



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:31 PM BST

PDB ID : 1JZU
Title : Cell transformation by the myc oncogene activates expression of a lipocalin: analysis of the gene (Q83) and solution structure of its protein product
Authors : Hartl, M.; Matt, T.; Schueler, W.; Siemeister, G.; Kontaxis, G.; Kloiber, K.; Konrat, R.; Bister, K.
Deposited on : 2001-09-17

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

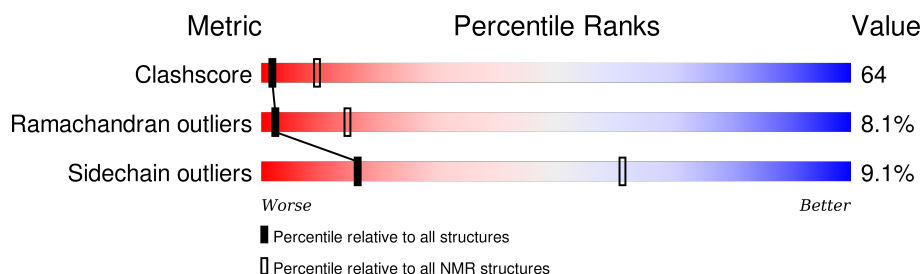
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 53%.

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 | 157 | |

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 15 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|--|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:5-A:54, A:59-A:147, A:152-A:154 (142) | 0.94 | 3 |

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 4 clusters and 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2528 atoms, of which 1262 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called lipocalin Q83.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|-------|
| 1 | A | 157 | Total | C | H | N | O | S | 0 |
| | | | 2528 | 799 | 1262 | 213 | 244 | 10 | |

There is a discrepancy between the modelled and reference sequences:

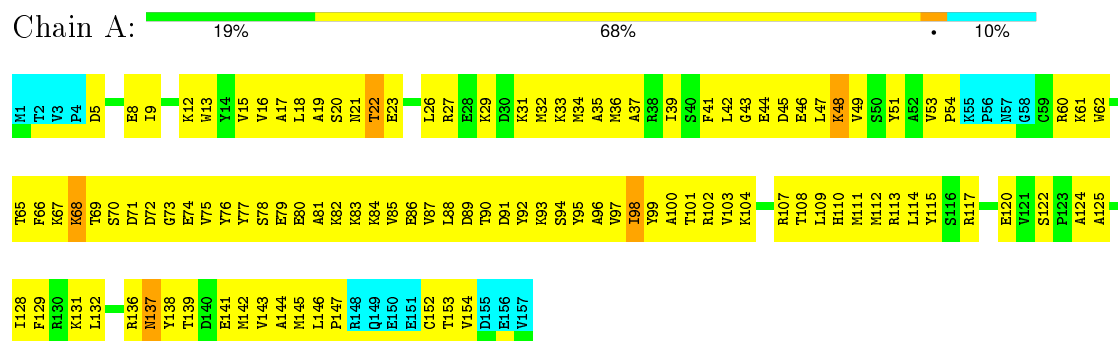
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|------------|
| A | 1 | MET | ALA | ENGINEERED | UNP Q9I9P7 |

4 Residue-property plots [i](#)

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: lipocalin Q83

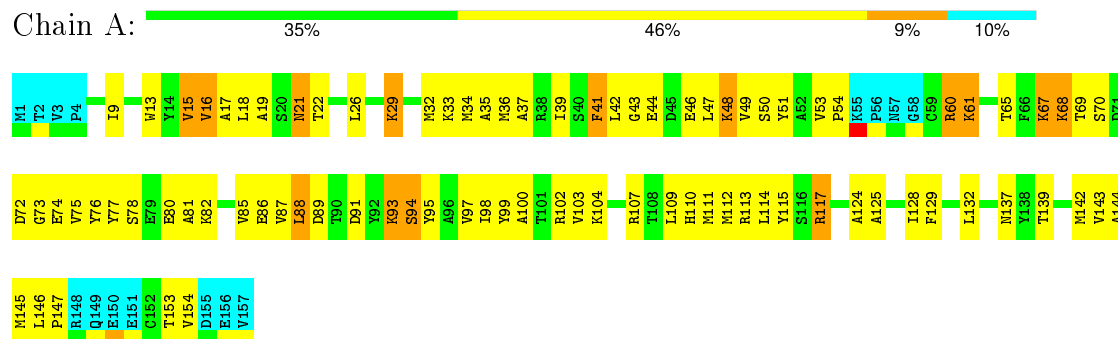


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

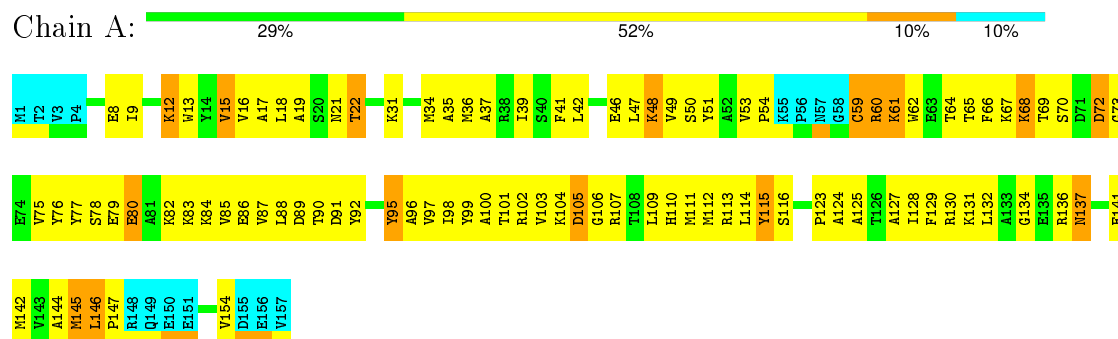
4.2.1 Score per residue for model 1

- Molecule 1: lipocalin Q83



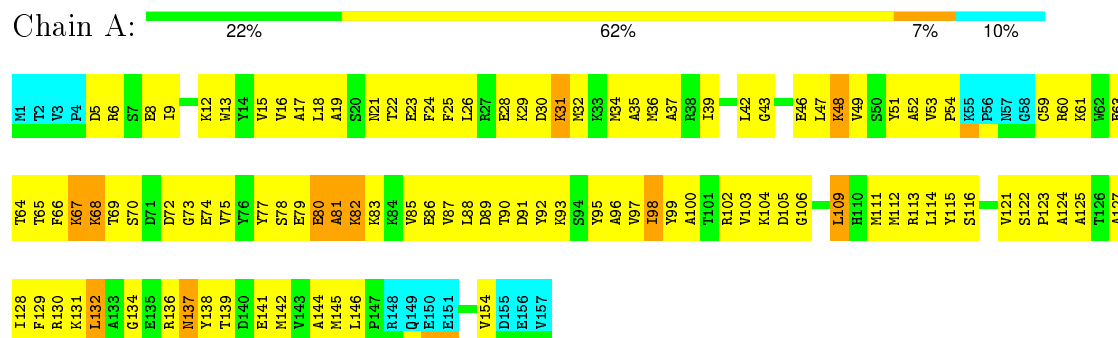
4.2.5 Score per residue for model 5

- Molecule 1: lipocalin Q83



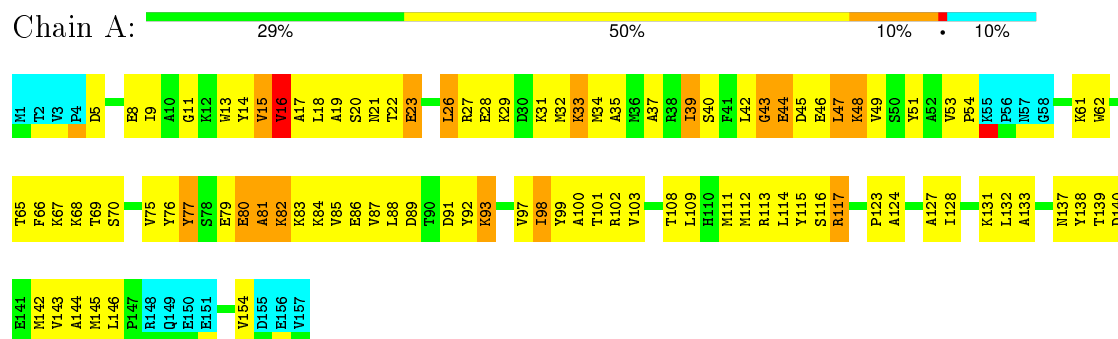
4.2.6 Score per residue for model 6

- Molecule 1: lipocalin Q83



4.2.7 Score per residue for model 7

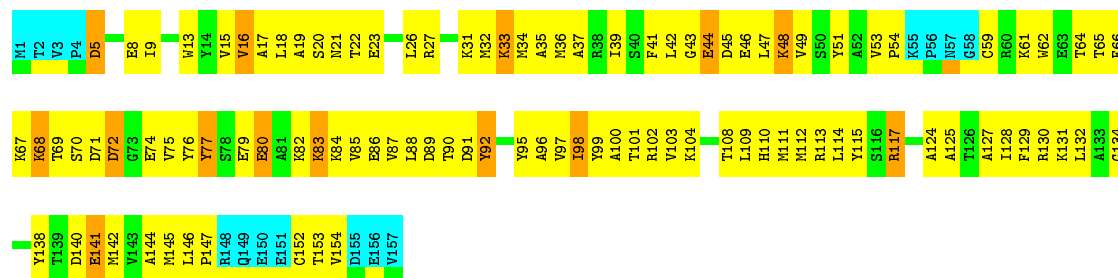
- Molecule 1: lipocalin Q83



4.2.8 Score per residue for model 8

- Molecule 1: lipocalin Q83

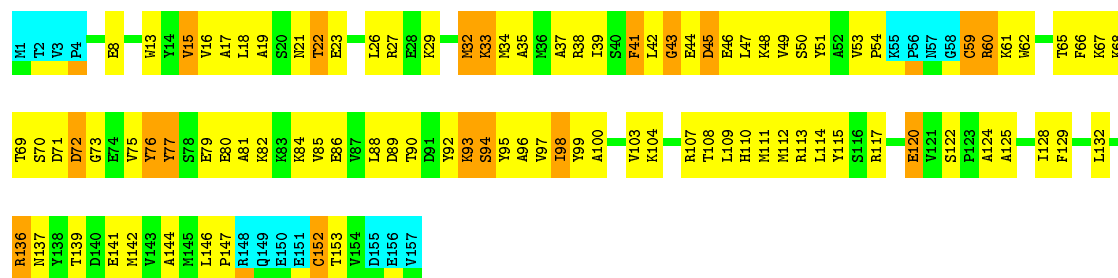
Chain A: 25% 57% 9% 10%



4.2.9 Score per residue for model 9

- Molecule 1: lipocalin Q83

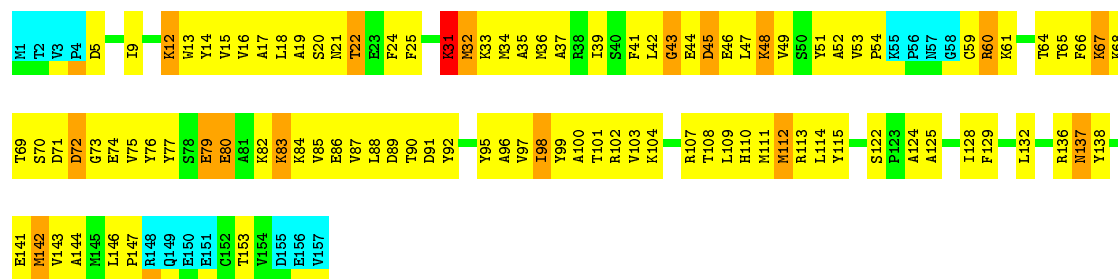
Chain A: 29% 50% 11% 10%



4.2.10 Score per residue for model 10

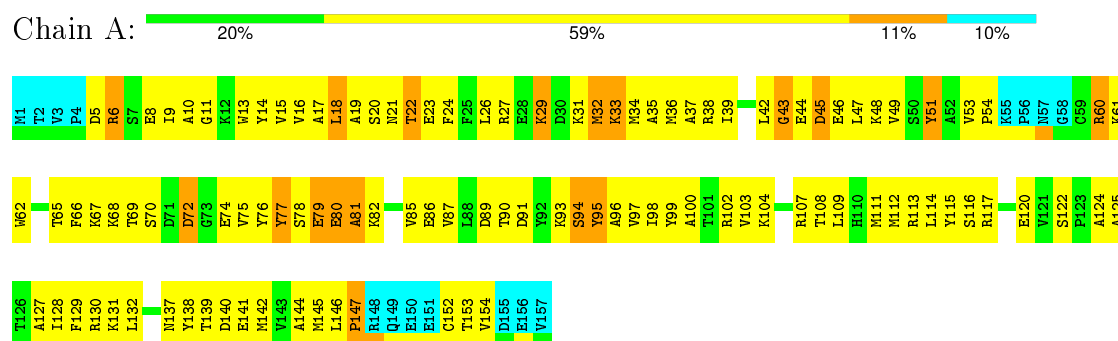
- Molecule 1: lipocalin Q83

Chain A: 26% 54% 10% • 10%



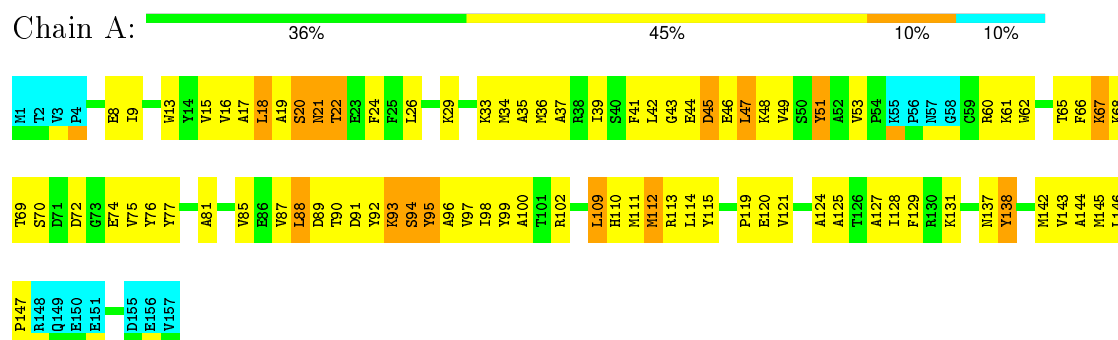
4.2.11 Score per residue for model 11

- Molecule 1: lipocalin Q83



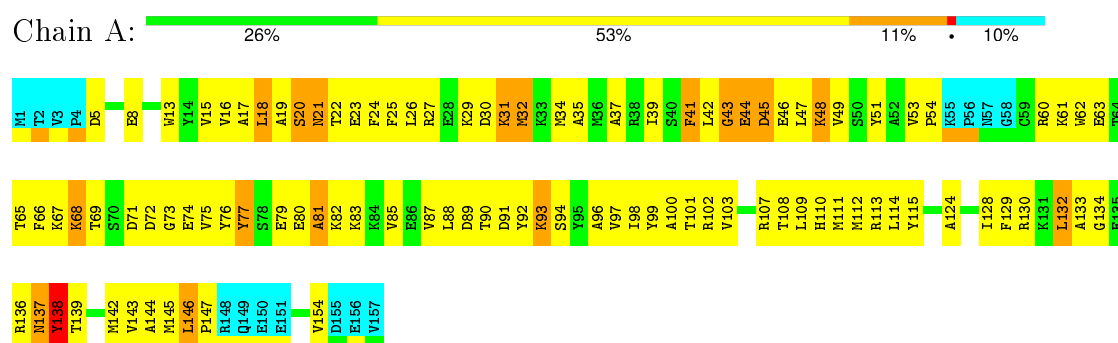
4.2.12 Score per residue for model 12

- Molecule 1: lipocalin Q83



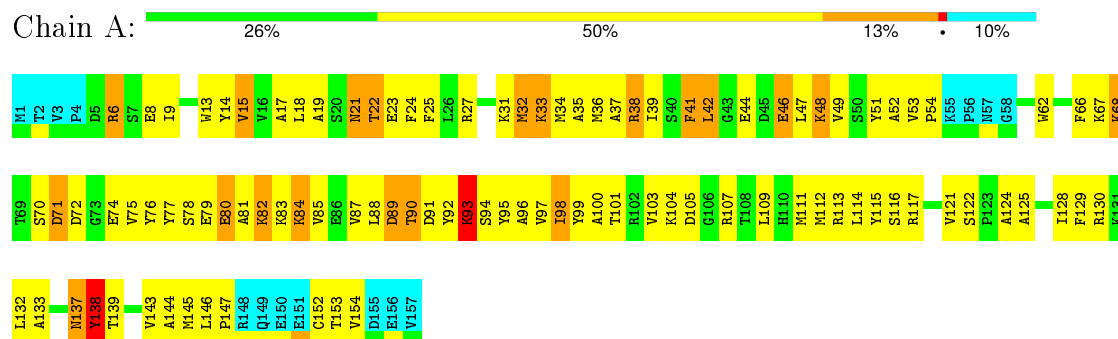
4.2.13 Score per residue for model 13

- Molecule 1: lipocalin Q83



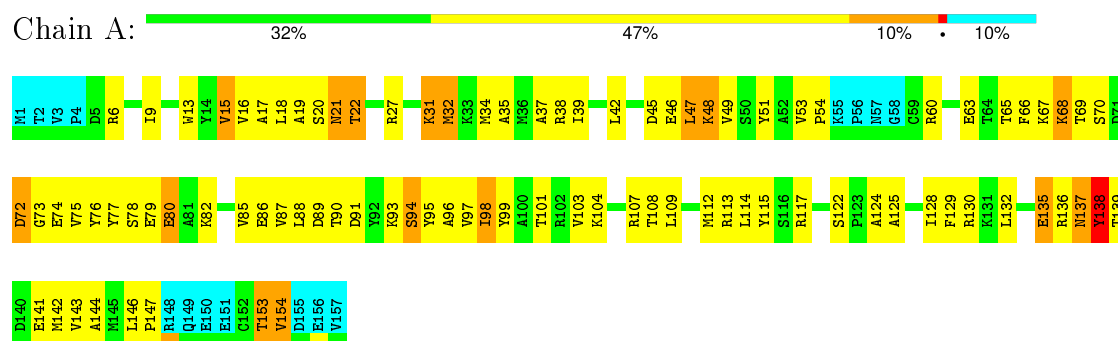
4.2.14 Score per residue for model 14

- Molecule 1: lipocalin Q83



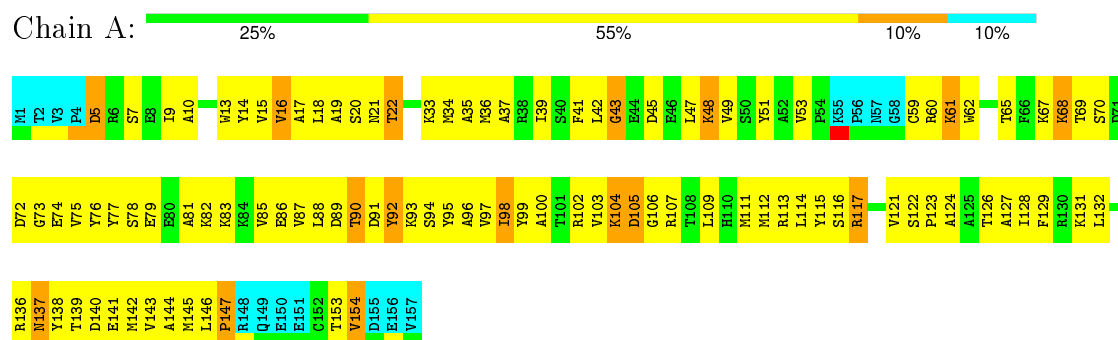
4.2.17 Score per residue for model 17

- Molecule 1: lipocalin Q83



4.2.18 Score per residue for model 18

- Molecule 1: lipocalin Q83



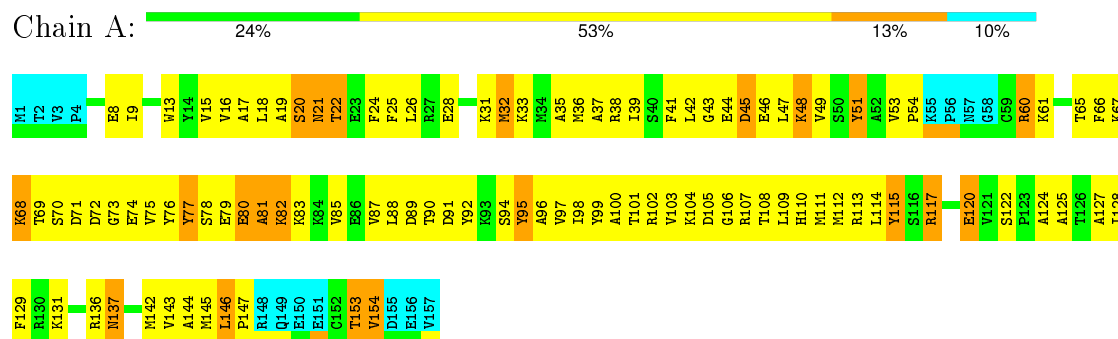
4.2.19 Score per residue for model 19

- Molecule 1: lipocalin Q83



4.2.20 Score per residue for model 20

- Molecule 1: lipocalin Q83



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA/CNS automated refinement using also ambiguous NOE distance constraints; simulated annealing (torsion angle dynamics)*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| ARIA/CNS | structure solution | 1.0 |
| 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 4664 |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1050 |
| Number of shifts mapped to atoms | 1050 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 53% |

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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 | 1146 | 1147 | 1146 | 146±15 |
| All | All | 22920 | 22940 | 22920 | 2915 |

