A:61:ILE:CG2 | 0.60 | 2.74 | 14 | 1 |
| 1:A:103:THR:O | 1:A:104:ARG:C | 0.60 | 2.40 | 14 | 8 |
| 1:A:45:TYR:C | 1:A:65:HIS:ND1 | 0.60 | 2.55 | 11 | 11 |
| 1:A:103:THR:CB | 1:A:106:ARG:HB2 | 0.60 | 2.27 | 15 | 2 |
| 1:A:88:PRO:C | 1:A:92:GLN:CD | 0.60 | 2.60 | 17 | 1 |
| 1:A:20:LYS:CD | 1:A:20:LYS:N | 0.60 | 2.63 | 5 | 1 |
| 1:A:17:SER:HB3 | 1:A:20:LYS:NZ | 0.60 | 2.11 | 16 | 2 |
| 1:A:11:TRP:CD2 | 1:A:34:PHE:CZ | 0.60 | 2.89 | 15 | 16 |
| 1:A:87:ILE:HG23 | 1:A:91:ILE:CD1 | 0.60 | 2.26 | 20 | 8 |
| 1:A:28:THR:HG21 | 1:A:30:LYS:HE3 | 0.60 | 1.72 | 14 | 2 |
| 1:A:21:ALA:C | 1:A:24:LEU:CD1 | 0.60 | 2.69 | 4 | 9 |
| 1:A:30:LYS:NZ | 1:A:107:TYR:HE2 | 0.60 | 1.93 | 19 | 5 |
| 1:A:24:LEU:HD11 | 1:A:25:LEU:HD12 | 0.60 | 1.67 | 7 | 1 |
| 1:A:103:THR:O | 1:A:106:ARG:CG | 0.60 | 2.50 | 13 | 1 |
| 1:A:97:ASN:O | 1:A:104:ARG:HD2 | 0.60 | 1.97 | 16 | 2 |
| 1:A:6:LEU:O | 1:A:7:GLU:OE2 | 0.60 | 2.19 | 10 | 1 |
| 1:A:78:VAL:HG21 | 1:A:94:HIS:CE1 | 0.60 | 2.32 | 18 | 4 |
| 1:A:84:PHE:CE2 | 1:A:93:TYR:CE2 | 0.60 | 2.88 | 2 | 3 |
| 1:A:85:ASP:OD1 | 1:A:85:ASP:C | 0.60 | 2.40 | 11 | 3 |
| 1:A:17:SER:N | 1:A:20:LYS:HE2 | 0.60 | 2.11 | 1 | 1 |
| 1:A:78:VAL:CG2 | 1:A:94:HIS:CE1 | 0.60 | 2.85 | 18 | 6 |
| 1:A:41:THR:C | 1:A:43:GLY:H | 0.60 | 2.00 | 4 | 20 |
| 1:A:25:LEU:HG | 1:A:35:MET:SD | 0.60 | 2.36 | 9 | 1 |
| 1:A:9:TYR:OH | 1:A:88:PRO:HG3 | 0.60 | 1.95 | 12 | 6 |
| 1:A:97:ASN:O | 1:A:104:ARG:HD3 | 0.60 | 1.97 | 8 | 4 |
| 1:A:32:GLY:H | 1:A:51:THR:HB | 0.60 | 1.57 | 4 | 3 |
| 1:A:103:THR:HG23 | 1:A:106:ARG:HG3 | 0.60 | 1.74 | 13 | 1 |
| 1:A:78:VAL:C | 1:A:81:LYS:HE2 | 0.60 | 2.17 | 13 | 1 |
| 1:A:11:TRP:O | 1:A:35:MET:CB | 0.60 | 2.50 | 9 | 2 |
| 1:A:103:THR:OG1 | 1:A:106:ARG:HB2 | 0.60 | 1.96 | 3 | 6 |
| 1:A:38:ASP:C | 1:A:38:ASP:OD1 | 0.60 | 2.40 | 17 | 1 |
| 1:A:20:LYS:CD | 1:A:20:LYS:H | 0.60 | 2.10 | 5 | 3 |
| 1:A:31:GLU:O | 1:A:106:ARG:HG2 | 0.60 | 1.96 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:22:GLU:HG2 | 1:A:61:ILE:CG2 | 0.60 | 2.27 | 8 | 4 |
| 1:A:103:THR:O | 1:A:106:ARG:HG3 | 0.60 | 1.97 | 13 | 1 |
| 1:A:74:LYS:CD | 1:A:83:VAL:HG23 | 0.60 | 2.26 | 14 | 1 |
| 1:A:62:LYS:CG | 1:A:64:TYR:CE1 | 0.59 | 2.85 | 11 | 11 |
| 1:A:21:ALA:O | 1:A:24:LEU:HG | 0.59 | 1.97 | 2 | 7 |
| 1:A:28:THR:CG2 | 1:A:30:LYS:HD2 | 0.59 | 2.26 | 14 | 2 |
| 1:A:18:ARG:CB | 1:A:63:HIS:CD2 | 0.59 | 2.85 | 18 | 3 |
| 1:A:25:LEU:CD1 | 1:A:48:SER:HB2 | 0.59 | 2.27 | 16 | 4 |
| 1:A:25:LEU:HB2 | 1:A:61:ILE:HG21 | 0.59 | 1.72 | 5 | 1 |
| 1:A:67:LYS:HA | 1:A:67:LYS:NZ | 0.59 | 2.11 | 1 | 1 |
| 1:A:20:LYS:N | 1:A:20:LYS:HD2 | 0.59 | 2.12 | 16 | 1 |
| 1:A:84:PHE:CZ | 1:A:93:TYR:CB | 0.59 | 2.85 | 18 | 11 |
| 1:A:14:LYS:C | 1:A:16:ILE:H | 0.59 | 2.01 | 15 | 13 |
| 1:A:21:ALA:C | 1:A:24:LEU:HG | 0.59 | 2.17 | 2 | 5 |
| 1:A:10:GLU:HG2 | 1:A:108:PRO:C | 0.59 | 2.18 | 16 | 8 |
| 1:A:81:LYS:NZ | 1:A:99:GLY:C | 0.59 | 2.56 | 5 | 5 |
| 1:A:84:PHE:HZ | 1:A:93:TYR:CD2 | 0.59 | 2.15 | 13 | 5 |
| 1:A:6:LEU:HD11 | 1:A:87:ILE:HG12 | 0.59 | 1.72 | 12 | 3 |
| 1:A:50:PHE:CD2 | 1:A:61:ILE:HG13 | 0.59 | 2.32 | 18 | 1 |
| 1:A:102:VAL:O | 1:A:103:THR:HB | 0.59 | 1.98 | 4 | 2 |
| 1:A:74:LYS:HB2 | 1:A:84:PHE:HA | 0.59 | 1.73 | 6 | 1 |
| 1:A:81:LYS:NZ | 1:A:101:LEU:HD11 | 0.59 | 2.12 | 12 | 1 |
| 1:A:49:VAL:O | 1:A:49:VAL:HG23 | 0.59 | 1.97 | 12 | 8 |
| 1:A:75:ARG:CZ | 1:A:85:ASP:CB | 0.59 | 2.80 | 7 | 2 |
| 1:A:20:LYS:HA | 1:A:23:LYS:CE | 0.59 | 2.27 | 15 | 2 |
| 1:A:17:SER:HB2 | 1:A:20:LYS:NZ | 0.59 | 2.13 | 15 | 4 |
| 1:A:24:LEU:O | 1:A:28:THR:HG23 | 0.59 | 1.98 | 18 | 1 |
| 1:A:69:THR:O | 1:A:75:ARG:CG | 0.59 | 2.51 | 17 | 2 |
| 1:A:92:GLN:NE2 | 1:A:92:GLN:HA | 0.59 | 2.10 | 11 | 7 |
| 1:A:33:ALA:HB1 | 1:A:109:VAL:HB | 0.59 | 1.73 | 3 | 4 |
| 1:A:85:ASP:OD1 | 1:A:85:ASP:O | 0.59 | 2.21 | 2 | 1 |
| 1:A:28:THR:HB | 1:A:30:LYS:HE2 | 0.59 | 1.73 | 4 | 1 |
| 1:A:25:LEU:HD21 | 1:A:48:SER:CB | 0.59 | 2.27 | 12 | 1 |
| 1:A:70:ASN:O | 1:A:74:LYS:HD3 | 0.59 | 1.98 | 20 | 1 |
| 1:A:64:TYR:HH | 1:A:101:LEU:HB3 | 0.59 | 1.57 | 1 | 1 |
| 1:A:95:GLN:HG3 | 1:A:105:LEU:HB3 | 0.59 | 1.74 | 4 | 11 |
| 1:A:81:LYS:O | 1:A:83:VAL:HG13 | 0.59 | 1.97 | 11 | 1 |
| 1:A:6:LEU:HB3 | 1:A:9:TYR:CE1 | 0.59 | 2.33 | 9 | 2 |
| 1:A:101:LEU:CD1 | 1:A:104:ARG:HA | 0.59 | 2.28 | 19 | 1 |
| 1:A:13:ASN:HD22 | 1:A:35:MET:CE | 0.59 | 2.09 | 1 | 5 |
| 1:A:13:ASN:CG | 1:A:16:ILE:HG13 | 0.59 | 2.18 | 17 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:6:LEU:HD21 | 1:A:45:TYR:HE2 | 0.59 | 1.54 | 17 | 1 |
| 1:A:74:LYS:HB3 | 1:A:83:VAL:C | 0.59 | 2.18 | 10 | 1 |
| 1:A:6:LEU:CD2 | 1:A:88:PRO:HD3 | 0.59 | 2.22 | 10 | 4 |
| 1:A:24:LEU:HD21 | 1:A:109:VAL:CG2 | 0.59 | 2.28 | 18 | 1 |
| 1:A:85:ASP:O | 1:A:85:ASP:CG | 0.59 | 2.40 | 6 | 2 |
| 1:A:109:VAL:O | 1:A:109:VAL:CG1 | 0.59 | 2.51 | 13 | 2 |
| 1:A:34:PHE:CE1 | 1:A:91:ILE:HD12 | 0.59 | 2.32 | 19 | 18 |
| 1:A:104:ARG:O | 1:A:104:ARG:HD2 | 0.59 | 1.97 | 5 | 3 |
| 1:A:68:GLU:HG2 | 1:A:76:TYR:CE1 | 0.59 | 2.32 | 5 | 2 |
| 1:A:52:LYS:HD2 | 1:A:52:LYS:O | 0.59 | 1.98 | 14 | 1 |
| 1:A:17:SER:HB2 | 1:A:20:LYS:HE2 | 0.59 | 1.75 | 19 | 7 |
| 1:A:35:MET:HB2 | 1:A:109:VAL:HG12 | 0.59 | 1.72 | 19 | 2 |
| 1:A:25:LEU:HD11 | 1:A:35:MET:CB | 0.59 | 2.28 | 8 | 1 |
| 1:A:70:ASN:N | 1:A:75:ARG:HG2 | 0.59 | 2.13 | 6 | 1 |
| 1:A:21:ALA:C | 1:A:24:LEU:HD12 | 0.59 | 2.18 | 4 | 5 |
| 1:A:34:PHE:CE2 | 1:A:105:LEU:CD1 | 0.59 | 2.85 | 20 | 3 |
| 1:A:81:LYS:HZ2 | 1:A:82:TYR:HE1 | 0.59 | 1.40 | 16 | 2 |
| 1:A:95:GLN:HA | 1:A:105:LEU:O | 0.59 | 1.97 | 14 | 10 |
| 1:A:74:LYS:HA | 1:A:83:VAL:O | 0.59 | 1.97 | 11 | 3 |
| 1:A:81:LYS:HZ1 | 1:A:99:GLY:C | 0.59 | 2.01 | 6 | 2 |
| 1:A:83:VAL:C | 1:A:84:PHE:CD1 | 0.59 | 2.76 | 5 | 2 |
| 1:A:11:TRP:CZ3 | 1:A:36:VAL:HB | 0.58 | 2.33 | 1 | 18 |
| 1:A:37:ARG:O | 1:A:46:THR:CB | 0.58 | 2.51 | 4 | 17 |
| 1:A:81:LYS:HD3 | 1:A:93:TYR:OH | 0.58 | 1.98 | 11 | 1 |
| 1:A:18:ARG:HB3 | 1:A:37:ARG:NH2 | 0.58 | 2.13 | 12 | 4 |
| 1:A:103:THR:OG1 | 1:A:103:THR:O | 0.58 | 2.21 | 19 | 6 |
| 1:A:62:LYS:HD3 | 1:A:64:TYR:CE1 | 0.58 | 2.32 | 16 | 2 |
| 1:A:25:LEU:CD2 | 1:A:50:PHE:HD1 | 0.58 | 2.03 | 8 | 3 |
| 1:A:98:GLY:CA | 1:A:104:ARG:HB2 | 0.58 | 2.28 | 20 | 2 |
| 1:A:66:ILE:HD13 | 1:A:66:ILE:H | 0.58 | 1.52 | 6 | 5 |
| 1:A:94:HIS:C | 1:A:105:LEU:HB2 | 0.58 | 2.19 | 15 | 15 |
| 1:A:37:ARG:O | 1:A:46:THR:OG1 | 0.58 | 2.21 | 4 | 12 |
| 1:A:84:PHE:CE1 | 1:A:90:LEU:HA | 0.58 | 2.33 | 18 | 6 |
| 1:A:84:PHE:CE1 | 1:A:93:TYR:CZ | 0.58 | 2.92 | 13 | 3 |
| 1:A:31:GLU:O | 1:A:106:ARG:HD2 | 0.58 | 1.96 | 16 | 4 |
| 1:A:17:SER:C | 1:A:37:ARG:NH1 | 0.58 | 2.56 | 5 | 1 |
| 1:A:11:TRP:CB | 1:A:35:MET:HA | 0.58 | 2.28 | 9 | 7 |
| 1:A:95:GLN:HA | 1:A:105:LEU:CB | 0.58 | 2.28 | 5 | 15 |
| 1:A:18:ARG:CA | 1:A:63:HIS:CE1 | 0.58 | 2.85 | 20 | 5 |
| 1:A:98:GLY:O | 1:A:104:ARG:HB3 | 0.58 | 1.98 | 5 | 5 |
| 1:A:95:GLN:HG2 | 1:A:105:LEU:HD23 | 0.58 | 1.75 | 3 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:ALA:O | 1:A:25:LEU:HD23 | 0.58 | 1.97 | 19 | 1 |
| 1:A:75:ARG:HB2 | 1:A:76:TYR:CD1 | 0.58 | 2.33 | 19 | 7 |
| 1:A:31:GLU:O | 1:A:106:ARG:HD3 | 0.58 | 1.98 | 6 | 4 |
| 1:A:49:VAL:CB | 1:A:102:VAL:CG1 | 0.58 | 2.82 | 13 | 1 |
| 1:A:101:LEU:O | 1:A:102:VAL:C | 0.58 | 2.42 | 10 | 8 |
| 1:A:12:TYR:CE2 | 1:A:14:LYS:HG2 | 0.58 | 2.32 | 15 | 7 |
| 1:A:11:TRP:HB2 | 1:A:35:MET:HA | 0.58 | 1.74 | 9 | 6 |
| 1:A:87:ILE:N | 1:A:87:ILE:CD1 | 0.58 | 2.66 | 3 | 4 |
| 1:A:99:GLY:O | 1:A:100:GLY:O | 0.58 | 2.20 | 13 | 2 |
| 1:A:29:GLY:HA3 | 1:A:52:LYS:NZ | 0.58 | 2.13 | 15 | 1 |
| 1:A:44:THR:HB | 1:A:68:GLU:OE2 | 0.58 | 1.98 | 20 | 1 |
| 1:A:37:ARG:CG | 1:A:46:THR:HB | 0.58 | 2.28 | 16 | 20 |
| 1:A:17:SER:CB | 1:A:20:LYS:HZ3 | 0.58 | 2.11 | 16 | 3 |
| 1:A:67:LYS:HG2 | 1:A:77:TYR:OH | 0.58 | 1.99 | 13 | 12 |
| 1:A:35:MET:SD | 1:A:109:VAL:HB | 0.58 | 2.38 | 9 | 1 |
| 1:A:64:TYR:HE2 | 1:A:101:LEU:CB | 0.58 | 2.12 | 20 | 2 |
| 1:A:64:TYR:CD2 | 1:A:101:LEU:CD1 | 0.58 | 2.86 | 7 | 1 |
| 1:A:74:LYS:HB2 | 1:A:83:VAL:C | 0.58 | 2.18 | 8 | 3 |
| 1:A:13:ASN:HD21 | 1:A:35:MET:CE | 0.58 | 2.11 | 13 | 5 |
| 1:A:37:ARG:HD3 | 1:A:46:THR:CB | 0.58 | 2.29 | 14 | 12 |
| 1:A:48:SER:HG | 1:A:63:HIS:CE1 | 0.58 | 2.16 | 11 | 1 |
| 1:A:64:TYR:OH | 1:A:101:LEU:HB3 | 0.58 | 1.97 | 1 | 2 |
| 1:A:109:VAL:CG1 | 1:A:109:VAL:O | 0.58 | 2.51 | 3 | 2 |
| 1:A:74:LYS:HG3 | 1:A:83:VAL:O | 0.58 | 1.98 | 1 | 2 |
| 1:A:19:ASP:O | 1:A:23:LYS:CD | 0.58 | 2.50 | 2 | 1 |
| 1:A:85:ASP:O | 1:A:86:SER:OG | 0.58 | 2.21 | 2 | 3 |
| 1:A:84:PHE:HE1 | 1:A:93:TYR:CE2 | 0.58 | 2.17 | 14 | 3 |
| 1:A:49:VAL:HB | 1:A:102:VAL:HG12 | 0.58 | 1.75 | 13 | 1 |
| 1:A:14:LYS:NZ | 1:A:38:ASP:CG | 0.58 | 2.57 | 20 | 1 |
| 1:A:51:THR:O | 1:A:51:THR:OG1 | 0.58 | 2.19 | 5 | 1 |
| 1:A:13:ASN:OD1 | 1:A:24:LEU:CD1 | 0.58 | 2.52 | 16 | 1 |
| 1:A:68:GLU:CG | 1:A:76:TYR:CD1 | 0.58 | 2.87 | 9 | 10 |
| 1:A:92:GLN:NE2 | 1:A:92:GLN:CA | 0.58 | 2.67 | 4 | 10 |
| 1:A:68:GLU:N | 1:A:68:GLU:OE1 | 0.58 | 2.37 | 9 | 3 |
| 1:A:50:PHE:C | 1:A:50:PHE:CD1 | 0.58 | 2.77 | 6 | 2 |
| 1:A:30:LYS:O | 1:A:51:THR:HA | 0.58 | 1.98 | 5 | 1 |
| 1:A:11:TRP:HA | 1:A:109:VAL:O | 0.58 | 1.99 | 12 | 4 |
| 1:A:106:ARG:O | 1:A:106:ARG:CD | 0.58 | 2.51 | 15 | 1 |
| 1:A:36:VAL:HG21 | 1:A:87:ILE:HG21 | 0.57 | 1.75 | 4 | 5 |
| 1:A:79:ALA:CB | 1:A:81:LYS:HE3 | 0.57 | 2.29 | 4 | 1 |
| 1:A:51:THR:OG1 | 1:A:103:THR:HG21 | 0.57 | 1.98 | 10 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:11:TRP:CG | 1:A:108:PRO:HB3 | 0.57 | 2.34 | 4 | 15 |
| 1:A:52:LYS:CD | 1:A:52:LYS:N | 0.57 | 2.67 | 11 | 1 |
| 1:A:22:GLU:CA | 1:A:61:ILE:HG21 | 0.57 | 2.19 | 19 | 2 |
| 1:A:21:ALA:CB | 1:A:35:MET:SD | 0.57 | 2.92 | 6 | 3 |
| 1:A:100:GLY:O | 1:A:101:LEU:HG | 0.57 | 1.99 | 12 | 1 |
| 1:A:49:VAL:CG2 | 1:A:102:VAL:HG13 | 0.57 | 2.29 | 16 | 2 |
| 1:A:98:GLY:CA | 1:A:104:ARG:HB3 | 0.57 | 2.29 | 20 | 1 |
| 1:A:64:TYR:HE2 | 1:A:101:LEU:CD1 | 0.57 | 2.11 | 10 | 1 |
| 1:A:17:SER:HB3 | 1:A:20:LYS:HD2 | 0.57 | 1.75 | 20 | 9 |
| 1:A:18:ARG:HA | 1:A:63:HIS:NE2 | 0.57 | 2.14 | 7 | 1 |
| 1:A:81:LYS:HZ2 | 1:A:99:GLY:HA2 | 0.57 | 1.58 | 17 | 2 |
| 1:A:62:LYS:HD3 | 1:A:102:VAL:CG1 | 0.57 | 2.29 | 17 | 1 |
| 1:A:78:VAL:CG2 | 1:A:94:HIS:NE2 | 0.57 | 2.67 | 12 | 5 |
| 1:A:22:GLU:CA | 1:A:22:GLU:OE1 | 0.57 | 2.51 | 4 | 1 |
| 1:A:28:THR:HB | 1:A:30:LYS:CD | 0.57 | 2.28 | 4 | 1 |
| 1:A:81:LYS:HZ3 | 1:A:94:HIS:CE1 | 0.57 | 2.17 | 13 | 1 |
| 1:A:75:ARG:HG2 | 1:A:84:PHE:O | 0.57 | 1.99 | 5 | 2 |
| 1:A:37:ARG:HG2 | 1:A:46:THR:HB | 0.57 | 1.75 | 3 | 20 |
| 1:A:49:VAL:CG2 | 1:A:102:VAL:HG12 | 0.57 | 2.29 | 13 | 2 |
| 1:A:47:VAL:O | 1:A:63:HIS:HA | 0.57 | 1.99 | 3 | 5 |
| 1:A:50:PHE:O | 1:A:50:PHE:CD1 | 0.57 | 2.57 | 6 | 3 |
| 1:A:74:LYS:HE2 | 1:A:74:LYS:CA | 0.57 | 2.28 | 8 | 1 |
| 1:A:110:CYS:O | 1:A:111:GLY:C | 0.57 | 2.42 | 17 | 1 |
| 1:A:29:GLY:O | 1:A:30:LYS:C | 0.57 | 2.41 | 13 | 3 |
| 1:A:67:LYS:NZ | 1:A:67:LYS:HB2 | 0.57 | 2.14 | 14 | 1 |
| 1:A:81:LYS:HE3 | 1:A:100:GLY:N | 0.57 | 2.14 | 16 | 1 |
| 1:A:25:LEU:HG | 1:A:61:ILE:HG23 | 0.57 | 1.76 | 19 | 2 |
| 1:A:86:SER:N | 1:A:89:LEU:HD12 | 0.57 | 2.14 | 15 | 4 |
| 1:A:94:HIS:NE2 | 1:A:99:GLY:HA2 | 0.57 | 2.14 | 17 | 1 |
| 1:A:13:ASN:OD1 | 1:A:16:ILE:HG13 | 0.57 | 1.98 | 4 | 4 |
| 1:A:28:THR:HB | 1:A:30:LYS:CE | 0.57 | 2.29 | 4 | 1 |
| 1:A:104:ARG:NH1 | 1:A:106:ARG:HA | 0.57 | 2.14 | 12 | 1 |
| 1:A:11:TRP:CD1 | 1:A:108:PRO:CB | 0.57 | 2.88 | 6 | 18 |
| 1:A:11:TRP:CZ3 | 1:A:36:VAL:CB | 0.57 | 2.87 | 1 | 18 |
| 1:A:46:THR:HA | 1:A:65:HIS:HD1 | 0.57 | 1.58 | 9 | 13 |
| 1:A:45:TYR:C | 1:A:66:ILE:HG12 | 0.57 | 2.20 | 7 | 8 |
| 1:A:23:LYS:HD2 | 1:A:24:LEU:N | 0.57 | 2.14 | 7 | 1 |
| 1:A:81:LYS:HZ2 | 1:A:93:TYR:HH | 0.57 | 1.41 | 13 | 1 |
| 1:A:75:ARG:HG3 | 1:A:85:ASP:HA | 0.57 | 1.75 | 3 | 3 |
| 1:A:77:TYR:CE2 | 1:A:80:GLU:HG2 | 0.57 | 2.34 | 8 | 1 |
| 1:A:20:LYS:O | 1:A:24:LEU:HD23 | 0.57 | 1.99 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:66:ILE:HG23 | 1:A:90:LEU:CG | 0.57 | 2.30 | 3 | 1 |
| 1:A:61:ILE:HD13 | 1:A:61:ILE:N | 0.57 | 2.15 | 16 | 1 |
| 1:A:6:LEU:C | 1:A:7:GLU:CG | 0.57 | 2.73 | 10 | 2 |
| 1:A:29:GLY:O | 1:A:30:LYS:HD2 | 0.57 | 1.99 | 3 | 3 |
| 1:A:69:THR:HG22 | 1:A:83:VAL:HG11 | 0.57 | 1.77 | 2 | 2 |
| 1:A:24:LEU:CD1 | 1:A:25:LEU:CD2 | 0.57 | 2.83 | 19 | 1 |
| 1:A:10:GLU:OE2 | 1:A:107:TYR:CE1 | 0.57 | 2.57 | 5 | 1 |
| 1:A:75:ARG:CG | 1:A:76:TYR:CE1 | 0.57 | 2.88 | 3 | 4 |
| 1:A:28:THR:CG2 | 1:A:109:VAL:HG11 | 0.57 | 2.28 | 2 | 3 |
| 1:A:10:GLU:CA | 1:A:110:CYS:HB3 | 0.57 | 2.29 | 19 | 2 |
| 1:A:90:LEU:O | 1:A:94:HIS:HB2 | 0.57 | 2.00 | 4 | 1 |
| 1:A:87:ILE:C | 1:A:91:ILE:HG12 | 0.57 | 2.19 | 17 | 18 |
| 1:A:91:ILE:CA | 1:A:105:LEU:CD2 | 0.57 | 2.83 | 12 | 11 |
| 1:A:6:LEU:CD1 | 1:A:45:TYR:CD2 | 0.57 | 2.80 | 16 | 6 |
| 1:A:68:GLU:CA | 1:A:68:GLU:OE1 | 0.57 | 2.53 | 20 | 2 |
| 1:A:20:LYS:O | 1:A:23:LYS:HD2 | 0.57 | 2.00 | 7 | 1 |
| 1:A:102:VAL:O | 1:A:103:THR:CB | 0.57 | 2.52 | 18 | 5 |
| 1:A:24:LEU:HD23 | 1:A:111:GLY:HA2 | 0.57 | 1.75 | 1 | 1 |
| 1:A:82:TYR:CE2 | 1:A:93:TYR:CE1 | 0.56 | 2.93 | 2 | 2 |
| 1:A:22:GLU:HG2 | 1:A:61:ILE:HB | 0.56 | 1.77 | 12 | 13 |
| 1:A:82:TYR:HD2 | 1:A:93:TYR:CE2 | 0.56 | 2.18 | 19 | 1 |
| 1:A:6:LEU:CB | 1:A:9:TYR:CE2 | 0.56 | 2.88 | 2 | 9 |
| 1:A:22:GLU:CB | 1:A:23:LYS:NZ | 0.56 | 2.68 | 2 | 1 |
| 1:A:66:ILE:CB | 1:A:87:ILE:CD1 | 0.56 | 2.83 | 3 | 2 |
| 1:A:45:TYR:CB | 1:A:87:ILE:HG12 | 0.56 | 2.31 | 11 | 13 |
| 1:A:64:TYR:CD2 | 1:A:101:LEU:CG | 0.56 | 2.87 | 7 | 2 |
| 1:A:24:LEU:HD12 | 1:A:25:LEU:CD2 | 0.56 | 2.30 | 19 | 1 |
| 1:A:64:TYR:CZ | 1:A:101:LEU:CB | 0.56 | 2.87 | 7 | 1 |
| 1:A:70:ASN:CG | 1:A:70:ASN:O | 0.56 | 2.43 | 2 | 1 |
| 1:A:66:ILE:HA | 1:A:78:VAL:HG12 | 0.56 | 1.77 | 6 | 1 |
| 1:A:95:GLN:OE1 | 1:A:108:PRO:HD3 | 0.56 | 2.00 | 14 | 2 |
| 1:A:97:ASN:O | 1:A:104:ARG:HG2 | 0.56 | 2.00 | 5 | 1 |
| 1:A:35:MET:O | 1:A:47:VAL:CA | 0.56 | 2.52 | 10 | 19 |
| 1:A:86:SER:CB | 1:A:88:PRO:HD2 | 0.56 | 2.31 | 20 | 6 |
| 1:A:84:PHE:CD2 | 1:A:90:LEU:CB | 0.56 | 2.88 | 7 | 5 |
| 1:A:11:TRP:O | 1:A:35:MET:HB2 | 0.56 | 1.99 | 9 | 1 |
| 1:A:91:ILE:HG22 | 1:A:95:GLN:HG3 | 0.56 | 1.77 | 5 | 2 |
| 1:A:81:LYS:HG3 | 1:A:82:TYR:CZ | 0.56 | 2.35 | 19 | 1 |
| 1:A:37:ARG:NH1 | 1:A:37:ARG:HG3 | 0.56 | 2.16 | 2 | 6 |
| 1:A:24:LEU:HB3 | 1:A:111:GLY:C | 0.56 | 2.21 | 6 | 1 |
| 1:A:74:LYS:O | 1:A:83:VAL:CG2 | 0.56 | 2.54 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:27:ASP:OD1 | 1:A:27:ASP:O | 0.56 | 2.22 | 4 | 2 |
| 1:A:31:GLU:HG3 | 1:A:106:ARG:CD | 0.56 | 2.30 | 12 | 1 |
| 1:A:94:HIS:O | 1:A:104:ARG:HD3 | 0.56 | 2.00 | 12 | 2 |
| 1:A:21:ALA:O | 1:A:25:LEU:CB | 0.56 | 2.53 | 3 | 5 |
| 1:A:35:MET:CE | 1:A:109:VAL:HG12 | 0.56 | 2.30 | 14 | 1 |
| 1:A:14:LYS:NZ | 1:A:14:LYS:HB3 | 0.56 | 2.15 | 1 | 1 |
| 1:A:16:ILE:CD1 | 1:A:24:LEU:HD13 | 0.56 | 2.30 | 16 | 1 |
| 1:A:62:LYS:HB3 | 1:A:64:TYR:HE1 | 0.56 | 1.60 | 9 | 20 |
| 1:A:98:GLY:O | 1:A:104:ARG:HG2 | 0.56 | 2.01 | 19 | 4 |
| 1:A:20:LYS:C | 1:A:23:LYS:HG3 | 0.56 | 2.19 | 7 | 1 |
| 1:A:33:ALA:HB2 | 1:A:50:PHE:CE1 | 0.56 | 2.36 | 8 | 1 |
| 1:A:74:LYS:O | 1:A:83:VAL:HB | 0.56 | 2.00 | 6 | 1 |
| 1:A:87:ILE:HG22 | 1:A:91:ILE:HG13 | 0.56 | 1.76 | 8 | 11 |
| 1:A:82:TYR:HB2 | 1:A:84:PHE:CE1 | 0.56 | 2.35 | 1 | 9 |
| 1:A:74:LYS:CG | 1:A:83:VAL:CG2 | 0.56 | 2.61 | 8 | 1 |
| 1:A:32:GLY:HA2 | 1:A:103:THR:HG21 | 0.56 | 1.77 | 6 | 4 |
| 1:A:40:ARG:CG | 1:A:41:THR:N | 0.56 | 2.68 | 4 | 1 |
| 1:A:43:GLY:O | 1:A:68:GLU:CD | 0.56 | 2.44 | 12 | 1 |
| 1:A:84:PHE:HE2 | 1:A:93:TYR:CD2 | 0.56 | 2.16 | 10 | 2 |
| 1:A:64:TYR:CZ | 1:A:101:LEU:HG | 0.56 | 2.34 | 9 | 2 |
| 1:A:92:GLN:CA | 1:A:92:GLN:NE2 | 0.56 | 2.68 | 13 | 8 |
| 1:A:10:GLU:HA | 1:A:110:CYS:HB3 | 0.56 | 1.77 | 19 | 3 |
| 1:A:7:GLU:OE1 | 1:A:14:LYS:CE | 0.56 | 2.54 | 14 | 1 |
| 1:A:10:GLU:HG3 | 1:A:10:GLU:O | 0.56 | 2.00 | 12 | 9 |
| 1:A:93:TYR:O | 1:A:97:ASN:N | 0.56 | 2.38 | 19 | 2 |
| 1:A:52:LYS:O | 1:A:52:LYS:CG | 0.56 | 2.54 | 18 | 1 |
| 1:A:106:ARG:HD3 | 1:A:106:ARG:O | 0.56 | 2.00 | 15 | 2 |
| 1:A:24:LEU:HD23 | 1:A:111:GLY:C | 0.56 | 2.20 | 1 | 2 |
| 1:A:98:GLY:HA3 | 1:A:104:ARG:HB3 | 0.56 | 1.77 | 20 | 2 |
| 1:A:47:VAL:HG12 | 1:A:49:VAL:HG12 | 0.56 | 1.78 | 14 | 3 |
| 1:A:19:ASP:HA | 1:A:22:GLU:OE1 | 0.56 | 2.00 | 12 | 2 |
| 1:A:30:LYS:NZ | 1:A:109:VAL:HG13 | 0.56 | 2.15 | 12 | 1 |
| 1:A:24:LEU:HD23 | 1:A:111:GLY:HA3 | 0.56 | 1.77 | 3 | 2 |
| 1:A:7:GLU:CG | 1:A:14:LYS:HE2 | 0.56 | 2.30 | 5 | 1 |
| 1:A:21:ALA:C | 1:A:24:LEU:CD2 | 0.56 | 2.74 | 16 | 1 |
| 1:A:21:ALA:CA | 1:A:24:LEU:HG | 0.56 | 2.31 | 13 | 11 |
| 1:A:31:GLU:O | 1:A:106:ARG:HG3 | 0.56 | 2.01 | 5 | 5 |
| 1:A:70:ASN:ND2 | 1:A:70:ASN:O | 0.56 | 2.37 | 9 | 1 |
| 1:A:86:SER:OG | 1:A:89:LEU:CD1 | 0.56 | 2.54 | 14 | 3 |
| 1:A:74:LYS:HE3 | 1:A:83:VAL:HB | 0.56 | 1.77 | 7 | 1 |
| 1:A:69:THR:O | 1:A:74:LYS:O | 0.56 | 2.23 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:66:ILE:HG13 | 1:A:87:ILE:HG12 | 0.56 | 1.77 | 17 | 3 |
| 1:A:30:LYS:NZ | 1:A:107:TYR:CD2 | 0.56 | 2.72 | 20 | 2 |
| 1:A:31:GLU:HA | 1:A:52:LYS:CE | 0.56 | 2.30 | 11 | 1 |
| 1:A:74:LYS:CE | 1:A:83:VAL:CB | 0.56 | 2.83 | 7 | 1 |
| 1:A:22:GLU:OE2 | 1:A:63:HIS:NE2 | 0.56 | 2.39 | 4 | 3 |
| 1:A:85:ASP:OD1 | 1:A:89:LEU:HD11 | 0.56 | 2.01 | 4 | 1 |
| 1:A:7:GLU:OE1 | 1:A:14:LYS:HE3 | 0.56 | 2.01 | 14 | 1 |
| 1:A:81:LYS:HZ2 | 1:A:99:GLY:C | 0.56 | 2.03 | 18 | 3 |
| 1:A:13:ASN:CB | 1:A:16:ILE:HD12 | 0.56 | 2.30 | 13 | 11 |
| 1:A:101:LEU:H | 1:A:101:LEU:CD1 | 0.56 | 2.14 | 11 | 1 |
| 1:A:45:TYR:HB2 | 1:A:66:ILE:CG1 | 0.56 | 2.31 | 8 | 2 |
| 1:A:89:LEU:HA | 1:A:92:GLN:CG | 0.56 | 2.30 | 17 | 1 |
| 1:A:69:THR:O | 1:A:75:ARG:HB3 | 0.56 | 2.01 | 4 | 3 |
| 1:A:104:ARG:NH2 | 1:A:106:ARG:HA | 0.56 | 2.16 | 13 | 1 |
| 1:A:76:TYR:O | 1:A:90:LEU:CD1 | 0.56 | 2.53 | 12 | 3 |
| 1:A:75:ARG:HB2 | 1:A:76:TYR:CE1 | 0.55 | 2.36 | 6 | 8 |
| 1:A:23:LYS:N | 1:A:23:LYS:HZ3 | 0.55 | 1.99 | 2 | 1 |
| 1:A:52:LYS:NZ | 1:A:52:LYS:HB2 | 0.55 | 2.16 | 17 | 1 |
| 1:A:35:MET:HG2 | 1:A:36:VAL:H | 0.55 | 1.61 | 14 | 3 |
| 1:A:64:TYR:CE2 | 1:A:101:LEU:HD11 | 0.55 | 2.36 | 10 | 1 |
| 1:A:13:ASN:OD1 | 1:A:35:MET:CG | 0.55 | 2.54 | 11 | 1 |
| 1:A:52:LYS:O | 1:A:53:ALA:HB2 | 0.55 | 2.02 | 1 | 5 |
| 1:A:34:PHE:O | 1:A:108:PRO:C | 0.55 | 2.44 | 9 | 2 |
| 1:A:74:LYS:HE3 | 1:A:83:VAL:CB | 0.55 | 2.31 | 7 | 1 |
| 1:A:95:GLN:CD | 1:A:105:LEU:HB3 | 0.55 | 2.21 | 20 | 1 |
| 1:A:45:TYR:CB | 1:A:87:ILE:CG1 | 0.55 | 2.85 | 19 | 10 |
| 1:A:81:LYS:HD3 | 1:A:82:TYR:HD1 | 0.55 | 1.59 | 11 | 2 |
| 1:A:82:TYR:CE1 | 1:A:99:GLY:HA2 | 0.55 | 2.37 | 11 | 2 |
| 1:A:49:VAL:O | 1:A:49:VAL:CG2 | 0.55 | 2.53 | 9 | 7 |
| 1:A:78:VAL:HG12 | 1:A:79:ALA:H | 0.55 | 1.54 | 9 | 2 |
| 1:A:74:LYS:CE | 1:A:74:LYS:CA | 0.55 | 2.84 | 8 | 1 |
| 1:A:21:ALA:HB1 | 1:A:48:SER:CB | 0.55 | 2.31 | 3 | 5 |
| 1:A:20:LYS:C | 1:A:20:LYS:HD2 | 0.55 | 2.22 | 18 | 1 |
| 1:A:49:VAL:HG21 | 1:A:64:TYR:OH | 0.55 | 2.01 | 20 | 1 |
| 1:A:7:GLU:HB2 | 1:A:14:LYS:HD3 | 0.55 | 1.79 | 1 | 1 |
| 1:A:17:SER:HB3 | 1:A:20:LYS:HD3 | 0.55 | 1.76 | 5 | 6 |
| 1:A:74:LYS:CE | 1:A:74:LYS:H | 0.55 | 2.13 | 8 | 1 |
| 1:A:64:TYR:CZ | 1:A:101:LEU:HD11 | 0.55 | 2.36 | 10 | 1 |
| 1:A:51:THR:O | 1:A:51:THR:HG22 | 0.55 | 2.02 | 10 | 2 |
| 1:A:6:LEU:CD1 | 1:A:11:TRP:CZ3 | 0.55 | 2.90 | 11 | 3 |
| 1:A:30:LYS:O | 1:A:52:LYS:NZ | 0.55 | 2.39 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:48:SER:OG | 1:A:63:HIS:CE1 | 0.55 | 2.59 | 11 | 2 |
| 1:A:100:GLY:O | 1:A:101:LEU:CD1 | 0.55 | 2.52 | 3 | 2 |
| 1:A:13:ASN:ND2 | 1:A:24:LEU:HD11 | 0.55 | 2.12 | 20 | 1 |
| 1:A:64:TYR:OH | 1:A:101:LEU:HA | 0.55 | 2.02 | 11 | 1 |
| 1:A:8:THR:HG23 | 1:A:9:TYR:CE1 | 0.55 | 2.37 | 3 | 2 |
| 1:A:84:PHE:HE1 | 1:A:93:TYR:CD2 | 0.55 | 2.18 | 18 | 5 |
| 1:A:35:MET:SD | 1:A:109:VAL:CG1 | 0.55 | 2.94 | 9 | 1 |
| 1:A:11:TRP:HD1 | 1:A:108:PRO:HB3 | 0.55 | 1.61 | 8 | 6 |
| 1:A:67:LYS:C | 1:A:68:GLU:CD | 0.55 | 2.65 | 7 | 1 |
| 1:A:10:GLU:O | 1:A:10:GLU:HG3 | 0.55 | 2.02 | 6 | 4 |
| 1:A:103:THR:O | 1:A:104:ARG:CD | 0.55 | 2.55 | 18 | 1 |
| 1:A:81:LYS:HD3 | 1:A:82:TYR:HD2 | 0.55 | 1.58 | 14 | 1 |
| 1:A:23:LYS:CG | 1:A:24:LEU:N | 0.55 | 2.69 | 3 | 10 |
| 1:A:91:ILE:O | 1:A:95:GLN:HB2 | 0.55 | 2.01 | 15 | 3 |
| 1:A:78:VAL:HG22 | 1:A:81:LYS:HZ1 | 0.55 | 1.61 | 13 | 1 |
| 1:A:66:ILE:CB | 1:A:87:ILE:HD12 | 0.55 | 2.31 | 3 | 1 |
| 1:A:17:SER:CA | 1:A:37:ARG:NH1 | 0.55 | 2.70 | 5 | 2 |
| 1:A:16:ILE:CG2 | 1:A:37:ARG:CB | 0.55 | 2.82 | 7 | 9 |
| 1:A:10:GLU:HB2 | 1:A:108:PRO:O | 0.55 | 2.02 | 3 | 7 |
| 1:A:34:PHE:HZ | 1:A:36:VAL:CG2 | 0.55 | 2.13 | 6 | 18 |
| 1:A:95:GLN:NE2 | 1:A:108:PRO:HG3 | 0.55 | 2.17 | 8 | 4 |
| 1:A:32:GLY:HA2 | 1:A:51:THR:HG1 | 0.55 | 1.61 | 12 | 6 |
| 1:A:11:TRP:N | 1:A:108:PRO:HB2 | 0.55 | 2.16 | 7 | 4 |
| 1:A:93:TYR:HA | 1:A:97:ASN:OD1 | 0.55 | 2.01 | 8 | 1 |
| 1:A:103:THR:O | 1:A:103:THR:OG1 | 0.55 | 2.22 | 3 | 3 |
| 1:A:87:ILE:N | 1:A:87:ILE:HD13 | 0.55 | 2.16 | 3 | 2 |
| 1:A:45:TYR:HD1 | 1:A:87:ILE:HD11 | 0.55 | 1.62 | 3 | 2 |
| 1:A:66:ILE:HG21 | 1:A:90:LEU:HD13 | 0.55 | 1.75 | 10 | 3 |
| 1:A:31:GLU:HA | 1:A:52:LYS:HE2 | 0.55 | 1.79 | 11 | 1 |
| 1:A:12:TYR:OH | 1:A:14:LYS:HG2 | 0.55 | 2.01 | 14 | 6 |
| 1:A:87:ILE:CG2 | 1:A:91:ILE:HG13 | 0.55 | 2.31 | 18 | 7 |
| 1:A:24:LEU:HD22 | 1:A:25:LEU:CA | 0.55 | 2.31 | 18 | 1 |
| 1:A:90:LEU:O | 1:A:93:TYR:HD1 | 0.55 | 1.79 | 1 | 4 |
| 1:A:28:THR:OG1 | 1:A:30:LYS:HD3 | 0.55 | 2.02 | 16 | 4 |
| 1:A:30:LYS:HE3 | 1:A:109:VAL:HG12 | 0.55 | 1.79 | 12 | 1 |
| 1:A:25:LEU:CB | 1:A:61:ILE:HG21 | 0.55 | 2.32 | 5 | 1 |
| 1:A:49:VAL:HG23 | 1:A:102:VAL:HG13 | 0.55 | 1.78 | 16 | 1 |
| 1:A:87:ILE:HD13 | 1:A:87:ILE:N | 0.55 | 2.17 | 19 | 5 |
| 1:A:13:ASN:CG | 1:A:35:MET:HE2 | 0.55 | 2.22 | 9 | 1 |
| 1:A:75:ARG:HG3 | 1:A:84:PHE:O | 0.55 | 2.01 | 19 | 5 |
| 1:A:85:ASP:C | 1:A:86:SER:OG | 0.55 | 2.45 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:25:LEU:HA | 1:A:109:VAL:HG11 | 0.55 | 1.78 | 20 | 1 |
| 1:A:34:PHE:CE1 | 1:A:35:MET:O | 0.54 | 2.61 | 12 | 9 |
| 1:A:24:LEU:O | 1:A:27:ASP:OD2 | 0.54 | 2.25 | 1 | 1 |
| 1:A:31:GLU:O | 1:A:31:GLU:OE1 | 0.54 | 2.25 | 1 | 1 |
| 1:A:84:PHE:HZ | 1:A:93:TYR:CG | 0.54 | 2.20 | 11 | 15 |
| 1:A:106:ARG:HD2 | 1:A:106:ARG:O | 0.54 | 2.02 | 19 | 1 |
| 1:A:53:ALA:C | 1:A:60:CYS:SG | 0.54 | 2.85 | 19 | 1 |
| 1:A:24:LEU:CD2 | 1:A:35:MET:HE1 | 0.54 | 2.31 | 1 | 6 |
| 1:A:74:LYS:CA | 1:A:83:VAL:CG2 | 0.54 | 2.85 | 13 | 1 |
| 1:A:100:GLY:O | 1:A:101:LEU:CG | 0.54 | 2.56 | 12 | 1 |
| 1:A:66:ILE:HB | 1:A:87:ILE:CD1 | 0.54 | 2.31 | 3 | 1 |
| 1:A:14:LYS:CG | 1:A:38:ASP:CB | 0.54 | 2.83 | 20 | 1 |
| 1:A:98:GLY:C | 1:A:104:ARG:HB3 | 0.54 | 2.23 | 5 | 2 |
| 1:A:7:GLU:HB3 | 1:A:14:LYS:HD2 | 0.54 | 1.79 | 1 | 1 |
| 1:A:18:ARG:CA | 1:A:63:HIS:NE2 | 0.54 | 2.70 | 18 | 2 |
| 1:A:39:SER:O | 1:A:40:ARG:HB2 | 0.54 | 2.03 | 18 | 1 |
| 1:A:24:LEU:HD22 | 1:A:35:MET:HE3 | 0.54 | 1.78 | 6 | 1 |
| 1:A:103:THR:OG1 | 1:A:106:ARG:HG2 | 0.54 | 2.03 | 3 | 1 |
| 1:A:29:GLY:C | 1:A:30:LYS:HD2 | 0.54 | 2.23 | 7 | 5 |
| 1:A:32:GLY:HA3 | 1:A:106:ARG:HB3 | 0.54 | 1.78 | 8 | 8 |
| 1:A:7:GLU:HB3 | 1:A:14:LYS:HD3 | 0.54 | 1.79 | 18 | 4 |
| 1:A:25:LEU:HG | 1:A:61:ILE:CG2 | 0.54 | 2.33 | 19 | 1 |
| 1:A:7:GLU:OE1 | 1:A:14:LYS:HD3 | 0.54 | 2.02 | 7 | 1 |
| 1:A:37:ARG:HH11 | 1:A:37:ARG:CG | 0.54 | 2.14 | 8 | 4 |
| 1:A:45:TYR:HD2 | 1:A:87:ILE:CD1 | 0.54 | 2.14 | 17 | 1 |
| 1:A:14:LYS:CE | 1:A:38:ASP:HB2 | 0.54 | 2.33 | 20 | 1 |
| 1:A:6:LEU:HA | 1:A:9:TYR:CD1 | 0.54 | 2.37 | 14 | 1 |
| 1:A:94:HIS:CD2 | 1:A:101:LEU:CD1 | 0.54 | 2.90 | 8 | 2 |
| 1:A:81:LYS:HD2 | 1:A:93:TYR:OH | 0.54 | 2.02 | 12 | 1 |
| 1:A:93:TYR:HE2 | 1:A:94:HIS:NE2 | 0.54 | 2.00 | 14 | 1 |
| 1:A:97:ASN:O | 1:A:104:ARG:HB2 | 0.54 | 2.03 | 5 | 2 |
| 1:A:69:THR:O | 1:A:75:ARG:HG2 | 0.54 | 2.02 | 17 | 1 |
| 1:A:49:VAL:HG22 | 1:A:62:LYS:O | 0.54 | 2.02 | 3 | 4 |
| 1:A:18:ARG:C | 1:A:18:ARG:HD3 | 0.54 | 2.23 | 14 | 1 |
| 1:A:98:GLY:HA2 | 1:A:104:ARG:HB2 | 0.54 | 1.79 | 4 | 5 |
| 1:A:49:VAL:CG2 | 1:A:49:VAL:O | 0.54 | 2.55 | 20 | 5 |
| 1:A:62:LYS:HD3 | 1:A:64:TYR:OH | 0.54 | 2.02 | 7 | 5 |
| 1:A:34:PHE:C | 1:A:108:PRO:HA | 0.54 | 2.23 | 6 | 8 |
| 1:A:24:LEU:O | 1:A:28:THR:HB | 0.54 | 2.02 | 6 | 2 |
| 1:A:98:GLY:O | 1:A:104:ARG:HD3 | 0.54 | 2.02 | 17 | 1 |
| 1:A:85:ASP:O | 1:A:86:SER:CB | 0.54 | 2.55 | 3 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:50:PHE:HB2 | 1:A:61:ILE:HG23 | 0.54 | 1.75 | 14 | 1 |
| 1:A:78:VAL:HG23 | 1:A:79:ALA:N | 0.54 | 2.16 | 10 | 4 |
| 1:A:98:GLY:HA2 | 1:A:104:ARG:HD3 | 0.54 | 1.79 | 10 | 5 |
| 1:A:13:ASN:CB | 1:A:16:ILE:HB | 0.54 | 2.30 | 3 | 7 |
| 1:A:86:SER:HB3 | 1:A:88:PRO:HD2 | 0.54 | 1.79 | 20 | 3 |
| 1:A:22:GLU:CG | 1:A:63:HIS:HE2 | 0.54 | 2.10 | 11 | 1 |
| 1:A:14:LYS:C | 1:A:16:ILE:N | 0.54 | 2.62 | 17 | 15 |
| 1:A:101:LEU:HD12 | 1:A:104:ARG:HA | 0.54 | 1.78 | 19 | 1 |
| 1:A:81:LYS:HB2 | 1:A:82:TYR:CD1 | 0.54 | 2.37 | 2 | 3 |
| 1:A:28:THR:HB | 1:A:30:LYS:NZ | 0.54 | 2.17 | 1 | 1 |
| 1:A:101:LEU:C | 1:A:103:THR:N | 0.54 | 2.60 | 3 | 10 |
| 1:A:12:TYR:OH | 1:A:38:ASP:HB2 | 0.54 | 2.02 | 17 | 5 |
| 1:A:74:LYS:HB3 | 1:A:84:PHE:HA | 0.54 | 1.79 | 8 | 1 |
| 1:A:34:PHE:HZ | 1:A:91:ILE:HD12 | 0.54 | 1.51 | 2 | 1 |
| 1:A:10:GLU:OE2 | 1:A:107:TYR:CE2 | 0.54 | 2.61 | 17 | 2 |
| 1:A:44:THR:HA | 1:A:68:GLU:OE2 | 0.54 | 2.03 | 20 | 1 |
| 1:A:21:ALA:O | 1:A:25:LEU:CD2 | 0.54 | 2.56 | 12 | 2 |
| 1:A:92:GLN:NE2 | 1:A:95:GLN:CD | 0.54 | 2.61 | 7 | 1 |
| 1:A:84:PHE:HE2 | 1:A:93:TYR:CE1 | 0.54 | 2.13 | 4 | 1 |
| 1:A:103:THR:O | 1:A:106:ARG:HB2 | 0.54 | 2.02 | 15 | 1 |
| 1:A:93:TYR:CE1 | 1:A:97:ASN:ND2 | 0.54 | 2.76 | 3 | 1 |
| 1:A:13:ASN:O | 1:A:37:ARG:HA | 0.53 | 2.04 | 6 | 3 |
| 1:A:69:THR:CG2 | 1:A:83:VAL:HG21 | 0.53 | 2.33 | 12 | 1 |
| 1:A:9:TYR:C | 1:A:11:TRP:N | 0.53 | 2.60 | 5 | 18 |
| 1:A:90:LEU:O | 1:A:93:TYR:HD2 | 0.53 | 1.86 | 14 | 5 |
| 1:A:45:TYR:CD1 | 1:A:45:TYR:N | 0.53 | 2.77 | 6 | 6 |
| 1:A:11:TRP:CD2 | 1:A:34:PHE:HE2 | 0.53 | 2.17 | 4 | 6 |
| 1:A:86:SER:HG | 1:A:88:PRO:HG2 | 0.53 | 1.61 | 6 | 1 |
| 1:A:25:LEU:HD12 | 1:A:109:VAL:HG21 | 0.53 | 1.72 | 12 | 1 |
| 1:A:25:LEU:CD2 | 1:A:109:VAL:HG23 | 0.53 | 2.32 | 5 | 1 |
| 1:A:37:ARG:HD3 | 1:A:46:THR:HB | 0.53 | 1.80 | 17 | 7 |
| 1:A:37:ARG:HG2 | 1:A:46:THR:OG1 | 0.53 | 2.04 | 11 | 12 |
| 1:A:67:LYS:HE3 | 1:A:67:LYS:CA | 0.53 | 2.34 | 7 | 1 |
| 1:A:66:ILE:CB | 1:A:87:ILE:HD11 | 0.53 | 2.33 | 2 | 4 |
| 1:A:52:LYS:O | 1:A:52:LYS:HD2 | 0.53 | 2.03 | 18 | 2 |
| 1:A:82:TYR:CE2 | 1:A:93:TYR:HE1 | 0.53 | 2.22 | 2 | 1 |
| 1:A:82:TYR:CD2 | 1:A:93:TYR:CZ | 0.53 | 2.97 | 2 | 2 |
| 1:A:24:LEU:CD1 | 1:A:25:LEU:HG | 0.53 | 2.33 | 13 | 1 |
| 1:A:39:SER:C | 1:A:40:ARG:HG2 | 0.53 | 2.23 | 1 | 1 |
| 1:A:104:ARG:HD2 | 1:A:104:ARG:O | 0.53 | 2.04 | 10 | 3 |
| 1:A:81:LYS:HE3 | 1:A:99:GLY:O | 0.53 | 2.03 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:28:THR:HG23 | 1:A:29:GLY:N | 0.53 | 2.17 | 12 | 4 |
| 1:A:69:THR:HG23 | 1:A:69:THR:O | 0.53 | 2.02 | 8 | 1 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:CB | 0.53 | 2.33 | 18 | 2 |
| 1:A:22:GLU:HA | 1:A:61:ILE:HG12 | 0.53 | 1.80 | 18 | 2 |
| 1:A:94:HIS:C | 1:A:104:ARG:HB2 | 0.53 | 2.23 | 17 | 1 |
| 1:A:26:LEU:HA | 1:A:50:PHE:CZ | 0.53 | 2.39 | 3 | 2 |
| 1:A:106:ARG:O | 1:A:106:ARG:HD2 | 0.53 | 2.03 | 1 | 2 |
| 1:A:69:THR:H | 1:A:75:ARG:C | 0.53 | 2.07 | 4 | 4 |
| 1:A:23:LYS:C | 1:A:23:LYS:HD2 | 0.53 | 2.24 | 19 | 1 |
| 1:A:37:ARG:HH11 | 1:A:37:ARG:HG2 | 0.53 | 1.64 | 8 | 3 |
| 1:A:101:LEU:HD12 | 1:A:101:LEU:N | 0.53 | 2.16 | 18 | 3 |
| 1:A:24:LEU:HB2 | 1:A:111:GLY:HA3 | 0.53 | 1.80 | 14 | 4 |
| 1:A:20:LYS:HB3 | 1:A:23:LYS:HE2 | 0.53 | 1.79 | 3 | 4 |
| 1:A:6:LEU:HD13 | 1:A:87:ILE:HG21 | 0.53 | 1.78 | 1 | 2 |