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 64.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:97:VAL:HG12 | 1:A:114:LEU:HD23 | 1.09 | 1.13 | 12 | 2 |
| 1:A:87:VAL:HG22 | 1:A:98:ILE:HD13 | 1.06 | 1.21 | 2 | 7 |
| 1:A:87:VAL:HG22 | 1:A:98:ILE:HD12 | 1.05 | 1.29 | 16 | 3 |
| 1:A:16:VAL:HG22 | 1:A:146:LEU:HD22 | 1.00 | 1.27 | 2 | 2 |
| 1:A:145:MET:HB2 | 1:A:154:VAL:HG22 | 0.95 | 1.38 | 5 | 1 |
| 1:A:18:LEU:O | 1:A:144:ALA:O | 0.95 | 1.85 | 13 | 13 |
| 1:A:88:LEU:HD11 | 1:A:132:LEU:HD11 | 0.94 | 1.35 | 18 | 1 |
| 1:A:97:VAL:HG12 | 1:A:114:LEU:HD13 | 0.93 | 1.35 | 14 | 2 |
| 1:A:17:ALA:O | 1:A:18:LEU:HD13 | 0.92 | 1.64 | 4 | 4 |
| 1:A:15:VAL:CG1 | 1:A:35:ALA:HB3 | 0.92 | 1.94 | 11 | 9 |
| 1:A:85:VAL:HG11 | 1:A:98:ILE:HD11 | 0.91 | 1.42 | 8 | 2 |
| 1:A:16:VAL:CG2 | 1:A:146:LEU:HD22 | 0.91 | 1.96 | 1 | 5 |
| 1:A:85:VAL:HG23 | 1:A:98:ILE:HD11 | 0.91 | 1.40 | 11 | 4 |
| 1:A:15:VAL:HG12 | 1:A:35:ALA:HB3 | 0.91 | 1.40 | 10 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:85:VAL:CG1 | 1:A:98:ILE:HD11 | 0.90 | 1.97 | 8 | 6 |
| 1:A:35:ALA:HB2 | 1:A:53:VAL:HG12 | 0.90 | 1.41 | 10 | 5 |
| 1:A:13:TRP:CH2 | 1:A:49:VAL:HG21 | 0.89 | 2.01 | 11 | 1 |
| 1:A:97:VAL:HG12 | 1:A:114:LEU:CD1 | 0.89 | 1.97 | 18 | 4 |
| 1:A:75:VAL:HG13 | 1:A:87:VAL:HB | 0.89 | 1.43 | 6 | 9 |
| 1:A:97:VAL:HG12 | 1:A:114:LEU:CD2 | 0.88 | 1.98 | 17 | 2 |
| 1:A:37:ALA:HB2 | 1:A:51:TYR:HB3 | 0.87 | 1.45 | 11 | 8 |
| 1:A:75:VAL:HG13 | 1:A:87:VAL:HG13 | 0.87 | 1.46 | 18 | 1 |
| 1:A:85:VAL:HG13 | 1:A:98:ILE:HD11 | 0.87 | 1.44 | 14 | 3 |
| 1:A:88:LEU:HD13 | 1:A:132:LEU:HD13 | 0.86 | 1.45 | 2 | 3 |
| 1:A:87:VAL:CG2 | 1:A:98:ILE:HD13 | 0.86 | 2.00 | 2 | 7 |
| 1:A:16:VAL:HG22 | 1:A:146:LEU:HD13 | 0.86 | 1.45 | 3 | 1 |
| 1:A:87:VAL:HG22 | 1:A:98:ILE:HG13 | 0.86 | 1.46 | 3 | 5 |
| 1:A:16:VAL:HG22 | 1:A:146:LEU:CB | 0.86 | 2.00 | 13 | 1 |
| 1:A:87:VAL:HG13 | 1:A:98:ILE:HB | 0.85 | 1.49 | 8 | 5 |
| 1:A:13:TRP:CZ2 | 1:A:39:ILE:HD12 | 0.85 | 2.05 | 19 | 6 |
| 1:A:15:VAL:HG13 | 1:A:35:ALA:HB1 | 0.85 | 1.47 | 19 | 5 |
| 1:A:18:LEU:HD23 | 1:A:19:ALA:N | 0.84 | 1.87 | 1 | 1 |
| 1:A:35:ALA:HB1 | 1:A:53:VAL:HG12 | 0.84 | 1.47 | 13 | 1 |
| 1:A:16:VAL:HG22 | 1:A:146:LEU:HB3 | 0.84 | 1.48 | 13 | 1 |
| 1:A:69:THR:O | 1:A:77:TYR:HA | 0.84 | 1.73 | 10 | 14 |
| 1:A:85:VAL:HG12 | 1:A:100:ALA:HA | 0.84 | 1.47 | 11 | 7 |
| 1:A:79:GLU:O | 1:A:80:GLU:O | 0.83 | 1.97 | 7 | 6 |
| 1:A:19:ALA:HB1 | 1:A:142:MET:O | 0.83 | 1.72 | 1 | 11 |
| 1:A:15:VAL:HG13 | 1:A:35:ALA:CB | 0.83 | 2.04 | 19 | 11 |
| 1:A:147:PRO:CB | 1:A:153:THR:HG21 | 0.82 | 2.03 | 20 | 1 |
| 1:A:85:VAL:CG2 | 1:A:98:ILE:HD11 | 0.81 | 2.04 | 19 | 7 |
| 1:A:85:VAL:HB | 1:A:98:ILE:HD11 | 0.81 | 1.52 | 6 | 4 |
| 1:A:13:TRP:CE3 | 1:A:49:VAL:HG21 | 0.80 | 2.11 | 7 | 2 |
| 1:A:95:TYR:CG | 1:A:125:ALA:HB2 | 0.80 | 2.12 | 14 | 13 |
| 1:A:17:ALA:C | 1:A:18:LEU:HD12 | 0.80 | 1.96 | 17 | 9 |
| 1:A:97:VAL:HG11 | 1:A:129:PHE:HB2 | 0.80 | 1.53 | 12 | 18 |
| 1:A:17:ALA:C | 1:A:18:LEU:HD22 | 0.80 | 1.97 | 3 | 5 |
| 1:A:17:ALA:HB3 | 1:A:114:LEU:CB | 0.80 | 2.07 | 18 | 15 |
| 1:A:69:THR:HG22 | 1:A:78:SER:O | 0.79 | 1.77 | 11 | 2 |
| 1:A:75:VAL:HB | 1:A:87:VAL:HG13 | 0.79 | 1.54 | 12 | 1 |
| 1:A:96:ALA:HB3 | 1:A:115:TYR:CE1 | 0.79 | 2.11 | 19 | 3 |
| 1:A:132:LEU:HD12 | 1:A:133:ALA:N | 0.79 | 1.92 | 7 | 2 |
| 1:A:85:VAL:HG12 | 1:A:98:ILE:HD11 | 0.79 | 1.55 | 12 | 3 |
| 1:A:77:TYR:CE2 | 1:A:85:VAL:HG21 | 0.79 | 2.13 | 2 | 2 |
| 1:A:95:TYR:CD1 | 1:A:125:ALA:HB2 | 0.78 | 2.12 | 10 | 11 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:47:LEU:O | 1:A:47:LEU:HD12 | 0.78 | 1.78 | 6 | 2 |
| 1:A:87:VAL:HG22 | 1:A:98:ILE:CG1 | 0.78 | 2.09 | 14 | 9 |
| 1:A:34:MET:O | 1:A:53:VAL:HG13 | 0.78 | 1.79 | 6 | 5 |
| 1:A:22:THR:HG23 | 1:A:109:LEU:HD12 | 0.78 | 1.55 | 10 | 1 |
| 1:A:154:VAL:HG13 | 1:A:154:VAL:O | 0.78 | 1.78 | 5 | 4 |
| 1:A:26:LEU:HD12 | 1:A:27:ARG:N | 0.78 | 1.92 | 13 | 1 |
| 1:A:15:VAL:HG11 | 1:A:35:ALA:HB3 | 0.78 | 1.54 | 6 | 2 |
| 1:A:75:VAL:HG21 | 1:A:91:ASP:OD2 | 0.77 | 1.80 | 3 | 3 |
| 1:A:108:THR:C | 1:A:109:LEU:HD12 | 0.77 | 2.00 | 9 | 4 |
| 1:A:68:LYS:HB3 | 1:A:78:SER:O | 0.77 | 1.80 | 19 | 7 |
| 1:A:35:ALA:CB | 1:A:53:VAL:HG12 | 0.77 | 2.10 | 13 | 6 |
| 1:A:23:GLU:O | 1:A:26:LEU:HD12 | 0.77 | 1.80 | 7 | 1 |
| 1:A:16:VAL:HG22 | 1:A:146:LEU:HB2 | 0.76 | 1.57 | 15 | 4 |
| 1:A:47:LEU:HD12 | 1:A:47:LEU:O | 0.76 | 1.81 | 16 | 2 |
| 1:A:108:THR:C | 1:A:109:LEU:HD22 | 0.76 | 2.01 | 17 | 7 |
| 1:A:146:LEU:HD12 | 1:A:147:PRO:HD2 | 0.76 | 1.58 | 15 | 7 |
| 1:A:109:LEU:HD22 | 1:A:109:LEU:O | 0.76 | 1.81 | 2 | 1 |
| 1:A:89:ASP:O | 1:A:90:THR:HG22 | 0.76 | 1.80 | 4 | 1 |
| 1:A:22:THR:HG21 | 1:A:109:LEU:HD23 | 0.76 | 1.58 | 20 | 1 |
| 1:A:9:ILE:HD11 | 1:A:91:ASP:OD1 | 0.76 | 1.80 | 10 | 2 |
| 1:A:147:PRO:HB2 | 1:A:153:THR:HG21 | 0.75 | 1.57 | 20 | 1 |
| 1:A:16:VAL:CG2 | 1:A:146:LEU:HD13 | 0.75 | 2.10 | 3 | 1 |
| 1:A:88:LEU:HD13 | 1:A:132:LEU:HD22 | 0.75 | 1.59 | 7 | 2 |
| 1:A:9:ILE:HD13 | 1:A:91:ASP:O | 0.75 | 1.82 | 1 | 5 |
| 1:A:9:ILE:HG22 | 1:A:39:ILE:CD1 | 0.75 | 2.11 | 19 | 1 |
| 1:A:19:ALA:HB3 | 1:A:112:MET:HB2 | 0.75 | 1.57 | 18 | 15 |
| 1:A:16:VAL:HB | 1:A:146:LEU:HD13 | 0.75 | 1.58 | 6 | 1 |
| 1:A:18:LEU:HD23 | 1:A:113:ARG:HA | 0.75 | 1.59 | 8 | 1 |
| 1:A:124:ALA:HB1 | 1:A:128:ILE:HD12 | 0.74 | 1.58 | 13 | 13 |
| 1:A:9:ILE:O | 1:A:9:ILE:HG22 | 0.74 | 1.82 | 4 | 4 |
| 1:A:17:ALA:HB3 | 1:A:114:LEU:HB3 | 0.74 | 1.58 | 16 | 17 |
| 1:A:47:LEU:O | 1:A:47:LEU:HD22 | 0.74 | 1.82 | 12 | 2 |
| 1:A:145:MET:O | 1:A:154:VAL:HG11 | 0.74 | 1.81 | 16 | 2 |
| 1:A:75:VAL:HG13 | 1:A:87:VAL:CB | 0.74 | 2.12 | 6 | 7 |
| 1:A:46:GLU:C | 1:A:47:LEU:HD12 | 0.74 | 2.03 | 14 | 4 |
| 1:A:109:LEU:HD23 | 1:A:110:HIS:N | 0.74 | 1.96 | 5 | 2 |
| 1:A:97:VAL:HG12 | 1:A:114:LEU:HG | 0.74 | 1.60 | 6 | 11 |
| 1:A:114:LEU:HD23 | 1:A:115:TYR:N | 0.73 | 1.99 | 16 | 10 |
| 1:A:124:ALA:HB1 | 1:A:128:ILE:CD1 | 0.73 | 2.13 | 3 | 18 |
| 1:A:53:VAL:O | 1:A:61:LYS:HA | 0.73 | 1.84 | 6 | 16 |
| 1:A:9:ILE:HG23 | 1:A:39:ILE:HD13 | 0.73 | 1.60 | 6 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:5:ASP:O | 1:A:8:GLU:HG2 | 0.73 | 1.83 | 8 | 6 |
| 1:A:19:ALA:O | 1:A:111:MET:HA | 0.73 | 1.83 | 2 | 12 |
| 1:A:88:LEU:HD23 | 1:A:89:ASP:N | 0.73 | 1.99 | 4 | 1 |
| 1:A:8:GLU:O | 1:A:9:ILE:HD13 | 0.73 | 1.84 | 12 | 1 |
| 1:A:17:ALA:C | 1:A:18:LEU:HD23 | 0.73 | 2.05 | 11 | 2 |
| 1:A:136:ARG:NH1 | 1:A:139:THR:HG21 | 0.72 | 1.99 | 18 | 1 |
| 1:A:15:VAL:CG2 | 1:A:18:LEU:HD11 | 0.72 | 2.15 | 13 | 2 |
| 1:A:85:VAL:HG12 | 1:A:98:ILE:CG1 | 0.72 | 2.14 | 1 | 5 |
| 1:A:86:GLU:OE2 | 1:A:88:LEU:HD21 | 0.72 | 1.84 | 10 | 1 |
| 1:A:87:VAL:HG22 | 1:A:98:ILE:CD1 | 0.72 | 2.15 | 5 | 9 |
| 1:A:47:LEU:HD22 | 1:A:47:LEU:O | 0.72 | 1.85 | 7 | 1 |
| 1:A:143:VAL:HG22 | 1:A:144:ALA:N | 0.71 | 1.99 | 4 | 5 |
| 1:A:18:LEU:HD23 | 1:A:147:PRO:HD2 | 0.71 | 1.61 | 18 | 1 |
| 1:A:88:LEU:CD1 | 1:A:132:LEU:HD22 | 0.71 | 2.15 | 15 | 2 |
| 1:A:9:ILE:HD12 | 1:A:91:ASP:O | 0.71 | 1.85 | 12 | 2 |
| 1:A:75:VAL:HG11 | 1:A:91:ASP:HB2 | 0.71 | 1.61 | 7 | 2 |
| 1:A:132:LEU:HD22 | 1:A:132:LEU:O | 0.71 | 1.86 | 13 | 1 |
| 1:A:98:ILE:HG23 | 1:A:113:ARG:HB3 | 0.70 | 1.64 | 19 | 5 |
| 1:A:143:VAL:HG22 | 1:A:144:ALA:H | 0.70 | 1.45 | 4 | 3 |
| 1:A:20:SER:HA | 1:A:142:MET:CB | 0.70 | 2.17 | 13 | 3 |
| 1:A:147:PRO:O | 1:A:154:VAL:HG23 | 0.70 | 1.85 | 5 | 1 |
| 1:A:101:THR:HG22 | 1:A:110:HIS:HA | 0.70 | 1.64 | 10 | 1 |
| 1:A:96:ALA:O | 1:A:114:LEU:HD22 | 0.70 | 1.86 | 12 | 2 |
| 1:A:88:LEU:CD1 | 1:A:132:LEU:HD11 | 0.70 | 2.17 | 13 | 1 |
| 1:A:32:MET:HB2 | 1:A:154:VAL:HG11 | 0.70 | 1.63 | 6 | 1 |
| 1:A:18:LEU:O | 1:A:144:ALA:HB3 | 0.70 | 1.87 | 1 | 1 |
| 1:A:9:ILE:HG22 | 1:A:39:ILE:HD13 | 0.70 | 1.64 | 20 | 6 |
| 1:A:98:ILE:HG21 | 1:A:115:TYR:CD2 | 0.70 | 2.21 | 17 | 3 |
| 1:A:98:ILE:HD13 | 1:A:99:TYR:N | 0.69 | 2.02 | 18 | 3 |
| 1:A:89:ASP:HB2 | 1:A:97:VAL:HG22 | 0.69 | 1.63 | 1 | 20 |
| 1:A:98:ILE:HD12 | 1:A:99:TYR:N | 0.69 | 2.01 | 7 | 4 |
| 1:A:9:ILE:HD11 | 1:A:91:ASP:OD2 | 0.69 | 1.87 | 3 | 2 |
| 1:A:146:LEU:O | 1:A:147:PRO:O | 0.69 | 2.08 | 18 | 2 |
| 1:A:37:ALA:HB1 | 1:A:49:VAL:HG22 | 0.69 | 1.64 | 11 | 6 |
| 1:A:91:ASP:N | 1:A:96:ALA:HB2 | 0.69 | 2.02 | 4 | 1 |
| 1:A:9:ILE:HG22 | 1:A:9:ILE:O | 0.69 | 1.86 | 10 | 3 |
| 1:A:75:VAL:HG11 | 1:A:91:ASP:OD2 | 0.69 | 1.86 | 18 | 3 |
| 1:A:15:VAL:HA | 1:A:114:LEU:O | 0.69 | 1.87 | 3 | 10 |
| 1:A:22:THR:CG2 | 1:A:109:LEU:HD12 | 0.69 | 2.17 | 13 | 3 |
| 1:A:88:LEU:HD12 | 1:A:132:LEU:HD11 | 0.69 | 1.64 | 13 | 1 |
| 1:A:9:ILE:HG23 | 1:A:39:ILE:CD1 | 0.68 | 2.17 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:15:VAL:HG13 | 1:A:35:ALA:HB3 | 0.68 | 1.64 | 5 | 8 |
| 1:A:16:VAL:HG21 | 1:A:146:LEU:HD12 | 0.68 | 1.62 | 20 | 1 |
| 1:A:42:LEU:HD23 | 1:A:43:GLY:N | 0.68 | 2.02 | 11 | 2 |
| 1:A:97:VAL:HG21 | 1:A:129:PHE:CD1 | 0.68 | 2.24 | 10 | 6 |
| 1:A:47:LEU:HD23 | 1:A:48:LYS:N | 0.68 | 2.04 | 19 | 1 |
| 1:A:9:ILE:HD13 | 1:A:91:ASP:OD1 | 0.68 | 1.87 | 4 | 1 |
| 1:A:48:LYS:HD3 | 1:A:65:THR:HG23 | 0.68 | 1.66 | 12 | 13 |
| 1:A:42:LEU:O | 1:A:46:GLU:O | 0.68 | 2.12 | 3 | 5 |
| 1:A:88:LEU:HD13 | 1:A:132:LEU:HD21 | 0.68 | 1.64 | 9 | 2 |
| 1:A:17:ALA:HB3 | 1:A:114:LEU:HB2 | 0.67 | 1.65 | 2 | 6 |
| 1:A:16:VAL:HG22 | 1:A:146:LEU:HG | 0.67 | 1.66 | 8 | 1 |
| 1:A:102:ARG:HD2 | 1:A:109:LEU:HD13 | 0.67 | 1.66 | 16 | 1 |
| 1:A:26:LEU:HD12 | 1:A:29:LYS:HE2 | 0.67 | 1.66 | 9 | 1 |
| 1:A:98:ILE:HD13 | 1:A:98:ILE:C | 0.67 | 2.09 | 8 | 4 |
| 1:A:91:ASP:HA | 1:A:96:ALA:HB2 | 0.67 | 1.64 | 19 | 9 |
| 1:A:36:MET:O | 1:A:51:TYR:HA | 0.67 | 1.89 | 11 | 15 |
| 1:A:42:LEU:HD22 | 1:A:46:GLU:O | 0.67 | 1.89 | 16 | 1 |
| 1:A:77:TYR:CZ | 1:A:85:VAL:HG11 | 0.67 | 2.23 | 18 | 1 |
| 1:A:89:ASP:CB | 1:A:97:VAL:HG22 | 0.67 | 2.19 | 14 | 1 |
| 1:A:143:VAL:HG12 | 1:A:144:ALA:N | 0.67 | 2.05 | 15 | 6 |
| 1:A:98:ILE:HG22 | 1:A:113:ARG:O | 0.67 | 1.87 | 18 | 1 |
| 1:A:130:ARG:CG | 1:A:139:THR:HG21 | 0.67 | 2.20 | 11 | 1 |
| 1:A:22:THR:HG22 | 1:A:111:MET:CE | 0.67 | 2.19 | 20 | 1 |
| 1:A:16:VAL:CG2 | 1:A:146:LEU:HD12 | 0.67 | 2.19 | 20 | 1 |
| 1:A:96:ALA:HB3 | 1:A:115:TYR:CD2 | 0.67 | 2.24 | 2 | 2 |
| 1:A:77:TYR:HB3 | 1:A:85:VAL:HG22 | 0.66 | 1.65 | 20 | 5 |
| 1:A:77:TYR:CZ | 1:A:85:VAL:HG21 | 0.66 | 2.26 | 8 | 4 |
| 1:A:87:VAL:HG13 | 1:A:98:ILE:HG22 | 0.66 | 1.66 | 7 | 1 |
| 1:A:18:LEU:C | 1:A:144:ALA:HB3 | 0.66 | 2.10 | 1 | 7 |
| 1:A:90:THR:O | 1:A:96:ALA:HB2 | 0.66 | 1.91 | 17 | 8 |
| 1:A:9:ILE:HD12 | 1:A:91:ASP:OD1 | 0.66 | 1.91 | 18 | 1 |
| 1:A:87:VAL:HG22 | 1:A:98:ILE:HB | 0.66 | 1.67 | 4 | 2 |
| 1:A:114:LEU:C | 1:A:114:LEU:HD23 | 0.66 | 2.11 | 3 | 9 |
| 1:A:146:LEU:HD23 | 1:A:147:PRO:N | 0.66 | 2.05 | 20 | 3 |
| 1:A:18:LEU:HD13 | 1:A:113:ARG:HA | 0.66 | 1.66 | 2 | 4 |
| 1:A:146:LEU:HD22 | 1:A:147:PRO:HD2 | 0.66 | 1.66 | 8 | 1 |
| 1:A:37:ALA:HB1 | 1:A:49:VAL:CG2 | 0.65 | 2.22 | 11 | 2 |
| 1:A:42:LEU:HD12 | 1:A:67:LYS:HD3 | 0.65 | 1.67 | 18 | 2 |
| 1:A:132:LEU:HD12 | 1:A:135:GLU:OE1 | 0.65 | 1.91 | 3 | 1 |
| 1:A:67:LYS:O | 1:A:68:LYS:HG3 | 0.65 | 1.91 | 3 | 1 |
| 1:A:85:VAL:HG11 | 1:A:98:ILE:HD13 | 0.65 | 1.67 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:35:ALA:CB | 1:A:53:VAL:HG22 | 0.65 | 2.21 | 2 | 2 |