| 1:A:82:TYR:OH | 1:A:99:GLY:HA2 | 0.53 | 2.04 | 4 | 2 |
| 1:A:81:LYS:HD2 | 1:A:82:TYR:HE1 | 0.53 | 1.59 | 13 | 1 |
| 1:A:39:SER:C | 1:A:41:THR:N | 0.53 | 2.61 | 5 | 2 |
| 1:A:11:TRP:C | 1:A:35:MET:HA | 0.53 | 2.24 | 17 | 8 |
| 1:A:86:SER:HB3 | 1:A:89:LEU:HG | 0.53 | 1.81 | 17 | 1 |
| 1:A:13:ASN:HD22 | 1:A:35:MET:CG | 0.53 | 2.16 | 14 | 3 |
| 1:A:84:PHE:CD1 | 1:A:90:LEU:CA | 0.53 | 2.90 | 15 | 6 |
| 1:A:20:LYS:HD3 | 1:A:23:LYS:CE | 0.53 | 2.33 | 18 | 1 |
| 1:A:93:TYR:O | 1:A:97:ASN:C | 0.53 | 2.47 | 4 | 1 |
| 1:A:74:LYS:CB | 1:A:83:VAL:O | 0.53 | 2.57 | 12 | 1 |
| 1:A:10:GLU:OE2 | 1:A:108:PRO:HG2 | 0.53 | 2.03 | 10 | 1 |
| 1:A:91:ILE:CG2 | 1:A:105:LEU:CD2 | 0.53 | 2.86 | 8 | 11 |
| 1:A:81:LYS:NZ | 1:A:99:GLY:HA2 | 0.53 | 2.19 | 1 | 3 |
| 1:A:22:GLU:OE1 | 1:A:61:ILE:HB | 0.53 | 2.04 | 2 | 1 |
| 1:A:91:ILE:CG2 | 1:A:105:LEU:HD12 | 0.53 | 2.31 | 4 | 1 |
| 1:A:37:ARG:HE | 1:A:46:THR:HG21 | 0.53 | 1.63 | 20 | 1 |
| 1:A:86:SER:H | 1:A:89:LEU:CD1 | 0.53 | 2.17 | 13 | 9 |
| 1:A:75:ARG:HB3 | 1:A:76:TYR:CE1 | 0.53 | 2.39 | 11 | 7 |
| 1:A:68:GLU:CD | 1:A:76:TYR:CZ | 0.53 | 2.82 | 3 | 2 |
| 1:A:7:GLU:HB3 | 1:A:14:LYS:HE2 | 0.53 | 1.81 | 7 | 1 |
| 1:A:81:LYS:CE | 1:A:94:HIS:HE1 | 0.53 | 2.16 | 12 | 2 |
| 1:A:103:THR:OG1 | 1:A:106:ARG:HD2 | 0.53 | 2.04 | 6 | 2 |
| 1:A:10:GLU:CD | 1:A:108:PRO:HG2 | 0.53 | 2.25 | 20 | 3 |
| 1:A:66:ILE:CD1 | 1:A:66:ILE:H | 0.53 | 2.15 | 12 | 4 |
| 1:A:104:ARG:HD2 | 1:A:104:ARG:C | 0.53 | 2.24 | 12 | 2 |
| 1:A:86:SER:HB3 | 1:A:89:LEU:CG | 0.53 | 2.34 | 17 | 1 |
| 1:A:92:GLN:HA | 1:A:95:GLN:HB2 | 0.53 | 1.82 | 17 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:32:GLY:O | 1:A:106:ARG:HB2 | 0.53 | 2.04 | 13 | 1 |
| 1:A:13:ASN:HD22 | 1:A:35:MET:HG3 | 0.52 | 1.63 | 3 | 3 |
| 1:A:95:GLN:CD | 1:A:108:PRO:HD3 | 0.52 | 2.24 | 20 | 1 |
| 1:A:52:LYS:HG2 | 1:A:52:LYS:O | 0.52 | 2.04 | 20 | 1 |
| 1:A:95:GLN:HE22 | 1:A:108:PRO:HD3 | 0.52 | 1.65 | 14 | 2 |
| 1:A:53:ALA:O | 1:A:60:CYS:HB2 | 0.52 | 2.05 | 11 | 1 |
| 1:A:81:LYS:HD3 | 1:A:93:TYR:HH | 0.52 | 1.63 | 11 | 1 |
| 1:A:35:MET:CG | 1:A:48:SER:HG | 0.52 | 2.16 | 9 | 2 |
| 1:A:12:TYR:C | 1:A:13:ASN:ND2 | 0.52 | 2.62 | 7 | 1 |
| 1:A:74:LYS:CB | 1:A:83:VAL:C | 0.52 | 2.78 | 8 | 1 |
| 1:A:21:ALA:HB1 | 1:A:48:SER:OG | 0.52 | 2.03 | 15 | 4 |
| 1:A:94:HIS:CD2 | 1:A:99:GLY:HA2 | 0.52 | 2.38 | 17 | 1 |
| 1:A:79:ALA:HB3 | 1:A:81:LYS:HE3 | 0.52 | 1.81 | 4 | 1 |
| 1:A:64:TYR:HE2 | 1:A:101:LEU:CG | 0.52 | 2.16 | 15 | 2 |
| 1:A:11:TRP:HB2 | 1:A:34:PHE:CD2 | 0.52 | 2.35 | 20 | 6 |
| 1:A:82:TYR:CD2 | 1:A:93:TYR:HE2 | 0.52 | 2.22 | 19 | 2 |
| 1:A:87:ILE:HG23 | 1:A:91:ILE:HG13 | 0.52 | 1.80 | 2 | 1 |
| 1:A:89:LEU:O | 1:A:92:GLN:HG2 | 0.52 | 2.05 | 17 | 1 |
| 1:A:10:GLU:HG3 | 1:A:108:PRO:O | 0.52 | 2.03 | 14 | 1 |
| 1:A:18:ARG:CG | 1:A:19:ASP:N | 0.52 | 2.71 | 16 | 1 |
| 1:A:45:TYR:HB2 | 1:A:66:ILE:HG12 | 0.52 | 1.80 | 8 | 2 |
| 1:A:103:THR:OG1 | 1:A:104:ARG:N | 0.52 | 2.43 | 7 | 1 |
| 1:A:74:LYS:HG2 | 1:A:83:VAL:CG2 | 0.52 | 2.30 | 8 | 1 |
| 1:A:99:GLY:O | 1:A:104:ARG:HB3 | 0.52 | 2.05 | 8 | 2 |
| 1:A:24:LEU:HD12 | 1:A:25:LEU:HG | 0.52 | 1.82 | 13 | 2 |
| 1:A:28:THR:OG1 | 1:A:30:LYS:HD2 | 0.52 | 2.04 | 4 | 1 |
| 1:A:29:GLY:CA | 1:A:50:PHE:HZ | 0.52 | 2.18 | 13 | 4 |
| 1:A:26:LEU:N | 1:A:61:ILE:HD11 | 0.52 | 2.19 | 15 | 2 |
| 1:A:96:TYR:O | 1:A:104:ARG:HD2 | 0.52 | 2.05 | 14 | 1 |
| 1:A:25:LEU:HD21 | 1:A:35:MET:HB2 | 0.52 | 1.80 | 5 | 1 |
| 1:A:7:GLU:CB | 1:A:14:LYS:CD | 0.52 | 2.87 | 1 | 1 |
| 1:A:98:GLY:CA | 1:A:104:ARG:HD3 | 0.52 | 2.34 | 10 | 1 |
| 1:A:24:LEU:O | 1:A:27:ASP:OD1 | 0.52 | 2.27 | 10 | 1 |
| 1:A:11:TRP:CE3 | 1:A:34:PHE:CZ | 0.52 | 2.98 | 15 | 4 |
| 1:A:65:HIS:O | 1:A:78:VAL:HA | 0.52 | 2.04 | 3 | 2 |
| 1:A:25:LEU:HD22 | 1:A:109:VAL:HG11 | 0.52 | 1.82 | 19 | 1 |
| 1:A:74:LYS:CE | 1:A:83:VAL:H | 0.52 | 2.18 | 7 | 1 |
| 1:A:69:THR:O | 1:A:69:THR:OG1 | 0.52 | 2.28 | 18 | 2 |
| 1:A:94:HIS:CD2 | 1:A:99:GLY:H | 0.52 | 2.22 | 20 | 1 |
| 1:A:93:TYR:CA | 1:A:97:ASN:ND2 | 0.52 | 2.72 | 1 | 1 |
| 1:A:51:THR:O | 1:A:51:THR:CG2 | 0.52 | 2.58 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:40:ARG:O | 1:A:41:THR:C | 0.52 | 2.48 | 10 | 2 |
| 1:A:37:ARG:CD | 1:A:46:THR:HG21 | 0.52 | 2.34 | 12 | 8 |
| 1:A:31:GLU:HG3 | 1:A:51:THR:HG23 | 0.52 | 1.79 | 7 | 2 |
| 1:A:94:HIS:HA | 1:A:98:GLY:O | 0.52 | 2.04 | 4 | 1 |
| 1:A:31:GLU:HG2 | 1:A:106:ARG:HD3 | 0.52 | 1.82 | 12 | 1 |
| 1:A:102:VAL:C | 1:A:103:THR:HG23 | 0.52 | 2.25 | 10 | 2 |
| 1:A:62:LYS:HB2 | 1:A:102:VAL:HG11 | 0.52 | 1.82 | 8 | 5 |
| 1:A:25:LEU:HD12 | 1:A:50:PHE:CB | 0.52 | 2.33 | 19 | 1 |
| 1:A:7:GLU:O | 1:A:8:THR:CB | 0.52 | 2.58 | 14 | 2 |
| 1:A:31:GLU:HG2 | 1:A:31:GLU:O | 0.52 | 2.02 | 1 | 2 |
| 1:A:65:HIS:N | 1:A:78:VAL:HG22 | 0.52 | 2.19 | 3 | 2 |
| 1:A:24:LEU:O | 1:A:27:ASP:HB3 | 0.52 | 2.05 | 2 | 1 |
| 1:A:24:LEU:HB3 | 1:A:111:GLY:CA | 0.52 | 2.35 | 6 | 1 |
| 1:A:67:LYS:HG3 | 1:A:68:GLU:N | 0.52 | 2.19 | 15 | 1 |
| 1:A:7:GLU:CA | 1:A:12:TYR:CE2 | 0.52 | 2.93 | 20 | 1 |
| 1:A:52:LYS:CG | 1:A:52:LYS:O | 0.52 | 2.58 | 20 | 1 |
| 1:A:75:ARG:HD3 | 1:A:76:TYR:CE1 | 0.52 | 2.40 | 10 | 1 |
| 1:A:18:ARG:O | 1:A:22:GLU:HG3 | 0.52 | 2.04 | 13 | 5 |
| 1:A:10:GLU:HG2 | 1:A:108:PRO:CG | 0.52 | 2.35 | 4 | 3 |
| 1:A:95:GLN:OE1 | 1:A:105:LEU:HB3 | 0.52 | 2.05 | 18 | 1 |
| 1:A:67:LYS:HA | 1:A:67:LYS:HE2 | 0.52 | 1.82 | 15 | 3 |
| 1:A:93:TYR:CE1 | 1:A:94:HIS:ND1 | 0.52 | 2.78 | 4 | 1 |
| 1:A:6:LEU:HB2 | 1:A:12:TYR:CE1 | 0.52 | 2.40 | 12 | 2 |
| 1:A:18:ARG:HG3 | 1:A:19:ASP:N | 0.52 | 2.18 | 15 | 2 |
| 1:A:83:VAL:O | 1:A:84:PHE:CG | 0.52 | 2.63 | 14 | 2 |
| 1:A:50:PHE:HB2 | 1:A:61:ILE:HG13 | 0.52 | 1.80 | 18 | 2 |
| 1:A:31:GLU:O | 1:A:31:GLU:HG2 | 0.52 | 2.05 | 10 | 1 |
| 1:A:67:LYS:CA | 1:A:67:LYS:HE2 | 0.52 | 2.34 | 2 | 1 |
| 1:A:32:GLY:HA2 | 1:A:103:THR:OG1 | 0.51 | 2.03 | 10 | 1 |
| 1:A:13:ASN:HD21 | 1:A:35:MET:HE1 | 0.51 | 1.65 | 10 | 2 |
| 1:A:16:ILE:CG2 | 1:A:17:SER:N | 0.51 | 2.72 | 11 | 8 |
| 1:A:22:GLU:HG2 | 1:A:63:HIS:CE1 | 0.51 | 2.40 | 11 | 1 |
| 1:A:50:PHE:CB | 1:A:61:ILE:HD12 | 0.51 | 2.35 | 7 | 4 |
| 1:A:74:LYS:HE3 | 1:A:83:VAL:C | 0.51 | 2.25 | 7 | 1 |
| 1:A:86:SER:H | 1:A:89:LEU:HD13 | 0.51 | 1.64 | 13 | 5 |
| 1:A:18:ARG:HB2 | 1:A:63:HIS:NE2 | 0.51 | 2.20 | 18 | 1 |
| 1:A:67:LYS:CA | 1:A:67:LYS:CE | 0.51 | 2.87 | 18 | 1 |
| 1:A:74:LYS:C | 1:A:83:VAL:CG1 | 0.51 | 2.79 | 17 | 1 |
| 1:A:30:LYS:N | 1:A:52:LYS:HD3 | 0.51 | 2.20 | 6 | 1 |
| 1:A:94:HIS:O | 1:A:98:GLY:HA2 | 0.51 | 2.04 | 4 | 1 |
| 1:A:31:GLU:CG | 1:A:106:ARG:CD | 0.51 | 2.87 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:GLU:CG | 1:A:76:TYR:CE1 | 0.51 | 2.93 | 17 | 8 |
| 1:A:67:LYS:HE3 | 1:A:67:LYS:HA | 0.51 | 1.82 | 7 | 3 |
| 1:A:28:THR:HG21 | 1:A:109:VAL:HB | 0.51 | 1.83 | 18 | 1 |
| 1:A:19:ASP:O | 1:A:23:LYS:HE2 | 0.51 | 2.02 | 2 | 1 |
| 1:A:101:LEU:CD1 | 1:A:101:LEU:H | 0.51 | 2.18 | 6 | 1 |
| 1:A:82:TYR:HB3 | 1:A:84:PHE:CZ | 0.51 | 2.40 | 7 | 3 |
| 1:A:22:GLU:OE2 | 1:A:61:ILE:HB | 0.51 | 2.05 | 4 | 3 |
| 1:A:49:VAL:CG2 | 1:A:64:TYR:CD1 | 0.51 | 2.94 | 15 | 5 |
| 1:A:34:PHE:CZ | 1:A:105:LEU:CD1 | 0.51 | 2.92 | 20 | 3 |
| 1:A:46:THR:OG1 | 1:A:65:HIS:CE1 | 0.51 | 2.64 | 9 | 4 |
| 1:A:20:LYS:CA | 1:A:23:LYS:HG2 | 0.51 | 2.35 | 9 | 8 |
| 1:A:25:LEU:HD22 | 1:A:50:PHE:CD1 | 0.51 | 2.40 | 16 | 1 |
| 1:A:17:SER:HB2 | 1:A:20:LYS:HE3 | 0.51 | 1.81 | 5 | 5 |
| 1:A:17:SER:CB | 1:A:20:LYS:HZ2 | 0.51 | 2.17 | 2 | 1 |
| 1:A:37:ARG:HG3 | 1:A:37:ARG:HH11 | 0.51 | 1.66 | 15 | 3 |
| 1:A:94:HIS:CG | 1:A:101:LEU:CD2 | 0.51 | 2.93 | 17 | 2 |
| 1:A:25:LEU:HD13 | 1:A:50:PHE:HB3 | 0.51 | 1.81 | 6 | 1 |
| 1:A:66:ILE:HA | 1:A:77:TYR:O | 0.51 | 2.05 | 13 | 1 |
| 1:A:85:ASP:H | 1:A:89:LEU:CD1 | 0.51 | 2.16 | 1 | 1 |
| 1:A:102:VAL:C | 1:A:103:THR:CG2 | 0.51 | 2.79 | 7 | 5 |
| 1:A:25:LEU:HD12 | 1:A:50:PHE:CG | 0.51 | 2.37 | 19 | 1 |
| 1:A:64:TYR:OH | 1:A:102:VAL:CG1 | 0.51 | 2.59 | 19 | 2 |
| 1:A:75:ARG:NH1 | 1:A:76:TYR:CE1 | 0.51 | 2.79 | 19 | 1 |
| 1:A:66:ILE:HG13 | 1:A:87:ILE:HD11 | 0.51 | 1.81 | 13 | 5 |
| 1:A:30:LYS:HE2 | 1:A:107:TYR:CE2 | 0.51 | 2.39 | 8 | 1 |
| 1:A:52:LYS:O | 1:A:52:LYS:HG3 | 0.51 | 2.05 | 18 | 1 |
| 1:A:6:LEU:C | 1:A:8:THR:H | 0.51 | 2.07 | 6 | 7 |
| 1:A:81:LYS:HG3 | 1:A:82:TYR:HD1 | 0.51 | 1.64 | 2 | 1 |
| 1:A:91:ILE:O | 1:A:105:LEU:CG | 0.51 | 2.58 | 17 | 1 |
| 1:A:35:MET:HB2 | 1:A:109:VAL:O | 0.51 | 2.06 | 1 | 1 |
| 1:A:95:GLN:HG2 | 1:A:105:LEU:CG | 0.51 | 2.36 | 9 | 3 |
| 1:A:49:VAL:N | 1:A:62:LYS:O | 0.51 | 2.38 | 18 | 4 |
| 1:A:25:LEU:CG | 1:A:109:VAL:CG1 | 0.51 | 2.88 | 20 | 3 |
| 1:A:86:SER:CA | 1:A:89:LEU:HD11 | 0.51 | 2.34 | 5 | 2 |
| 1:A:16:ILE:HD13 | 1:A:21:ALA:CB | 0.51 | 2.33 | 9 | 2 |
| 1:A:82:TYR:CD2 | 1:A:93:TYR:CD1 | 0.51 | 2.99 | 9 | 1 |
| 1:A:32:GLY:H | 1:A:51:THR:CB | 0.51 | 2.17 | 2 | 3 |
| 1:A:32:GLY:O | 1:A:33:ALA:C | 0.51 | 2.49 | 5 | 5 |
| 1:A:25:LEU:CD1 | 1:A:61:ILE:HG23 | 0.51 | 2.36 | 6 | 1 |
| 1:A:28:THR:CG2 | 1:A:109:VAL:HG12 | 0.51 | 2.26 | 4 | 1 |
| 1:A:40:ARG:HG3 | 1:A:41:THR:N | 0.51 | 2.21 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:41:THR:C | 1:A:43:GLY:N | 0.51 | 2.63 | 4 | 20 |
| 1:A:22:GLU:HG2 | 1:A:61:ILE:HG21 | 0.51 | 1.83 | 8 | 2 |
| 1:A:82:TYR:CE1 | 1:A:93:TYR:CZ | 0.51 | 2.95 | 8 | 2 |
| 1:A:86:SER:C | 1:A:89:LEU:CD1 | 0.51 | 2.79 | 5 | 5 |
| 1:A:32:GLY:HA2 | 1:A:103:THR:HG23 | 0.51 | 1.81 | 5 | 3 |
| 1:A:20:LYS:CB | 1:A:23:LYS:HE2 | 0.51 | 2.36 | 3 | 3 |
| 1:A:67:LYS:HA | 1:A:67:LYS:CE | 0.51 | 2.36 | 15 | 1 |
| 1:A:18:ARG:N | 1:A:37:ARG:NH1 | 0.51 | 2.59 | 5 | 1 |
| 1:A:7:GLU:HG2 | 1:A:14:LYS:HD3 | 0.51 | 1.82 | 5 | 1 |
| 1:A:45:TYR:CG | 1:A:87:ILE:CG1 | 0.51 | 2.92 | 8 | 4 |
| 1:A:74:LYS:N | 1:A:83:VAL:HG23 | 0.51 | 2.21 | 6 | 1 |
| 1:A:24:LEU:HB2 | 1:A:111:GLY:O | 0.51 | 2.06 | 15 | 1 |
| 1:A:74:LYS:H | 1:A:83:VAL:CG2 | 0.51 | 2.18 | 14 | 1 |
| 1:A:49:VAL:HG22 | 1:A:62:LYS:CB | 0.50 | 2.36 | 9 | 1 |
| 1:A:53:ALA:HB3 | 1:A:60:CYS:HG | 0.50 | 1.65 | 19 | 1 |
| 1:A:104:ARG:NH2 | 1:A:106:ARG:CD | 0.50 | 2.75 | 10 | 1 |
| 1:A:14:LYS:CG | 1:A:15:SER:H | 0.50 | 2.18 | 19 | 5 |
| 1:A:35:MET:CG | 1:A:36:VAL:N | 0.50 | 2.73 | 5 | 11 |
| 1:A:81:LYS:HB3 | 1:A:81:LYS:HZ3 | 0.50 | 1.67 | 11 | 1 |
| 1:A:53:ALA:HB3 | 1:A:60:CYS:HB2 | 0.50 | 1.82 | 20 | 2 |
| 1:A:69:THR:H | 1:A:75:ARG:CA | 0.50 | 2.19 | 6 | 1 |
| 1:A:18:ARG:HD3 | 1:A:19:ASP:OD1 | 0.50 | 2.05 | 10 | 1 |
| 1:A:75:ARG:N | 1:A:83:VAL:HG23 | 0.50 | 2.22 | 13 | 2 |
| 1:A:86:SER:HB3 | 1:A:89:LEU:CD1 | 0.50 | 2.36 | 20 | 1 |
| 1:A:10:GLU:HA | 1:A:110:CYS:CB | 0.50 | 2.36 | 10 | 5 |
| 1:A:35:MET:C | 1:A:48:SER:H | 0.50 | 2.10 | 12 | 11 |
| 1:A:86:SER:C | 1:A:88:PRO:HD2 | 0.50 | 2.26 | 7 | 6 |
| 1:A:31:GLU:OE2 | 1:A:51:THR:HG23 | 0.50 | 2.07 | 7 | 1 |
| 1:A:64:TYR:CG | 1:A:101:LEU:HG | 0.50 | 2.40 | 7 | 1 |
| 1:A:25:LEU:HG | 1:A:50:PHE:HB3 | 0.50 | 1.82 | 18 | 1 |
| 1:A:69:THR:CG2 | 1:A:75:ARG:HA | 0.50 | 2.36 | 2 | 1 |
| 1:A:75:ARG:HG2 | 1:A:85:ASP:HA | 0.50 | 1.82 | 2 | 1 |
| 1:A:94:HIS:NE2 | 1:A:99:GLY:C | 0.50 | 2.65 | 16 | 1 |
| 1:A:25:LEU:HD13 | 1:A:109:VAL:CG2 | 0.50 | 2.25 | 18 | 1 |
| 1:A:20:LYS:C | 1:A:20:LYS:CD | 0.50 | 2.79 | 12 | 2 |
| 1:A:81:LYS:CG | 1:A:82:TYR:HD1 | 0.50 | 2.18 | 2 | 1 |
| 1:A:13:ASN:HB2 | 1:A:16:ILE:HD12 | 0.50 | 1.82 | 13 | 1 |
| 1:A:36:VAL:HA | 1:A:47:VAL:HA | 0.50 | 1.84 | 10 | 18 |
| 1:A:11:TRP:HD1 | 1:A:108:PRO:CB | 0.50 | 2.20 | 8 | 15 |
| 1:A:52:LYS:HD2 | 1:A:52:LYS:N | 0.50 | 2.22 | 11 | 1 |
| 1:A:77:TYR:HE2 | 1:A:80:GLU:CA | 0.50 | 2.18 | 8 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:74:LYS:HG2 | 1:A:85:ASP:HB2 | 0.50 | 1.83 | 6 | 1 |
| 1:A:6:LEU:O | 1:A:9:TYR:N | 0.50 | 2.37 | 12 | 1 |
| 1:A:68:GLU:OE1 | 1:A:76:TYR:HA | 0.50 | 2.05 | 20 | 1 |
| 1:A:74:LYS:H | 1:A:83:VAL:HG21 | 0.50 | 1.66 | 14 | 1 |
| 1:A:93:TYR:CE1 | 1:A:97:ASN:OD1 | 0.50 | 2.64 | 14 | 1 |
| 1:A:25:LEU:HD12 | 1:A:50:PHE:HB3 | 0.50 | 1.84 | 19 | 1 |
| 1:A:20:LYS:HA | 1:A:23:LYS:HE2 | 0.50 | 1.83 | 15 | 2 |
| 1:A:79:ALA:CB | 1:A:81:LYS:CG | 0.50 | 2.89 | 6 | 3 |
| 1:A:49:VAL:CB | 1:A:102:VAL:HG12 | 0.50 | 2.36 | 13 | 1 |
| 1:A:30:LYS:HZ2 | 1:A:109:VAL:HG13 | 0.50 | 1.65 | 12 | 1 |
| 1:A:22:GLU:O | 1:A:26:LEU:HB2 | 0.50 | 2.07 | 20 | 2 |
| 1:A:94:HIS:O | 1:A:104:ARG:O | 0.50 | 2.29 | 15 | 2 |
| 1:A:33:ALA:O | 1:A:50:PHE:N | 0.50 | 2.44 | 3 | 12 |
| 1:A:106:ARG:HD3 | 1:A:106:ARG:C | 0.50 | 2.27 | 18 | 2 |
| 1:A:101:LEU:H | 1:A:101:LEU:HD13 | 0.50 | 1.67 | 5 | 2 |
| 1:A:10:GLU:HG3 | 1:A:108:PRO:HB2 | 0.50 | 1.84 | 20 | 1 |
| 1:A:14:LYS:HG2 | 1:A:38:ASP:HB3 | 0.50 | 1.83 | 20 | 1 |
| 1:A:23:LYS:O | 1:A:27:ASP:OD1 | 0.50 | 2.30 | 14 | 1 |
| 1:A:81:LYS:HE3 | 1:A:99:GLY:HA2 | 0.50 | 1.84 | 16 | 1 |
| 1:A:6:LEU:CD1 | 1:A:12:TYR:CE1 | 0.50 | 2.89 | 10 | 8 |
| 1:A:12:TYR:C | 1:A:13:ASN:OD1 | 0.50 | 2.49 | 11 | 1 |
| 1:A:31:GLU:OE2 | 1:A:106:ARG:HG3 | 0.50 | 2.07 | 18 | 1 |
| 1:A:81:LYS:HB2 | 1:A:82:TYR:CE1 | 0.50 | 2.42 | 2 | 1 |
| 1:A:86:SER:CB | 1:A:89:LEU:HG | 0.50 | 2.36 | 17 | 1 |
| 1:A:81:LYS:CG | 1:A:82:TYR:H | 0.50 | 2.17 | 13 | 1 |
| 1:A:77:TYR:HB3 | 1:A:83:VAL:HB | 0.50 | 1.83 | 12 | 1 |
| 1:A:24:LEU:CB | 1:A:111:GLY:HA3 | 0.50 | 2.37 | 14 | 1 |
| 1:A:7:GLU:OE2 | 1:A:14:LYS:HE2 | 0.50 | 2.07 | 5 | 1 |
| 1:A:81:LYS:HZ2 | 1:A:99:GLY:CA | 0.49 | 2.20 | 18 | 3 |
| 1:A:49:VAL:CG2 | 1:A:102:VAL:HG11 | 0.49 | 2.37 | 6 | 2 |
| 1:A:75:ARG:NH2 | 1:A:85:ASP:HB3 | 0.49 | 2.22 | 7 | 2 |
| 1:A:62:LYS:CB | 1:A:102:VAL:CG1 | 0.49 | 2.90 | 3 | 2 |
| 1:A:20:LYS:HD3 | 1:A:23:LYS:HE3 | 0.49 | 1.83 | 18 | 2 |
| 1:A:23:LYS:HE2 | 1:A:23:LYS:N | 0.49 | 2.17 | 2 | 1 |
| 1:A:84:PHE:CD1 | 1:A:90:LEU:HG | 0.49 | 2.43 | 6 | 2 |
| 1:A:7:GLU:O | 1:A:9:TYR:N | 0.49 | 2.44 | 12 | 1 |
| 1:A:16:ILE:CD1 | 1:A:21:ALA:HB2 | 0.49 | 2.37 | 3 | 2 |
| 1:A:92:GLN:N | 1:A:92:GLN:NE2 | 0.49 | 2.59 | 10 | 3 |
| 1:A:52:LYS:CD | 1:A:52:LYS:H | 0.49 | 2.19 | 11 | 1 |
| 1:A:17:SER:N | 1:A:20:LYS:CE | 0.49 | 2.75 | 3 | 4 |
| 1:A:98:GLY:HA2 | 1:A:104:ARG:HG2 | 0.49 | 1.83 | 1 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:37:ARG:CG | 1:A:37:ARG:NH1 | 0.49 | 2.73 | 8 | 2 |
| 1:A:20:LYS:HG2 | 1:A:23:LYS:HE2 | 0.49 | 1.84 | 18 | 1 |
| 1:A:81:LYS:NZ | 1:A:94:HIS:HE1 | 0.49 | 2.01 | 2 | 1 |
| 1:A:28:THR:HB | 1:A:30:LYS:HD2 | 0.49 | 1.83 | 4 | 1 |
| 1:A:67:LYS:HE2 | 1:A:67:LYS:CA | 0.49 | 2.37 | 13 | 2 |
| 1:A:93:TYR:C | 1:A:93:TYR:CD1 | 0.49 | 2.85 | 3 | 3 |
| 1:A:81:LYS:CE | 1:A:99:GLY:O | 0.49 | 2.60 | 5 | 1 |
| 1:A:18:ARG:HD3 | 1:A:19:ASP:CG | 0.49 | 2.27 | 10 | 1 |
| 1:A:49:VAL:HG22 | 1:A:64:TYR:CE1 | 0.49 | 2.42 | 10 | 2 |
| 1:A:47:VAL:CB | 1:A:64:TYR:O | 0.49 | 2.61 | 15 | 11 |
| 1:A:7:GLU:OE1 | 1:A:14:LYS:CD | 0.49 | 2.60 | 7 | 1 |
| 1:A:22:GLU:HG2 | 1:A:61:ILE:CB | 0.49 | 2.37 | 8 | 3 |
| 1:A:9:TYR:O | 1:A:12:TYR:N | 0.49 | 2.46 | 14 | 7 |
| 1:A:75:ARG:HD2 | 1:A:85:ASP:OD1 | 0.49 | 2.08 | 3 | 2 |
| 1:A:6:LEU:C | 1:A:7:GLU:HG3 | 0.49 | 2.27 | 5 | 1 |
| 1:A:16:ILE:HD11 | 1:A:21:ALA:HA | 0.49 | 1.83 | 9 | 2 |
| 1:A:34:PHE:CZ | 1:A:91:ILE:CG1 | 0.49 | 2.96 | 19 | 2 |
| 1:A:18:ARG:HA | 1:A:63:HIS:CD2 | 0.49 | 2.43 | 7 | 1 |
| 1:A:66:ILE:HB | 1:A:87:ILE:HD11 | 0.49 | 1.82 | 3 | 3 |
| 1:A:68:GLU:OE1 | 1:A:68:GLU:CA | 0.49 | 2.60 | 16 | 3 |
| 1:A:69:THR:O | 1:A:75:ARG:CB | 0.49 | 2.60 | 4 | 2 |
| 1:A:49:VAL:HG11 | 1:A:64:TYR:CE2 | 0.49 | 2.42 | 20 | 1 |
| 1:A:20:LYS:HD2 | 1:A:20:LYS:N | 0.49 | 2.22 | 5 | 1 |
| 1:A:75:ARG:NH2 | 1:A:85:ASP:CG | 0.49 | 2.65 | 1 | 1 |
| 1:A:98:GLY:C | 1:A:104:ARG:HG2 | 0.49 | 2.28 | 1 | 1 |
| 1:A:84:PHE:HE2 | 1:A:93:TYR:CE2 | 0.49 | 2.25 | 2 | 3 |
| 1:A:9:TYR:CD2 | 1:A:11:TRP:CE2 | 0.49 | 3.01 | 14 | 2 |
| 1:A:18:ARG:HA | 1:A:37:ARG:NH1 | 0.49 | 2.22 | 18 | 1 |
| 1:A:24:LEU:HB3 | 1:A:111:GLY:O | 0.49 | 2.06 | 2 | 1 |
| 1:A:94:HIS:CB | 1:A:105:LEU:HG | 0.49 | 2.37 | 14 | 2 |
| 1:A:105:LEU:H | 1:A:105:LEU:CD2 | 0.49 | 2.20 | 14 | 1 |
| 1:A:82:TYR:CB | 1:A:93:TYR:OH | 0.49 | 2.58 | 14 | 1 |
| 1:A:104:ARG:NH2 | 1:A:106:ARG:CZ | 0.49 | 2.75 | 10 | 1 |
| 1:A:78:VAL:CG2 | 1:A:94:HIS:HE1 | 0.49 | 2.20 | 20 | 4 |
| 1:A:79:ALA:C | 1:A:81:LYS:H | 0.49 | 2.11 | 11 | 11 |
| 1:A:31:GLU:OE1 | 1:A:31:GLU:N | 0.49 | 2.46 | 1 | 1 |
| 1:A:70:ASN:ND2 | 1:A:70:ASN:N | 0.49 | 2.61 | 16 | 1 |
| 1:A:82:TYR:CZ | 1:A:93:TYR:CE1 | 0.49 | 3.01 | 8 | 2 |
| 1:A:39:SER:OG | 1:A:41:THR:HB | 0.49 | 2.08 | 18 | 1 |
| 1:A:97:ASN:O | 1:A:98:GLY:C | 0.49 | 2.49 | 17 | 1 |
| 1:A:6:LEU:HD11 | 1:A:87:ILE:CG1 | 0.49 | 2.38 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:86:SER:HB3 | 1:A:88:PRO:HG2 | 0.49 | 1.84 | 13 | 5 |
| 1:A:87:ILE:HA | 1:A:90:LEU:HB3 | 0.49 | 1.84 | 20 | 3 |
| 1:A:28:THR:HG22 | 1:A:50:PHE:HE1 | 0.49 | 1.68 | 17 | 1 |
| 1:A:81:LYS:HE3 | 1:A:94:HIS:CE1 | 0.49 | 2.43 | 12 | 1 |
| 1:A:9:TYR:HB2 | 1:A:12:TYR:CB | 0.49 | 2.37 | 20 | 1 |
| 1:A:81:LYS:HB3 | 1:A:81:LYS:NZ | 0.49 | 2.23 | 11 | 1 |
| 1:A:16:ILE:HD11 | 1:A:24:LEU:HD22 | 0.49 | 1.84 | 17 | 3 |
| 1:A:16:ILE:HG22 | 1:A:37:ARG:HD2 | 0.49 | 1.83 | 13 | 3 |
| 1:A:25:LEU:CD2 | 1:A:50:PHE:CD1 | 0.49 | 2.90 | 8 | 2 |
| 1:A:38:ASP:OD1 | 1:A:40:ARG:HG2 | 0.49 | 2.08 | 18 | 1 |
| 1:A:6:LEU:CD2 | 1:A:45:TYR:CE2 | 0.49 | 2.87 | 17 | 1 |
| 1:A:17:SER:HB3 | 1:A:20:LYS:HE2 | 0.49 | 1.84 | 4 | 2 |
| 1:A:7:GLU:CA | 1:A:12:TYR:CD2 | 0.49 | 2.96 | 20 | 2 |
| 1:A:22:GLU:HA | 1:A:61:ILE:CG2 | 0.49 | 2.29 | 15 | 3 |
| 1:A:37:ARG:HG2 | 1:A:37:ARG:HH11 | 0.48 | 1.68 | 10 | 2 |
| 1:A:13:ASN:OD1 | 1:A:35:MET:CE | 0.48 | 2.61 | 9 | 2 |
| 1:A:46:THR:HA | 1:A:65:HIS:ND1 | 0.48 | 2.23 | 9 | 10 |
| 1:A:82:TYR:CZ | 1:A:99:GLY:HA2 | 0.48 | 2.43 | 2 | 1 |
| 1:A:86:SER:HG | 1:A:88:PRO:CG | 0.48 | 2.21 | 6 | 2 |
| 1:A:78:VAL:HG22 | 1:A:81:LYS:NZ | 0.48 | 2.22 | 13 | 1 |
| 1:A:18:ARG:HD3 | 1:A:63:HIS:CD2 | 0.48 | 2.43 | 15 | 1 |
| 1:A:41:THR:CG2 | 1:A:42:PRO:N | 0.48 | 2.76 | 2 | 4 |
| 1:A:76:TYR:CD2 | 1:A:87:ILE:HD12 | 0.48 | 2.44 | 17 | 2 |
| 1:A:52:LYS:HZ3 | 1:A:52:LYS:HB2 | 0.48 | 1.68 | 17 | 1 |
| 1:A:62:LYS:CB | 1:A:102:VAL:HG11 | 0.48 | 2.38 | 3 | 2 |
| 1:A:94:HIS:CE1 | 1:A:101:LEU:HD21 | 0.48 | 2.43 | 7 | 2 |
| 1:A:74:LYS:O | 1:A:83:VAL:CB | 0.48 | 2.62 | 6 | 1 |
| 1:A:25:LEU:CG | 1:A:50:PHE:CD1 | 0.48 | 2.96 | 12 | 1 |
| 1:A:53:ALA:CB | 1:A:60:CYS:HG | 0.48 | 2.21 | 19 | 1 |
| 1:A:9:TYR:CB | 1:A:11:TRP:CZ2 | 0.48 | 2.95 | 12 | 5 |
| 1:A:47:VAL:HG23 | 1:A:66:ILE:HD12 | 0.48 | 1.86 | 13 | 2 |
| 1:A:69:THR:N | 1:A:75:ARG:HD2 | 0.48 | 2.23 | 17 | 1 |
| 1:A:44:THR:C | 1:A:45:TYR:CD1 | 0.48 | 2.86 | 6 | 4 |
| 1:A:86:SER:CA | 1:A:89:LEU:HD12 | 0.48 | 2.38 | 12 | 2 |
| 1:A:7:GLU:C | 1:A:9:TYR:N | 0.48 | 2.66 | 12 | 1 |
| 1:A:23:LYS:O | 1:A:27:ASP:HB3 | 0.48 | 2.09 | 3 | 1 |
| 1:A:96:TYR:C | 1:A:98:GLY:N | 0.48 | 2.65 | 3 | 1 |
| 1:A:95:GLN:CA | 1:A:105:LEU:CB | 0.48 | 2.91 | 10 | 4 |
| 1:A:35:MET:HE3 | 1:A:109:VAL:HG23 | 0.48 | 1.86 | 10 | 2 |
| 1:A:21:ALA:HB3 | 1:A:48:SER:OG | 0.48 | 2.08 | 18 | 1 |
| 1:A:6:LEU:CA | 1:A:9:TYR:CE2 | 0.48 | 2.96 | 2 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:28:THR:CB | 1:A:109:VAL:HG21 | 0.48 | 2.38 | 17 | 1 |
| 1:A:29:GLY:O | 1:A:52:LYS:HD2 | 0.48 | 2.07 | 15 | 1 |
| 1:A:91:ILE:HG22 | 1:A:95:GLN:HG2 | 0.48 | 1.85 | 20 | 1 |
| 1:A:25:LEU:CB | 1:A:61:ILE:CG2 | 0.48 | 2.90 | 5 | 1 |
| 1:A:19:ASP:HB2 | 1:A:20:LYS:NZ | 0.48 | 2.23 | 10 | 1 |
| 1:A:66:ILE:HG22 | 1:A:76:TYR:CB | 0.48 | 2.30 | 19 | 2 |
| 1:A:87:ILE:CD1 | 1:A:87:ILE:N | 0.48 | 2.77 | 19 | 2 |
| 1:A:6:LEU:C | 1:A:8:THR:N | 0.48 | 2.64 | 7 | 9 |
| 1:A:25:LEU:HB3 | 1:A:61:ILE:HD12 | 0.48 | 1.84 | 2 | 1 |
| 1:A:78:VAL:HG21 | 1:A:101:LEU:HD21 | 0.48 | 1.85 | 17 | 2 |
| 1:A:91:ILE:C | 1:A:95:GLN:HG3 | 0.48 | 2.28 | 16 | 2 |
| 1:A:75:ARG:CD | 1:A:76:TYR:CE1 | 0.48 | 2.97 | 10 | 1 |
| 1:A:102:VAL:HG13 | 1:A:103:THR:N | 0.48 | 2.23 | 11 | 1 |
| 1:A:37:ARG:NE | 1:A:46:THR:HG21 | 0.48 | 2.22 | 20 | 1 |
| 1:A:22:GLU:OE1 | 1:A:22:GLU:CA | 0.48 | 2.62 | 14 | 1 |
| 1:A:9:TYR:HB3 | 1:A:11:TRP:CD2 | 0.48 | 2.43 | 14 | 4 |
| 1:A:37:ARG:HG3 | 1:A:37:ARG:NH1 | 0.48 | 2.24 | 15 | 2 |
| 1:A:39:SER:O | 1:A:41:THR:HB | 0.48 | 2.08 | 9 | 1 |
| 1:A:64:TYR:C | 1:A:78:VAL:CG2 | 0.48 | 2.82 | 8 | 1 |
| 1:A:84:PHE:CD1 | 1:A:90:LEU:CG | 0.48 | 2.96 | 6 | 2 |
| 1:A:81:LYS:HD2 | 1:A:82:TYR:CD1 | 0.48 | 2.40 | 12 | 1 |
| 1:A:94:HIS:CB | 1:A:105:LEU:CG | 0.48 | 2.92 | 14 | 1 |
| 1:A:6:LEU:CB | 1:A:9:TYR:HD2 | 0.48 | 2.22 | 6 | 6 |
| 1:A:24:LEU:CD2 | 1:A:111:GLY:CA | 0.48 | 2.87 | 1 | 1 |
| 1:A:102:VAL:CG1 | 1:A:103:THR:N | 0.48 | 2.77 | 10 | 2 |
| 1:A:104:ARG:NH2 | 1:A:106:ARG:HD2 | 0.48 | 2.23 | 10 | 1 |
| 1:A:49:VAL:CG2 | 1:A:64:TYR:HE1 | 0.48 | 2.19 | 8 | 1 |
| 1:A:74:LYS:HB3 | 1:A:84:PHE:CA | 0.48 | 2.39 | 8 | 1 |
| 1:A:103:THR:HB | 1:A:106:ARG:HB2 | 0.47 | 1.86 | 9 | 3 |
| 1:A:82:TYR:CZ | 1:A:93:TYR:HE1 | 0.47 | 2.27 | 8 | 2 |
| 1:A:84:PHE:CD2 | 1:A:90:LEU:CG | 0.47 | 2.97 | 7 | 2 |
| 1:A:18:ARG:CA | 1:A:37:ARG:NH1 | 0.47 | 2.77 | 18 | 1 |
| 1:A:7:GLU:OE1 | 1:A:14:LYS:HG3 | 0.47 | 2.09 | 12 | 1 |
| 1:A:25:LEU:HG | 1:A:50:PHE:CD1 | 0.47 | 2.43 | 12 | 1 |
| 1:A:106:ARG:C | 1:A:106:ARG:CD | 0.47 | 2.83 | 15 | 1 |
| 1:A:74:LYS:HD3 | 1:A:74:LYS:O | 0.47 | 2.08 | 20 | 1 |
| 1:A:52:LYS:HD3 | 1:A:52:LYS:O | 0.47 | 2.07 | 14 | 1 |
| 1:A:7:GLU:CD | 1:A:14:LYS:HE2 | 0.47 | 2.29 | 5 | 1 |
| 1:A:49:VAL:CG2 | 1:A:102:VAL:HG22 | 0.47 | 2.39 | 5 | 1 |
| 1:A:90:LEU:HA | 1:A:93:TYR:CD1 | 0.47 | 2.43 | 19 | 2 |
| 1:A:67:LYS:CA | 1:A:67:LYS:HE3 | 0.47 | 2.38 | 18 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:12:TYR:HE2 | 1:A:14:LYS:CG | 0.47 | 2.22 | 15 | 6 |
| 1:A:6:LEU:CG | 1:A:12:TYR:CD1 | 0.47 | 2.97 | 14 | 1 |
| 1:A:17:SER:N | 1:A:20:LYS:HD3 | 0.47 | 2.23 | 3 | 2 |
| 1:A:86:SER:OG | 1:A:89:LEU:HG | 0.47 | 2.09 | 16 | 1 |
| 1:A:12:TYR:OH | 1:A:38:ASP:CB | 0.47 | 2.63 | 19 | 1 |
| 1:A:95:GLN:HG3 | 1:A:105:LEU:HB2 | 0.47 | 1.79 | 17 | 1 |
| 1:A:82:TYR:CE1 | 1:A:93:TYR:HE1 | 0.47 | 2.28 | 20 | 1 |
| 1:A:78:VAL:HG22 | 1:A:94:HIS:NE2 | 0.47 | 2.24 | 14 | 1 |
| 1:A:24:LEU:CD2 | 1:A:35:MET:SD | 0.47 | 3.02 | 16 | 3 |
| 1:A:75:ARG:C | 1:A:83:VAL:CG1 | 0.47 | 2.82 | 17 | 2 |
| 1:A:10:GLU:HG2 | 1:A:108:PRO:HG2 | 0.47 | 1.85 | 4 | 3 |
| 1:A:10:GLU:HG3 | 1:A:108:PRO:C | 0.47 | 2.30 | 4 | 1 |
| 1:A:43:GLY:C | 1:A:68:GLU:OE2 | 0.47 | 2.53 | 10 | 1 |
| 1:A:24:LEU:HB2 | 1:A:111:GLY:CA | 0.47 | 2.40 | 18 | 3 |
| 1:A:105:LEU:H | 1:A:105:LEU:HD22 | 0.47 | 1.70 | 14 | 2 |
| 1:A:13:ASN:CB | 1:A:16:ILE:CD1 | 0.47 | 2.93 | 13 | 1 |
| 1:A:97:ASN:C | 1:A:97:ASN:ND2 | 0.47 | 2.67 | 3 | 1 |
| 1:A:77:TYR:CB | 1:A:81:LYS:O | 0.47 | 2.62 | 5 | 1 |
| 1:A:13:ASN:CB | 1:A:16:ILE:CG1 | 0.47 | 2.91 | 10 | 2 |
| 1:A:26:LEU:HD23 | 1:A:61:ILE:HD11 | 0.47 | 1.84 | 10 | 1 |
| 1:A:68:GLU:OE1 | 1:A:76:TYR:CE1 | 0.47 | 2.67 | 10 | 1 |
| 1:A:37:ARG:CG | 1:A:37:ARG:HH11 | 0.47 | 2.22 | 17 | 3 |
| 1:A:44:THR:OG1 | 1:A:65:HIS:NE2 | 0.47 | 2.32 | 8 | 2 |
| 1:A:36:VAL:CB | 1:A:46:THR:O | 0.47 | 2.62 | 12 | 14 |
| 1:A:102:VAL:CG2 | 1:A:103:THR:N | 0.47 | 2.78 | 1 | 3 |
| 1:A:41:THR:HG22 | 1:A:44:THR:H | 0.47 | 1.69 | 2 | 2 |
| 1:A:67:LYS:HE2 | 1:A:67:LYS:HA | 0.47 | 1.85 | 2 | 2 |
| 1:A:83:VAL:C | 1:A:84:PHE:CG | 0.47 | 2.88 | 14 | 2 |
| 1:A:30:LYS:HE3 | 1:A:107:TYR:HD2 | 0.47 | 1.64 | 6 | 1 |
| 1:A:21:ALA:O | 1:A:25:LEU:CG | 0.47 | 2.63 | 3 | 1 |
| 1:A:24:LEU:C | 1:A:24:LEU:HD13 | 0.47 | 2.26 | 5 | 1 |
| 1:A:76:TYR:CD2 | 1:A:86:SER:CA | 0.47 | 2.97 | 5 | 1 |
| 1:A:77:TYR:HE2 | 1:A:80:GLU:H | 0.47 | 1.53 | 11 | 1 |
| 1:A:45:TYR:CD1 | 1:A:87:ILE:CG1 | 0.47 | 2.97 | 5 | 2 |
| 1:A:9:TYR:C | 1:A:11:TRP:H | 0.47 | 2.12 | 5 | 3 |
| 1:A:17:SER:HB3 | 1:A:20:LYS:HE3 | 0.47 | 1.85 | 15 | 2 |
| 1:A:28:THR:CG2 | 1:A:109:VAL:CG1 | 0.47 | 2.72 | 4 | 1 |
| 1:A:99:GLY:C | 1:A:101:LEU:HD12 | 0.47 | 2.30 | 12 | 1 |
| 1:A:25:LEU:HD23 | 1:A:61:ILE:CG2 | 0.47 | 2.39 | 12 | 1 |
| 1:A:12:TYR:CE2 | 1:A:14:LYS:CG | 0.47 | 2.98 | 15 | 2 |
| 1:A:10:GLU:O | 1:A:109:VAL:CA | 0.47 | 2.62 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:82:TYR:HB2 | 1:A:84:PHE:CE2 | 0.47 | 2.45 | 9 | 2 |
| 1:A:90:LEU:C | 1:A:93:TYR:CD1 | 0.47 | 2.88 | 19 | 2 |
| 1:A:49:VAL:HG23 | 1:A:62:LYS:HB3 | 0.47 | 1.86 | 18 | 3 |
| 1:A:38:ASP:OD1 | 1:A:39:SER:O | 0.47 | 2.32 | 8 | 1 |
| 1:A:98:GLY:N | 1:A:104:ARG:CD | 0.47 | 2.78 | 2 | 1 |
| 1:A:95:GLN:HB3 | 1:A:96:TYR:CD1 | 0.47 | 2.45 | 2 | 1 |
| 1:A:69:THR:HG21 | 1:A:83:VAL:CG1 | 0.47 | 2.31 | 4 | 1 |
| 1:A:6:LEU:H | 1:A:6:LEU:HD23 | 0.47 | 1.70 | 11 | 1 |
| 1:A:11:TRP:O | 1:A:35:MET:C | 0.47 | 2.53 | 9 | 1 |
| 1:A:82:TYR:O | 1:A:83:VAL:CG1 | 0.47 | 2.63 | 8 | 1 |
| 1:A:10:GLU:HG3 | 1:A:108:PRO:CG | 0.47 | 2.40 | 20 | 1 |
| 1:A:75:ARG:NH1 | 1:A:76:TYR:OH | 0.46 | 2.48 | 10 | 1 |
| 1:A:28:THR:HG22 | 1:A:50:PHE:HE2 | 0.46 | 1.70 | 11 | 1 |
| 1:A:74:LYS:HE3 | 1:A:83:VAL:N | 0.46 | 2.24 | 7 | 1 |
| 1:A:40:ARG:NE | 1:A:41:THR:H | 0.46 | 2.08 | 4 | 1 |
| 1:A:34:PHE:CB | 1:A:108:PRO:HA | 0.46 | 2.41 | 15 | 3 |
| 1:A:87:ILE:HD13 | 1:A:87:ILE:H | 0.46 | 1.70 | 3 | 1 |
| 1:A:50:PHE:CZ | 1:A:52:LYS:NZ | 0.46 | 2.83 | 11 | 1 |
| 1:A:95:GLN:HE22 | 1:A:108:PRO:CD | 0.46 | 2.24 | 9 | 1 |
| 1:A:36:VAL:HG11 | 1:A:87:ILE:HG21 | 0.46 | 1.87 | 19 | 1 |
| 1:A:24:LEU:HD12 | 1:A:25:LEU:H | 0.46 | 1.69 | 8 | 5 |
| 1:A:69:THR:O | 1:A:75:ARG:HD2 | 0.46 | 2.09 | 17 | 1 |
| 1:A:69:THR:O | 1:A:69:THR:CG2 | 0.46 | 2.63 | 11 | 1 |
| 1:A:35:MET:HE1 | 1:A:111:GLY:H | 0.46 | 1.69 | 9 | 1 |
| 1:A:100:GLY:C | 1:A:101:LEU:HD23 | 0.46 | 2.22 | 2 | 1 |
| 1:A:78:VAL:O | 1:A:81:LYS:HE3 | 0.46 | 2.10 | 2 | 1 |
| 1:A:29:GLY:C | 1:A:30:LYS:HG2 | 0.46 | 2.30 | 20 | 1 |
| 1:A:28:THR:CB | 1:A:30:LYS:HD3 | 0.46 | 2.41 | 1 | 1 |
| 1:A:6:LEU:O | 1:A:7:GLU:CG | 0.46 | 2.64 | 10 | 1 |
| 1:A:85:ASP:CG | 1:A:85:ASP:O | 0.46 | 2.53 | 19 | 1 |
| 1:A:74:LYS:CD | 1:A:74:LYS:N | 0.46 | 2.75 | 7 | 1 |
| 1:A:97:ASN:ND2 | 1:A:97:ASN:N | 0.46 | 2.63 | 12 | 1 |
| 1:A:35:MET:HG3 | 1:A:109:VAL:O | 0.46 | 2.11 | 16 | 2 |
| 1:A:106:ARG:C | 1:A:106:ARG:HD3 | 0.46 | 2.31 | 15 | 1 |
| 1:A:98:GLY:C | 1:A:100:GLY:N | 0.46 | 2.69 | 5 | 1 |
| 1:A:32:GLY:N | 1:A:51:THR:HG1 | 0.46 | 2.04 | 18 | 4 |
| 1:A:7:GLU:N | 1:A:12:TYR:HD2 | 0.46 | 2.07 | 9 | 1 |
| 1:A:67:LYS:HB3 | 1:A:77:TYR:CZ | 0.46 | 2.45 | 8 | 4 |
| 1:A:49:VAL:HG22 | 1:A:64:TYR:CD1 | 0.46 | 2.45 | 15 | 1 |
| 1:A:100:GLY:N | 1:A:101:LEU:HD13 | 0.46 | 2.25 | 20 | 1 |
| 1:A:106:ARG:O | 1:A:106:ARG:HD3 | 0.46 | 2.11 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:62:LYS:CB | 1:A:64:TYR:HE1 | 0.46 | 2.23 | 20 | 7 |
| 1:A:81:LYS:CB | 1:A:82:TYR:HD1 | 0.46 | 2.23 | 3 | 6 |
| 1:A:17:SER:H | 1:A:20:LYS:HD3 | 0.46 | 1.69 | 3 | 3 |
| 1:A:20:LYS:C | 1:A:23:LYS:HG2 | 0.46 | 2.31 | 9 | 4 |
| 1:A:41:THR:HG23 | 1:A:42:PRO:CG | 0.46 | 2.40 | 2 | 1 |
| 1:A:81:LYS:CD | 1:A:82:TYR:HD1 | 0.46 | 2.15 | 12 | 1 |
| 1:A:81:LYS:CE | 1:A:82:TYR:HE1 | 0.46 | 2.23 | 3 | 3 |
| 1:A:93:TYR:CD1 | 1:A:93:TYR:C | 0.46 | 2.87 | 17 | 2 |
| 1:A:46:THR:CA | 1:A:65:HIS:HD1 | 0.46 | 2.24 | 9 | 3 |
| 1:A:84:PHE:CZ | 1:A:93:TYR:HB3 | 0.46 | 2.45 | 18 | 2 |
| 1:A:66:ILE:H | 1:A:66:ILE:CD1 | 0.46 | 2.13 | 6 | 2 |
| 1:A:10:GLU:OE1 | 1:A:107:TYR:OH | 0.46 | 2.30 | 4 | 1 |
| 1:A:103:THR:O | 1:A:106:ARG:N | 0.46 | 2.49 | 15 | 1 |
| 1:A:95:GLN:HG2 | 1:A:105:LEU:CD2 | 0.46 | 2.40 | 3 | 1 |
| 1:A:97:ASN:HD22 | 1:A:98:GLY:N | 0.46 | 2.08 | 3 | 1 |
| 1:A:6:LEU:CG | 1:A:12:TYR:CE1 | 0.46 | 2.99 | 14 | 1 |
| 1:A:75:ARG:N | 1:A:83:VAL:HG12 | 0.46 | 2.26 | 17 | 1 |
| 1:A:84:PHE:CD1 | 1:A:90:LEU:CB | 0.46 | 2.99 | 15 | 2 |
| 1:A:91:ILE:CA | 1:A:105:LEU:HD21 | 0.46 | 2.38 | 12 | 1 |
| 1:A:30:LYS:HD2 | 1:A:109:VAL:HG13 | 0.46 | 1.80 | 12 | 1 |
| 1:A:81:LYS:CE | 1:A:82:TYR:CE2 | 0.46 | 2.99 | 14 | 1 |
| 1:A:22:GLU:CA | 1:A:61:ILE:HG13 | 0.46 | 2.41 | 5 | 1 |
| 1:A:75:ARG:HD3 | 1:A:76:TYR:CZ | 0.46 | 2.46 | 10 | 1 |
| 1:A:77:TYR:CD1 | 1:A:83:VAL:CG1 | 0.46 | 2.99 | 18 | 3 |
| 1:A:83:VAL:HG23 | 1:A:83:VAL:O | 0.46 | 2.11 | 18 | 1 |
| 1:A:22:GLU:CB | 1:A:23:LYS:HZ1 | 0.46 | 2.23 | 2 | 1 |
| 1:A:28:THR:HB | 1:A:109:VAL:CG2 | 0.46 | 2.41 | 17 | 1 |
| 1:A:6:LEU:CD2 | 1:A:87:ILE:HB | 0.46 | 2.41 | 1 | 2 |
| 1:A:30:LYS:CG | 1:A:107:TYR:HD2 | 0.46 | 2.16 | 15 | 2 |
| 1:A:18:ARG:O | 1:A:18:ARG:HD3 | 0.46 | 2.11 | 14 | 1 |
| 1:A:67:LYS:HA | 1:A:67:LYS:HE3 | 0.46 | 1.88 | 14 | 1 |
| 1:A:106:ARG:NH1 | 1:A:106:ARG:O | 0.46 | 2.49 | 5 | 1 |
| 1:A:91:ILE:HG23 | 1:A:105:LEU:HD21 | 0.46 | 1.86 | 8 | 3 |
| 1:A:39:SER:O | 1:A:40:ARG:CB | 0.46 | 2.62 | 18 | 1 |
| 1:A:103:THR:C | 1:A:104:ARG:HG2 | 0.46 | 2.31 | 17 | 2 |
| 1:A:84:PHE:HD1 | 1:A:90:LEU:CG | 0.46 | 2.24 | 6 | 2 |
| 1:A:66:ILE:HA | 1:A:78:VAL:HG13 | 0.46 | 1.88 | 4 | 1 |
| 1:A:6:LEU:CB | 1:A:12:TYR:CE1 | 0.46 | 2.99 | 14 | 1 |
| 1:A:40:ARG:O | 1:A:41:THR:CG2 | 0.46 | 2.58 | 1 | 1 |
| 1:A:77:TYR:HD2 | 1:A:80:GLU:N | 0.45 | 2.09 | 3 | 4 |
| 1:A:11:TRP:HE3 | 1:A:36:VAL:HG23 | 0.45 | 1.69 | 14 | 7 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:12:TYR:CE1 | 1:A:45:TYR:HD2 | 0.45 | 2.29 | 9 | 2 |
| 1:A:25:LEU:CG | 1:A:50:PHE:HB3 | 0.45 | 2.41 | 19 | 1 |
| 1:A:74:LYS:HB3 | 1:A:84:PHE:C | 0.45 | 2.31 | 6 | 1 |
| 1:A:12:TYR:HA | 1:A:36:VAL:HB | 0.45 | 1.88 | 20 | 3 |
| 1:A:23:LYS:HG3 | 1:A:24:LEU:H | 0.45 | 1.71 | 4 | 3 |
| 1:A:84:PHE:CG | 1:A:90:LEU:HA | 0.45 | 2.46 | 13 | 1 |
| 1:A:103:THR:OG1 | 1:A:106:ARG:CB | 0.45 | 2.65 | 3 | 1 |
| 1:A:70:ASN:ND2 | 1:A:70:ASN:H | 0.45 | 2.09 | 14 | 2 |
| 1:A:22:GLU:CG | 1:A:63:HIS:CE1 | 0.45 | 2.98 | 16 | 2 |
| 1:A:35:MET:CB | 1:A:109:VAL:O | 0.45 | 2.62 | 9 | 1 |
| 1:A:25:LEU:CD1 | 1:A:48:SER:HG | 0.45 | 2.19 | 9 | 1 |
| 1:A:20:LYS:HB3 | 1:A:23:LYS:HE3 | 0.45 | 1.86 | 3 | 3 |
| 1:A:37:ARG:CD | 1:A:46:THR:HB | 0.45 | 2.41 | 17 | 5 |
| 1:A:50:PHE:HB2 | 1:A:60:CYS:C | 0.45 | 2.32 | 7 | 3 |
| 1:A:86:SER:HB2 | 1:A:88:PRO:HG2 | 0.45 | 1.89 | 7 | 1 |
| 1:A:84:PHE:CE1 | 1:A:93:TYR:HD2 | 0.45 | 2.24 | 20 | 3 |
| 1:A:11:TRP:CD1 | 1:A:34:PHE:CD2 | 0.45 | 3.04 | 6 | 2 |
| 1:A:82:TYR:CE1 | 1:A:93:TYR:HE2 | 0.45 | 2.27 | 4 | 1 |
| 1:A:34:PHE:HB3 | 1:A:108:PRO:HA | 0.45 | 1.86 | 15 | 3 |
| 1:A:14:LYS:HG2 | 1:A:38:ASP:HB2 | 0.45 | 1.81 | 20 | 1 |
| 1:A:28:THR:HG22 | 1:A:50:PHE:CZ | 0.45 | 2.47 | 20 | 1 |
| 1:A:84:PHE:HZ | 1:A:93:TYR:CE2 | 0.45 | 2.28 | 5 | 1 |
| 1:A:77:TYR:HE2 | 1:A:80:GLU:N | 0.45 | 2.07 | 11 | 3 |
| 1:A:24:LEU:CD1 | 1:A:25:LEU:CD1 | 0.45 | 2.91 | 8 | 2 |
| 1:A:84:PHE:HD1 | 1:A:84:PHE:N | 0.45 | 2.07 | 5 | 2 |
| 1:A:44:THR:HG23 | 1:A:65:HIS:HE2 | 0.45 | 1.70 | 15 | 1 |
| 1:A:81:LYS:HE3 | 1:A:99:GLY:C | 0.45 | 2.32 | 20 | 1 |
| 1:A:11:TRP:HB3 | 1:A:34:PHE:O | 0.45 | 2.11 | 1 | 1 |
| 1:A:36:VAL:HG21 | 1:A:87:ILE:CG2 | 0.45 | 2.42 | 9 | 3 |
| 1:A:64:TYR:HD2 | 1:A:78:VAL:CG1 | 0.45 | 2.25 | 8 | 1 |
| 1:A:32:GLY:CA | 1:A:106:ARG:HB3 | 0.45 | 2.42 | 18 | 1 |
| 1:A:75:ARG:CG | 1:A:76:TYR:HE1 | 0.45 | 2.25 | 3 | 1 |
| 1:A:68:GLU:HA | 1:A:68:GLU:OE1 | 0.45 | 2.11 | 20 | 1 |
| 1:A:67:LYS:HZ2 | 1:A:67:LYS:HA | 0.45 | 1.72 | 1 | 1 |
| 1:A:98:GLY:CA | 1:A:104:ARG:HG2 | 0.45 | 2.42 | 1 | 1 |
| 1:A:77:TYR:CB | 1:A:83:VAL:HA | 0.45 | 2.41 | 9 | 1 |
| 1:A:98:GLY:CA | 1:A:104:ARG:CD | 0.45 | 2.94 | 2 | 1 |
| 1:A:23:LYS:N | 1:A:23:LYS:NZ | 0.45 | 2.64 | 2 | 1 |
| 1:A:32:GLY:H | 1:A:51:THR:CA | 0.45 | 2.24 | 5 | 2 |
| 1:A:24:LEU:CD2 | 1:A:25:LEU:HD22 | 0.45 | 2.41 | 12 | 1 |
| 1:A:44:THR:CA | 1:A:68:GLU:HG3 | 0.45 | 2.41 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:12:TYR:CD1 | 1:A:36:VAL:CG1 | 0.45 | 2.99 | 5 | 1 |
| 1:A:22:GLU:CG | 1:A:63:HIS:HE1 | 0.45 | 2.24 | 8 | 2 |
| 1:A:65:HIS:C | 1:A:78:VAL:HG23 | 0.45 | 2.32 | 8 | 1 |
| 1:A:67:LYS:CB | 1:A:77:TYR:CZ | 0.45 | 2.99 | 5 | 3 |
| 1:A:45:TYR:HB2 | 1:A:66:ILE:HG13 | 0.45 | 1.89 | 18 | 1 |
| 1:A:81:LYS:HG2 | 1:A:82:TYR:H | 0.45 | 1.65 | 4 | 1 |
| 1:A:68:GLU:OE2 | 1:A:76:TYR:CD2 | 0.45 | 2.70 | 13 | 2 |
| 1:A:30:LYS:HD2 | 1:A:109:VAL:HG11 | 0.45 | 1.86 | 12 | 1 |
| 1:A:29:GLY:O | 1:A:52:LYS:HG3 | 0.45 | 2.12 | 15 | 1 |
| 1:A:91:ILE:CG2 | 1:A:95:GLN:HE21 | 0.45 | 2.25 | 20 | 1 |
| 1:A:26:LEU:HD13 | 1:A:61:ILE:HG13 | 0.45 | 1.86 | 1 | 1 |
| 1:A:11:TRP:CB | 1:A:34:PHE:O | 0.45 | 2.64 | 1 | 1 |
| 1:A:103:THR:C | 1:A:104:ARG:O | 0.45 | 2.55 | 19 | 5 |
| 1:A:74:LYS:HE2 | 1:A:74:LYS:HA | 0.45 | 1.86 | 8 | 1 |
| 1:A:106:ARG:HH11 | 1:A:106:ARG:CG | 0.45 | 2.25 | 6 | 1 |
| 1:A:11:TRP:CE3 | 1:A:12:TYR:CA | 0.45 | 3.00 | 20 | 2 |
| 1:A:87:ILE:CG2 | 1:A:91:ILE:HD11 | 0.45 | 2.38 | 4 | 1 |
| 1:A:37:ARG:CG | 1:A:46:THR:CB | 0.45 | 2.94 | 16 | 3 |
| 1:A:43:GLY:O | 1:A:45:TYR:CE1 | 0.45 | 2.69 | 3 | 1 |
| 1:A:51:THR:O | 1:A:60:CYS:HB3 | 0.45 | 2.11 | 20 | 1 |
| 1:A:64:TYR:CD1 | 1:A:64:TYR:N | 0.45 | 2.84 | 10 | 2 |
| 1:A:62:LYS:HG2 | 1:A:64:TYR:CZ | 0.45 | 2.47 | 11 | 1 |
| 1:A:16:ILE:HA | 1:A:20:LYS:HE3 | 0.45 | 1.87 | 3 | 2 |
| 1:A:33:ALA:CB | 1:A:109:VAL:HG21 | 0.45 | 2.27 | 9 | 1 |
| 1:A:93:TYR:HE2 | 1:A:94:HIS:CE1 | 0.45 | 2.24 | 19 | 1 |
| 1:A:34:PHE:CG | 1:A:35:MET:N | 0.45 | 2.84 | 17 | 5 |
| 1:A:74:LYS:O | 1:A:83:VAL:HG11 | 0.45 | 2.12 | 17 | 1 |
| 1:A:12:TYR:HE2 | 1:A:14:LYS:CD | 0.45 | 2.25 | 5 | 1 |
| 1:A:62:LYS:CG | 1:A:64:TYR:HE1 | 0.45 | 2.25 | 15 | 5 |
| 1:A:24:LEU:HD12 | 1:A:35:MET:SD | 0.45 | 2.49 | 9 | 1 |
| 1:A:64:TYR:CG | 1:A:101:LEU:HD23 | 0.45 | 2.43 | 6 | 2 |
| 1:A:25:LEU:HB3 | 1:A:61:ILE:CD1 | 0.45 | 2.42 | 2 | 2 |
| 1:A:44:THR:HG1 | 1:A:45:TYR:N | 0.45 | 2.09 | 6 | 1 |
| 1:A:62:LYS:CE | 1:A:64:TYR:OH | 0.45 | 2.65 | 16 | 1 |
| 1:A:104:ARG:HH22 | 1:A:106:ARG:CZ | 0.45 | 2.25 | 10 | 1 |
| 1:A:94:HIS:HD2 | 1:A:101:LEU:CD2 | 0.45 | 2.24 | 8 | 2 |
| 1:A:18:ARG:N | 1:A:37:ARG:CZ | 0.45 | 2.79 | 5 | 3 |
| 1:A:29:GLY:C | 1:A:52:LYS:HD3 | 0.45 | 2.33 | 6 | 1 |
| 1:A:76:TYR:HD2 | 1:A:87:ILE:HD13 | 0.45 | 1.71 | 12 | 1 |
| 1:A:6:LEU:HD11 | 1:A:87:ILE:CB | 0.45 | 2.42 | 12 | 1 |
| 1:A:22:GLU:OE2 | 1:A:63:HIS:CE1 | 0.45 | 2.70 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:97:ASN:HD21 | 1:A:99:GLY:N | 0.45 | 2.10 | 3 | 1 |
| 1:A:81:LYS:HE3 | 1:A:99:GLY:CA | 0.45 | 2.41 | 20 | 1 |
| 1:A:31:GLU:CD | 1:A:31:GLU:O | 0.45 | 2.55 | 1 | 1 |
| 1:A:9:TYR:O | 1:A:10:GLU:C | 0.44 | 2.55 | 10 | 8 |
| 1:A:109:VAL:CG1 | 1:A:110:CYS:N | 0.44 | 2.81 | 14 | 2 |
| 1:A:27:ASP:OD1 | 1:A:27:ASP:C | 0.44 | 2.54 | 9 | 1 |
| 1:A:94:HIS:CE1 | 1:A:101:LEU:CD1 | 0.44 | 2.98 | 8 | 1 |
| 1:A:31:GLU:CD | 1:A:106:ARG:HG3 | 0.44 | 2.32 | 18 | 1 |
| 1:A:35:MET:CB | 1:A:48:SER:HB2 | 0.44 | 2.35 | 20 | 2 |
| 1:A:24:LEU:HB2 | 1:A:111:GLY:HA2 | 0.44 | 1.89 | 4 | 1 |
| 1:A:25:LEU:CD1 | 1:A:50:PHE:HB3 | 0.44 | 2.42 | 19 | 1 |
| 1:A:18:ARG:CA | 1:A:63:HIS:CD2 | 0.44 | 3.00 | 7 | 1 |
| 1:A:21:ALA:C | 1:A:24:LEU:CG | 0.44 | 2.85 | 2 | 1 |
| 1:A:28:THR:HG22 | 1:A:50:PHE:CE1 | 0.44 | 2.47 | 20 | 2 |
| 1:A:104:ARG:CZ | 1:A:106:ARG:HA | 0.44 | 2.42 | 12 | 1 |
| 1:A:25:LEU:HD23 | 1:A:61:ILE:HG21 | 0.44 | 1.87 | 12 | 1 |
| 1:A:47:VAL:CG2 | 1:A:91:ILE:HD11 | 0.44 | 2.42 | 12 | 3 |
| 1:A:29:GLY:C | 1:A:30:LYS:CD | 0.44 | 2.86 | 3 | 1 |
| 1:A:24:LEU:CD2 | 1:A:111:GLY:N | 0.44 | 2.81 | 1 | 1 |
| 1:A:28:THR:HG23 | 1:A:30:LYS:N | 0.44 | 2.27 | 16 | 1 |
| 1:A:98:GLY:HA2 | 1:A:104:ARG:HB3 | 0.44 | 1.87 | 7 | 1 |
| 1:A:74:LYS:HG2 | 1:A:85:ASP:N | 0.44 | 2.27 | 6 | 1 |
| 1:A:91:ILE:HA | 1:A:105:LEU:HD23 | 0.44 | 1.89 | 15 | 1 |
| 1:A:49:VAL:HB | 1:A:102:VAL:HG22 | 0.44 | 1.89 | 16 | 1 |
| 1:A:13:ASN:HD21 | 1:A:35:MET:HB2 | 0.44 | 1.70 | 9 | 1 |
| 1:A:93:TYR:CE1 | 1:A:99:GLY:CA | 0.44 | 3.00 | 9 | 1 |
| 1:A:20:LYS:HA | 1:A:23:LYS:HD3 | 0.44 | 1.89 | 17 | 4 |
| 1:A:67:LYS:CA | 1:A:68:GLU:OE1 | 0.44 | 2.65 | 7 | 1 |
| 1:A:38:ASP:OD1 | 1:A:38:ASP:C | 0.44 | 2.55 | 8 | 1 |
| 1:A:105:LEU:HD23 | 1:A:105:LEU:H | 0.44 | 1.72 | 4 | 1 |
| 1:A:69:THR:HG22 | 1:A:77:TYR:CE1 | 0.44 | 2.47 | 14 | 1 |
| 1:A:16:ILE:CD1 | 1:A:21:ALA:HA | 0.44 | 2.42 | 9 | 1 |
| 1:A:6:LEU:HD23 | 1:A:6:LEU:H | 0.44 | 1.71 | 7 | 1 |
| 1:A:46:THR:HA | 1:A:65:HIS:HA | 0.44 | 1.89 | 15 | 6 |
| 1:A:92:GLN:N | 1:A:92:GLN:HE21 | 0.44 | 2.10 | 3 | 5 |
| 1:A:6:LEU:HA | 1:A:9:TYR:HE2 | 0.44 | 1.71 | 18 | 6 |
| 1:A:40:ARG:O | 1:A:44:THR:HG22 | 0.44 | 2.12 | 4 | 1 |
| 1:A:84:PHE:HZ | 1:A:93:TYR:CZ | 0.44 | 2.30 | 4 | 1 |
| 1:A:30:LYS:H | 1:A:30:LYS:CD | 0.44 | 2.25 | 13 | 2 |
| 1:A:22:GLU:HG3 | 1:A:61:ILE:CG2 | 0.44 | 2.43 | 12 | 1 |
| 1:A:23:LYS:HG2 | 1:A:24:LEU:H | 0.44 | 1.71 | 3 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:12:TYR:OH | 1:A:14:LYS:CB | 0.44 | 2.66 | 20 | 1 |
| 1:A:26:LEU:HD13 | 1:A:61:ILE:CG1 | 0.44 | 2.42 | 20 | 1 |
| 1:A:51:THR:HG1 | 1:A:103:THR:HG21 | 0.44 | 1.72 | 10 | 1 |
| 1:A:10:GLU:OE1 | 1:A:108:PRO:HG2 | 0.44 | 2.12 | 11 | 3 |
| 1:A:84:PHE:HD2 | 1:A:90:LEU:CG | 0.44 | 2.26 | 2 | 2 |
| 1:A:37:ARG:HH11 | 1:A:37:ARG:HG3 | 0.44 | 1.70 | 6 | 2 |
| 1:A:49:VAL:CB | 1:A:102:VAL:HG11 | 0.44 | 2.43 | 13 | 1 |
| 1:A:87:ILE:HB | 1:A:88:PRO:HD3 | 0.44 | 1.90 | 3 | 2 |
| 1:A:45:TYR:N | 1:A:45:TYR:HD1 | 0.44 | 2.10 | 20 | 1 |
| 1:A:6:LEU:HA | 1:A:9:TYR:HE1 | 0.44 | 1.66 | 14 | 1 |
| 1:A:81:LYS:CE | 1:A:82:TYR:HE2 | 0.44 | 2.26 | 14 | 1 |
| 1:A:49:VAL:O | 1:A:61:ILE:HA | 0.44 | 2.13 | 9 | 1 |
| 1:A:64:TYR:OH | 1:A:101:LEU:CB | 0.44 | 2.66 | 19 | 1 |
| 1:A:92:GLN:HE22 | 1:A:95:GLN:NE2 | 0.44 | 2.10 | 7 | 1 |
| 1:A:48:SER:HA | 1:A:62:LYS:O | 0.44 | 2.13 | 18 | 1 |
| 1:A:47:VAL:CG1 | 1:A:49:VAL:CG1 | 0.44 | 2.95 | 17 | 1 |
| 1:A:32:GLY:HA3 | 1:A:106:ARG:HD2 | 0.44 | 1.90 | 12 | 1 |
| 1:A:44:THR:HB | 1:A:68:GLU:HG3 | 0.44 | 1.89 | 12 | 1 |
| 1:A:30:LYS:CD | 1:A:30:LYS:H | 0.44 | 2.26 | 15 | 1 |
| 1:A:64:TYR:HE2 | 1:A:101:LEU:HB3 | 0.44 | 1.72 | 19 | 2 |
| 1:A:6:LEU:CD2 | 1:A:6:LEU:H | 0.44 | 2.25 | 7 | 1 |
| 1:A:52:LYS:O | 1:A:52:LYS:CD | 0.44 | 2.66 | 18 | 1 |
| 1:A:19:ASP:HB2 | 1:A:20:LYS:HE3 | 0.44 | 1.89 | 2 | 1 |
| 1:A:78:VAL:CG2 | 1:A:81:LYS:NZ | 0.44 | 2.81 | 13 | 1 |
| 1:A:13:ASN:ND2 | 1:A:35:MET:HG2 | 0.44 | 2.21 | 12 | 1 |
| 1:A:20:LYS:HD3 | 1:A:20:LYS:O | 0.44 | 2.13 | 12 | 1 |
| 1:A:47:VAL:CB | 1:A:64:TYR:HB2 | 0.44 | 2.41 | 15 | 1 |
| 1:A:81:LYS:O | 1:A:82:TYR:O | 0.44 | 2.34 | 5 | 1 |
| 1:A:68:GLU:OE1 | 1:A:75:ARG:NE | 0.44 | 2.47 | 6 | 1 |
| 1:A:74:LYS:CB | 1:A:85:ASP:N | 0.44 | 2.81 | 6 | 1 |
| 1:A:93:TYR:HB2 | 1:A:97:ASN:OD1 | 0.44 | 2.12 | 12 | 1 |
| 1:A:16:ILE:C | 1:A:20:LYS:HE3 | 0.44 | 2.34 | 3 | 1 |
| 1:A:11:TRP:HB3 | 1:A:108:PRO:CA | 0.43 | 2.42 | 20 | 6 |
| 1:A:35:MET:CE | 1:A:111:GLY:H | 0.43 | 2.26 | 19 | 2 |
| 1:A:26:LEU:HD11 | 1:A:61:ILE:HG13 | 0.43 | 1.90 | 7 | 1 |
| 1:A:92:GLN:NE2 | 1:A:92:GLN:N | 0.43 | 2.65 | 18 | 2 |
| 1:A:24:LEU:HD12 | 1:A:35:MET:HE3 | 0.43 | 1.90 | 2 | 1 |
| 1:A:98:GLY:CA | 1:A:104:ARG:HE | 0.43 | 2.26 | 2 | 1 |
| 1:A:77:TYR:CB | 1:A:83:VAL:CG1 | 0.43 | 2.94 | 6 | 1 |
| 1:A:84:PHE:HD1 | 1:A:90:LEU:HD12 | 0.43 | 1.72 | 15 | 1 |
| 1:A:40:ARG:HH11 | 1:A:40:ARG:CG | 0.43 | 2.26 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:84:PHE:CE2 | 1:A:90:LEU:HG | 0.43 | 2.48 | 3 | 1 |
| 1:A:105:LEU:N | 1:A:105:LEU:HD22 | 0.43 | 2.27 | 14 | 1 |
| 1:A:12:TYR:HE2 | 1:A:14:LYS:HG3 | 0.43 | 1.71 | 18 | 2 |
| 1:A:74:LYS:O | 1:A:83:VAL:HG21 | 0.43 | 2.13 | 6 | 1 |
| 1:A:30:LYS:HE2 | 1:A:109:VAL:HG12 | 0.43 | 1.89 | 4 | 1 |
| 1:A:78:VAL:HG21 | 1:A:94:HIS:NE2 | 0.43 | 2.28 | 12 | 1 |
| 1:A:26:LEU:HD12 | 1:A:61:ILE:CG1 | 0.43 | 2.43 | 14 | 1 |
| 1:A:47:VAL:CG1 | 1:A:49:VAL:HG12 | 0.43 | 2.42 | 14 | 1 |
| 1:A:9:TYR:CB | 1:A:11:TRP:CD2 | 0.43 | 3.01 | 11 | 4 |
| 1:A:10:GLU:C | 1:A:110:CYS:HB3 | 0.43 | 2.33 | 19 | 1 |
| 1:A:64:TYR:HE2 | 1:A:101:LEU:CD2 | 0.43 | 2.27 | 15 | 2 |
| 1:A:98:GLY:O | 1:A:104:ARG:CD | 0.43 | 2.65 | 17 | 1 |
| 1:A:98:GLY:HA2 | 1:A:104:ARG:NE | 0.43 | 2.28 | 6 | 2 |
| 1:A:76:TYR:CD2 | 1:A:87:ILE:HD13 | 0.43 | 2.47 | 12 | 1 |
| 1:A:60:CYS:O | 1:A:60:CYS:SG | 0.43 | 2.76 | 15 | 1 |
| 1:A:76:TYR:HD2 | 1:A:87:ILE:HD12 | 0.43 | 1.72 | 7 | 2 |
| 1:A:75:ARG:HH21 | 1:A:85:ASP:CB | 0.43 | 2.26 | 15 | 1 |
| 1:A:20:LYS:CG | 1:A:23:LYS:NZ | 0.43 | 2.81 | 20 | 1 |
| 1:A:20:LYS:H | 1:A:20:LYS:HD3 | 0.43 | 1.73 | 16 | 1 |
| 1:A:37:ARG:NH1 | 1:A:37:ARG:CG | 0.43 | 2.81 | 14 | 3 |
| 1:A:77:TYR:HB3 | 1:A:83:VAL:HG13 | 0.43 | 1.90 | 9 | 1 |
| 1:A:25:LEU:HD11 | 1:A:109:VAL:CG1 | 0.43 | 2.42 | 8 | 1 |
| 1:A:25:LEU:HD12 | 1:A:109:VAL:CG1 | 0.43 | 2.41 | 8 | 1 |
| 1:A:77:TYR:HB3 | 1:A:82:TYR:O | 0.43 | 2.10 | 8 | 1 |
| 1:A:21:ALA:HB1 | 1:A:35:MET:SD | 0.43 | 2.54 | 6 | 1 |
| 1:A:24:LEU:CD2 | 1:A:109:VAL:HG13 | 0.43 | 2.28 | 15 | 1 |
| 1:A:17:SER:N | 1:A:20:LYS:NZ | 0.43 | 2.67 | 20 | 1 |
| 1:A:7:GLU:N | 1:A:12:TYR:CE2 | 0.43 | 2.86 | 20 | 1 |
| 1:A:31:GLU:OE2 | 1:A:106:ARG:CZ | 0.43 | 2.65 | 1 | 1 |
| 1:A:46:THR:CA | 1:A:65:HIS:ND1 | 0.43 | 2.81 | 9 | 1 |
| 1:A:24:LEU:HG | 1:A:111:GLY:H | 0.43 | 1.74 | 18 | 1 |
| 1:A:11:TRP:HH2 | 1:A:87:ILE:CG2 | 0.43 | 2.19 | 2 | 1 |
| 1:A:106:ARG:CG | 1:A:106:ARG:NH1 | 0.43 | 2.81 | 6 | 1 |
| 1:A:13:ASN:HD22 | 1:A:35:MET:HG2 | 0.43 | 1.73 | 12 | 1 |
| 1:A:25:LEU:HG | 1:A:35:MET:HE3 | 0.43 | 1.91 | 20 | 1 |
| 1:A:69:THR:HG23 | 1:A:75:ARG:HA | 0.43 | 1.89 | 20 | 2 |
| 1:A:25:LEU:CD2 | 1:A:109:VAL:HG12 | 0.43 | 2.44 | 1 | 2 |
| 1:A:78:VAL:HG22 | 1:A:94:HIS:CE1 | 0.43 | 2.48 | 14 | 1 |
| 1:A:99:GLY:C | 1:A:101:LEU:H | 0.43 | 2.17 | 5 | 1 |
| 1:A:62:LYS:HD3 | 1:A:64:TYR:CZ | 0.43 | 2.49 | 16 | 1 |
| 1:A:92:GLN:HE21 | 1:A:92:GLN:HA | 0.43 | 1.74 | 19 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:18:ARG:CB | 1:A:63:HIS:NE2 | 0.43 | 2.82 | 18 | 1 |
| 1:A:20:LYS:C | 1:A:24:LEU:HD23 | 0.43 | 2.31 | 2 | 1 |
| 1:A:22:GLU:HB2 | 1:A:23:LYS:HZ1 | 0.43 | 1.68 | 2 | 1 |
| 1:A:49:VAL:HB | 1:A:102:VAL:HG11 | 0.43 | 1.87 | 13 | 1 |
| 1:A:30:LYS:HZ2 | 1:A:109:VAL:HG23 | 0.43 | 1.69 | 3 | 1 |
| 1:A:78:VAL:HG23 | 1:A:101:LEU:HD11 | 0.43 | 1.91 | 16 | 1 |
| 1:A:81:LYS:NZ | 1:A:81:LYS:C | 0.43 | 2.71 | 19 | 1 |
| 1:A:11:TRP:HB2 | 1:A:35:MET:CA | 0.43 | 2.43 | 17 | 2 |
| 1:A:25:LEU:HD12 | 1:A:48:SER:OG | 0.43 | 2.11 | 6 | 1 |
| 1:A:69:THR:O | 1:A:75:ARG:CA | 0.43 | 2.66 | 16 | 2 |
| 1:A:84:PHE:HE1 | 1:A:93:TYR:CZ | 0.43 | 2.30 | 12 | 2 |
| 1:A:28:THR:CB | 1:A:30:LYS:HE3 | 0.43 | 2.43 | 14 | 2 |
| 1:A:14:LYS:HE2 | 1:A:38:ASP:HB2 | 0.43 | 1.89 | 20 | 1 |
| 1:A:90:LEU:C | 1:A:93:TYR:HD1 | 0.43 | 2.15 | 19 | 1 |
| 1:A:94:HIS:CD2 | 1:A:101:LEU:HD11 | 0.43 | 2.48 | 19 | 1 |
| 1:A:44:THR:CG2 | 1:A:65:HIS:CD2 | 0.43 | 3.02 | 4 | 1 |
| 1:A:96:TYR:CD1 | 1:A:96:TYR:N | 0.43 | 2.86 | 13 | 1 |
| 1:A:75:ARG:NE | 1:A:85:ASP:HB2 | 0.43 | 2.28 | 12 | 1 |
| 1:A:20:LYS:CB | 1:A:23:LYS:CE | 0.43 | 2.96 | 3 | 1 |
| 1:A:37:ARG:CD | 1:A:46:THR:CB | 0.43 | 2.97 | 16 | 2 |
| 1:A:35:MET:HE3 | 1:A:109:VAL:HG12 | 0.43 | 1.90 | 14 | 1 |
| 1:A:25:LEU:HD21 | 1:A:35:MET:HB3 | 0.43 | 1.89 | 5 | 1 |
| 1:A:24:LEU:CB | 1:A:111:GLY:HA2 | 0.43 | 2.44 | 19 | 1 |
| 1:A:20:LYS:CA | 1:A:23:LYS:CG | 0.43 | 2.96 | 7 | 2 |
| 1:A:74:LYS:CE | 1:A:83:VAL:N | 0.43 | 2.82 | 7 | 1 |
| 1:A:92:GLN:HE21 | 1:A:92:GLN:N | 0.43 | 2.12 | 18 | 2 |
| 1:A:74:LYS:CG | 1:A:85:ASP:HB2 | 0.43 | 2.44 | 6 | 1 |
| 1:A:20:LYS:N | 1:A:20:LYS:HZ3 | 0.43 | 2.12 | 4 | 1 |
| 1:A:62:LYS:CE | 1:A:64:TYR:HE1 | 0.42 | 2.25 | 10 | 1 |
| 1:A:16:ILE:HG22 | 1:A:37:ARG:HB3 | 0.42 | 1.87 | 7 | 1 |
| 1:A:48:SER:OG | 1:A:63:HIS:ND1 | 0.42 | 2.52 | 18 | 1 |
| 1:A:104:ARG:NH1 | 1:A:105:LEU:O | 0.42 | 2.52 | 12 | 1 |
| 1:A:75:ARG:CZ | 1:A:85:ASP:OD2 | 0.42 | 2.67 | 15 | 1 |
| 1:A:10:GLU:HG3 | 1:A:108:PRO:CB | 0.42 | 2.44 | 20 | 1 |
| 1:A:85:ASP:OD1 | 1:A:86:SER:HB2 | 0.42 | 2.14 | 11 | 1 |
| 1:A:31:GLU:CG | 1:A:51:THR:HG23 | 0.42 | 2.43 | 19 | 1 |
| 1:A:21:ALA:O | 1:A:24:LEU:HD11 | 0.42 | 2.11 | 8 | 1 |
| 1:A:25:LEU:CB | 1:A:50:PHE:CD1 | 0.42 | 2.99 | 8 | 1 |
| 1:A:74:LYS:N | 1:A:85:ASP:OD1 | 0.42 | 2.52 | 15 | 1 |
| 1:A:68:GLU:HG2 | 1:A:76:TYR:CG | 0.42 | 2.48 | 3 | 1 |
| 1:A:34:PHE:CZ | 1:A:105:LEU:HD11 | 0.42 | 2.45 | 20 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:ASN:OD1 | 1:A:24:LEU:HD11 | 0.42 | 2.13 | 16 | 1 |
| 1:A:10:GLU:C | 1:A:110:CYS:HB2 | 0.42 | 2.35 | 11 | 3 |
| 1:A:109:VAL:HG12 | 1:A:110:CYS:N | 0.42 | 2.28 | 9 | 1 |
| 1:A:91:ILE:CA | 1:A:105:LEU:HD23 | 0.42 | 2.43 | 6 | 3 |
| 1:A:87:ILE:CG2 | 1:A:91:ILE:CD1 | 0.42 | 2.96 | 4 | 1 |
| 1:A:26:LEU:N | 1:A:61:ILE:CD1 | 0.42 | 2.82 | 15 | 2 |
| 1:A:40:ARG:NH1 | 1:A:40:ARG:CG | 0.42 | 2.82 | 3 | 1 |
| 1:A:6:LEU:N | 1:A:6:LEU:HD23 | 0.42 | 2.28 | 3 | 1 |
| 1:A:109:VAL:O | 1:A:109:VAL:HG12 | 0.42 | 2.13 | 20 | 1 |
| 1:A:67:LYS:CB | 1:A:67:LYS:NZ | 0.42 | 2.83 | 14 | 1 |
| 1:A:98:GLY:CA | 1:A:104:ARG:CG | 0.42 | 2.97 | 10 | 1 |
| 1:A:103:THR:O | 1:A:104:ARG:NE | 0.42 | 2.50 | 11 | 1 |
| 1:A:24:LEU:HD11 | 1:A:25:LEU:CD1 | 0.42 | 2.42 | 7 | 1 |
| 1:A:35:MET:CB | 1:A:48:SER:HB3 | 0.42 | 2.41 | 7 | 1 |
| 1:A:6:LEU:CD2 | 1:A:6:LEU:N | 0.42 | 2.82 | 7 | 1 |
| 1:A:24:LEU:HA | 1:A:27:ASP:OD2 | 0.42 | 2.14 | 17 | 1 |
| 1:A:34:PHE:CE1 | 1:A:47:VAL:HG22 | 0.42 | 2.49 | 3 | 3 |
| 1:A:78:VAL:O | 1:A:79:ALA:HB3 | 0.42 | 2.13 | 12 | 1 |
| 1:A:64:TYR:N | 1:A:64:TYR:CD1 | 0.42 | 2.86 | 15 | 1 |
| 1:A:10:GLU:C | 1:A:108:PRO:HB2 | 0.42 | 2.34 | 4 | 1 |
| 1:A:64:TYR:HE2 | 1:A:101:LEU:HD23 | 0.42 | 1.70 | 15 | 1 |
| 1:A:94:HIS:CD2 | 1:A:99:GLY:C | 0.42 | 2.93 | 17 | 1 |
| 1:A:41:THR:HG1 | 1:A:42:PRO:HD2 | 0.42 | 1.74 | 6 | 1 |
| 1:A:9:TYR:CD2 | 1:A:11:TRP:NE1 | 0.42 | 2.87 | 14 | 1 |
| 1:A:14:LYS:HG2 | 1:A:15:SER:H | 0.42 | 1.75 | 6 | 5 |
| 1:A:25:LEU:HD21 | 1:A:109:VAL:CG2 | 0.42 | 2.45 | 6 | 3 |
| 1:A:98:GLY:O | 1:A:104:ARG:CG | 0.42 | 2.68 | 11 | 1 |
| 1:A:10:GLU:HG3 | 1:A:108:PRO:HG2 | 0.42 | 1.90 | 8 | 1 |
| 1:A:98:GLY:C | 1:A:100:GLY:H | 0.42 | 2.18 | 5 | 1 |
| 1:A:99:GLY:O | 1:A:101:LEU:CD1 | 0.42 | 2.61 | 5 | 1 |
| 1:A:64:TYR:CZ | 1:A:101:LEU:CA | 0.42 | 3.01 | 11 | 1 |
| 1:A:101:LEU:HD12 | 1:A:104:ARG:CA | 0.42 | 2.44 | 19 | 1 |
| 1:A:52:LYS:CB | 1:A:52:LYS:NZ | 0.42 | 2.81 | 17 | 1 |
| 1:A:105:LEU:HD23 | 1:A:105:LEU:N | 0.42 | 2.30 | 4 | 1 |
| 1:A:49:VAL:CG2 | 1:A:102:VAL:HB | 0.42 | 2.45 | 4 | 1 |
| 1:A:40:ARG:NH1 | 1:A:40:ARG:HG3 | 0.42 | 2.29 | 14 | 1 |
| 1:A:85:ASP:CA | 1:A:89:LEU:HD11 | 0.42 | 2.44 | 1 | 1 |
| 1:A:7:GLU:CB | 1:A:14:LYS:CE | 0.42 | 2.96 | 11 | 2 |
| 1:A:45:TYR:HD1 | 1:A:87:ILE:CD1 | 0.42 | 2.28 | 9 | 1 |
| 1:A:12:TYR:CE1 | 1:A:45:TYR:CD2 | 0.42 | 3.07 | 5 | 2 |
| 1:A:104:ARG:C | 1:A:106:ARG:N | 0.42 | 2.73 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:95:GLN:HB3 | 1:A:96:TYR:CE1 | 0.42 | 2.50 | 2 | 1 |
| 1:A:6:LEU:O | 1:A:8:THR:HG23 | 0.42 | 2.14 | 12 | 1 |
| 1:A:25:LEU:CD2 | 1:A:35:MET:HE3 | 0.42 | 2.45 | 5 | 1 |
| 1:A:28:THR:HG23 | 1:A:30:LYS:CE | 0.42 | 2.45 | 6 | 2 |
| 1:A:34:PHE:CA | 1:A:108:PRO:HA | 0.42 | 2.45 | 6 | 1 |
| 1:A:13:ASN:HB3 | 1:A:16:ILE:HD12 | 0.42 | 1.90 | 4 | 2 |
| 1:A:32:GLY:CA | 1:A:106:ARG:HB2 | 0.42 | 2.44 | 13 | 2 |
| 1:A:68:GLU:C | 1:A:75:ARG:O | 0.42 | 2.55 | 3 | 1 |
| 1:A:93:TYR:CD1 | 1:A:97:ASN:CG | 0.42 | 2.93 | 3 | 1 |
| 1:A:14:LYS:O | 1:A:15:SER:C | 0.42 | 2.59 | 5 | 2 |
| 1:A:106:ARG:HD2 | 1:A:106:ARG:C | 0.42 | 2.36 | 1 | 1 |
| 1:A:33:ALA:CB | 1:A:50:PHE:HD2 | 0.42 | 2.17 | 1 | 1 |
| 1:A:49:VAL:HB | 1:A:102:VAL:CG2 | 0.41 | 2.45 | 18 | 1 |
| 1:A:74:LYS:CE | 1:A:84:PHE:HA | 0.41 | 2.45 | 6 | 1 |
| 1:A:81:LYS:NZ | 1:A:101:LEU:CD1 | 0.41 | 2.79 | 12 | 1 |
| 1:A:76:TYR:CD2 | 1:A:87:ILE:CD1 | 0.41 | 3.03 | 12 | 1 |
| 1:A:76:TYR:O | 1:A:83:VAL:C | 0.41 | 2.58 | 12 | 2 |
| 1:A:86:SER:HB2 | 1:A:89:LEU:CG | 0.41 | 2.45 | 15 | 1 |
| 1:A:25:LEU:HD22 | 1:A:50:PHE:HB3 | 0.41 | 1.92 | 3 | 1 |
| 1:A:17:SER:HB3 | 1:A:20:LYS:HZ3 | 0.41 | 1.75 | 10 | 1 |
| 1:A:6:LEU:HB2 | 1:A:12:TYR:CE2 | 0.41 | 2.50 | 11 | 1 |
| 1:A:7:GLU:O | 1:A:8:THR:HG23 | 0.41 | 2.14 | 9 | 1 |
| 1:A:67:LYS:CA | 1:A:77:TYR:O | 0.41 | 2.68 | 3 | 3 |
| 1:A:25:LEU:CG | 1:A:61:ILE:HG23 | 0.41 | 2.45 | 19 | 1 |
| 1:A:100:GLY:C | 1:A:101:LEU:O | 0.41 | 2.59 | 7 | 3 |
| 1:A:25:LEU:HD21 | 1:A:48:SER:HB3 | 0.41 | 1.92 | 18 | 1 |
| 1:A:18:ARG:H | 1:A:37:ARG:CZ | 0.41 | 2.28 | 2 | 1 |
| 1:A:74:LYS:HB3 | 1:A:83:VAL:HB | 0.41 | 1.91 | 2 | 1 |
| 1:A:24:LEU:HB3 | 1:A:111:GLY:HA2 | 0.41 | 1.90 | 6 | 1 |
| 1:A:30:LYS:CD | 1:A:107:TYR:HE2 | 0.41 | 2.28 | 6 | 1 |
| 1:A:103:THR:CB | 1:A:106:ARG:HG3 | 0.41 | 2.45 | 13 | 1 |
| 1:A:40:ARG:NE | 1:A:40:ARG:HA | 0.41 | 2.31 | 13 | 1 |
| 1:A:7:GLU:CA | 1:A:12:TYR:HD2 | 0.41 | 2.28 | 12 | 1 |
| 1:A:31:GLU:HG2 | 1:A:106:ARG:HD2 | 0.41 | 1.91 | 5 | 1 |
| 1:A:11:TRP:HE3 | 1:A:36:VAL:CB | 0.41 | 2.28 | 10 | 3 |
| 1:A:81:LYS:O | 1:A:83:VAL:CG1 | 0.41 | 2.66 | 11 | 1 |
| 1:A:9:TYR:CD1 | 1:A:11:TRP:CE2 | 0.41 | 3.08 | 19 | 1 |
| 1:A:6:LEU:HD13 | 1:A:87:ILE:CG2 | 0.41 | 2.45 | 7 | 2 |
| 1:A:92:GLN:NE2 | 1:A:95:GLN:NE2 | 0.41 | 2.69 | 7 | 1 |
| 1:A:18:ARG:C | 1:A:63:HIS:NE2 | 0.41 | 2.72 | 18 | 1 |
| 1:A:22:GLU:HB2 | 1:A:23:LYS:HE2 | 0.41 | 1.91 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:31:GLU:HG3 | 1:A:106:ARG:HD3 | 0.41 | 1.88 | 12 | 1 |
| 1:A:12:TYR:CZ | 1:A:14:LYS:HG2 | 0.41 | 2.50 | 16 | 2 |
| 1:A:34:PHE:HD2 | 1:A:95:GLN:NE2 | 0.41 | 2.11 | 20 | 1 |
| 1:A:78:VAL:HG22 | 1:A:94:HIS:HE2 | 0.41 | 1.74 | 14 | 1 |
| 1:A:40:ARG:C | 1:A:41:THR:O | 0.41 | 2.56 | 9 | 3 |
| 1:A:67:LYS:O | 1:A:76:TYR:C | 0.41 | 2.58 | 9 | 3 |
| 1:A:66:ILE:CG2 | 1:A:87:ILE:CD1 | 0.41 | 2.90 | 5 | 2 |
| 1:A:45:TYR:CA | 1:A:66:ILE:HG12 | 0.41 | 2.45 | 7 | 1 |
| 1:A:74:LYS:HE2 | 1:A:84:PHE:HA | 0.41 | 1.91 | 17 | 1 |
| 1:A:67:LYS:CG | 1:A:77:TYR:HE1 | 0.41 | 2.22 | 4 | 1 |
| 1:A:90:LEU:HG | 1:A:93:TYR:CE1 | 0.41 | 2.50 | 12 | 1 |
| 1:A:97:ASN:HD22 | 1:A:97:ASN:N | 0.41 | 2.13 | 12 | 1 |
| 1:A:89:LEU:O | 1:A:93:TYR:N | 0.41 | 2.51 | 3 | 1 |
| 1:A:14:LYS:CD | 1:A:38:ASP:HB2 | 0.41 | 2.45 | 20 | 1 |
| 1:A:62:LYS:CD | 1:A:64:TYR:CZ | 0.41 | 3.03 | 16 | 1 |
| 1:A:25:LEU:C | 1:A:50:PHE:CE2 | 0.41 | 2.94 | 10 | 1 |
| 1:A:33:ALA:HB2 | 1:A:50:PHE:CE2 | 0.41 | 2.49 | 10 | 1 |
| 1:A:42:PRO:HB2 | 1:A:68:GLU:HB2 | 0.41 | 1.91 | 10 | 1 |
| 1:A:34:PHE:HD2 | 1:A:108:PRO:HB3 | 0.41 | 1.75 | 13 | 6 |
| 1:A:34:PHE:HE1 | 1:A:47:VAL:HG22 | 0.41 | 1.75 | 3 | 3 |
| 1:A:21:ALA:C | 1:A:25:LEU:HD23 | 0.41 | 2.35 | 19 | 1 |
| 1:A:79:ALA:O | 1:A:81:LYS:CG | 0.41 | 2.62 | 8 | 1 |
| 1:A:89:LEU:CA | 1:A:92:GLN:HG2 | 0.41 | 2.46 | 17 | 1 |
| 1:A:17:SER:CB | 1:A:20:LYS:HZ1 | 0.41 | 2.29 | 15 | 1 |
| 1:A:82:TYR:CG | 1:A:93:TYR:HE2 | 0.41 | 2.29 | 5 | 1 |
| 1:A:52:LYS:O | 1:A:53:ALA:CB | 0.41 | 2.67 | 1 | 1 |
| 1:A:12:TYR:HD1 | 1:A:36:VAL:CG1 | 0.41 | 2.28 | 19 | 1 |
| 1:A:25:LEU:CD2 | 1:A:48:SER:HB3 | 0.41 | 2.45 | 18 | 1 |
| 1:A:49:VAL:HG23 | 1:A:102:VAL:HB | 0.41 | 1.92 | 13 | 1 |
| 1:A:86:SER:HB2 | 1:A:89:LEU:HG | 0.41 | 1.93 | 15 | 1 |
| 1:A:94:HIS:CD2 | 1:A:99:GLY:N | 0.41 | 2.88 | 20 | 1 |
| 1:A:20:LYS:HD3 | 1:A:20:LYS:H | 0.41 | 1.74 | 5 | 1 |
| 1:A:25:LEU:CD1 | 1:A:50:PHE:HD1 | 0.41 | 2.28 | 5 | 1 |
| 1:A:20:LYS:H | 1:A:20:LYS:HD2 | 0.41 | 1.76 | 10 | 1 |
| 1:A:16:ILE:HG23 | 1:A:17:SER:O | 0.41 | 2.15 | 11 | 1 |
| 1:A:98:GLY:O | 1:A:104:ARG:CB | 0.41 | 2.69 | 16 | 2 |
| 1:A:35:MET:CE | 1:A:109:VAL:HG13 | 0.41 | 2.38 | 8 | 1 |
| 1:A:30:LYS:H | 1:A:30:LYS:HD2 | 0.41 | 1.74 | 13 | 1 |
| 1:A:21:ALA:HB1 | 1:A:48:SER:HB2 | 0.41 | 1.92 | 12 | 1 |
| 1:A:37:ARG:NH1 | 1:A:63:HIS:HB3 | 0.41 | 2.31 | 12 | 1 |
| 1:A:34:PHE:HB3 | 1:A:108:PRO:CA | 0.41 | 2.46 | 15 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:GLU:CD | 1:A:76:TYR:CG | 0.41 | 2.90 | 16 | 1 |
| 1:A:93:TYR:CA | 1:A:97:ASN:OD1 | 0.41 | 2.69 | 8 | 1 |
| 1:A:93:TYR:CA | 1:A:97:ASN:HD22 | 0.41 | 2.29 | 18 | 1 |
| 1:A:6:LEU:CA | 1:A:9:TYR:CD2 | 0.41 | 3.03 | 2 | 1 |
| 1:A:64:TYR:CE1 | 1:A:102:VAL:HG13 | 0.41 | 2.51 | 17 | 1 |
| 1:A:11:TRP:CE2 | 1:A:91:ILE:HG21 | 0.41 | 2.50 | 6 | 2 |
| 1:A:14:LYS:HD2 | 1:A:14:LYS:N | 0.41 | 2.30 | 13 | 1 |
| 1:A:6:LEU:O | 1:A:12:TYR:CZ | 0.41 | 2.72 | 15 | 1 |
| 1:A:18:ARG:HD2 | 1:A:63:HIS:HE2 | 0.41 | 1.75 | 15 | 1 |
| 1:A:75:ARG:CG | 1:A:76:TYR:CD1 | 0.41 | 3.00 | 3 | 1 |
| 1:A:50:PHE:CD1 | 1:A:50:PHE:O | 0.41 | 2.74 | 14 | 1 |
| 1:A:6:LEU:O | 1:A:9:TYR:HD2 | 0.41 | 1.99 | 1 | 1 |
| 1:A:11:TRP:CE3 | 1:A:12:TYR:HB2 | 0.41 | 2.50 | 19 | 1 |
| 1:A:83:VAL:CG2 | 1:A:83:VAL:O | 0.41 | 2.69 | 18 | 1 |
| 1:A:68:GLU:CD | 1:A:76:TYR:HE1 | 0.41 | 2.17 | 6 | 1 |
| 1:A:7:GLU:HA | 1:A:12:TYR:HD2 | 0.41 | 1.76 | 6 | 1 |
| 1:A:76:TYR:HD2 | 1:A:87:ILE:CD1 | 0.41 | 2.28 | 12 | 1 |
| 1:A:83:VAL:O | 1:A:83:VAL:CG2 | 0.41 | 2.67 | 12 | 1 |
| 1:A:29:GLY:HA3 | 1:A:52:LYS:HZ1 | 0.41 | 1.74 | 15 | 1 |
| 1:A:7:GLU:CG | 1:A:14:LYS:HD3 | 0.41 | 2.44 | 5 | 1 |
| 1:A:75:ARG:NE | 1:A:85:ASP:OD1 | 0.41 | 2.53 | 1 | 1 |
| 1:A:28:THR:OG1 | 1:A:30:LYS:CD | 0.41 | 2.68 | 16 | 1 |
| 1:A:9:TYR:HB2 | 1:A:11:TRP:CE2 | 0.41 | 2.49 | 8 | 1 |
| 1:A:90:LEU:HG | 1:A:93:TYR:HE1 | 0.41 | 1.76 | 12 | 1 |
| 1:A:14:LYS:HZ3 | 1:A:38:ASP:CG | 0.41 | 2.16 | 20 | 1 |
| 1:A:8:THR:O | 1:A:8:THR:OG1 | 0.40 | 2.38 | 10 | 1 |
| 1:A:69:THR:H | 1:A:75:ARG:HA | 0.40 | 1.75 | 7 | 1 |
| 1:A:96:TYR:C | 1:A:97:ASN:O | 0.40 | 2.59 | 8 | 1 |
| 1:A:24:LEU:HD21 | 1:A:109:VAL:HG23 | 0.40 | 1.92 | 18 | 1 |
| 1:A:101:LEU:HB2 | 1:A:104:ARG:HA | 0.40 | 1.93 | 17 | 1 |
| 1:A:82:TYR:CD1 | 1:A:93:TYR:HE1 | 0.40 | 2.28 | 17 | 1 |
| 1:A:25:LEU:HD12 | 1:A:61:ILE:CG2 | 0.40 | 2.45 | 6 | 1 |
| 1:A:40:ARG:CG | 1:A:41:THR:H | 0.40 | 2.27 | 4 | 1 |
| 1:A:44:THR:HG21 | 1:A:67:LYS:NZ | 0.40 | 2.31 | 15 | 1 |
| 1:A:66:ILE:HG13 | 1:A:87:ILE:HD12 | 0.40 | 1.92 | 14 | 1 |
| 1:A:88:PRO:CA | 1:A:92:GLN:OE1 | 0.40 | 2.69 | 5 | 1 |
| 1:A:85:ASP:N | 1:A:89:LEU:HD12 | 0.40 | 2.28 | 1 | 1 |
| 1:A:102:VAL:HG13 | 1:A:103:THR:HG23 | 0.40 | 1.92 | 10 | 1 |
| 1:A:40:ARG:O | 1:A:43:GLY:N | 0.40 | 2.54 | 10 | 1 |
| 1:A:6:LEU:HD11 | 1:A:87:ILE:HB | 0.40 | 1.93 | 11 | 1 |
| 1:A:23:LYS:CD | 1:A:24:LEU:N | 0.40 | 2.84 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:82:TYR:HD1 | 1:A:93:TYR:OH | 0.40 | 1.96 | 17 | 1 |
| 1:A:70:ASN:O | 1:A:74:LYS:CE | 0.40 | 2.70 | 20 | 1 |
| 1:A:92:GLN:O | 1:A:96:TYR:CD1 | 0.40 | 2.74 | 16 | 1 |
| 1:A:92:GLN:HE21 | 1:A:95:GLN:CD | 0.40 | 2.19 | 7 | 1 |
| 1:A:74:LYS:HB2 | 1:A:84:PHE:N | 0.40 | 2.31 | 8 | 1 |
| 1:A:11:TRP:HH2 | 1:A:87:ILE:HG22 | 0.40 | 1.61 | 2 | 1 |
| 1:A:81:LYS:NZ | 1:A:99:GLY:N | 0.40 | 2.69 | 17 | 1 |
| 1:A:75:ARG:NE | 1:A:76:TYR:CE1 | 0.40 | 2.89 | 4 | 1 |
| 1:A:81:LYS:CE | 1:A:100:GLY:N | 0.40 | 2.84 | 16 | 1 |
| 1:A:25:LEU:CB | 1:A:61:ILE:HG23 | 0.40 | 2.47 | 19 | 1 |
| 1:A:103:THR:OG1 | 1:A:104:ARG:HG3 | 0.40 | 2.16 | 7 | 1 |
| 1:A:25:LEU:HD12 | 1:A:33:ALA:HB3 | 0.40 | 1.92 | 18 | 1 |
| 1:A:22:GLU:CD | 1:A:61:ILE:O | 0.40 | 2.60 | 2 | 1 |
| 1:A:31:GLU:HA | 1:A:51:THR:HG23 | 0.40 | 1.92 | 17 | 1 |
| 1:A:24:LEU:CB | 1:A:111:GLY:CA | 0.40 | 2.99 | 6 | 1 |
| 1:A:13:ASN:CB | 1:A:16:ILE:CB | 0.40 | 2.97 | 3 | 1 |
| 1:A:74:LYS:CD | 1:A:83:VAL:HB | 0.40 | 2.46 | 7 | 1 |
| 1:A:84:PHE:CD2 | 1:A:90:LEU:HG | 0.40 | 2.52 | 7 | 1 |
| 1:A:74:LYS:HB2 | 1:A:83:VAL:O | 0.40 | 2.15 | 17 | 1 |
| 1:A:88:PRO:HA | 1:A:91:ILE:HB | 0.40 | 1.93 | 17 | 1 |
| 1:A:30:LYS:HE3 | 1:A:107:TYR:HE2 | 0.40 | 1.68 | 4 | 1 |
| 1:A:30:LYS:CB | 1:A:33:ALA:HB2 | 0.40 | 2.44 | 15 | 1 |
| 1:A:13:ASN:HD22 | 1:A:24:LEU:CD1 | 0.40 | 2.22 | 20 | 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 | 97/110 (88%) | 67±2 (69±2%) | 14±2 (15±3%) | 16±2 (17±2%) | 0 | 4 |
| All | All | 1940/2200 (88%) | 1333 (69%) | 283 (15%) | 324 (17%) | 0 | 4 |