| 1:A:47:LEU:HD12 | 1:A:70:SER:HB3 | 0.65 | 1.68 | 10 | 1 |
| 1:A:34:MET:SD | 1:A:146:LEU:HD21 | 0.65 | 2.31 | 1 | 1 |
| 1:A:143:VAL:CG2 | 1:A:144:ALA:H | 0.65 | 2.03 | 4 | 4 |
| 1:A:146:LEU:HB3 | 1:A:147:PRO:HD3 | 0.65 | 1.68 | 5 | 1 |
| 1:A:96:ALA:HB3 | 1:A:115:TYR:CZ | 0.65 | 2.26 | 16 | 1 |
| 1:A:88:LEU:HD11 | 1:A:132:LEU:CD1 | 0.65 | 2.20 | 18 | 2 |
| 1:A:77:TYR:O | 1:A:85:VAL:HG22 | 0.65 | 1.91 | 2 | 2 |
| 1:A:88:LEU:N | 1:A:88:LEU:HD12 | 0.64 | 2.07 | 17 | 3 |
| 1:A:88:LEU:HD13 | 1:A:132:LEU:CD2 | 0.64 | 2.21 | 4 | 2 |
| 1:A:95:TYR:CB | 1:A:125:ALA:HB2 | 0.64 | 2.22 | 5 | 3 |
| 1:A:18:LEU:N | 1:A:18:LEU:HD23 | 0.64 | 2.07 | 15 | 2 |
| 1:A:26:LEU:C | 1:A:26:LEU:HD22 | 0.64 | 2.12 | 7 | 1 |
| 1:A:109:LEU:N | 1:A:109:LEU:HD23 | 0.64 | 2.06 | 6 | 3 |
| 1:A:16:VAL:HG23 | 1:A:146:LEU:HD22 | 0.64 | 1.70 | 12 | 3 |
| 1:A:90:THR:O | 1:A:95:TYR:O | 0.64 | 2.16 | 4 | 8 |
| 1:A:18:LEU:N | 1:A:18:LEU:HD22 | 0.64 | 2.07 | 12 | 3 |
| 1:A:75:VAL:HG11 | 1:A:91:ASP:CB | 0.64 | 2.22 | 7 | 2 |
| 1:A:15:VAL:HG23 | 1:A:113:ARG:HG3 | 0.64 | 1.70 | 8 | 1 |
| 1:A:147:PRO:HG3 | 1:A:154:VAL:HG12 | 0.64 | 1.69 | 4 | 1 |
| 1:A:13:TRP:CG | 1:A:115:TYR:CE1 | 0.64 | 2.86 | 5 | 1 |
| 1:A:75:VAL:HG22 | 1:A:87:VAL:CG2 | 0.64 | 2.22 | 16 | 1 |
| 1:A:43:GLY:O | 1:A:45:ASP:N | 0.64 | 2.31 | 7 | 5 |
| 1:A:87:VAL:CG2 | 1:A:98:ILE:HD12 | 0.64 | 2.22 | 1 | 3 |
| 1:A:85:VAL:CG1 | 1:A:98:ILE:HD13 | 0.64 | 2.23 | 7 | 1 |
| 1:A:70:SER:HA | 1:A:76:TYR:O | 0.64 | 1.93 | 16 | 10 |
| 1:A:88:LEU:HD13 | 1:A:132:LEU:CD1 | 0.64 | 2.22 | 10 | 2 |
| 1:A:34:MET:SD | 1:A:146:LEU:HD11 | 0.64 | 2.33 | 1 | 1 |
| 1:A:71:ASP:O | 1:A:72:ASP:CB | 0.63 | 2.47 | 9 | 3 |
| 1:A:98:ILE:C | 1:A:98:ILE:HD13 | 0.63 | 2.14 | 6 | 2 |
| 1:A:16:VAL:HG12 | 1:A:146:LEU:HD22 | 0.63 | 1.69 | 5 | 1 |
| 1:A:9:ILE:CG2 | 1:A:39:ILE:HD13 | 0.63 | 2.24 | 3 | 5 |
| 1:A:85:VAL:HG22 | 1:A:100:ALA:HB1 | 0.63 | 1.70 | 18 | 2 |
| 1:A:95:TYR:CZ | 1:A:124:ALA:HB3 | 0.63 | 2.29 | 6 | 1 |
| 1:A:114:LEU:C | 1:A:114:LEU:HD13 | 0.63 | 2.14 | 12 | 2 |
| 1:A:132:LEU:O | 1:A:132:LEU:HD23 | 0.63 | 1.94 | 16 | 3 |
| 1:A:47:LEU:HD23 | 1:A:47:LEU:H | 0.63 | 1.52 | 5 | 1 |
| 1:A:130:ARG:HG3 | 1:A:139:THR:HG21 | 0.63 | 1.70 | 11 | 1 |
| 1:A:143:VAL:HG12 | 1:A:144:ALA:H | 0.63 | 1.54 | 15 | 5 |
| 1:A:79:GLU:O | 1:A:81:ALA:N | 0.63 | 2.32 | 15 | 6 |
| 1:A:88:LEU:HD12 | 1:A:88:LEU:N | 0.63 | 2.08 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:139:THR:O | 1:A:143:VAL:HG23 | 0.63 | 1.94 | 2 | 4 |
| 1:A:75:VAL:HG22 | 1:A:87:VAL:HB | 0.63 | 1.69 | 8 | 2 |
| 1:A:85:VAL:CB | 1:A:98:ILE:HD11 | 0.62 | 2.24 | 6 | 7 |
| 1:A:18:LEU:HD22 | 1:A:18:LEU:N | 0.62 | 2.09 | 13 | 4 |
| 1:A:14:TYR:O | 1:A:115:TYR:HA | 0.62 | 1.94 | 16 | 4 |
| 1:A:85:VAL:HG12 | 1:A:98:ILE:CD1 | 0.62 | 2.23 | 12 | 3 |
| 1:A:15:VAL:HG12 | 1:A:35:ALA:CB | 0.62 | 2.22 | 10 | 2 |
| 1:A:89:ASP:OD2 | 1:A:97:VAL:HG13 | 0.62 | 1.95 | 18 | 8 |
| 1:A:116:SER:HB2 | 1:A:121:VAL:HG22 | 0.62 | 1.70 | 14 | 1 |
| 1:A:41:PHE:CD2 | 1:A:47:LEU:HD22 | 0.62 | 2.29 | 13 | 1 |
| 1:A:75:VAL:O | 1:A:87:VAL:CG1 | 0.62 | 2.47 | 18 | 1 |
| 1:A:47:LEU:HB2 | 1:A:77:TYR:OH | 0.62 | 1.95 | 3 | 1 |
| 1:A:42:LEU:HD13 | 1:A:42:LEU:N | 0.62 | 2.10 | 16 | 1 |
| 1:A:77:TYR:O | 1:A:85:VAL:O | 0.62 | 2.18 | 5 | 4 |
| 1:A:109:LEU:HD22 | 1:A:109:LEU:N | 0.62 | 2.10 | 10 | 2 |
| 1:A:13:TRP:HB2 | 1:A:37:ALA:HB3 | 0.62 | 1.68 | 18 | 4 |
| 1:A:91:ASP:HB3 | 1:A:96:ALA:HB2 | 0.62 | 1.70 | 18 | 1 |
| 1:A:146:LEU:HD13 | 1:A:147:PRO:N | 0.62 | 2.10 | 8 | 1 |
| 1:A:19:ALA:HB1 | 1:A:142:MET:C | 0.62 | 2.15 | 8 | 2 |
| 1:A:85:VAL:HG22 | 1:A:100:ALA:CB | 0.62 | 2.24 | 18 | 5 |
| 1:A:89:ASP:HB3 | 1:A:96:ALA:HA | 0.62 | 1.72 | 18 | 4 |
| 1:A:9:ILE:HD12 | 1:A:91:ASP:OD2 | 0.62 | 1.95 | 16 | 2 |
| 1:A:132:LEU:HD23 | 1:A:132:LEU:O | 0.62 | 1.95 | 10 | 2 |
| 1:A:17:ALA:C | 1:A:18:LEU:HD13 | 0.62 | 2.15 | 4 | 2 |
| 1:A:17:ALA:HB3 | 1:A:114:LEU:HD13 | 0.61 | 1.70 | 13 | 6 |
| 1:A:22:THR:HG23 | 1:A:111:MET:HB3 | 0.61 | 1.72 | 19 | 1 |
| 1:A:143:VAL:CG2 | 1:A:144:ALA:N | 0.61 | 2.63 | 4 | 5 |
| 1:A:46:GLU:HA | 1:A:68:LYS:O | 0.61 | 1.95 | 5 | 6 |
| 1:A:16:VAL:HB | 1:A:146:LEU:HD12 | 0.61 | 1.72 | 9 | 1 |
| 1:A:32:MET:HE2 | 1:A:154:VAL:HG12 | 0.61 | 1.73 | 14 | 1 |
| 1:A:42:LEU:HD11 | 1:A:48:LYS:HG2 | 0.61 | 1.72 | 19 | 2 |
| 1:A:102:ARG:HD2 | 1:A:109:LEU:HD22 | 0.61 | 1.70 | 11 | 1 |
| 1:A:20:SER:HA | 1:A:142:MET:HB2 | 0.61 | 1.71 | 13 | 1 |
| 1:A:48:LYS:CB | 1:A:67:LYS:HB3 | 0.61 | 2.25 | 6 | 3 |
| 1:A:109:LEU:HD12 | 1:A:109:LEU:N | 0.61 | 2.11 | 20 | 3 |
| 1:A:71:ASP:OD1 | 1:A:76:TYR:N | 0.61 | 2.33 | 15 | 3 |
| 1:A:53:VAL:HG23 | 1:A:53:VAL:O | 0.61 | 1.96 | 10 | 8 |
| 1:A:16:VAL:HG22 | 1:A:146:LEU:CD1 | 0.61 | 2.25 | 3 | 1 |
| 1:A:81:ALA:O | 1:A:83:LYS:N | 0.61 | 2.34 | 14 | 4 |
| 1:A:22:THR:HG23 | 1:A:109:LEU:CD1 | 0.61 | 2.26 | 10 | 1 |
| 1:A:47:LEU:C | 1:A:47:LEU:HD22 | 0.61 | 2.16 | 17 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:20:SER:OG | 1:A:142:MET:HA | 0.61 | 1.96 | 19 | 1 |
| 1:A:89:ASP:HB3 | 1:A:97:VAL:HG22 | 0.61 | 1.72 | 14 | 1 |
| 1:A:146:LEU:HD12 | 1:A:146:LEU:N | 0.61 | 2.11 | 16 | 1 |
| 1:A:42:LEU:HD12 | 1:A:67:LYS:CD | 0.60 | 2.26 | 18 | 1 |
| 1:A:42:LEU:HD13 | 1:A:43:GLY:N | 0.60 | 2.11 | 4 | 3 |
| 1:A:49:VAL:HG13 | 1:A:51:TYR:CZ | 0.60 | 2.31 | 16 | 2 |
| 1:A:42:LEU:HD22 | 1:A:67:LYS:CE | 0.60 | 2.26 | 15 | 1 |
| 1:A:77:TYR:OH | 1:A:85:VAL:HG21 | 0.60 | 1.95 | 7 | 2 |
| 1:A:19:ALA:HB3 | 1:A:112:MET:SD | 0.60 | 2.36 | 7 | 7 |
| 1:A:88:LEU:HD23 | 1:A:132:LEU:HD13 | 0.60 | 1.74 | 5 | 1 |
| 1:A:133:ALA:HB1 | 1:A:139:THR:CB | 0.60 | 2.26 | 15 | 1 |
| 1:A:47:LEU:HD21 | 1:A:70:SER:CB | 0.60 | 2.27 | 15 | 3 |
| 1:A:85:VAL:HG12 | 1:A:100:ALA:CB | 0.60 | 2.27 | 19 | 3 |
| 1:A:79:GLU:HG3 | 1:A:83:LYS:HB2 | 0.60 | 1.73 | 6 | 2 |
| 1:A:85:VAL:HG22 | 1:A:100:ALA:HA | 0.60 | 1.73 | 12 | 4 |
| 1:A:47:LEU:HD12 | 1:A:47:LEU:N | 0.60 | 2.11 | 2 | 3 |
| 1:A:18:LEU:HG | 1:A:112:MET:O | 0.60 | 1.97 | 1 | 1 |
| 1:A:32:MET:SD | 1:A:154:VAL:HG11 | 0.60 | 2.37 | 3 | 2 |
| 1:A:75:VAL:HB | 1:A:87:VAL:CG1 | 0.60 | 2.25 | 12 | 1 |
| 1:A:82:LYS:O | 1:A:102:ARG:HA | 0.60 | 1.96 | 15 | 5 |
| 1:A:42:LEU:HB3 | 1:A:46:GLU:O | 0.59 | 1.97 | 11 | 10 |
| 1:A:21:ASN:O | 1:A:22:THR:OG1 | 0.59 | 2.19 | 18 | 3 |
| 1:A:39:ILE:HD12 | 1:A:40:SER:N | 0.59 | 2.12 | 7 | 1 |
| 1:A:47:LEU:HD12 | 1:A:70:SER:CB | 0.59 | 2.26 | 1 | 1 |
| 1:A:99:TYR:O | 1:A:99:TYR:CD1 | 0.59 | 2.55 | 8 | 8 |
| 1:A:146:LEU:N | 1:A:146:LEU:HD23 | 0.59 | 2.13 | 13 | 3 |
| 1:A:22:THR:HG22 | 1:A:109:LEU:HD12 | 0.59 | 1.73 | 13 | 2 |
| 1:A:134:GLY:CA | 1:A:139:THR:HG23 | 0.59 | 2.27 | 13 | 1 |
| 1:A:20:SER:HA | 1:A:141:GLU:O | 0.59 | 1.97 | 19 | 1 |
| 1:A:85:VAL:HG13 | 1:A:99:TYR:O | 0.59 | 1.98 | 1 | 3 |
| 1:A:147:PRO:HB3 | 1:A:153:THR:HG21 | 0.59 | 1.74 | 20 | 1 |
| 1:A:146:LEU:HD12 | 1:A:147:PRO:CD | 0.59 | 2.27 | 4 | 2 |
| 1:A:109:LEU:N | 1:A:109:LEU:HD22 | 0.59 | 2.11 | 7 | 5 |
| 1:A:82:LYS:HB2 | 1:A:103:VAL:HG13 | 0.59 | 1.74 | 17 | 1 |
| 1:A:22:THR:CB | 1:A:109:LEU:HD12 | 0.59 | 2.27 | 13 | 1 |
| 1:A:21:ASN:O | 1:A:22:THR:CB | 0.59 | 2.50 | 15 | 1 |
| 1:A:97:VAL:CG1 | 1:A:114:LEU:HD23 | 0.59 | 2.08 | 12 | 1 |
| 1:A:42:LEU:HD13 | 1:A:42:LEU:C | 0.59 | 2.17 | 7 | 2 |
| 1:A:102:ARG:HD3 | 1:A:109:LEU:HD22 | 0.59 | 1.73 | 20 | 1 |
| 1:A:15:VAL:HB | 1:A:35:ALA:CB | 0.59 | 2.27 | 15 | 4 |
| 1:A:154:VAL:CG1 | 1:A:154:VAL:O | 0.59 | 2.49 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:ASN:O | 1:A:22:THR:HG23 | 0.59 | 1.98 | 1 | 2 |
| 1:A:75:VAL:O | 1:A:87:VAL:HB | 0.59 | 1.98 | 17 | 10 |
| 1:A:47:LEU:HD23 | 1:A:70:SER:OG | 0.58 | 1.97 | 20 | 1 |
| 1:A:102:ARG:HB2 | 1:A:109:LEU:HD23 | 0.58 | 1.73 | 19 | 4 |
| 1:A:102:ARG:HD3 | 1:A:109:LEU:HD11 | 0.58 | 1.74 | 1 | 2 |
| 1:A:33:LYS:HD3 | 1:A:53:VAL:HG11 | 0.58 | 1.73 | 4 | 1 |
| 1:A:77:TYR:CE1 | 1:A:85:VAL:HG11 | 0.58 | 2.33 | 18 | 1 |
| 1:A:19:ALA:O | 1:A:112:MET:N | 0.58 | 2.35 | 1 | 18 |
| 1:A:91:ASP:CA | 1:A:96:ALA:HB2 | 0.58 | 2.27 | 16 | 5 |
| 1:A:53:VAL:O | 1:A:53:VAL:HG23 | 0.58 | 1.98 | 13 | 5 |
| 1:A:26:LEU:HD12 | 1:A:29:LYS:CE | 0.58 | 2.29 | 9 | 1 |
| 1:A:15:VAL:HG22 | 1:A:18:LEU:HD11 | 0.58 | 1.73 | 13 | 1 |
| 1:A:88:LEU:HD12 | 1:A:132:LEU:HD22 | 0.58 | 1.73 | 15 | 1 |
| 1:A:20:SER:HB2 | 1:A:111:MET:HA | 0.58 | 1.75 | 19 | 4 |
| 1:A:109:LEU:C | 1:A:109:LEU:HD23 | 0.58 | 2.17 | 16 | 2 |
| 1:A:102:ARG:O | 1:A:109:LEU:HD23 | 0.58 | 1.98 | 18 | 1 |
| 1:A:26:LEU:HD13 | 1:A:27:ARG:N | 0.58 | 2.13 | 7 | 1 |
| 1:A:101:THR:HG23 | 1:A:109:LEU:O | 0.58 | 1.98 | 14 | 1 |
| 1:A:22:THR:HB | 1:A:109:LEU:HD12 | 0.58 | 1.75 | 13 | 1 |
| 1:A:75:VAL:HG22 | 1:A:87:VAL:HG21 | 0.58 | 1.74 | 16 | 1 |
| 1:A:79:GLU:HB3 | 1:A:83:LYS:HB2 | 0.58 | 1.74 | 14 | 1 |
| 1:A:22:THR:HG21 | 1:A:109:LEU:CD2 | 0.58 | 2.27 | 20 | 1 |
| 1:A:22:THR:HG21 | 1:A:25:PHE:CD2 | 0.58 | 2.33 | 6 | 1 |
| 1:A:15:VAL:CG1 | 1:A:35:ALA:HB1 | 0.58 | 2.27 | 7 | 5 |
| 1:A:146:LEU:C | 1:A:146:LEU:HD23 | 0.58 | 2.18 | 9 | 2 |
| 1:A:98:ILE:HG21 | 1:A:115:TYR:CE2 | 0.58 | 2.33 | 17 | 2 |
| 1:A:26:LEU:N | 1:A:26:LEU:HD12 | 0.58 | 2.14 | 12 | 1 |
| 1:A:85:VAL:HG12 | 1:A:100:ALA:CA | 0.58 | 2.28 | 19 | 3 |
| 1:A:85:VAL:HG11 | 1:A:100:ALA:HB1 | 0.58 | 1.75 | 2 | 1 |
| 1:A:85:VAL:CG1 | 1:A:100:ALA:HB1 | 0.58 | 2.29 | 2 | 1 |
| 1:A:81:ALA:O | 1:A:103:VAL:HG12 | 0.58 | 1.98 | 6 | 2 |
| 1:A:13:TRP:CE2 | 1:A:39:ILE:HG21 | 0.58 | 2.33 | 15 | 4 |
| 1:A:19:ALA:O | 1:A:20:SER:CB | 0.58 | 2.52 | 13 | 4 |
| 1:A:82:LYS:O | 1:A:103:VAL:HG12 | 0.58 | 1.98 | 18 | 2 |
| 1:A:13:TRP:HZ2 | 1:A:39:ILE:HD12 | 0.58 | 1.57 | 19 | 1 |
| 1:A:42:LEU:HD13 | 1:A:42:LEU:H | 0.58 | 1.59 | 16 | 1 |
| 1:A:21:ASN:HB3 | 1:A:141:GLU:O | 0.58 | 1.98 | 6 | 2 |
| 1:A:95:TYR:HB3 | 1:A:125:ALA:HB2 | 0.58 | 1.75 | 5 | 1 |
| 1:A:39:ILE:HD11 | 1:A:47:LEU:HD13 | 0.58 | 1.75 | 4 | 1 |
| 1:A:37:ALA:CB | 1:A:51:TYR:HB3 | 0.57 | 2.29 | 6 | 2 |
| 1:A:47:LEU:H | 1:A:47:LEU:HD23 | 0.57 | 1.58 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:127:ALA:O | 1:A:131:LYS:N | 0.57 | 2.38 | 6 | 10 |
| 1:A:88:LEU:H | 1:A:88:LEU:HD23 | 0.57 | 1.59 | 14 | 2 |
| 1:A:32:MET:SD | 1:A:144:ALA:HB1 | 0.57 | 2.38 | 6 | 1 |
| 1:A:65:THR:HG22 | 1:A:67:LYS:HD2 | 0.57 | 1.75 | 6 | 1 |
| 1:A:146:LEU:N | 1:A:147:PRO:CD | 0.57 | 2.66 | 18 | 2 |
| 1:A:18:LEU:HD11 | 1:A:32:MET:SD | 0.57 | 2.39 | 11 | 1 |
| 1:A:34:MET:HG3 | 1:A:54:PRO:HD2 | 0.57 | 1.77 | 9 | 1 |
| 1:A:18:LEU:HD23 | 1:A:19:ALA:H | 0.57 | 1.56 | 1 | 1 |
| 1:A:32:MET:CB | 1:A:154:VAL:HG11 | 0.57 | 2.29 | 6 | 1 |
| 1:A:15:VAL:CG2 | 1:A:18:LEU:HD21 | 0.57 | 2.30 | 8 | 1 |
| 1:A:35:ALA:HB2 | 1:A:53:VAL:HG22 | 0.57 | 1.76 | 2 | 3 |
| 1:A:146:LEU:N | 1:A:146:LEU:HD12 | 0.57 | 2.14 | 19 | 1 |
| 1:A:21:ASN:OD1 | 1:A:142:MET:HB2 | 0.57 | 2.00 | 4 | 1 |
| 1:A:95:TYR:CE2 | 1:A:122:SER:HB3 | 0.57 | 2.34 | 17 | 8 |
| 1:A:16:VAL:O | 1:A:18:LEU:CD2 | 0.57 | 2.53 | 6 | 2 |
| 1:A:98:ILE:C | 1:A:98:ILE:HD12 | 0.57 | 2.20 | 7 | 1 |
| 1:A:103:VAL:HG13 | 1:A:103:VAL:O | 0.57 | 2.00 | 10 | 2 |
| 1:A:87:VAL:CG2 | 1:A:96:ALA:HB1 | 0.57 | 2.30 | 12 | 1 |
| 1:A:13:TRP:NE1 | 1:A:39:ILE:HD12 | 0.57 | 2.15 | 2 | 1 |
| 1:A:133:ALA:HB1 | 1:A:139:THR:HB | 0.57 | 1.76 | 15 | 1 |
| 1:A:34:MET:HA | 1:A:146:LEU:HD12 | 0.57 | 1.76 | 17 | 1 |
| 1:A:16:VAL:HG22 | 1:A:146:LEU:CD2 | 0.57 | 2.19 | 2 | 1 |
| 1:A:47:LEU:C | 1:A:47:LEU:HD12 | 0.56 | 2.21 | 15 | 4 |
| 1:A:75:VAL:O | 1:A:87:VAL:CB | 0.56 | 2.53 | 16 | 3 |
| 1:A:26:LEU:N | 1:A:26:LEU:HD22 | 0.56 | 2.15 | 20 | 2 |
| 1:A:23:GLU:OE1 | 1:A:26:LEU:HD12 | 0.56 | 2.01 | 8 | 2 |
| 1:A:47:LEU:HD22 | 1:A:47:LEU:C | 0.56 | 2.21 | 7 | 1 |
| 1:A:26:LEU:HD13 | 1:A:27:ARG:H | 0.56 | 1.59 | 7 | 1 |
| 1:A:16:VAL:HG13 | 1:A:146:LEU:HD13 | 0.56 | 1.76 | 7 | 1 |
| 1:A:17:ALA:CB | 1:A:114:LEU:HD13 | 0.56 | 2.30 | 3 | 5 |
| 1:A:77:TYR:HB3 | 1:A:85:VAL:HB | 0.56 | 1.76 | 10 | 1 |
| 1:A:116:SER:CB | 1:A:121:VAL:HG22 | 0.56 | 2.30 | 14 | 2 |
| 1:A:146:LEU:HD23 | 1:A:146:LEU:C | 0.56 | 2.20 | 20 | 1 |
| 1:A:88:LEU:HD23 | 1:A:132:LEU:HD22 | 0.56 | 1.77 | 6 | 1 |
| 1:A:102:ARG:HB3 | 1:A:109:LEU:HD13 | 0.56 | 1.77 | 8 | 1 |
| 1:A:86:GLU:C | 1:A:98:ILE:HD12 | 0.56 | 2.20 | 19 | 3 |
| 1:A:21:ASN:HA | 1:A:111:MET:HG2 | 0.56 | 1.78 | 20 | 1 |
| 1:A:34:MET:O | 1:A:54:PRO:HD2 | 0.56 | 2.00 | 13 | 14 |
| 1:A:13:TRP:O | 1:A:37:ALA:HB3 | 0.56 | 2.01 | 2 | 2 |
| 1:A:77:TYR:CE2 | 1:A:85:VAL:HG11 | 0.56 | 2.36 | 8 | 1 |
| 1:A:8:GLU:C | 1:A:9:ILE:HD13 | 0.56 | 2.21 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:8:GLU:HG3 | 1:A:9:ILE:HG12 | 0.56 | 1.75 | 12 | 1 |
| 1:A:76:TYR:C | 1:A:76:TYR:CD1 | 0.56 | 2.78 | 15 | 2 |
| 1:A:82:LYS:N | 1:A:103:VAL:O | 0.56 | 2.39 | 20 | 13 |
| 1:A:21:ASN:HB2 | 1:A:141:GLU:O | 0.56 | 2.00 | 11 | 4 |
| 1:A:132:LEU:C | 1:A:132:LEU:HD23 | 0.56 | 2.22 | 16 | 2 |
| 1:A:90:THR:C | 1:A:96:ALA:HB2 | 0.56 | 2.22 | 4 | 1 |
| 1:A:98:ILE:HD12 | 1:A:99:TYR:H | 0.56 | 1.61 | 2 | 1 |
| 1:A:41:PHE:CD2 | 1:A:47:LEU:HD12 | 0.55 | 2.36 | 19 | 1 |
| 1:A:128:ILE:O | 1:A:132:LEU:HD13 | 0.55 | 2.01 | 11 | 1 |
| 1:A:42:LEU:HD21 | 1:A:48:LYS:CG | 0.55 | 2.31 | 20 | 1 |
| 1:A:77:TYR:HB3 | 1:A:85:VAL:CG2 | 0.55 | 2.31 | 4 | 2 |
| 1:A:89:ASP:O | 1:A:90:THR:CG2 | 0.55 | 2.52 | 4 | 1 |
| 1:A:16:VAL:CG1 | 1:A:146:LEU:HD22 | 0.55 | 2.32 | 17 | 1 |
| 1:A:70:SER:HB2 | 1:A:75:VAL:HG13 | 0.55 | 1.78 | 2 | 2 |
| 1:A:47:LEU:HD13 | 1:A:68:LYS:O | 0.55 | 2.01 | 7 | 1 |
| 1:A:80:GLU:O | 1:A:81:ALA:C | 0.55 | 2.44 | 7 | 2 |
| 1:A:13:TRP:CE2 | 1:A:115:TYR:CZ | 0.55 | 2.94 | 5 | 2 |
| 1:A:13:TRP:CZ3 | 1:A:49:VAL:HG11 | 0.55 | 2.37 | 19 | 1 |
| 1:A:13:TRP:HB3 | 1:A:115:TYR:HB3 | 0.55 | 1.78 | 20 | 4 |
| 1:A:26:LEU:HD23 | 1:A:26:LEU:C | 0.55 | 2.22 | 6 | 1 |
| 1:A:13:TRP:CZ3 | 1:A:115:TYR:CE2 | 0.55 | 2.95 | 14 | 3 |
| 1:A:95:TYR:HB2 | 1:A:125:ALA:HB2 | 0.55 | 1.79 | 6 | 2 |
| 1:A:32:MET:HA | 1:A:32:MET:CE | 0.55 | 2.31 | 6 | 2 |
| 1:A:84:LYS:HG3 | 1:A:103:VAL:HG21 | 0.55 | 1.77 | 5 | 1 |
| 1:A:109:LEU:C | 1:A:109:LEU:HD22 | 0.55 | 2.21 | 2 | 1 |
| 1:A:88:LEU:HD23 | 1:A:88:LEU:H | 0.55 | 1.61 | 15 | 2 |
| 1:A:41:PHE:CE2 | 1:A:47:LEU:HD22 | 0.55 | 2.37 | 16 | 2 |
| 1:A:68:LYS:CB | 1:A:78:SER:O | 0.55 | 2.54 | 18 | 4 |
| 1:A:47:LEU:N | 1:A:47:LEU:HD12 | 0.55 | 2.17 | 3 | 1 |
| 1:A:87:VAL:HG22 | 1:A:98:ILE:CB | 0.55 | 2.31 | 4 | 1 |
| 1:A:75:VAL:CG1 | 1:A:87:VAL:HG13 | 0.55 | 2.29 | 18 | 1 |
| 1:A:68:LYS:HD3 | 1:A:68:LYS:N | 0.55 | 2.17 | 13 | 1 |
| 1:A:96:ALA:HB3 | 1:A:117:ARG:NH2 | 0.54 | 2.17 | 20 | 2 |
| 1:A:75:VAL:HG12 | 1:A:87:VAL:CG2 | 0.54 | 2.32 | 3 | 2 |
| 1:A:6:ARG:N | 1:A:6:ARG:NE | 0.54 | 2.55 | 15 | 1 |
| 1:A:114:LEU:HD23 | 1:A:114:LEU:C | 0.54 | 2.21 | 6 | 6 |
| 1:A:74:GLU:N | 1:A:74:GLU:OE1 | 0.54 | 2.40 | 17 | 5 |
| 1:A:11:GLY:N | 1:A:39:ILE:HG23 | 0.54 | 2.17 | 7 | 2 |
| 1:A:97:VAL:HB | 1:A:129:PHE:CG | 0.54 | 2.37 | 4 | 2 |
| 1:A:13:TRP:CH2 | 1:A:39:ILE:HD12 | 0.54 | 2.38 | 20 | 9 |
| 1:A:98:ILE:HG23 | 1:A:113:ARG:O | 0.54 | 2.03 | 2 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:88:LEU:HD23 | 1:A:88:LEU:N | 0.54 | 2.16 | 15 | 3 |
| 1:A:49:VAL:HG13 | 1:A:49:VAL:O | 0.54 | 2.03 | 9 | 8 |
| 1:A:24:PHE:CD1 | 1:A:25:PHE:N | 0.54 | 2.75 | 6 | 6 |
| 1:A:18:LEU:HD12 | 1:A:113:ARG:HA | 0.54 | 1.79 | 4 | 2 |
| 1:A:17:ALA:HB3 | 1:A:114:LEU:CD1 | 0.54 | 2.33 | 3 | 5 |
| 1:A:104:LYS:O | 1:A:106:GLY:N | 0.54 | 2.41 | 5 | 5 |
| 1:A:70:SER:OG | 1:A:75:VAL:HG13 | 0.54 | 2.02 | 10 | 1 |
| 1:A:99:TYR:CD1 | 1:A:99:TYR:O | 0.54 | 2.61 | 6 | 3 |
| 1:A:51:TYR:CD1 | 1:A:51:TYR:O | 0.54 | 2.61 | 8 | 6 |
| 1:A:98:ILE:HG21 | 1:A:115:TYR:CE1 | 0.54 | 2.38 | 20 | 3 |
| 1:A:48:LYS:HB3 | 1:A:67:LYS:HB2 | 0.54 | 1.80 | 18 | 5 |
| 1:A:49:VAL:O | 1:A:49:VAL:HG13 | 0.54 | 2.02 | 7 | 9 |
| 1:A:54:PRO:HA | 1:A:61:LYS:HA | 0.54 | 1.80 | 2 | 4 |
| 1:A:147:PRO:HA | 1:A:154:VAL:HA | 0.54 | 1.80 | 1 | 2 |
| 1:A:13:TRP:CE3 | 1:A:115:TYR:CG | 0.54 | 2.95 | 11 | 1 |
| 1:A:67:LYS:C | 1:A:68:LYS:HD2 | 0.54 | 2.23 | 7 | 1 |
| 1:A:72:ASP:O | 1:A:74:GLU:N | 0.54 | 2.40 | 15 | 12 |
| 1:A:88:LEU:HD12 | 1:A:88:LEU:H | 0.54 | 1.62 | 12 | 1 |
| 1:A:42:LEU:HB2 | 1:A:46:GLU:O | 0.54 | 2.03 | 9 | 4 |
| 1:A:85:VAL:HG13 | 1:A:100:ALA:HA | 0.54 | 1.78 | 8 | 3 |
| 1:A:123:PRO:O | 1:A:127:ALA:CB | 0.53 | 2.56 | 5 | 5 |
| 1:A:147:PRO:CG | 1:A:154:VAL:HG12 | 0.53 | 2.33 | 4 | 1 |
| 1:A:136:ARG:HH12 | 1:A:139:THR:HG21 | 0.53 | 1.63 | 18 | 1 |
| 1:A:79:GLU:CB | 1:A:83:LYS:O | 0.53 | 2.56 | 14 | 1 |
| 1:A:85:VAL:CG1 | 1:A:98:ILE:CG1 | 0.53 | 2.86 | 1 | 3 |
| 1:A:23:GLU:H | 1:A:109:LEU:HD12 | 0.53 | 1.62 | 19 | 1 |
| 1:A:77:TYR:CZ | 1:A:85:VAL:CG2 | 0.53 | 2.91 | 19 | 4 |
| 1:A:154:VAL:O | 1:A:154:VAL:HG23 | 0.53 | 2.03 | 18 | 1 |
| 1:A:146:LEU:C | 1:A:146:LEU:HD13 | 0.53 | 2.24 | 8 | 1 |
| 1:A:35:ALA:HA | 1:A:53:VAL:HG12 | 0.53 | 1.80 | 19 | 2 |
| 1:A:75:VAL:O | 1:A:87:VAL:HG23 | 0.53 | 2.04 | 6 | 1 |
| 1:A:116:SER:OG | 1:A:121:VAL:HG22 | 0.53 | 2.03 | 6 | 1 |
| 1:A:13:TRP:CE3 | 1:A:115:TYR:CD2 | 0.53 | 2.97 | 7 | 8 |
| 1:A:77:TYR:CD1 | 1:A:77:TYR:O | 0.53 | 2.62 | 1 | 5 |
| 1:A:79:GLU:O | 1:A:80:GLU:HG2 | 0.53 | 2.04 | 19 | 1 |
| 1:A:98:ILE:O | 1:A:113:ARG:HB3 | 0.53 | 2.03 | 16 | 6 |
| 1:A:24:PHE:CZ | 1:A:25:PHE:CE1 | 0.53 | 2.97 | 10 | 1 |
| 1:A:43:GLY:O | 1:A:44:GLU:CB | 0.53 | 2.57 | 19 | 2 |
| 1:A:53:VAL:HG22 | 1:A:62:TRP:O | 0.53 | 2.03 | 11 | 2 |
| 1:A:16:VAL:O | 1:A:146:LEU:HB2 | 0.53 | 2.04 | 5 | 1 |
| 1:A:130:ARG:O | 1:A:139:THR:HG21 | 0.53 | 2.04 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:TRP:CE2 | 1:A:115:TYR:CD2 | 0.53 | 2.97 | 2 | 1 |
| 1:A:18:LEU:N | 1:A:18:LEU:HD12 | 0.53 | 2.19 | 20 | 2 |
| 1:A:26:LEU:HD23 | 1:A:26:LEU:O | 0.53 | 2.04 | 6 | 1 |
| 1:A:32:MET:HB3 | 1:A:154:VAL:HG21 | 0.53 | 1.80 | 17 | 1 |
| 1:A:15:VAL:N | 1:A:115:TYR:CD2 | 0.53 | 2.77 | 11 | 1 |
| 1:A:79:GLU:HB2 | 1:A:83:LYS:CB | 0.53 | 2.34 | 20 | 2 |
| 1:A:13:TRP:CD1 | 1:A:115:TYR:CE1 | 0.53 | 2.97 | 2 | 2 |
| 1:A:109:LEU:HD13 | 1:A:109:LEU:H | 0.53 | 1.63 | 2 | 1 |
| 1:A:77:TYR:O | 1:A:85:VAL:HB | 0.53 | 2.04 | 14 | 2 |
| 1:A:145:MET:O | 1:A:154:VAL:HG21 | 0.53 | 2.04 | 15 | 3 |
| 1:A:103:VAL:O | 1:A:103:VAL:HG23 | 0.53 | 2.04 | 8 | 2 |
| 1:A:85:VAL:CG1 | 1:A:100:ALA:CB | 0.52 | 2.86 | 2 | 3 |
| 1:A:15:VAL:CG1 | 1:A:35:ALA:CB | 0.52 | 2.87 | 8 | 4 |
| 1:A:18:LEU:HD23 | 1:A:111:MET:HE2 | 0.52 | 1.80 | 5 | 1 |
| 1:A:51:TYR:OH | 1:A:66:PHE:CG | 0.52 | 2.62 | 12 | 1 |
| 1:A:15:VAL:HG23 | 1:A:18:LEU:HD11 | 0.52 | 1.81 | 2 | 1 |
| 1:A:22:THR:HG21 | 1:A:109:LEU:HB3 | 0.52 | 1.80 | 18 | 1 |
| 1:A:143:VAL:CG1 | 1:A:144:ALA:N | 0.52 | 2.71 | 15 | 5 |
| 1:A:132:LEU:HD23 | 1:A:132:LEU:C | 0.52 | 2.24 | 14 | 3 |
| 1:A:123:PRO:O | 1:A:127:ALA:HB3 | 0.52 | 2.03 | 5 | 3 |
| 1:A:11:GLY:H | 1:A:39:ILE:HG23 | 0.52 | 1.63 | 19 | 1 |
| 1:A:145:MET:N | 1:A:145:MET:SD | 0.52 | 2.83 | 5 | 1 |
| 1:A:87:VAL:HB | 1:A:98:ILE:HB | 0.52 | 1.80 | 12 | 2 |
| 1:A:13:TRP:CE3 | 1:A:115:TYR:CE2 | 0.52 | 2.98 | 16 | 4 |
| 1:A:89:ASP:O | 1:A:90:THR:CB | 0.52 | 2.58 | 18 | 2 |
| 1:A:102:ARG:HB2 | 1:A:109:LEU:HD13 | 0.52 | 1.80 | 11 | 1 |
| 1:A:16:VAL:CG1 | 1:A:146:LEU:HD13 | 0.52 | 2.35 | 7 | 1 |
| 1:A:77:TYR:CB | 1:A:85:VAL:HG22 | 0.52 | 2.35 | 20 | 2 |
| 1:A:143:VAL:CG1 | 1:A:144:ALA:H | 0.52 | 2.17 | 15 | 4 |
| 1:A:20:SER:O | 1:A:142:MET:HB3 | 0.52 | 2.04 | 15 | 3 |
| 1:A:9:ILE:O | 1:A:9:ILE:CG2 | 0.52 | 2.54 | 4 | 2 |
| 1:A:49:VAL:HG13 | 1:A:51:TYR:CE1 | 0.52 | 2.40 | 5 | 1 |
| 1:A:115:TYR:CD1 | 1:A:115:TYR:O | 0.52 | 2.63 | 19 | 1 |
| 1:A:21:ASN:ND2 | 1:A:110:HIS:HB2 | 0.52 | 2.19 | 9 | 1 |
| 1:A:153:THR:O | 1:A:153:THR:HG23 | 0.52 | 2.05 | 15 | 3 |
| 1:A:109:LEU:N | 1:A:109:LEU:HD13 | 0.52 | 2.19 | 2 | 1 |
| 1:A:108:THR:O | 1:A:109:LEU:HD13 | 0.52 | 2.05 | 7 | 5 |
| 1:A:82:LYS:HA | 1:A:103:VAL:O | 0.52 | 2.05 | 15 | 8 |
| 1:A:68:LYS:HD3 | 1:A:77:TYR:CD1 | 0.52 | 2.40 | 7 | 1 |
| 1:A:98:ILE:CG2 | 1:A:115:TYR:CD1 | 0.52 | 2.93 | 15 | 1 |
| 1:A:16:VAL:HG23 | 1:A:146:LEU:HD13 | 0.52 | 1.81 | 15 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:LYS:HG3 | 1:A:79:GLU:CG | 0.52 | 2.34 | 20 | 1 |
| 1:A:154:VAL:HG23 | 1:A:154:VAL:O | 0.52 | 2.05 | 20 | 1 |
| 1:A:88:LEU:HD23 | 1:A:132:LEU:HD11 | 0.52 | 1.82 | 17 | 1 |
| 1:A:13:TRP:CD2 | 1:A:115:TYR:CE2 | 0.52 | 2.97 | 5 | 1 |
| 1:A:9:ILE:HG23 | 1:A:91:ASP:O | 0.52 | 2.04 | 19 | 1 |
| 1:A:79:GLU:O | 1:A:83:LYS:HB2 | 0.52 | 2.04 | 7 | 1 |
| 1:A:68:LYS:HG3 | 1:A:77:TYR:CD1 | 0.52 | 2.39 | 13 | 1 |
| 1:A:77:TYR:CE1 | 1:A:85:VAL:CG2 | 0.52 | 2.93 | 8 | 2 |
| 1:A:146:LEU:O | 1:A:154:VAL:HG13 | 0.52 | 2.05 | 18 | 1 |
| 1:A:98:ILE:CG2 | 1:A:115:TYR:CE1 | 0.52 | 2.93 | 20 | 3 |
| 1:A:137:ASN:O | 1:A:138:TYR:CD1 | 0.52 | 2.63 | 4 | 6 |
| 1:A:77:TYR:CE2 | 1:A:85:VAL:CG2 | 0.52 | 2.93 | 13 | 3 |
| 1:A:9:ILE:HG23 | 1:A:91:ASP:OD1 | 0.52 | 2.05 | 18 | 1 |
| 1:A:42:LEU:HD23 | 1:A:42:LEU:C | 0.52 | 2.25 | 11 | 2 |
| 1:A:37:ALA:HA | 1:A:51:TYR:HA | 0.51 | 1.82 | 15 | 7 |
| 1:A:18:LEU:CB | 1:A:112:MET:O | 0.51 | 2.58 | 15 | 6 |
| 1:A:95:TYR:CE2 | 1:A:125:ALA:CA | 0.51 | 2.93 | 3 | 1 |
| 1:A:66:PHE:CE2 | 1:A:77:TYR:CE2 | 0.51 | 2.98 | 9 | 1 |
| 1:A:104:LYS:O | 1:A:107:ARG:HG2 | 0.51 | 2.05 | 11 | 8 |
| 1:A:13:TRP:CE2 | 1:A:115:TYR:CE1 | 0.51 | 2.99 | 19 | 2 |
| 1:A:21:ASN:ND2 | 1:A:140:ASP:O | 0.51 | 2.44 | 2 | 3 |
| 1:A:132:LEU:HD12 | 1:A:132:LEU:C | 0.51 | 2.26 | 7 | 2 |
| 1:A:16:VAL:HG23 | 1:A:146:LEU:HG | 0.51 | 1.83 | 20 | 1 |
| 1:A:13:TRP:HB3 | 1:A:115:TYR:CD2 | 0.51 | 2.40 | 13 | 2 |
| 1:A:66:PHE:O | 1:A:66:PHE:CD1 | 0.51 | 2.63 | 8 | 1 |
| 1:A:13:TRP:CE2 | 1:A:115:TYR:CE2 | 0.51 | 2.99 | 5 | 2 |
| 1:A:75:VAL:CG1 | 1:A:87:VAL:CG1 | 0.51 | 2.89 | 12 | 2 |
| 1:A:107:ARG:HH12 | 1:A:109:LEU:HD11 | 0.51 | 1.65 | 14 | 1 |
| 1:A:70:SER:OG | 1:A:77:TYR:CB | 0.51 | 2.58 | 19 | 1 |
| 1:A:14:TYR:CB | 1:A:36:MET:HA | 0.51 | 2.35 | 11 | 1 |
| 1:A:15:VAL:O | 1:A:35:ALA:O | 0.51 | 2.27 | 19 | 4 |
| 1:A:13:TRP:CZ3 | 1:A:115:TYR:CZ | 0.51 | 2.99 | 14 | 1 |
| 1:A:27:ARG:HD3 | 1:A:28:GLU:N | 0.51 | 2.20 | 15 | 1 |
| 1:A:98:ILE:O | 1:A:113:ARG:O | 0.51 | 2.29 | 15 | 6 |
| 1:A:75:VAL:HG22 | 1:A:87:VAL:CB | 0.51 | 2.36 | 8 | 1 |
| 1:A:68:LYS:HB2 | 1:A:77:TYR:CD2 | 0.51 | 2.40 | 3 | 2 |
| 1:A:75:VAL:HG23 | 1:A:91:ASP:OD2 | 0.51 | 2.05 | 12 | 1 |
| 1:A:146:LEU:HB3 | 1:A:147:PRO:HD2 | 0.51 | 1.83 | 19 | 1 |
| 1:A:71:ASP:O | 1:A:72:ASP:HB3 | 0.51 | 2.05 | 2 | 2 |
| 1:A:33:LYS:HD2 | 1:A:33:LYS:N | 0.51 | 2.20 | 9 | 1 |