All 31 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 | 52 | LYS | 20 |
| 1 | A | 41 | THR | 20 |
| 1 | A | 42 | PRO | 20 |
| 1 | A | 80 | GLU | 19 |
| 1 | A | 104 | ARG | 19 |
| 1 | A | 105 | LEU | 19 |
| 1 | A | 7 | GLU | 18 |
| 1 | A | 103 | THR | 17 |
| 1 | A | 70 | ASN | 14 |
| 1 | A | 15 | SER | 14 |
| 1 | A | 97 | ASN | 14 |
| 1 | A | 10 | GLU | 13 |
| 1 | A | 99 | GLY | 13 |
| 1 | A | 79 | ALA | 12 |
| 1 | A | 74 | LYS | 11 |
| 1 | A | 100 | GLY | 10 |
| 1 | A | 102 | VAL | 10 |
| 1 | A | 101 | LEU | 9 |
| 1 | A | 14 | LYS | 8 |
| 1 | A | 53 | ALA | 7 |
| 1 | A | 6 | LEU | 6 |
| 1 | A | 82 | TYR | 6 |
| 1 | A | 8 | THR | 5 |
| 1 | A | 40 | ARG | 3 |
| 1 | A | 98 | GLY | 3 |
| 1 | A | 86 | SER | 3 |
| 1 | A | 111 | GLY | 3 |
| 1 | A | 30 | LYS | 3 |
| 1 | A | 75 | ARG | 2 |
| 1 | A | 44 | THR | 2 |
| 1 | A | 29 | GLY | 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 | 86/97 (89%) | 45±3 (52±3%) | 42±3 (48±3%) | 0 | 1 |
| All | All | 1720/1940 (89%) | 890 (52%) | 830 (48%) | 0 | 1 |