| 1:A:132:LEU:HD13 | 1:A:132:LEU:C | 0.51 | 2.26 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:47:LEU:HD12 | 1:A:70:SER:HB2 | 0.51 | 1.83 | 1 | 1 |
| 1:A:75:VAL:O | 1:A:87:VAL:N | 0.51 | 2.43 | 1 | 10 |
| 1:A:9:ILE:CG2 | 1:A:9:ILE:O | 0.51 | 2.58 | 10 | 2 |
| 1:A:82:LYS:HA | 1:A:104:LYS:HB3 | 0.51 | 1.82 | 10 | 2 |
| 1:A:137:ASN:O | 1:A:139:THR:N | 0.51 | 2.44 | 6 | 3 |
| 1:A:13:TRP:CD2 | 1:A:115:TYR:CZ | 0.51 | 2.98 | 5 | 1 |
| 1:A:87:VAL:HG11 | 1:A:115:TYR:OH | 0.51 | 2.05 | 14 | 1 |
| 1:A:124:ALA:HB1 | 1:A:128:ILE:HD11 | 0.51 | 1.83 | 3 | 4 |
| 1:A:32:MET:HG2 | 1:A:154:VAL:HG12 | 0.51 | 1.82 | 2 | 2 |
| 1:A:88:LEU:N | 1:A:88:LEU:HD23 | 0.51 | 2.20 | 19 | 2 |
| 1:A:9:ILE:O | 1:A:39:ILE:HD13 | 0.51 | 2.06 | 19 | 1 |
| 1:A:20:SER:HB3 | 1:A:111:MET:HA | 0.51 | 1.81 | 8 | 2 |
| 1:A:95:TYR:CD2 | 1:A:125:ALA:HB1 | 0.50 | 2.41 | 3 | 1 |
| 1:A:85:VAL:CG1 | 1:A:98:ILE:HG12 | 0.50 | 2.36 | 1 | 3 |
| 1:A:108:THR:HG22 | 1:A:110:HIS:CE1 | 0.50 | 2.40 | 19 | 1 |
| 1:A:74:GLU:O | 1:A:75:VAL:CG2 | 0.50 | 2.59 | 19 | 2 |
| 1:A:77:TYR:CD2 | 1:A:85:VAL:HG21 | 0.50 | 2.40 | 2 | 2 |
| 1:A:47:LEU:HD12 | 1:A:70:SER:OG | 0.50 | 2.07 | 11 | 2 |
| 1:A:136:ARG:HD2 | 1:A:136:ARG:N | 0.50 | 2.22 | 9 | 1 |
| 1:A:88:LEU:HD13 | 1:A:132:LEU:HD11 | 0.50 | 1.82 | 10 | 1 |
| 1:A:48:LYS:HA | 1:A:66:PHE:O | 0.50 | 2.06 | 5 | 8 |
| 1:A:19:ALA:HB3 | 1:A:112:MET:CB | 0.50 | 2.35 | 6 | 2 |
| 1:A:85:VAL:HG22 | 1:A:100:ALA:CA | 0.50 | 2.36 | 7 | 4 |
| 1:A:146:LEU:HD12 | 1:A:147:PRO:HD3 | 0.50 | 1.81 | 4 | 1 |
| 1:A:19:ALA:CB | 1:A:112:MET:HB2 | 0.50 | 2.35 | 18 | 1 |
| 1:A:75:VAL:O | 1:A:87:VAL:O | 0.50 | 2.29 | 8 | 3 |
| 1:A:15:VAL:HG13 | 1:A:113:ARG:CG | 0.50 | 2.36 | 18 | 1 |
| 1:A:14:TYR:CE1 | 1:A:116:SER:OG | 0.50 | 2.64 | 11 | 1 |
| 1:A:28:GLU:O | 1:A:31:LYS:HG2 | 0.50 | 2.06 | 7 | 1 |
| 1:A:84:LYS:O | 1:A:101:THR:O | 0.50 | 2.30 | 10 | 3 |
| 1:A:136:ARG:O | 1:A:137:ASN:CB | 0.50 | 2.59 | 6 | 1 |
| 1:A:146:LEU:HD23 | 1:A:146:LEU:N | 0.50 | 2.21 | 3 | 1 |
| 1:A:104:LYS:O | 1:A:105:ASP:C | 0.50 | 2.50 | 5 | 3 |
| 1:A:102:ARG:CG | 1:A:109:LEU:HD23 | 0.50 | 2.37 | 15 | 1 |
| 1:A:77:TYR:CD1 | 1:A:77:TYR:C | 0.50 | 2.85 | 13 | 3 |
| 1:A:49:VAL:CG1 | 1:A:66:PHE:CZ | 0.50 | 2.95 | 8 | 1 |
| 1:A:16:VAL:HA | 1:A:146:LEU:HD22 | 0.50 | 1.81 | 5 | 1 |
| 1:A:76:TYR:O | 1:A:76:TYR:CD1 | 0.50 | 2.64 | 13 | 2 |
| 1:A:33:LYS:N | 1:A:33:LYS:CD | 0.50 | 2.75 | 9 | 1 |
| 1:A:44:GLU:O | 1:A:46:GLU:OE1 | 0.50 | 2.29 | 14 | 2 |
| 1:A:48:LYS:HD2 | 1:A:65:THR:HG23 | 0.50 | 1.82 | 15 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:99:TYR:CZ | 1:A:101:THR:CG2 | 0.50 | 2.95 | 20 | 4 |
| 1:A:98:ILE:CD1 | 1:A:98:ILE:C | 0.50 | 2.80 | 8 | 4 |
| 1:A:80:GLU:O | 1:A:81:ALA:HB2 | 0.50 | 2.06 | 19 | 4 |
| 1:A:114:LEU:HD23 | 1:A:114:LEU:O | 0.50 | 2.06 | 3 | 1 |
| 1:A:21:ASN:O | 1:A:22:THR:HB | 0.50 | 2.06 | 14 | 5 |
| 1:A:19:ALA:N | 1:A:144:ALA:HB3 | 0.50 | 2.22 | 5 | 3 |
| 1:A:76:TYR:CZ | 1:A:78:SER:OG | 0.50 | 2.64 | 5 | 1 |
| 1:A:88:LEU:CD1 | 1:A:88:LEU:N | 0.50 | 2.74 | 5 | 1 |
| 1:A:13:TRP:NE1 | 1:A:115:TYR:CE2 | 0.50 | 2.79 | 2 | 1 |
| 1:A:21:ASN:O | 1:A:22:THR:CG2 | 0.50 | 2.59 | 1 | 2 |
| 1:A:16:VAL:CG1 | 1:A:146:LEU:HD12 | 0.50 | 2.36 | 9 | 1 |
| 1:A:15:VAL:O | 1:A:35:ALA:HB3 | 0.50 | 2.07 | 19 | 1 |
| 1:A:20:SER:O | 1:A:21:ASN:ND2 | 0.50 | 2.45 | 11 | 4 |
| 1:A:89:ASP:O | 1:A:90:THR:HB | 0.50 | 2.07 | 18 | 1 |
| 1:A:98:ILE:CG2 | 1:A:113:ARG:HB3 | 0.50 | 2.37 | 18 | 1 |
| 1:A:47:LEU:HD12 | 1:A:47:LEU:C | 0.50 | 2.26 | 18 | 1 |
| 1:A:15:VAL:HB | 1:A:35:ALA:HB1 | 0.50 | 1.84 | 15 | 1 |
| 1:A:47:LEU:HD23 | 1:A:68:LYS:O | 0.50 | 2.06 | 8 | 1 |
| 1:A:135:GLU:OE1 | 1:A:136:ARG:N | 0.50 | 2.44 | 17 | 1 |
| 1:A:51:TYR:N | 1:A:51:TYR:CD1 | 0.50 | 2.80 | 16 | 2 |
| 1:A:26:LEU:C | 1:A:26:LEU:HD12 | 0.50 | 2.26 | 13 | 1 |
| 1:A:41:PHE:CG | 1:A:47:LEU:HD13 | 0.50 | 2.42 | 20 | 1 |
| 1:A:95:TYR:CD2 | 1:A:122:SER:HB3 | 0.50 | 2.42 | 2 | 4 |
| 1:A:34:MET:O | 1:A:53:VAL:HA | 0.50 | 2.07 | 16 | 6 |
| 1:A:47:LEU:HD21 | 1:A:70:SER:OG | 0.50 | 2.07 | 18 | 1 |
| 1:A:145:MET:O | 1:A:146:LEU:C | 0.49 | 2.49 | 20 | 4 |
| 1:A:88:LEU:N | 1:A:88:LEU:CD1 | 0.49 | 2.74 | 17 | 2 |
| 1:A:66:PHE:CD2 | 1:A:79:GLU:OE2 | 0.49 | 2.64 | 19 | 3 |
| 1:A:13:TRP:CD1 | 1:A:115:TYR:CZ | 0.49 | 3.00 | 2 | 2 |
| 1:A:79:GLU:O | 1:A:83:LYS:HB3 | 0.49 | 2.06 | 18 | 2 |
| 1:A:99:TYR:CE1 | 1:A:112:MET:CE | 0.49 | 2.94 | 7 | 1 |
| 1:A:134:GLY:N | 1:A:139:THR:HG23 | 0.49 | 2.21 | 13 | 1 |
| 1:A:93:LYS:HD3 | 1:A:94:SER:N | 0.49 | 2.22 | 1 | 1 |
| 1:A:24:PHE:CE1 | 1:A:25:PHE:CE1 | 0.49 | 2.99 | 10 | 1 |
| 1:A:15:VAL:HG22 | 1:A:115:TYR:CD1 | 0.49 | 2.42 | 20 | 2 |
| 1:A:21:ASN:N | 1:A:110:HIS:O | 0.49 | 2.45 | 12 | 4 |
| 1:A:136:ARG:O | 1:A:137:ASN:HB3 | 0.49 | 2.07 | 6 | 2 |
| 1:A:17:ALA:O | 1:A:18:LEU:HD23 | 0.49 | 2.07 | 8 | 1 |
| 1:A:72:ASP:OD1 | 1:A:73:GLY:N | 0.49 | 2.45 | 4 | 1 |
| 1:A:75:VAL:CG1 | 1:A:87:VAL:HB | 0.49 | 2.32 | 16 | 2 |
| 1:A:32:MET:O | 1:A:147:PRO:CG | 0.49 | 2.60 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:45:ASP:O | 1:A:46:GLU:CG | 0.49 | 2.60 | 12 | 3 |
| 1:A:60:ARG:NH2 | 1:A:147:PRO:CG | 0.49 | 2.75 | 10 | 1 |
| 1:A:13:TRP:HB3 | 1:A:115:TYR:CD1 | 0.49 | 2.43 | 6 | 7 |
| 1:A:77:TYR:CE1 | 1:A:85:VAL:HG21 | 0.49 | 2.42 | 8 | 1 |
| 1:A:41:PHE:CE2 | 1:A:47:LEU:HD12 | 0.49 | 2.43 | 19 | 1 |
| 1:A:9:ILE:HD13 | 1:A:91:ASP:OD2 | 0.49 | 2.07 | 19 | 1 |
| 1:A:71:ASP:CB | 1:A:76:TYR:CZ | 0.49 | 2.95 | 13 | 1 |
| 1:A:88:LEU:N | 1:A:97:VAL:O | 0.49 | 2.44 | 6 | 8 |
| 1:A:32:MET:HE3 | 1:A:153:THR:N | 0.49 | 2.22 | 10 | 1 |
| 1:A:20:SER:O | 1:A:142:MET:O | 0.49 | 2.30 | 4 | 1 |
| 1:A:79:GLU:HB2 | 1:A:83:LYS:HB2 | 0.49 | 1.83 | 20 | 1 |
| 1:A:13:TRP:O | 1:A:37:ALA:N | 0.49 | 2.46 | 2 | 14 |
| 1:A:98:ILE:N | 1:A:113:ARG:O | 0.49 | 2.45 | 6 | 10 |
| 1:A:124:ALA:O | 1:A:128:ILE:N | 0.49 | 2.43 | 3 | 18 |
| 1:A:94:SER:HB2 | 1:A:117:ARG:NE | 0.49 | 2.22 | 2 | 1 |
| 1:A:41:PHE:CD1 | 1:A:47:LEU:HD13 | 0.49 | 2.43 | 20 | 1 |
| 1:A:48:LYS:HB3 | 1:A:67:LYS:HB3 | 0.49 | 1.83 | 12 | 7 |
| 1:A:96:ALA:HB3 | 1:A:115:TYR:O | 0.49 | 2.06 | 17 | 1 |
| 1:A:95:TYR:CD2 | 1:A:125:ALA:CB | 0.49 | 2.96 | 3 | 1 |
| 1:A:115:TYR:O | 1:A:115:TYR:CD1 | 0.49 | 2.66 | 14 | 2 |
| 1:A:27:ARG:NH1 | 1:A:111:MET:HE1 | 0.49 | 2.22 | 9 | 1 |
| 1:A:17:ALA:CB | 1:A:114:LEU:HD23 | 0.49 | 2.37 | 14 | 1 |
| 1:A:47:LEU:HD11 | 1:A:77:TYR:CE1 | 0.49 | 2.42 | 15 | 1 |
| 1:A:18:LEU:O | 1:A:144:ALA:CB | 0.49 | 2.60 | 1 | 1 |
| 1:A:128:ILE:HA | 1:A:131:LYS:HG2 | 0.49 | 1.82 | 3 | 2 |
| 1:A:95:TYR:CD2 | 1:A:125:ALA:HB2 | 0.49 | 2.42 | 12 | 2 |
| 1:A:51:TYR:O | 1:A:51:TYR:CD1 | 0.49 | 2.65 | 17 | 4 |
| 1:A:95:TYR:CD1 | 1:A:125:ALA:HB1 | 0.49 | 2.42 | 3 | 1 |
| 1:A:18:LEU:HB2 | 1:A:144:ALA:HB3 | 0.49 | 1.84 | 4 | 2 |
| 1:A:91:ASP:OD1 | 1:A:91:ASP:O | 0.49 | 2.31 | 7 | 1 |
| 1:A:146:LEU:CD2 | 1:A:146:LEU:N | 0.49 | 2.76 | 13 | 2 |
| 1:A:29:LYS:O | 1:A:32:MET:HG3 | 0.49 | 2.08 | 7 | 1 |
| 1:A:32:MET:HG3 | 1:A:154:VAL:HG12 | 0.49 | 1.84 | 14 | 1 |
| 1:A:93:LYS:C | 1:A:93:LYS:HD3 | 0.48 | 2.28 | 17 | 2 |
| 1:A:25:PHE:CD1 | 1:A:26:LEU:N | 0.48 | 2.81 | 4 | 2 |
| 1:A:77:TYR:CB | 1:A:85:VAL:O | 0.48 | 2.61 | 11 | 2 |
| 1:A:68:LYS:N | 1:A:68:LYS:HD3 | 0.48 | 2.22 | 8 | 1 |
| 1:A:16:VAL:HB | 1:A:146:LEU:HD22 | 0.48 | 1.85 | 17 | 1 |
| 1:A:107:ARG:O | 1:A:107:ARG:CG | 0.48 | 2.60 | 17 | 1 |
| 1:A:42:LEU:HD23 | 1:A:67:LYS:HD2 | 0.48 | 1.85 | 5 | 1 |
| 1:A:93:LYS:O | 1:A:94:SER:OG | 0.48 | 2.23 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:96:ALA:HB3 | 1:A:115:TYR:HD2 | 0.48 | 1.65 | 2 | 1 |
| 1:A:15:VAL:HG22 | 1:A:115:TYR:CE1 | 0.48 | 2.43 | 20 | 1 |
| 1:A:42:LEU:N | 1:A:42:LEU:HD22 | 0.48 | 2.23 | 20 | 1 |
| 1:A:32:MET:O | 1:A:32:MET:SD | 0.48 | 2.72 | 20 | 1 |
| 1:A:43:GLY:O | 1:A:44:GLU:HB2 | 0.48 | 2.08 | 19 | 2 |
| 1:A:75:VAL:HG11 | 1:A:91:ASP:CG | 0.48 | 2.28 | 17 | 2 |
| 1:A:76:TYR:CD1 | 1:A:86:GLU:HG2 | 0.48 | 2.43 | 5 | 1 |
| 1:A:75:VAL:O | 1:A:87:VAL:HG13 | 0.48 | 2.08 | 18 | 1 |
| 1:A:42:LEU:HD12 | 1:A:42:LEU:N | 0.48 | 2.23 | 15 | 1 |
| 1:A:68:LYS:HD2 | 1:A:77:TYR:CD2 | 0.48 | 2.43 | 10 | 2 |
| 1:A:68:LYS:CD | 1:A:68:LYS:N | 0.48 | 2.77 | 8 | 1 |
| 1:A:153:THR:HG23 | 1:A:153:THR:O | 0.48 | 2.08 | 2 | 3 |
| 1:A:44:GLU:O | 1:A:45:ASP:HB2 | 0.48 | 2.07 | 12 | 1 |
| 1:A:13:TRP:CD2 | 1:A:115:TYR:CE1 | 0.48 | 3.02 | 16 | 3 |
| 1:A:121:VAL:CG1 | 1:A:126:THR:HG23 | 0.48 | 2.38 | 15 | 3 |
| 1:A:36:MET:O | 1:A:51:TYR:CA | 0.48 | 2.61 | 15 | 2 |
| 1:A:93:LYS:HD2 | 1:A:93:LYS:C | 0.48 | 2.28 | 9 | 2 |
| 1:A:97:VAL:HG11 | 1:A:129:PHE:CB | 0.48 | 2.36 | 15 | 1 |
| 1:A:98:ILE:CG2 | 1:A:115:TYR:CD2 | 0.48 | 2.96 | 17 | 3 |
| 1:A:67:LYS:O | 1:A:68:LYS:HG2 | 0.48 | 2.09 | 20 | 1 |
| 1:A:95:TYR:CG | 1:A:125:ALA:HB1 | 0.48 | 2.42 | 3 | 1 |
| 1:A:47:LEU:CD1 | 1:A:68:LYS:O | 0.48 | 2.61 | 7 | 1 |
| 1:A:32:MET:CE | 1:A:154:VAL:HG12 | 0.48 | 2.38 | 14 | 1 |
| 1:A:115:TYR:N | 1:A:115:TYR:CD1 | 0.48 | 2.82 | 20 | 1 |
| 1:A:19:ALA:O | 1:A:20:SER:HB2 | 0.48 | 2.09 | 12 | 4 |
| 1:A:75:VAL:HG12 | 1:A:87:VAL:HG12 | 0.48 | 1.86 | 12 | 1 |
| 1:A:91:ASP:OD1 | 1:A:117:ARG:NH2 | 0.48 | 2.47 | 11 | 2 |
| 1:A:112:MET:CE | 1:A:133:ALA:HB1 | 0.48 | 2.38 | 13 | 1 |
| 1:A:100:ALA:N | 1:A:111:MET:O | 0.48 | 2.47 | 20 | 13 |
| 1:A:146:LEU:CD2 | 1:A:146:LEU:C | 0.48 | 2.82 | 9 | 2 |
| 1:A:10:ALA:HA | 1:A:39:ILE:HG23 | 0.48 | 1.85 | 11 | 1 |
| 1:A:95:TYR:CE2 | 1:A:122:SER:CB | 0.48 | 2.97 | 18 | 4 |
| 1:A:31:LYS:HD2 | 1:A:31:LYS:N | 0.48 | 2.23 | 4 | 2 |
| 1:A:145:MET:O | 1:A:154:VAL:HG23 | 0.48 | 2.09 | 8 | 2 |
| 1:A:95:TYR:CE2 | 1:A:125:ALA:HB1 | 0.48 | 2.44 | 3 | 1 |
| 1:A:77:TYR:CD2 | 1:A:85:VAL:CG2 | 0.48 | 2.97 | 2 | 2 |
| 1:A:42:LEU:CD1 | 1:A:42:LEU:N | 0.48 | 2.77 | 16 | 1 |
| 1:A:93:LYS:O | 1:A:93:LYS:HG2 | 0.48 | 2.08 | 13 | 1 |
| 1:A:41:PHE:CD2 | 1:A:47:LEU:CD2 | 0.47 | 2.97 | 9 | 4 |
| 1:A:9:ILE:O | 1:A:39:ILE:CG2 | 0.47 | 2.61 | 5 | 1 |
| 1:A:76:TYR:CD1 | 1:A:76:TYR:O | 0.47 | 2.67 | 15 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:101:THR:HG22 | 1:A:110:HIS:HD1 | 0.47 | 1.67 | 4 | 1 |
| 1:A:81:ALA:O | 1:A:82:LYS:C | 0.47 | 2.52 | 14 | 2 |
| 1:A:32:MET:HG2 | 1:A:152:CYS:HA | 0.47 | 1.85 | 9 | 1 |
| 1:A:133:ALA:HB1 | 1:A:139:THR:CG2 | 0.47 | 2.39 | 14 | 1 |
| 1:A:42:LEU:HD21 | 1:A:48:LYS:HG2 | 0.47 | 1.86 | 6 | 2 |
| 1:A:87:VAL:CB | 1:A:98:ILE:HB | 0.47 | 2.39 | 12 | 1 |
| 1:A:10:ALA:HA | 1:A:39:ILE:HG22 | 0.47 | 1.86 | 2 | 1 |
| 1:A:21:ASN:ND2 | 1:A:142:MET:HG2 | 0.47 | 2.23 | 9 | 1 |
| 1:A:99:TYR:HA | 1:A:112:MET:HA | 0.47 | 1.85 | 6 | 3 |
| 1:A:88:LEU:HD11 | 1:A:132:LEU:HD13 | 0.47 | 1.84 | 19 | 1 |
| 1:A:66:PHE:CE2 | 1:A:68:LYS:HE3 | 0.47 | 2.44 | 11 | 1 |
| 1:A:38:ARG:O | 1:A:49:VAL:HA | 0.47 | 2.09 | 14 | 2 |
| 1:A:41:PHE:HA | 1:A:47:LEU:HD22 | 0.47 | 1.86 | 10 | 1 |
| 1:A:77:TYR:O | 1:A:77:TYR:CD1 | 0.47 | 2.68 | 6 | 2 |
| 1:A:67:LYS:O | 1:A:68:LYS:HB2 | 0.47 | 2.09 | 17 | 3 |
| 1:A:75:VAL:HG13 | 1:A:87:VAL:CG1 | 0.47 | 2.39 | 4 | 1 |
| 1:A:34:MET:HA | 1:A:34:MET:CE | 0.47 | 2.39 | 7 | 1 |
| 1:A:67:LYS:HA | 1:A:77:TYR:OH | 0.47 | 2.10 | 15 | 1 |
| 1:A:102:ARG:CG | 1:A:109:LEU:HD21 | 0.47 | 2.39 | 1 | 1 |
| 1:A:109:LEU:N | 1:A:109:LEU:CD2 | 0.47 | 2.77 | 6 | 5 |
| 1:A:91:ASP:C | 1:A:92:TYR:CD1 | 0.47 | 2.88 | 8 | 4 |
| 1:A:15:VAL:HG23 | 1:A:18:LEU:HD21 | 0.47 | 1.87 | 8 | 1 |
| 1:A:95:TYR:CE1 | 1:A:125:ALA:HB1 | 0.47 | 2.45 | 3 | 1 |
| 1:A:16:VAL:CG1 | 1:A:17:ALA:N | 0.47 | 2.77 | 3 | 2 |
| 1:A:47:LEU:C | 1:A:47:LEU:HD23 | 0.47 | 2.29 | 19 | 1 |
| 1:A:90:THR:HG21 | 1:A:93:LYS:HD3 | 0.47 | 1.86 | 2 | 1 |
| 1:A:16:VAL:CB | 1:A:146:LEU:HD12 | 0.47 | 2.38 | 9 | 1 |
| 1:A:16:VAL:CG2 | 1:A:146:LEU:CD1 | 0.47 | 2.91 | 20 | 1 |
| 1:A:97:VAL:CG2 | 1:A:129:PHE:CD1 | 0.47 | 2.98 | 12 | 5 |
| 1:A:47:LEU:HD21 | 1:A:70:SER:HB2 | 0.47 | 1.86 | 6 | 1 |
| 1:A:13:TRP:CD1 | 1:A:117:ARG:NH1 | 0.47 | 2.82 | 1 | 2 |
| 1:A:49:VAL:CG1 | 1:A:66:PHE:CE1 | 0.47 | 2.97 | 8 | 1 |
| 1:A:18:LEU:CB | 1:A:144:ALA:HB3 | 0.47 | 2.39 | 3 | 2 |
| 1:A:41:PHE:CD2 | 1:A:47:LEU:HD21 | 0.47 | 2.45 | 3 | 1 |
| 1:A:31:LYS:N | 1:A:31:LYS:HD2 | 0.47 | 2.25 | 3 | 1 |
| 1:A:114:LEU:O | 1:A:114:LEU:HD13 | 0.47 | 2.10 | 12 | 1 |
| 1:A:98:ILE:CG2 | 1:A:113:ARG:O | 0.47 | 2.61 | 18 | 2 |
| 1:A:89:ASP:O | 1:A:90:THR:O | 0.47 | 2.33 | 14 | 1 |
| 1:A:124:ALA:O | 1:A:128:ILE:HB | 0.47 | 2.10 | 3 | 15 |
| 1:A:91:ASP:OD1 | 1:A:92:TYR:CE1 | 0.47 | 2.68 | 10 | 1 |
| 1:A:80:GLU:O | 1:A:82:LYS:N | 0.47 | 2.48 | 10 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:109:LEU:N | 1:A:109:LEU:HD12 | 0.47 | 2.23 | 8 | 1 |
| 1:A:34:MET:HG3 | 1:A:146:LEU:HD11 | 0.47 | 1.85 | 17 | 1 |
| 1:A:15:VAL:CG2 | 1:A:115:TYR:CE2 | 0.47 | 2.97 | 12 | 1 |
| 1:A:76:TYR:CD2 | 1:A:86:GLU:CB | 0.47 | 2.98 | 2 | 1 |
| 1:A:98:ILE:HG13 | 1:A:113:ARG:O | 0.47 | 2.10 | 7 | 1 |
| 1:A:145:MET:O | 1:A:154:VAL:HG22 | 0.47 | 2.10 | 13 | 1 |
| 1:A:41:PHE:CG | 1:A:47:LEU:HD22 | 0.47 | 2.44 | 13 | 1 |
| 1:A:71:ASP:HB3 | 1:A:76:TYR:CE2 | 0.47 | 2.45 | 15 | 2 |
| 1:A:77:TYR:CD2 | 1:A:79:GLU:OE2 | 0.47 | 2.68 | 20 | 1 |
| 1:A:47:LEU:O | 1:A:77:TYR:OH | 0.47 | 2.33 | 20 | 4 |
| 1:A:51:TYR:OH | 1:A:66:PHE:CZ | 0.47 | 2.67 | 6 | 2 |
| 1:A:145:MET:HG3 | 1:A:154:VAL:HG21 | 0.47 | 1.86 | 19 | 1 |
| 1:A:147:PRO:HB2 | 1:A:153:THR:HB | 0.47 | 1.86 | 19 | 1 |
| 1:A:115:TYR:CD1 | 1:A:115:TYR:C | 0.47 | 2.87 | 2 | 1 |
| 1:A:87:VAL:HG13 | 1:A:98:ILE:CG2 | 0.47 | 2.38 | 7 | 1 |
| 1:A:51:TYR:OH | 1:A:66:PHE:CE1 | 0.47 | 2.68 | 15 | 2 |
| 1:A:32:MET:HG3 | 1:A:154:VAL:HG13 | 0.47 | 1.85 | 1 | 1 |
| 1:A:13:TRP:CZ2 | 1:A:39:ILE:HD13 | 0.47 | 2.45 | 15 | 2 |
| 1:A:75:VAL:O | 1:A:87:VAL:HG12 | 0.47 | 2.07 | 18 | 1 |
| 1:A:113:ARG:HD3 | 1:A:115:TYR:OH | 0.47 | 2.10 | 11 | 1 |
| 1:A:99:TYR:CE2 | 1:A:101:THR:CG2 | 0.47 | 2.98 | 19 | 4 |
| 1:A:41:PHE:C | 1:A:42:LEU:HD22 | 0.47 | 2.30 | 9 | 2 |
| 1:A:92:TYR:N | 1:A:92:TYR:CD1 | 0.47 | 2.82 | 4 | 3 |
| 1:A:146:LEU:CD1 | 1:A:146:LEU:N | 0.47 | 2.78 | 19 | 2 |
| 1:A:13:TRP:CE2 | 1:A:39:ILE:HD12 | 0.47 | 2.45 | 2 | 1 |
| 1:A:15:VAL:HB | 1:A:115:TYR:CE2 | 0.47 | 2.45 | 11 | 1 |
| 1:A:19:ALA:HB3 | 1:A:112:MET:CE | 0.47 | 2.40 | 11 | 1 |
| 1:A:93:LYS:CG | 1:A:93:LYS:O | 0.47 | 2.62 | 13 | 1 |
| 1:A:145:MET:O | 1:A:146:LEU:O | 0.46 | 2.32 | 20 | 2 |
| 1:A:66:PHE:CE2 | 1:A:83:LYS:CG | 0.46 | 2.97 | 6 | 1 |
| 1:A:95:TYR:CE2 | 1:A:125:ALA:HA | 0.46 | 2.45 | 3 | 1 |
| 1:A:33:LYS:HD3 | 1:A:33:LYS:N | 0.46 | 2.25 | 3 | 2 |
| 1:A:74:GLU:OE1 | 1:A:74:GLU:N | 0.46 | 2.48 | 4 | 1 |
| 1:A:117:ARG:N | 1:A:117:ARG:CD | 0.46 | 2.79 | 2 | 1 |
| 1:A:84:LYS:HD2 | 1:A:85:VAL:N | 0.46 | 2.25 | 14 | 1 |
| 1:A:133:ALA:HB1 | 1:A:139:THR:OG1 | 0.46 | 2.10 | 15 | 1 |
| 1:A:19:ALA:N | 1:A:112:MET:HB2 | 0.46 | 2.24 | 19 | 3 |
| 1:A:77:TYR:CZ | 1:A:85:VAL:HG22 | 0.46 | 2.44 | 6 | 1 |
| 1:A:88:LEU:HB2 | 1:A:97:VAL:HG23 | 0.46 | 1.87 | 6 | 2 |
| 1:A:82:LYS:CB | 1:A:103:VAL:HG13 | 0.46 | 2.40 | 17 | 1 |
| 1:A:95:TYR:CZ | 1:A:125:ALA:HB1 | 0.46 | 2.45 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:59:CYS:O | 1:A:60:ARG:HB2 | 0.46 | 2.10 | 5 | 1 |
| 1:A:33:LYS:HD3 | 1:A:53:VAL:HG23 | 0.46 | 1.87 | 19 | 1 |
| 1:A:9:ILE:HD11 | 1:A:92:TYR:CE1 | 0.46 | 2.45 | 4 | 1 |
| 1:A:18:LEU:N | 1:A:18:LEU:CD2 | 0.46 | 2.78 | 15 | 3 |
| 1:A:82:LYS:HE3 | 1:A:82:LYS:HA | 0.46 | 1.86 | 2 | 1 |
| 1:A:24:PHE:CE2 | 1:A:27:ARG:NH2 | 0.46 | 2.83 | 11 | 1 |
| 1:A:88:LEU:CD2 | 1:A:132:LEU:HD22 | 0.46 | 2.40 | 6 | 1 |
| 1:A:22:THR:HG22 | 1:A:109:LEU:HB3 | 0.46 | 1.87 | 13 | 2 |
| 1:A:99:TYR:CD1 | 1:A:112:MET:HG3 | 0.46 | 2.45 | 2 | 1 |
| 1:A:15:VAL:N | 1:A:35:ALA:O | 0.46 | 2.48 | 11 | 1 |
| 1:A:87:VAL:CG1 | 1:A:98:ILE:HG22 | 0.46 | 2.37 | 7 | 1 |
| 1:A:41:PHE:CD1 | 1:A:41:PHE:O | 0.46 | 2.68 | 15 | 1 |
| 1:A:85:VAL:CG1 | 1:A:100:ALA:HA | 0.46 | 2.40 | 13 | 3 |
| 1:A:15:VAL:CG2 | 1:A:115:TYR:CZ | 0.46 | 2.99 | 6 | 2 |
| 1:A:77:TYR:O | 1:A:85:VAL:N | 0.46 | 2.48 | 10 | 2 |
| 1:A:68:LYS:HE3 | 1:A:77:TYR:CG | 0.46 | 2.45 | 8 | 1 |
| 1:A:62:TRP:CZ2 | 1:A:64:THR:OG1 | 0.46 | 2.69 | 5 | 2 |
| 1:A:80:GLU:OE1 | 1:A:80:GLU:N | 0.46 | 2.48 | 2 | 2 |
| 1:A:34:MET:HA | 1:A:146:LEU:CD2 | 0.46 | 2.40 | 5 | 1 |
| 1:A:49:VAL:O | 1:A:51:TYR:CE1 | 0.46 | 2.69 | 19 | 2 |
| 1:A:14:TYR:CB | 1:A:116:SER:O | 0.46 | 2.64 | 18 | 1 |
| 1:A:6:ARG:HD2 | 1:A:6:ARG:N | 0.46 | 2.26 | 11 | 1 |
| 1:A:32:MET:CG | 1:A:154:VAL:HG12 | 0.46 | 2.40 | 14 | 1 |
| 1:A:42:LEU:HD22 | 1:A:44:GLU:HB2 | 0.46 | 1.86 | 1 | 1 |
| 1:A:72:ASP:O | 1:A:73:GLY:C | 0.46 | 2.53 | 17 | 4 |
| 1:A:114:LEU:C | 1:A:114:LEU:CD1 | 0.46 | 2.84 | 17 | 2 |
| 1:A:23:GLU:N | 1:A:23:GLU:OE1 | 0.46 | 2.49 | 3 | 1 |
| 1:A:85:VAL:HG11 | 1:A:100:ALA:CB | 0.46 | 2.41 | 2 | 1 |
| 1:A:107:ARG:NH1 | 1:A:109:LEU:HD11 | 0.46 | 2.26 | 14 | 1 |
| 1:A:17:ALA:HB3 | 1:A:114:LEU:HD23 | 0.46 | 1.87 | 14 | 1 |
| 1:A:19:ALA:O | 1:A:112:MET:SD | 0.46 | 2.74 | 14 | 3 |
| 1:A:68:LYS:N | 1:A:68:LYS:CD | 0.46 | 2.78 | 13 | 1 |
| 1:A:13:TRP:CZ2 | 1:A:39:ILE:HG21 | 0.46 | 2.45 | 15 | 1 |
| 1:A:92:TYR:CD1 | 1:A:92:TYR:N | 0.46 | 2.84 | 8 | 2 |
| 1:A:20:SER:O | 1:A:21:ASN:CG | 0.46 | 2.54 | 2 | 1 |
| 1:A:94:SER:O | 1:A:117:ARG:HD2 | 0.46 | 2.10 | 2 | 1 |
| 1:A:48:LYS:HD2 | 1:A:48:LYS:C | 0.46 | 2.31 | 19 | 7 |
| 1:A:97:VAL:HG12 | 1:A:114:LEU:CG | 0.46 | 2.39 | 16 | 5 |
| 1:A:37:ALA:HB2 | 1:A:51:TYR:CB | 0.46 | 2.37 | 10 | 1 |
| 1:A:112:MET:HB3 | 1:A:129:PHE:CZ | 0.46 | 2.46 | 4 | 1 |
| 1:A:97:VAL:CG1 | 1:A:114:LEU:HD13 | 0.46 | 2.25 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:95:TYR:CD1 | 1:A:95:TYR:O | 0.46 | 2.69 | 8 | 3 |
| 1:A:68:LYS:CG | 1:A:78:SER:O | 0.46 | 2.64 | 14 | 6 |
| 1:A:97:VAL:HG23 | 1:A:97:VAL:O | 0.46 | 2.11 | 6 | 3 |
| 1:A:114:LEU:C | 1:A:114:LEU:CD2 | 0.46 | 2.84 | 11 | 6 |
| 1:A:15:VAL:O | 1:A:16:VAL:HG13 | 0.46 | 2.10 | 19 | 1 |
| 1:A:17:ALA:O | 1:A:18:LEU:HD12 | 0.46 | 2.10 | 19 | 1 |
| 1:A:152:CYS:O | 1:A:153:THR:CG2 | 0.46 | 2.64 | 19 | 1 |
| 1:A:147:PRO:O | 1:A:154:VAL:HG12 | 0.46 | 2.10 | 19 | 1 |
| 1:A:99:TYR:CD1 | 1:A:112:MET:SD | 0.46 | 3.09 | 13 | 3 |
| 1:A:85:VAL:HG23 | 1:A:98:ILE:CD1 | 0.45 | 2.33 | 20 | 1 |
| 1:A:124:ALA:O | 1:A:128:ILE:CB | 0.45 | 2.64 | 5 | 8 |
| 1:A:93:LYS:O | 1:A:94:SER:HB3 | 0.45 | 2.12 | 9 | 3 |
| 1:A:145:MET:O | 1:A:154:VAL:CG2 | 0.45 | 2.64 | 3 | 3 |
| 1:A:115:TYR:C | 1:A:115:TYR:CD1 | 0.45 | 2.89 | 5 | 1 |
| 1:A:41:PHE:O | 1:A:41:PHE:CD1 | 0.45 | 2.70 | 5 | 1 |
| 1:A:82:LYS:HD2 | 1:A:82:LYS:N | 0.45 | 2.26 | 15 | 2 |
| 1:A:42:LEU:HD22 | 1:A:67:LYS:HE2 | 0.45 | 1.86 | 15 | 1 |
| 1:A:82:LYS:HG2 | 1:A:83:LYS:HD3 | 0.45 | 1.88 | 15 | 1 |
| 1:A:75:VAL:O | 1:A:87:VAL:CG2 | 0.45 | 2.64 | 6 | 1 |
| 1:A:20:SER:HB2 | 1:A:110:HIS:O | 0.45 | 2.11 | 8 | 1 |
| 1:A:21:ASN:HB3 | 1:A:142:MET:HB2 | 0.45 | 1.88 | 17 | 1 |
| 1:A:137:ASN:O | 1:A:138:TYR:CB | 0.45 | 2.65 | 17 | 2 |
| 1:A:77:TYR:CE1 | 1:A:85:VAL:HB | 0.45 | 2.47 | 7 | 2 |
| 1:A:38:ARG:C | 1:A:49:VAL:HG23 | 0.45 | 2.32 | 19 | 1 |
| 1:A:14:TYR:CD1 | 1:A:116:SER:O | 0.45 | 2.70 | 2 | 1 |
| 1:A:82:LYS:O | 1:A:103:VAL:CG1 | 0.45 | 2.65 | 18 | 1 |
| 1:A:59:CYS:O | 1:A:60:ARG:CB | 0.45 | 2.64 | 9 | 1 |
| 1:A:13:TRP:N | 1:A:37:ALA:O | 0.45 | 2.47 | 13 | 4 |
| 1:A:109:LEU:C | 1:A:109:LEU:CD2 | 0.45 | 2.84 | 16 | 2 |
| 1:A:21:ASN:CG | 1:A:142:MET:HB2 | 0.45 | 2.32 | 15 | 1 |
| 1:A:48:LYS:HB3 | 1:A:67:LYS:CB | 0.45 | 2.42 | 16 | 2 |
| 1:A:42:LEU:O | 1:A:43:GLY:O | 0.45 | 2.35 | 11 | 4 |
| 1:A:86:GLU:HB3 | 1:A:99:TYR:CZ | 0.45 | 2.47 | 6 | 1 |
| 1:A:113:ARG:CD | 1:A:115:TYR:CZ | 0.45 | 3.00 | 8 | 3 |
| 1:A:23:GLU:CD | 1:A:26:LEU:HD12 | 0.45 | 2.31 | 8 | 1 |
| 1:A:19:ALA:HA | 1:A:144:ALA:N | 0.45 | 2.26 | 14 | 6 |
| 1:A:102:ARG:CD | 1:A:109:LEU:HD13 | 0.45 | 2.42 | 5 | 1 |
| 1:A:48:LYS:HB2 | 1:A:66:PHE:O | 0.45 | 2.10 | 19 | 1 |
| 1:A:88:LEU:HB2 | 1:A:97:VAL:CG2 | 0.45 | 2.40 | 2 | 1 |
| 1:A:14:TYR:HB2 | 1:A:116:SER:OG | 0.45 | 2.11 | 2 | 2 |
| 1:A:53:VAL:O | 1:A:53:VAL:CG2 | 0.45 | 2.65 | 11 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:93:LYS:NZ | 1:A:93:LYS:HB3 | 0.45 | 2.27 | 9 | 1 |
| 1:A:26:LEU:HD22 | 1:A:142:MET:CE | 0.45 | 2.41 | 13 | 1 |
| 1:A:89:ASP:CB | 1:A:97:VAL:HG13 | 0.45 | 2.41 | 16 | 2 |
| 1:A:18:LEU:CD2 | 1:A:111:MET:HE2 | 0.45 | 2.41 | 5 | 1 |
| 1:A:47:LEU:HD21 | 1:A:70:SER:HB3 | 0.45 | 1.87 | 4 | 1 |
| 1:A:14:TYR:HB3 | 1:A:36:MET:HA | 0.45 | 1.89 | 11 | 1 |
| 1:A:11:GLY:O | 1:A:38:ARG:HG3 | 0.45 | 2.12 | 11 | 1 |
| 1:A:133:ALA:O | 1:A:137:ASN:O | 0.45 | 2.35 | 15 | 1 |
| 1:A:105:ASP:O | 1:A:105:ASP:OD1 | 0.45 | 2.35 | 15 | 1 |
| 1:A:109:LEU:CD1 | 1:A:109:LEU:N | 0.45 | 2.79 | 2 | 2 |
| 1:A:31:LYS:CD | 1:A:31:LYS:N | 0.45 | 2.79 | 10 | 3 |
| 1:A:98:ILE:O | 1:A:113:ARG:N | 0.45 | 2.49 | 12 | 3 |
| 1:A:87:VAL:C | 1:A:88:LEU:HD12 | 0.45 | 2.32 | 5 | 1 |
| 1:A:103:VAL:HA | 1:A:107:ARG:O | 0.45 | 2.11 | 14 | 1 |
| 1:A:44:GLU:O | 1:A:45:ASP:HB3 | 0.45 | 2.12 | 10 | 4 |
| 1:A:99:TYR:CD1 | 1:A:99:TYR:C | 0.45 | 2.90 | 9 | 2 |
| 1:A:39:ILE:HD11 | 1:A:47:LEU:HD12 | 0.45 | 1.87 | 5 | 1 |
| 1:A:100:ALA:HB3 | 1:A:111:MET:HG3 | 0.45 | 1.86 | 19 | 1 |
| 1:A:97:VAL:HB | 1:A:129:PHE:CD1 | 0.45 | 2.47 | 13 | 2 |
| 1:A:93:LYS:HD2 | 1:A:93:LYS:N | 0.45 | 2.26 | 2 | 2 |
| 1:A:77:TYR:CE1 | 1:A:85:VAL:CG1 | 0.45 | 2.99 | 18 | 1 |
| 1:A:36:MET:O | 1:A:51:TYR:CB | 0.45 | 2.65 | 20 | 2 |
| 1:A:51:TYR:CE1 | 1:A:64:THR:HB | 0.45 | 2.47 | 10 | 1 |
| 1:A:16:VAL:CB | 1:A:146:LEU:HD13 | 0.45 | 2.36 | 6 | 1 |
| 1:A:47:LEU:CD1 | 1:A:47:LEU:N | 0.45 | 2.80 | 2 | 4 |
| 1:A:77:TYR:N | 1:A:85:VAL:O | 0.45 | 2.50 | 5 | 2 |
| 1:A:66:PHE:CZ | 1:A:68:LYS:CE | 0.45 | 2.99 | 11 | 1 |
| 1:A:98:ILE:O | 1:A:113:ARG:CB | 0.45 | 2.65 | 10 | 1 |
| 1:A:68:LYS:CG | 1:A:77:TYR:CD1 | 0.45 | 3.00 | 12 | 1 |
| 1:A:29:LYS:HE2 | 1:A:29:LYS:HA | 0.45 | 1.89 | 12 | 1 |
| 1:A:70:SER:OG | 1:A:77:TYR:HB2 | 0.45 | 2.12 | 19 | 1 |
| 1:A:33:LYS:HB2 | 1:A:53:VAL:CG1 | 0.45 | 2.42 | 14 | 1 |
| 1:A:105:ASP:OD1 | 1:A:105:ASP:O | 0.45 | 2.35 | 14 | 1 |
| 1:A:85:VAL:HG13 | 1:A:99:TYR:C | 0.45 | 2.31 | 1 | 1 |
| 1:A:15:VAL:HG23 | 1:A:115:TYR:CD1 | 0.45 | 2.47 | 6 | 1 |
| 1:A:13:TRP:NE1 | 1:A:39:ILE:CG2 | 0.45 | 2.80 | 5 | 2 |
| 1:A:75:VAL:HG11 | 1:A:91:ASP:HB3 | 0.45 | 1.87 | 5 | 1 |
| 1:A:119:PRO:O | 1:A:121:VAL:N | 0.45 | 2.48 | 12 | 3 |
| 1:A:41:PHE:CE2 | 1:A:47:LEU:CD2 | 0.45 | 3.00 | 16 | 1 |
| 1:A:89:ASP:CG | 1:A:97:VAL:HG13 | 0.45 | 2.32 | 14 | 1 |