All 68 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 | 92 | GLN | 20 |
| 1 | A | 76 | TYR | 20 |
| 1 | A | 37 | ARG | 20 |
| 1 | A | 16 | ILE | 20 |
| 1 | A | 66 | ILE | 20 |
| 1 | A | 89 | LEU | 20 |
| 1 | A | 10 | GLU | 19 |
| 1 | A | 105 | LEU | 19 |
| 1 | A | 61 | ILE | 19 |
| 1 | A | 82 | TYR | 19 |
| 1 | A | 106 | ARG | 18 |
| 1 | A | 50 | PHE | 18 |
| 1 | A | 14 | LYS | 18 |
| 1 | A | 20 | LYS | 18 |
| 1 | A | 41 | THR | 18 |
| 1 | A | 44 | THR | 18 |
| 1 | A | 6 | LEU | 17 |
| 1 | A | 17 | SER | 17 |
| 1 | A | 67 | LYS | 17 |
| 1 | A | 48 | SER | 16 |
| 1 | A | 93 | TYR | 15 |
| 1 | A | 18 | ARG | 15 |
| 1 | A | 74 | LYS | 15 |
| 1 | A | 69 | THR | 15 |
| 1 | A | 24 | LEU | 15 |
| 1 | A | 94 | HIS | 15 |
| 1 | A | 110 | CYS | 15 |
| 1 | A | 87 | ILE | 14 |
| 1 | A | 81 | LYS | 14 |
| 1 | A | 52 | LYS | 14 |
| 1 | A | 86 | SER | 14 |
| 1 | A | 104 | ARG | 14 |
| 1 | A | 103 | THR | 14 |
| 1 | A | 7 | GLU | 14 |
| 1 | A | 101 | LEU | 13 |
| 1 | A | 70 | ASN | 13 |
| 1 | A | 65 | HIS | 13 |
| 1 | A | 15 | SER | 13 |
| 1 | A | 30 | LYS | 13 |
| 1 | A | 40 | ARG | 12 |
| 1 | A | 25 | LEU | 12 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 8 | THR | 11 |
| 1 | A | 75 | ARG | 11 |
| 1 | A | 23 | LYS | 11 |
| 1 | A | 26 | LEU | 11 |
| 1 | A | 28 | THR | 11 |
| 1 | A | 27 | ASP | 10 |
| 1 | A | 109 | VAL | 9 |
| 1 | A | 68 | GLU | 9 |
| 1 | A | 95 | GLN | 8 |
| 1 | A | 60 | CYS | 8 |
| 1 | A | 85 | ASP | 8 |
| 1 | A | 31 | GLU | 7 |
| 1 | A | 102 | VAL | 7 |
| 1 | A | 97 | ASN | 6 |
| 1 | A | 39 | SER | 5 |
| 1 | A | 62 | LYS | 5 |
| 1 | A | 45 | TYR | 4 |
| 1 | A | 19 | ASP | 3 |
| 1 | A | 49 | VAL | 3 |
| 1 | A | 83 | VAL | 3 |
| 1 | A | 38 | ASP | 3 |
| 1 | A | 51 | THR | 3 |
| 1 | A | 22 | GLU | 3 |
| 1 | A | 13 | ASN | 2 |
| 1 | A | 80 | GLU | 2 |
| 1 | A | 84 | PHE | 2 |
| 1 | A | 78 | VAL | 2 |