| 1:A:52:ALA:HA | 1:A:62:TRP:O | 0.45 | 2.12 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:79:GLU:OE1 | 1:A:83:LYS:HB3 | 0.44 | 2.12 | 20 | 1 |
| 1:A:8:GLU:OE2 | 1:A:92:TYR:CD2 | 0.44 | 2.70 | 9 | 4 |
| 1:A:29:LYS:O | 1:A:32:MET:CE | 0.44 | 2.65 | 6 | 2 |
| 1:A:49:VAL:CG1 | 1:A:49:VAL:O | 0.44 | 2.65 | 15 | 2 |
| 1:A:22:THR:OG1 | 1:A:23:GLU:N | 0.44 | 2.50 | 11 | 3 |
| 1:A:18:LEU:HD23 | 1:A:111:MET:CE | 0.44 | 2.42 | 5 | 1 |
| 1:A:68:LYS:CD | 1:A:77:TYR:CE1 | 0.44 | 3.00 | 12 | 1 |
| 1:A:8:GLU:OE2 | 1:A:92:TYR:CE2 | 0.44 | 2.70 | 7 | 2 |
| 1:A:76:TYR:CE2 | 1:A:86:GLU:HB2 | 0.44 | 2.48 | 2 | 1 |
| 1:A:39:ILE:HD12 | 1:A:40:SER:H | 0.44 | 1.71 | 7 | 1 |
| 1:A:138:TYR:O | 1:A:138:TYR:CG | 0.44 | 2.70 | 7 | 1 |
| 1:A:130:ARG:O | 1:A:134:GLY:N | 0.44 | 2.49 | 5 | 3 |
| 1:A:66:PHE:CG | 1:A:79:GLU:OE2 | 0.44 | 2.70 | 19 | 1 |
| 1:A:13:TRP:CE2 | 1:A:39:ILE:CD1 | 0.44 | 3.01 | 2 | 1 |
| 1:A:77:TYR:HB2 | 1:A:85:VAL:O | 0.44 | 2.13 | 9 | 1 |
| 1:A:41:PHE:CD1 | 1:A:41:PHE:N | 0.44 | 2.84 | 16 | 7 |
| 1:A:85:VAL:HG12 | 1:A:86:GLU:N | 0.44 | 2.27 | 10 | 1 |
| 1:A:69:THR:O | 1:A:76:TYR:O | 0.44 | 2.36 | 9 | 2 |
| 1:A:109:LEU:HD23 | 1:A:109:LEU:H | 0.44 | 1.72 | 6 | 1 |
| 1:A:51:TYR:CE1 | 1:A:64:THR:HG22 | 0.44 | 2.47 | 6 | 1 |
| 1:A:99:TYR:CB | 1:A:112:MET:HG2 | 0.44 | 2.42 | 9 | 3 |
| 1:A:115:TYR:CD1 | 1:A:116:SER:N | 0.44 | 2.85 | 5 | 1 |
| 1:A:90:THR:OG1 | 1:A:92:TYR:CD1 | 0.44 | 2.68 | 4 | 1 |
| 1:A:86:GLU:C | 1:A:98:ILE:HD13 | 0.44 | 2.32 | 4 | 1 |
| 1:A:88:LEU:CD1 | 1:A:132:LEU:HD13 | 0.44 | 2.31 | 2 | 2 |
| 1:A:13:TRP:CG | 1:A:115:TYR:CD1 | 0.44 | 3.05 | 16 | 1 |
| 1:A:41:PHE:C | 1:A:42:LEU:HD12 | 0.44 | 2.33 | 15 | 1 |
| 1:A:71:ASP:OD1 | 1:A:76:TYR:CD2 | 0.44 | 2.70 | 15 | 1 |
| 1:A:20:SER:HA | 1:A:142:MET:HB3 | 0.44 | 1.89 | 20 | 2 |
| 1:A:51:TYR:CE1 | 1:A:64:THR:CG2 | 0.44 | 3.01 | 6 | 1 |
| 1:A:13:TRP:CZ2 | 1:A:39:ILE:CD1 | 0.44 | 3.01 | 8 | 5 |
| 1:A:113:ARG:HD3 | 1:A:115:TYR:CZ | 0.44 | 2.48 | 8 | 1 |
| 1:A:37:ALA:HA | 1:A:50:SER:O | 0.44 | 2.13 | 5 | 3 |
| 1:A:26:LEU:N | 1:A:26:LEU:CD1 | 0.44 | 2.80 | 12 | 1 |
| 1:A:22:THR:OG1 | 1:A:109:LEU:CB | 0.44 | 2.65 | 18 | 3 |
| 1:A:85:VAL:HG13 | 1:A:100:ALA:HB2 | 0.44 | 1.88 | 18 | 1 |
| 1:A:68:LYS:CG | 1:A:77:TYR:HB2 | 0.44 | 2.43 | 13 | 1 |
| 1:A:33:LYS:HE3 | 1:A:53:VAL:HG11 | 0.44 | 1.87 | 10 | 1 |
| 1:A:72:ASP:OD2 | 1:A:76:TYR:CE1 | 0.44 | 2.70 | 10 | 1 |
| 1:A:15:VAL:CG1 | 1:A:35:ALA:O | 0.44 | 2.66 | 13 | 2 |
| 1:A:86:GLU:O | 1:A:98:ILE:HD12 | 0.44 | 2.12 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:88:LEU:HD23 | 1:A:97:VAL:O | 0.44 | 2.13 | 18 | 1 |
| 1:A:30:ASP:O | 1:A:32:MET:N | 0.44 | 2.50 | 13 | 1 |
| 1:A:29:LYS:HE3 | 1:A:29:LYS:HA | 0.44 | 1.90 | 13 | 1 |
| 1:A:18:LEU:HA | 1:A:112:MET:O | 0.44 | 2.13 | 6 | 1 |
| 1:A:84:LYS:N | 1:A:101:THR:O | 0.44 | 2.50 | 5 | 1 |
| 1:A:76:TYR:CD1 | 1:A:76:TYR:C | 0.44 | 2.90 | 9 | 2 |
| 1:A:93:LYS:HE2 | 1:A:95:TYR:CZ | 0.44 | 2.47 | 18 | 1 |
| 1:A:21:ASN:HD22 | 1:A:110:HIS:HB2 | 0.44 | 1.73 | 1 | 1 |
| 1:A:42:LEU:N | 1:A:46:GLU:O | 0.44 | 2.50 | 20 | 3 |
| 1:A:34:MET:O | 1:A:54:PRO:CD | 0.44 | 2.66 | 3 | 6 |
| 1:A:128:ILE:O | 1:A:131:LYS:HB3 | 0.44 | 2.13 | 8 | 1 |
| 1:A:75:VAL:CG1 | 1:A:87:VAL:HG12 | 0.44 | 2.42 | 12 | 1 |
| 1:A:102:ARG:NH1 | 1:A:111:MET:CE | 0.44 | 2.81 | 4 | 1 |
| 1:A:138:TYR:CG | 1:A:138:TYR:O | 0.44 | 2.70 | 2 | 1 |
| 1:A:26:LEU:HD22 | 1:A:27:ARG:N | 0.44 | 2.28 | 7 | 1 |
| 1:A:16:VAL:HG13 | 1:A:17:ALA:N | 0.44 | 2.28 | 10 | 2 |
| 1:A:15:VAL:HG23 | 1:A:115:TYR:CE1 | 0.44 | 2.47 | 6 | 1 |
| 1:A:75:VAL:CB | 1:A:87:VAL:CG1 | 0.44 | 2.96 | 12 | 1 |
| 1:A:69:THR:O | 1:A:77:TYR:CA | 0.44 | 2.63 | 2 | 3 |
| 1:A:61:LYS:C | 1:A:62:TRP:CD1 | 0.44 | 2.91 | 16 | 1 |
| 1:A:59:CYS:O | 1:A:60:ARG:CG | 0.44 | 2.66 | 18 | 1 |
| 1:A:15:VAL:HG22 | 1:A:35:ALA:HB3 | 0.44 | 1.89 | 7 | 1 |
| 1:A:76:TYR:CD1 | 1:A:86:GLU:OE2 | 0.44 | 2.70 | 9 | 1 |
| 1:A:41:PHE:CD2 | 1:A:47:LEU:HD23 | 0.44 | 2.48 | 14 | 2 |
| 1:A:42:LEU:HB3 | 1:A:46:GLU:HG2 | 0.44 | 1.88 | 14 | 1 |
| 1:A:44:GLU:O | 1:A:45:ASP:CG | 0.44 | 2.56 | 20 | 1 |
| 1:A:54:PRO:HA | 1:A:60:ARG:O | 0.44 | 2.13 | 17 | 1 |
| 1:A:45:ASP:O | 1:A:46:GLU:HG3 | 0.44 | 2.13 | 9 | 4 |
| 1:A:32:MET:HB3 | 1:A:154:VAL:HG11 | 0.44 | 1.88 | 17 | 1 |
| 1:A:12:LYS:NZ | 1:A:12:LYS:HB3 | 0.44 | 2.28 | 4 | 2 |
| 1:A:53:VAL:N | 1:A:62:TRP:O | 0.44 | 2.50 | 16 | 4 |
| 1:A:133:ALA:O | 1:A:137:ASN:N | 0.44 | 2.51 | 16 | 1 |
| 1:A:41:PHE:N | 1:A:41:PHE:CD1 | 0.44 | 2.86 | 14 | 3 |
| 1:A:13:TRP:CE2 | 1:A:39:ILE:HB | 0.44 | 2.48 | 7 | 1 |
| 1:A:13:TRP:O | 1:A:37:ALA:O | 0.44 | 2.36 | 1 | 1 |
| 1:A:48:LYS:C | 1:A:48:LYS:HD2 | 0.43 | 2.34 | 17 | 3 |
| 1:A:13:TRP:CG | 1:A:115:TYR:CZ | 0.43 | 3.06 | 5 | 1 |
| 1:A:42:LEU:CB | 1:A:46:GLU:O | 0.43 | 2.65 | 12 | 1 |
| 1:A:15:VAL:HA | 1:A:115:TYR:HA | 0.43 | 1.88 | 11 | 1 |
| 1:A:13:TRP:CD1 | 1:A:39:ILE:CG2 | 0.43 | 3.01 | 7 | 1 |
| 1:A:96:ALA:O | 1:A:114:LEU:HD12 | 0.43 | 2.13 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:16:VAL:HG13 | 1:A:146:LEU:HB2 | 0.43 | 1.89 | 8 | 1 |
| 1:A:93:LYS:CD | 1:A:93:LYS:O | 0.43 | 2.65 | 3 | 1 |
| 1:A:88:LEU:HD23 | 1:A:132:LEU:CD1 | 0.43 | 2.41 | 5 | 1 |
| 1:A:102:ARG:CZ | 1:A:111:MET:HE1 | 0.43 | 2.43 | 2 | 1 |
| 1:A:76:TYR:CE1 | 1:A:85:VAL:O | 0.43 | 2.71 | 14 | 1 |
| 1:A:28:GLU:O | 1:A:32:MET:CG | 0.43 | 2.66 | 20 | 1 |
| 1:A:83:LYS:N | 1:A:83:LYS:HD3 | 0.43 | 2.28 | 8 | 1 |
| 1:A:71:ASP:OD1 | 1:A:72:ASP:N | 0.43 | 2.51 | 16 | 2 |
| 1:A:27:ARG:NE | 1:A:27:ARG:HA | 0.43 | 2.28 | 17 | 1 |
| 1:A:95:TYR:OH | 1:A:114:LEU:CD1 | 0.43 | 2.66 | 3 | 1 |
| 1:A:88:LEU:CD2 | 1:A:132:LEU:HD13 | 0.43 | 2.42 | 5 | 1 |
| 1:A:13:TRP:NE1 | 1:A:39:ILE:HG21 | 0.43 | 2.28 | 5 | 1 |
| 1:A:39:ILE:HA | 1:A:49:VAL:HA | 0.43 | 1.90 | 5 | 1 |
| 1:A:17:ALA:HB3 | 1:A:114:LEU:CG | 0.43 | 2.43 | 12 | 1 |
| 1:A:147:PRO:CB | 1:A:154:VAL:HG12 | 0.43 | 2.44 | 4 | 1 |
| 1:A:53:VAL:O | 1:A:62:TRP:N | 0.43 | 2.49 | 4 | 1 |
| 1:A:53:VAL:CG2 | 1:A:62:TRP:HB2 | 0.43 | 2.43 | 16 | 1 |
| 1:A:85:VAL:HG13 | 1:A:100:ALA:CA | 0.43 | 2.44 | 7 | 3 |
| 1:A:136:ARG:NH1 | 1:A:136:ARG:HB3 | 0.43 | 2.28 | 13 | 1 |
| 1:A:100:ALA:HB2 | 1:A:113:ARG:HH12 | 0.43 | 1.73 | 15 | 1 |
| 1:A:21:ASN:HB2 | 1:A:110:HIS:HB2 | 0.43 | 1.91 | 15 | 1 |
| 1:A:82:LYS:O | 1:A:82:LYS:HD3 | 0.43 | 2.14 | 10 | 1 |
| 1:A:60:ARG:NH2 | 1:A:147:PRO:HG3 | 0.43 | 2.28 | 10 | 1 |
| 1:A:31:LYS:O | 1:A:32:MET:CG | 0.43 | 2.66 | 10 | 1 |
| 1:A:13:TRP:CZ2 | 1:A:91:ASP:OD1 | 0.43 | 2.71 | 6 | 1 |
| 1:A:16:VAL:O | 1:A:18:LEU:HD22 | 0.43 | 2.14 | 4 | 2 |
| 1:A:42:LEU:C | 1:A:42:LEU:HD13 | 0.43 | 2.34 | 8 | 1 |
| 1:A:102:ARG:HD2 | 1:A:102:ARG:N | 0.43 | 2.28 | 3 | 1 |
| 1:A:27:ARG:NH1 | 1:A:27:ARG:HB3 | 0.43 | 2.27 | 3 | 1 |
| 1:A:67:LYS:N | 1:A:77:TYR:OH | 0.43 | 2.51 | 5 | 1 |
| 1:A:76:TYR:CD2 | 1:A:86:GLU:OE2 | 0.43 | 2.71 | 16 | 1 |
| 1:A:7:SER:O | 1:A:10:ALA:O | 0.43 | 2.36 | 18 | 1 |
| 1:A:66:PHE:HB3 | 1:A:77:TYR:CE2 | 0.43 | 2.48 | 14 | 1 |
| 1:A:42:LEU:O | 1:A:44:GLU:N | 0.43 | 2.52 | 12 | 3 |
| 1:A:33:LYS:N | 1:A:33:LYS:HD2 | 0.43 | 2.29 | 19 | 1 |
| 1:A:66:PHE:CD2 | 1:A:68:LYS:NZ | 0.43 | 2.86 | 7 | 1 |
| 1:A:67:LYS:O | 1:A:68:LYS:CG | 0.43 | 2.66 | 20 | 3 |
| 1:A:131:LYS:NZ | 1:A:131:LYS:HB3 | 0.43 | 2.29 | 3 | 1 |
| 1:A:42:LEU:C | 1:A:42:LEU:CD1 | 0.43 | 2.86 | 7 | 1 |
| 1:A:42:LEU:O | 1:A:43:GLY:C | 0.43 | 2.56 | 7 | 1 |
| 1:A:26:LEU:HD22 | 1:A:26:LEU:N | 0.43 | 2.28 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:146:LEU:CD2 | 1:A:147:PRO:O | 0.43 | 2.67 | 20 | 1 |
| 1:A:26:LEU:N | 1:A:26:LEU:CD2 | 0.43 | 2.82 | 20 | 1 |
| 1:A:66:PHE:CE2 | 1:A:83:LYS:HG2 | 0.43 | 2.49 | 6 | 1 |
| 1:A:13:TRP:CZ2 | 1:A:91:ASP:OD2 | 0.43 | 2.72 | 8 | 2 |
| 1:A:102:ARG:HB2 | 1:A:109:LEU:HD11 | 0.43 | 1.91 | 12 | 1 |
| 1:A:29:LYS:CE | 1:A:29:LYS:HA | 0.43 | 2.44 | 12 | 2 |
| 1:A:51:TYR:CD2 | 1:A:113:ARG:NH1 | 0.43 | 2.87 | 9 | 1 |
| 1:A:16:VAL:CG2 | 1:A:146:LEU:HB2 | 0.43 | 2.38 | 15 | 1 |
| 1:A:21:ASN:N | 1:A:21:ASN:ND2 | 0.43 | 2.66 | 1 | 1 |
| 1:A:76:TYR:CD1 | 1:A:86:GLU:HB3 | 0.43 | 2.48 | 1 | 1 |
| 1:A:22:THR:HG22 | 1:A:111:MET:HE2 | 0.43 | 1.90 | 20 | 1 |
| 1:A:68:LYS:HG2 | 1:A:78:SER:O | 0.43 | 2.13 | 6 | 4 |
| 1:A:25:PHE:CE1 | 1:A:28:GLU:HB2 | 0.43 | 2.49 | 6 | 1 |
| 1:A:68:LYS:N | 1:A:68:LYS:HD2 | 0.43 | 2.29 | 12 | 1 |
| 1:A:18:LEU:HD12 | 1:A:18:LEU:N | 0.43 | 2.27 | 9 | 1 |
| 1:A:38:ARG:C | 1:A:38:ARG:HD3 | 0.43 | 2.33 | 14 | 1 |
| 1:A:6:ARG:HB2 | 1:A:6:ARG:NH1 | 0.43 | 2.29 | 14 | 1 |
| 1:A:68:LYS:HE3 | 1:A:77:TYR:HB3 | 0.43 | 1.90 | 3 | 1 |
| 1:A:18:LEU:CD2 | 1:A:18:LEU:N | 0.43 | 2.79 | 12 | 1 |
| 1:A:75:VAL:HG12 | 1:A:76:TYR:CD2 | 0.43 | 2.49 | 19 | 1 |
| 1:A:93:LYS:HE3 | 1:A:95:TYR:CE1 | 0.43 | 2.49 | 4 | 1 |
| 1:A:128:ILE:HG22 | 1:A:132:LEU:HD13 | 0.43 | 1.90 | 11 | 1 |
| 1:A:24:PHE:CZ | 1:A:27:ARG:NH2 | 0.43 | 2.87 | 11 | 1 |
| 1:A:32:MET:O | 1:A:147:PRO:HG3 | 0.43 | 2.13 | 9 | 1 |
| 1:A:18:LEU:HB2 | 1:A:144:ALA:O | 0.43 | 2.13 | 16 | 2 |
| 1:A:146:LEU:C | 1:A:146:LEU:CD2 | 0.43 | 2.88 | 10 | 1 |
| 1:A:18:LEU:CD1 | 1:A:112:MET:O | 0.43 | 2.66 | 6 | 1 |
| 1:A:61:LYS:HB2 | 1:A:61:LYS:NZ | 0.43 | 2.29 | 8 | 1 |
| 1:A:16:VAL:HA | 1:A:146:LEU:HB2 | 0.43 | 1.90 | 5 | 1 |
| 1:A:68:LYS:HB2 | 1:A:77:TYR:CE1 | 0.43 | 2.49 | 4 | 1 |
| 1:A:133:ALA:HB3 | 1:A:139:THR:HG22 | 0.43 | 1.90 | 4 | 1 |
| 1:A:13:TRP:CZ2 | 1:A:39:ILE:HB | 0.43 | 2.49 | 11 | 1 |
| 1:A:19:ALA:HB3 | 1:A:112:MET:HE2 | 0.43 | 1.91 | 11 | 1 |
| 1:A:29:LYS:NZ | 1:A:29:LYS:HB3 | 0.43 | 2.29 | 11 | 1 |
| 1:A:85:VAL:HG12 | 1:A:98:ILE:HG13 | 0.43 | 1.89 | 15 | 1 |
| 1:A:42:LEU:HD23 | 1:A:48:LYS:H | 0.42 | 1.74 | 10 | 1 |
| 1:A:20:SER:OG | 1:A:27:ARG:NH2 | 0.42 | 2.52 | 2 | 2 |
| 1:A:114:LEU:CD2 | 1:A:114:LEU:C | 0.42 | 2.88 | 1 | 3 |
| 1:A:24:PHE:CE1 | 1:A:107:ARG:CZ | 0.42 | 3.02 | 16 | 1 |
| 1:A:61:LYS:HD3 | 1:A:61:LYS:N | 0.42 | 2.29 | 1 | 1 |
| 1:A:29:LYS:HB3 | 1:A:29:LYS:NZ | 0.42 | 2.29 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:66:PHE:CZ | 1:A:79:GLU:OE2 | 0.42 | 2.72 | 20 | 1 |
| 1:A:67:LYS:NZ | 1:A:67:LYS:HB3 | 0.42 | 2.29 | 20 | 1 |
| 1:A:75:VAL:HB | 1:A:87:VAL:HB | 0.42 | 1.89 | 20 | 1 |
| 1:A:68:LYS:HB2 | 1:A:77:TYR:CZ | 0.42 | 2.49 | 10 | 1 |
| 1:A:18:LEU:HD12 | 1:A:112:MET:O | 0.42 | 2.14 | 6 | 1 |
| 1:A:76:TYR:CD2 | 1:A:86:GLU:OE1 | 0.42 | 2.72 | 8 | 1 |
| 1:A:130:ARG:O | 1:A:139:THR:CG2 | 0.42 | 2.68 | 17 | 1 |
| 1:A:9:ILE:HD11 | 1:A:92:TYR:CD1 | 0.42 | 2.49 | 12 | 1 |
| 1:A:147:PRO:O | 1:A:154:VAL:CG1 | 0.42 | 2.67 | 19 | 1 |
| 1:A:113:ARG:CZ | 1:A:115:TYR:OH | 0.42 | 2.68 | 4 | 1 |
| 1:A:139:THR:O | 1:A:142:MET:C | 0.42 | 2.57 | 9 | 1 |
| 1:A:66:PHE:CE2 | 1:A:77:TYR:CD2 | 0.42 | 3.07 | 20 | 2 |
| 1:A:86:GLU:O | 1:A:88:LEU:CD1 | 0.42 | 2.67 | 17 | 1 |
| 1:A:6:ARG:HA | 1:A:6:ARG:NE | 0.42 | 2.28 | 17 | 1 |
| 1:A:98:ILE:HG23 | 1:A:98:ILE:O | 0.42 | 2.13 | 3 | 1 |
| 1:A:77:TYR:CE2 | 1:A:79:GLU:OE1 | 0.42 | 2.73 | 16 | 1 |
| 1:A:8:GLU:OE1 | 1:A:92:TYR:CD2 | 0.42 | 2.72 | 16 | 2 |
| 1:A:109:LEU:N | 1:A:109:LEU:CD1 | 0.42 | 2.83 | 11 | 1 |
| 1:A:99:TYR:CE1 | 1:A:112:MET:SD | 0.42 | 3.13 | 14 | 2 |
| 1:A:87:VAL:N | 1:A:98:ILE:HD13 | 0.42 | 2.30 | 13 | 1 |
| 1:A:121:VAL:HG12 | 1:A:126:THR:HG23 | 0.42 | 1.91 | 15 | 1 |