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 ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5461

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|------|
| Total number of shifts | 1213 |
| Number of shifts mapped to atoms | 1150 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 63 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 5 |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 63 occurrences are reported below.

| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|------------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| A | 116 | HIS | HD2 | 6.982 | -1.0 | 2 |
| A | 115 | ILE | HG23 | 0.824 | -1.0 | 4 |
| A | 115 | ILE | HD12 | 0.821 | -1.0 | 1 |
| A | 116 | HIS | CD2 | 116.712 | -1.0 | 1 |
| A | 114 | GLY | HA2 | 4.221 | -1.0 | 2 |
| A | 114 | GLY | HA3 | 3.707 | -1.0 | 2 |
| A | 117 | ARG | CD | 43.48 | -1.0 | 1 |
| A | 117 | ARG | CA | 55.943 | -1.0 | 1 |
| A | 113 | PRO | HD2 | 3.937 | -1.0 | 2 |
| A | 114 | GLY | CA | 45.397 | -1.0 | 1 |
| A | 115 | ILE | HG13 | 1.132 | -1.0 | 9 |
| A | 115 | ILE | HD13 | 0.821 | -1.0 | 1 |
| A | 115 | ILE | HB | 1.808 | -1.0 | 1 |
| A | 114 | GLY | N | 109.559 | -1.0 | 1 |

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| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|------------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| A | 117 | ARG | HB3 | 1.728 | -1.0 | 2 |
| A | 116 | HIS | CE1 | 135.637 | -1.0 | 1 |
| A | 116 | HIS | CB | 30.879 | -1.0 | 1 |
| A | 115 | ILE | N | 119.987 | -1.0 | 1 |
| A | 115 | ILE | CA | 61.146 | -1.0 | 1 |
| A | 116 | HIS | HB2 | 3.072 | -1.0 | 2 |
| A | 112 | SER | HA | 4.813 | -1.0 | 1 |
| A | 117 | ARG | HA | 4.399 | -1.0 | 1 |
| A | 118 | ASP | N | 127.786 | -1.0 | 1 |
| A | 115 | ILE | CG2 | 17.467 | -1.0 | 2 |
| A | 117 | ARG | H | 8.214 | -1.0 | 1 |
| A | 117 | ARG | CG | 26.983 | -1.0 | 1 |
| A | 115 | ILE | HG22 | 0.824 | -1.0 | 4 |
| A | 115 | ILE | H | 7.832 | -1.0 | 1 |
| A | 117 | ARG | HB2 | 1.878 | -1.0 | 2 |
| A | 112 | SER | H | 8.091 | -1.0 | 1 |
| A | 117 | ARG | HG2 | 1.606 | -1.0 | 2 |
| A | 115 | ILE | CB | 38.959 | -1.0 | 1 |
| A | 117 | ARG | HD2 | 3.198 | -1.0 | 2 |
| A | 113 | PRO | HB3 | 2.032 | -1.0 | 2 |
| A | 112 | SER | CA | 56.089 | -1.0 | 1 |
| A | 116 | HIS | HE1 | 7.79 | -1.0 | 2 |
| A | 113 | PRO | HB2 | 2.399 | -1.0 | 2 |
| A | 115 | ILE | CD1 | 12.943 | -1.0 | 1 |
| A | 113 | PRO | CG | 27.474 | -1.0 | 1 |
| A | 112 | SER | HB3 | 3.837 | -1.0 | 2 |
| A | 112 | SER | HB2 | 3.869 | -1.0 | 2 |
| A | 113 | PRO | CD | 50.953 | -1.0 | 1 |
| A | 117 | ARG | N | 124.475 | -1.0 | 1 |
| A | 113 | PRO | CB | 32.313 | -1.0 | 1 |
| A | 113 | PRO | HA | 4.556 | -1.0 | 1 |
| A | 113 | PRO | HG2 | 2.121 | -1.0 | 2 |
| A | 114 | GLY | H | 8.461 | -1.0 | 1 |
| A | 113 | PRO | HD3 | 3.868 | -1.0 | 2 |
| A | 115 | ILE | HA | 4.168 | -1.0 | 1 |
| A | 118 | ASP | CB | 42.423 | -1.0 | 1 |
| A | 116 | HIS | HA | 4.654 | -1.0 | 1 |
| A | 116 | HIS | N | 124.354 | -1.0 | 1 |
| A | 112 | SER | CB | 63.495 | -1.0 | 1 |
| A | 116 | HIS | CA | 56.424 | -1.0 | 1 |
| A | 115 | ILE | HG12 | 1.315 | -1.0 | 9 |

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| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|------------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| A | 116 | HIS | H | 8.42 | -1.0 | 1 |
| A | 115 | ILE | HD11 | 0.821 | -1.0 | 1 |
| A | 117 | ARG | CB | 31.416 | -1.0 | 1 |
| A | 113 | PRO | CA | 63.806 | -1.0 | 1 |
| A | 118 | ASP | H | 8.025 | -1.0 | 1 |
| A | 115 | ILE | HG21 | 0.824 | -1.0 | 4 |
| A | 115 | ILE | CG1 | 27.161 | -1.0 | 2 |
| A | 112 | SER | N | 117.006 | -1.0 | 1 |

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 113 | -0.34 ± 0.29 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 106 | -0.23 ± 0.26 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | — |
| ^{15}N | 107 | -0.17 ± 0.41 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 997 atoms were assigned a chemical shift out of a possible 1250. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone | 379/479 (79%) | 189/191 (99%) | 96/194 (49%) | 94/94 (100%) |
| Sidechain | 517/630 (82%) | 324/371 (87%) | 186/227 (82%) | 7/32 (22%) |
| Aromatic | 101/141 (72%) | 71/73 (97%) | 30/63 (48%) | 0/5 (0%) |
| Overall | 997/1250 (80%) | 584/635 (92%) | 312/484 (64%) | 101/131 (77%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1098 atoms were assigned a chemical shift out of a possible 1375. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 415/530 (78%) | 207/211 (98%) | 107/216 (50%) | 101/103 (98%) |
| Sidechain | 582/704 (83%) | 366/415 (88%) | 206/254 (81%) | 10/35 (29%) |
| Aromatic | 101/141 (72%) | 71/73 (97%) | 30/63 (48%) | 0/5 (0%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|---------|-----------------|----------------|-----------------|-----------------|
| Overall | 1098/1375 (80%) | 644/699 (92%) | 343/533 (64%) | 111/143 (78%) |

7.1.4 Statistically unusual chemical shifts ⓘ

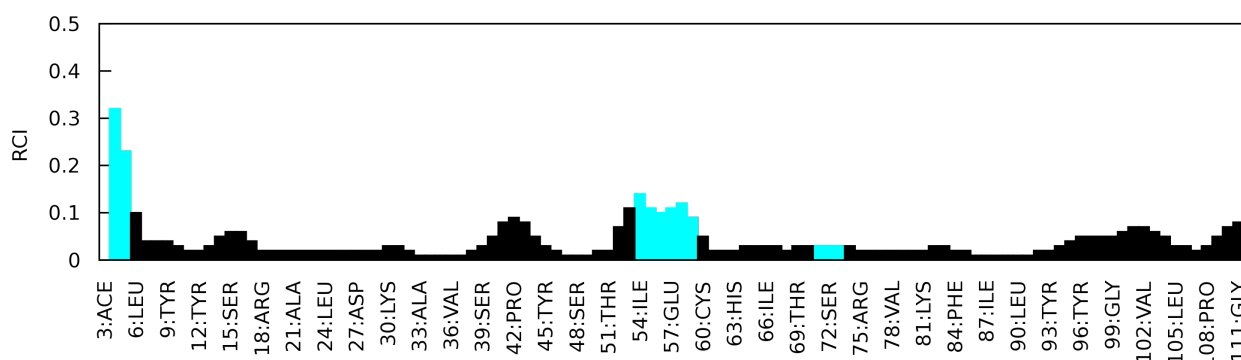
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 75 | ARG | NE | 121.48 | 92.63 – 76.73 | 23.1 |
| 1 | A | 37 | ARG | NE | 117.93 | 92.63 – 76.73 | 20.9 |
| 1 | A | 105 | LEU | HB3 | -1.01 | 3.34 – -0.26 | -7.1 |
| 1 | A | 9 | TYR | HB3 | 0.65 | 4.75 – 0.95 | -5.8 |
| 1 | A | 67 | LYS | HB3 | 0.29 | 3.10 – 0.40 | -5.4 |

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5461

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|------|
| Total number of shifts | 1228 |
| Number of shifts mapped to atoms | 1165 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 63 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 6 |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 63 occurrences are reported below.

| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|------------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| A | 116 | HIS | HD2 | 6.982 | -1.0 | 2 |
| A | 115 | ILE | HG23 | 0.824 | -1.0 | 4 |
| A | 115 | ILE | HD12 | 0.821 | -1.0 | 1 |
| A | 116 | HIS | CD2 | 116.712 | -1.0 | 1 |
| A | 114 | GLY | HA2 | 4.221 | -1.0 | 2 |
| A | 114 | GLY | HA3 | 3.707 | -1.0 | 2 |
| A | 117 | ARG | CD | 43.48 | -1.0 | 1 |
| A | 117 | ARG | CA | 55.943 | -1.0 | 1 |
| A | 113 | PRO | HD2 | 3.937 | -1.0 | 2 |
| A | 114 | GLY | CA | 45.397 | -1.0 | 1 |
| A | 115 | ILE | HG13 | 1.132 | -1.0 | 9 |
| A | 115 | ILE | HD13 | 0.821 | -1.0 | 1 |
| A | 115 | ILE | HB | 1.808 | -1.0 | 1 |
| A | 114 | GLY | N | 109.664 | -1.0 | 1 |
| A | 117 | ARG | HB3 | 1.728 | -1.0 | 2 |
| A | 116 | HIS | CE1 | 135.637 | -1.0 | 1 |
| A | 116 | HIS | CB | 30.879 | -1.0 | 1 |
| A | 115 | ILE | N | 120.026 | -1.0 | 1 |
| A | 115 | ILE | CA | 61.146 | -1.0 | 1 |
| A | 116 | HIS | HB2 | 3.072 | -1.0 | 2 |
| A | 112 | SER | HA | 4.813 | -1.0 | 1 |
| A | 117 | ARG | HA | 4.399 | -1.0 | 1 |
| A | 118 | ASP | N | 127.859 | -1.0 | 1 |
| A | 115 | ILE | CG2 | 17.467 | -1.0 | 2 |
| A | 117 | ARG | H | 8.169 | -1.0 | 1 |
| A | 117 | ARG | CG | 26.983 | -1.0 | 1 |

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| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|------------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| A | 115 | ILE | HG22 | 0.824 | -1.0 | 4 |
| A | 115 | ILE | H | 7.828 | -1.0 | 1 |
| A | 117 | ARG | HB2 | 1.878 | -1.0 | 2 |
| A | 112 | SER | H | 8.105 | -1.0 | 1 |
| A | 117 | ARG | HG2 | 1.606 | -1.0 | 2 |
| A | 115 | ILE | CB | 38.959 | -1.0 | 1 |
| A | 117 | ARG | HD2 | 3.198 | -1.0 | 2 |
| A | 113 | PRO | HB3 | 2.032 | -1.0 | 2 |
| A | 112 | SER | CA | 56.089 | -1.0 | 1 |
| A | 116 | HIS | HE1 | 7.79 | -1.0 | 2 |
| A | 113 | PRO | HB2 | 2.399 | -1.0 | 2 |
| A | 115 | ILE | CD1 | 12.943 | -1.0 | 1 |
| A | 113 | PRO | CG | 27.474 | -1.0 | 1 |
| A | 112 | SER | HB3 | 3.837 | -1.0 | 2 |
| A | 112 | SER | HB2 | 3.869 | -1.0 | 2 |
| A | 113 | PRO | CD | 50.953 | -1.0 | 1 |
| A | 117 | ARG | N | 124.39 | -1.0 | 1 |
| A | 113 | PRO | CB | 32.313 | -1.0 | 1 |
| A | 113 | PRO | HA | 4.556 | -1.0 | 1 |
| A | 113 | PRO | HG2 | 2.121 | -1.0 | 2 |
| A | 114 | GLY | H | 8.457 | -1.0 | 1 |
| A | 113 | PRO | HD3 | 3.868 | -1.0 | 2 |
| A | 115 | ILE | HA | 4.168 | -1.0 | 1 |
| A | 118 | ASP | CB | 42.423 | -1.0 | 1 |
| A | 116 | HIS | HA | 4.654 | -1.0 | 1 |
| A | 116 | HIS | N | 124.554 | -1.0 | 1 |
| A | 112 | SER | CB | 63.495 | -1.0 | 1 |
| A | 116 | HIS | CA | 56.424 | -1.0 | 1 |
| A | 115 | ILE | HG12 | 1.315 | -1.0 | 9 |
| A | 116 | HIS | H | 8.385 | -1.0 | 1 |
| A | 115 | ILE | HD11 | 0.821 | -1.0 | 1 |
| A | 117 | ARG | CB | 31.416 | -1.0 | 1 |
| A | 113 | PRO | CA | 63.806 | -1.0 | 1 |
| A | 118 | ASP | H | 8.013 | -1.0 | 1 |
| A | 115 | ILE | HG21 | 0.824 | -1.0 | 4 |
| A | 115 | ILE | CG1 | 27.161 | -1.0 | 2 |
| A | 112 | SER | N | 117.132 | -1.0 | 1 |

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 114 | -0.31 ± 0.13 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 107 | -0.21 ± 0.13 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | — |
| ^{15}N | 107 | -0.34 ± 0.42 | None needed (< 0.5 ppm) |

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1009 atoms were assigned a chemical shift out of a possible 1250. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone | 380/479 (79%) | 189/191 (99%) | 97/194 (50%) | 94/94 (100%) |
| Sidechain | 528/630 (84%) | 328/371 (88%) | 193/227 (85%) | 7/32 (22%) |
| Aromatic | 101/141 (72%) | 71/73 (97%) | 30/63 (48%) | 0/5 (0%) |
| Overall | 1009/1250 (81%) | 588/635 (93%) | 320/484 (66%) | 101/131 (77%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1114 atoms were assigned a chemical shift out of a possible 1375. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone | 416/530 (78%) | 207/211 (98%) | 108/216 (50%) | 101/103 (98%) |
| Sidechain | 597/704 (85%) | 372/415 (90%) | 215/254 (85%) | 10/35 (29%) |
| Aromatic | 101/141 (72%) | 71/73 (97%) | 30/63 (48%) | 0/5 (0%) |
| Overall | 1114/1375 (81%) | 650/699 (93%) | 353/533 (66%) | 111/143 (78%) |

7.2.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 75 | ARG | NE | 121.48 | 92.63 – 76.73 | 23.1 |
| 1 | A | 37 | ARG | NE | 117.93 | 92.63 – 76.73 | 20.9 |
| 1 | A | 105 | LEU | HB3 | -1.01 | 3.34 – -0.26 | -7.1 |
| 1 | A | 26 | LEU | HG | 3.64 | 3.16 – -0.14 | 6.5 |
| 1 | A | 9 | TYR | HB3 | 0.65 | 4.75 – 0.95 | -5.8 |
| 1 | A | 67 | LYS | HB3 | 0.29 | 3.10 – 0.40 | -5.4 |

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