| 1:A:33:LYS:N | 1:A:147:PRO:HG3 | 0.42 | 2.29 | 1 | 1 |
| 1:A:16:VAL:CG2 | 1:A:146:LEU:CG | 0.42 | 2.97 | 20 | 1 |
| 1:A:48:LYS:HG3 | 1:A:65:THR:HG23 | 0.42 | 1.91 | 10 | 1 |
| 1:A:52:ALA:CB | 1:A:63:GLU:OE2 | 0.42 | 2.66 | 6 | 1 |
| 1:A:67:LYS:HB3 | 1:A:67:LYS:NZ | 0.42 | 2.29 | 3 | 1 |
| 1:A:136:ARG:O | 1:A:137:ASN:O | 0.42 | 2.38 | 5 | 1 |
| 1:A:85:VAL:CG1 | 1:A:98:ILE:CD1 | 0.42 | 2.98 | 15 | 2 |
| 1:A:27:ARG:CZ | 1:A:111:MET:CE | 0.42 | 2.98 | 9 | 1 |
| 1:A:84:LYS:O | 1:A:101:THR:N | 0.42 | 2.49 | 14 | 1 |
| 1:A:90:THR:CG2 | 1:A:93:LYS:HB3 | 0.42 | 2.45 | 15 | 1 |
| 1:A:94:SER:O | 1:A:117:ARG:HD3 | 0.42 | 2.14 | 1 | 1 |
| 1:A:17:ALA:O | 1:A:114:LEU:N | 0.42 | 2.52 | 20 | 2 |
| 1:A:9:ILE:HD11 | 1:A:92:TYR:CE2 | 0.42 | 2.49 | 8 | 1 |
| 1:A:76:TYR:CD2 | 1:A:86:GLU:CG | 0.42 | 3.02 | 18 | 1 |
| 1:A:66:PHE:CE2 | 1:A:68:LYS:CE | 0.42 | 3.01 | 11 | 1 |
| 1:A:98:ILE:C | 1:A:98:ILE:CD1 | 0.42 | 2.86 | 14 | 1 |
| 1:A:84:LYS:HB2 | 1:A:101:THR:O | 0.42 | 2.14 | 15 | 1 |
| 1:A:49:VAL:O | 1:A:49:VAL:CG1 | 0.42 | 2.68 | 20 | 1 |
| 1:A:82:LYS:CA | 1:A:103:VAL:O | 0.42 | 2.68 | 15 | 4 |
| 1:A:97:VAL:CG2 | 1:A:97:VAL:O | 0.42 | 2.67 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:TRP:CH2 | 1:A:91:ASP:OD2 | 0.42 | 2.72 | 8 | 1 |
| 1:A:146:LEU:CD1 | 1:A:146:LEU:C | 0.42 | 2.88 | 8 | 1 |
| 1:A:124:ALA:O | 1:A:128:ILE:HG13 | 0.42 | 2.15 | 5 | 1 |
| 1:A:41:PHE:CE2 | 1:A:47:LEU:CD1 | 0.42 | 3.03 | 19 | 1 |
| 1:A:147:PRO:HB2 | 1:A:153:THR:CB | 0.42 | 2.44 | 19 | 1 |
| 1:A:98:ILE:HD12 | 1:A:98:ILE:C | 0.42 | 2.35 | 4 | 1 |
| 1:A:43:GLY:O | 1:A:44:GLU:CG | 0.42 | 2.68 | 7 | 4 |
| 1:A:70:SER:CB | 1:A:75:VAL:HG13 | 0.42 | 2.45 | 2 | 1 |
| 1:A:42:LEU:HD11 | 1:A:48:LYS:HB3 | 0.42 | 1.92 | 2 | 1 |
| 1:A:36:MET:O | 1:A:51:TYR:HB2 | 0.42 | 2.13 | 18 | 2 |
| 1:A:26:LEU:C | 1:A:26:LEU:CD2 | 0.42 | 2.84 | 7 | 1 |
| 1:A:27:ARG:O | 1:A:31:LYS:N | 0.42 | 2.52 | 14 | 1 |
| 1:A:61:LYS:HB3 | 1:A:61:LYS:NZ | 0.42 | 2.28 | 13 | 1 |
| 1:A:66:PHE:CD2 | 1:A:79:GLU:OE1 | 0.42 | 2.73 | 15 | 1 |
| 1:A:77:TYR:CE2 | 1:A:79:GLU:OE2 | 0.42 | 2.73 | 20 | 1 |
| 1:A:53:VAL:CG2 | 1:A:53:VAL:O | 0.42 | 2.66 | 10 | 3 |
| 1:A:68:LYS:HD3 | 1:A:77:TYR:CE1 | 0.42 | 2.49 | 12 | 1 |
| 1:A:42:LEU:HD12 | 1:A:67:LYS:HG3 | 0.42 | 1.91 | 19 | 1 |
| 1:A:145:MET:HG3 | 1:A:145:MET:O | 0.42 | 2.15 | 18 | 1 |
| 1:A:91:ASP:O | 1:A:92:TYR:CB | 0.42 | 2.67 | 14 | 1 |
| 1:A:130:ARG:NH1 | 1:A:139:THR:OG1 | 0.42 | 2.53 | 14 | 1 |
| 1:A:17:ALA:C | 1:A:18:LEU:CD2 | 0.42 | 2.87 | 15 | 1 |
| 1:A:68:LYS:HG3 | 1:A:79:GLU:HG2 | 0.42 | 1.90 | 20 | 1 |
| 1:A:68:LYS:N | 1:A:77:TYR:OH | 0.42 | 2.53 | 20 | 1 |
| 1:A:19:ALA:HB2 | 1:A:129:PHE:HZ | 0.42 | 1.74 | 6 | 1 |
| 1:A:35:ALA:N | 1:A:146:LEU:HD11 | 0.42 | 2.30 | 5 | 1 |
| 1:A:97:VAL:O | 1:A:97:VAL:HG23 | 0.42 | 2.15 | 5 | 1 |
| 1:A:124:ALA:O | 1:A:128:ILE:CG1 | 0.42 | 2.68 | 5 | 1 |
| 1:A:47:LEU:H | 1:A:47:LEU:HD13 | 0.42 | 1.74 | 12 | 1 |
| 1:A:68:LYS:HG2 | 1:A:69:THR:N | 0.42 | 2.30 | 19 | 1 |
| 1:A:34:MET:HA | 1:A:34:MET:HE2 | 0.42 | 1.92 | 7 | 1 |
| 1:A:29:LYS:O | 1:A:32:MET:HE3 | 0.42 | 2.15 | 6 | 1 |
| 1:A:75:VAL:CG2 | 1:A:87:VAL:HB | 0.42 | 2.43 | 8 | 1 |
| 1:A:68:LYS:HG2 | 1:A:79:GLU:HA | 0.42 | 1.90 | 5 | 3 |
| 1:A:20:SER:HB2 | 1:A:111:MET:CA | 0.42 | 2.44 | 19 | 1 |
| 1:A:38:ARG:N | 1:A:50:SER:O | 0.42 | 2.52 | 9 | 1 |
| 1:A:136:ARG:N | 1:A:136:ARG:CD | 0.42 | 2.83 | 9 | 1 |
| 1:A:82:LYS:O | 1:A:103:VAL:HB | 0.42 | 2.15 | 9 | 1 |
| 1:A:18:LEU:O | 1:A:144:ALA:CA | 0.42 | 2.68 | 1 | 1 |
| 1:A:17:ALA:C | 1:A:18:LEU:CD1 | 0.42 | 2.83 | 10 | 1 |
| 1:A:48:LYS:HB3 | 1:A:48:LYS:NZ | 0.42 | 2.30 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:32:MET:SD | 1:A:144:ALA:CB | 0.42 | 3.07 | 6 | 1 |
| 1:A:89:ASP:OD1 | 1:A:90:THR:N | 0.42 | 2.53 | 6 | 4 |
| 1:A:128:ILE:HA | 1:A:131:LYS:HB3 | 0.42 | 1.91 | 8 | 1 |
| 1:A:84:LYS:HB2 | 1:A:84:LYS:NZ | 0.42 | 2.30 | 3 | 1 |
| 1:A:109:LEU:CD2 | 1:A:109:LEU:N | 0.42 | 2.83 | 4 | 1 |
| 1:A:112:MET:N | 1:A:112:MET:CE | 0.42 | 2.83 | 2 | 1 |
| 1:A:68:LYS:HG2 | 1:A:77:TYR:CD1 | 0.42 | 2.50 | 2 | 1 |
| 1:A:34:MET:O | 1:A:53:VAL:CA | 0.42 | 2.67 | 16 | 1 |
| 1:A:91:ASP:HB2 | 1:A:95:TYR:CE1 | 0.42 | 2.50 | 14 | 1 |
| 1:A:79:GLU:HB2 | 1:A:83:LYS:O | 0.41 | 2.15 | 20 | 1 |
| 1:A:74:GLU:O | 1:A:92:TYR:OH | 0.41 | 2.38 | 10 | 1 |
| 1:A:129:PHE:O | 1:A:132:LEU:HG | 0.41 | 2.15 | 6 | 1 |
| 1:A:90:THR:CG2 | 1:A:93:LYS:HD3 | 0.41 | 2.45 | 2 | 2 |
| 1:A:31:LYS:N | 1:A:31:LYS:HD3 | 0.41 | 2.30 | 6 | 1 |
| 1:A:95:TYR:CE2 | 1:A:97:VAL:CG1 | 0.41 | 3.03 | 3 | 1 |
| 1:A:84:LYS:NZ | 1:A:84:LYS:HB3 | 0.41 | 2.29 | 19 | 1 |
| 1:A:34:MET:HG3 | 1:A:147:PRO:CG | 0.41 | 2.45 | 4 | 1 |
| 1:A:8:GLU:OE2 | 1:A:92:TYR:CZ | 0.41 | 2.73 | 14 | 1 |
| 1:A:82:LYS:O | 1:A:102:ARG:CB | 0.41 | 2.68 | 6 | 1 |
| 1:A:16:VAL:CB | 1:A:146:LEU:HD22 | 0.41 | 2.44 | 17 | 1 |
| 1:A:114:LEU:HD12 | 1:A:129:PHE:CD2 | 0.41 | 2.50 | 19 | 1 |
| 1:A:13:TRP:HE3 | 1:A:115:TYR:CD2 | 0.41 | 2.32 | 11 | 1 |
| 1:A:87:VAL:HG22 | 1:A:98:ILE:HG12 | 0.41 | 1.87 | 14 | 1 |
| 1:A:113:ARG:HD2 | 1:A:115:TYR:CE1 | 0.41 | 2.50 | 15 | 1 |
| 1:A:136:ARG:O | 1:A:137:ASN:HB2 | 0.41 | 2.15 | 20 | 1 |
| 1:A:99:TYR:CB | 1:A:112:MET:HA | 0.41 | 2.45 | 5 | 1 |
| 1:A:71:ASP:HB2 | 1:A:75:VAL:CB | 0.41 | 2.45 | 19 | 1 |
| 1:A:102:ARG:CZ | 1:A:111:MET:CE | 0.41 | 2.98 | 2 | 1 |
| 1:A:97:VAL:CG1 | 1:A:129:PHE:HB2 | 0.41 | 2.44 | 2 | 1 |
| 1:A:95:TYR:CE1 | 1:A:125:ALA:HB2 | 0.41 | 2.49 | 16 | 1 |
| 1:A:85:VAL:HA | 1:A:100:ALA:CB | 0.41 | 2.46 | 18 | 1 |
| 1:A:100:ALA:O | 1:A:111:MET:O | 0.41 | 2.38 | 13 | 1 |
| 1:A:34:MET:HB2 | 1:A:147:PRO:HG3 | 0.41 | 1.92 | 13 | 1 |
| 1:A:91:ASP:OD1 | 1:A:92:TYR:CD1 | 0.41 | 2.74 | 20 | 1 |
| 1:A:12:LYS:N | 1:A:12:LYS:HD2 | 0.41 | 2.30 | 10 | 1 |
| 1:A:21:ASN:OD1 | 1:A:140:ASP:O | 0.41 | 2.38 | 8 | 1 |
| 1:A:23:GLU:O | 1:A:28:GLU:N | 0.41 | 2.51 | 3 | 1 |
| 1:A:145:MET:CB | 1:A:154:VAL:HG22 | 0.41 | 2.27 | 5 | 1 |
| 1:A:76:TYR:CE1 | 1:A:78:SER:OG | 0.41 | 2.73 | 5 | 1 |
| 1:A:121:VAL:HG12 | 1:A:121:VAL:O | 0.41 | 2.15 | 12 | 1 |
| 1:A:71:ASP:OD2 | 1:A:76:TYR:CZ | 0.41 | 2.74 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:51:TYR:CD1 | 1:A:53:VAL:CG2 | 0.41 | 3.03 | 4 | 1 |
| 1:A:132:LEU:C | 1:A:132:LEU:CD2 | 0.41 | 2.88 | 16 | 1 |
| 1:A:13:TRP:CD1 | 1:A:117:ARG:NH2 | 0.41 | 2.88 | 18 | 1 |
| 1:A:93:LYS:NZ | 1:A:93:LYS:HB2 | 0.41 | 2.30 | 7 | 1 |
| 1:A:8:GLU:OE2 | 1:A:92:TYR:CE1 | 0.41 | 2.73 | 14 | 1 |
| 1:A:83:LYS:NZ | 1:A:83:LYS:HB2 | 0.41 | 2.30 | 15 | 1 |
| 1:A:9:ILE:HD11 | 1:A:91:ASP:O | 0.41 | 2.15 | 15 | 1 |
| 1:A:69:THR:O | 1:A:77:TYR:CD1 | 0.41 | 2.73 | 3 | 2 |
| 1:A:18:LEU:CD1 | 1:A:113:ARG:HA | 0.41 | 2.46 | 12 | 1 |
| 1:A:48:LYS:CB | 1:A:66:PHE:O | 0.41 | 2.69 | 19 | 1 |
| 1:A:16:VAL:HA | 1:A:34:MET:CE | 0.41 | 2.46 | 4 | 1 |
| 1:A:88:LEU:CD2 | 1:A:89:ASP:N | 0.41 | 2.79 | 4 | 1 |
| 1:A:89:ASP:OD1 | 1:A:128:ILE:HD12 | 0.41 | 2.15 | 2 | 1 |
| 1:A:146:LEU:N | 1:A:147:PRO:HD3 | 0.41 | 2.31 | 16 | 1 |
| 1:A:91:ASP:HB3 | 1:A:96:ALA:CB | 0.41 | 2.45 | 18 | 1 |
| 1:A:60:ARG:CD | 1:A:60:ARG:N | 0.41 | 2.83 | 11 | 1 |
| 1:A:120:GLU:HG3 | 1:A:120:GLU:O | 0.41 | 2.14 | 9 | 1 |
| 1:A:13:TRP:CH2 | 1:A:39:ILE:CD1 | 0.41 | 3.03 | 15 | 1 |
| 1:A:18:LEU:HG | 1:A:113:ARG:HA | 0.41 | 1.92 | 20 | 1 |
| 1:A:51:TYR:CZ | 1:A:66:PHE:HB2 | 0.41 | 2.51 | 20 | 1 |
| 1:A:76:TYR:CE2 | 1:A:86:GLU:OE1 | 0.41 | 2.74 | 10 | 1 |
| 1:A:32:MET:CG | 1:A:154:VAL:HG11 | 0.41 | 2.45 | 6 | 1 |
| 1:A:27:ARG:NH1 | 1:A:31:LYS:CE | 0.41 | 2.83 | 3 | 1 |
| 1:A:117:ARG:CD | 1:A:117:ARG:H | 0.41 | 2.27 | 2 | 1 |
| 1:A:9:ILE:HG12 | 1:A:91:ASP:O | 0.41 | 2.15 | 7 | 1 |
| 1:A:117:ARG:N | 1:A:117:ARG:HD2 | 0.41 | 2.29 | 7 | 1 |
| 1:A:81:ALA:HA | 1:A:103:VAL:CG2 | 0.41 | 2.46 | 14 | 1 |
| 1:A:22:THR:CG2 | 1:A:27:ARG:NH2 | 0.41 | 2.84 | 14 | 1 |
| 1:A:18:LEU:HG | 1:A:144:ALA:O | 0.41 | 2.16 | 15 | 1 |
| 1:A:85:VAL:CG1 | 1:A:98:ILE:HG13 | 0.41 | 2.45 | 15 | 1 |
| 1:A:84:LYS:N | 1:A:103:VAL:HG12 | 0.41 | 2.31 | 10 | 1 |
| 1:A:70:SER:OG | 1:A:75:VAL:HG23 | 0.41 | 2.15 | 6 | 1 |
| 1:A:67:LYS:CA | 1:A:77:TYR:OH | 0.41 | 2.69 | 5 | 1 |
| 1:A:13:TRP:CZ2 | 1:A:115:TYR:CZ | 0.41 | 3.09 | 19 | 1 |
| 1:A:27:ARG:NH1 | 1:A:109:LEU:HD11 | 0.41 | 2.30 | 4 | 1 |
| 1:A:31:LYS:O | 1:A:32:MET:O | 0.41 | 2.38 | 2 | 1 |
| 1:A:77:TYR:CB | 1:A:85:VAL:CG2 | 0.41 | 2.99 | 9 | 1 |
| 1:A:26:LEU:CD2 | 1:A:142:MET:CE | 0.41 | 2.99 | 13 | 1 |
| 1:A:102:ARG:HB2 | 1:A:109:LEU:HB3 | 0.41 | 1.91 | 15 | 1 |
| 1:A:87:VAL:HG23 | 1:A:98:ILE:HD13 | 0.41 | 1.90 | 15 | 1 |
| 1:A:88:LEU:HD12 | 1:A:132:LEU:HD13 | 0.41 | 1.93 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:81:ALA:HB1 | 1:A:103:VAL:HB | 0.41 | 1.91 | 1 | 1 |
| 1:A:120:GLU:O | 1:A:120:GLU:HG2 | 0.41 | 2.15 | 20 | 1 |
| 1:A:69:THR:CG2 | 1:A:78:SER:HB3 | 0.41 | 2.45 | 20 | 1 |
| 1:A:77:TYR:C | 1:A:77:TYR:CD1 | 0.41 | 2.94 | 2 | 3 |
| 1:A:19:ALA:HA | 1:A:143:VAL:HA | 0.41 | 1.92 | 17 | 2 |
| 1:A:152:CYS:O | 1:A:153:THR:HG23 | 0.41 | 2.15 | 19 | 1 |
| 1:A:87:VAL:CG2 | 1:A:98:ILE:HB | 0.41 | 2.44 | 4 | 1 |
| 1:A:33:LYS:NZ | 1:A:33:LYS:HB3 | 0.41 | 2.30 | 2 | 1 |
| 1:A:41:PHE:CE1 | 1:A:47:LEU:HD21 | 0.41 | 2.51 | 2 | 1 |
| 1:A:120:GLU:HG2 | 1:A:120:GLU:O | 0.41 | 2.15 | 2 | 1 |
| 1:A:146:LEU:O | 1:A:146:LEU:CD2 | 0.41 | 2.68 | 18 | 1 |
| 1:A:86:GLU:OE1 | 1:A:88:LEU:CD2 | 0.41 | 2.69 | 7 | 1 |
| 1:A:21:ASN:OD1 | 1:A:142:MET:CG | 0.41 | 2.69 | 15 | 1 |
| 1:A:82:LYS:CD | 1:A:82:LYS:H | 0.41 | 2.28 | 6 | 1 |
| 1:A:9:ILE:CD1 | 1:A:91:ASP:O | 0.41 | 2.68 | 17 | 1 |
| 1:A:34:MET:HB3 | 1:A:54:PRO:HD2 | 0.41 | 1.93 | 17 | 1 |
| 1:A:22:THR:HG21 | 1:A:31:LYS:NZ | 0.41 | 2.31 | 17 | 1 |
| 1:A:146:LEU:N | 1:A:146:LEU:CD2 | 0.41 | 2.84 | 3 | 1 |
| 1:A:48:LYS:HB2 | 1:A:65:THR:HG23 | 0.41 | 1.92 | 3 | 1 |
| 1:A:43:GLY:O | 1:A:46:GLU:OE2 | 0.41 | 2.38 | 19 | 1 |
| 1:A:86:GLU:OE1 | 1:A:86:GLU:O | 0.41 | 2.39 | 4 | 1 |
| 1:A:128:ILE:HG23 | 1:A:131:LYS:HE2 | 0.41 | 1.93 | 4 | 1 |
| 1:A:31:LYS:HB2 | 1:A:31:LYS:NZ | 0.41 | 2.31 | 16 | 1 |
| 1:A:25:PHE:C | 1:A:25:PHE:CD1 | 0.41 | 2.94 | 16 | 1 |
| 1:A:61:LYS:NZ | 1:A:61:LYS:HB2 | 0.41 | 2.31 | 11 | 1 |
| 1:A:138:TYR:CD2 | 1:A:140:ASP:HB3 | 0.41 | 2.49 | 11 | 1 |
| 1:A:22:THR:O | 1:A:23:GLU:CG | 0.41 | 2.69 | 9 | 1 |
| 1:A:74:GLU:O | 1:A:75:VAL:HG23 | 0.41 | 2.15 | 15 | 1 |
| 1:A:67:LYS:CB | 1:A:67:LYS:NZ | 0.41 | 2.84 | 15 | 1 |
| 1:A:107:ARG:HH12 | 1:A:109:LEU:HD21 | 0.41 | 1.76 | 20 | 1 |
| 1:A:82:LYS:HB3 | 1:A:83:LYS:HD3 | 0.41 | 1.91 | 10 | 1 |
| 1:A:9:ILE:CD1 | 1:A:91:ASP:OD2 | 0.41 | 2.69 | 6 | 1 |
| 1:A:33:LYS:CD | 1:A:33:LYS:N | 0.41 | 2.84 | 3 | 1 |
| 1:A:20:SER:CB | 1:A:111:MET:HG2 | 0.41 | 2.46 | 2 | 1 |
| 1:A:146:LEU:N | 1:A:147:PRO:HD2 | 0.41 | 2.30 | 18 | 1 |
| 1:A:17:ALA:HB3 | 1:A:114:LEU:CD2 | 0.41 | 2.45 | 14 | 1 |
| 1:A:32:MET:SD | 1:A:32:MET:N | 0.41 | 2.94 | 13 | 1 |
| 1:A:9:ILE:CG2 | 1:A:39:ILE:CD1 | 0.40 | 2.95 | 6 | 1 |
| 1:A:93:LYS:C | 1:A:93:LYS:CD | 0.40 | 2.90 | 17 | 1 |
| 1:A:6:ARG:N | 1:A:6:ARG:HD3 | 0.40 | 2.31 | 3 | 1 |
| 1:A:61:LYS:NZ | 1:A:61:LYS:HB3 | 0.40 | 2.31 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:TRP:N | 1:A:13:TRP:CD1 | 0.40 | 2.89 | 5 | 1 |
| 1:A:98:ILE:CG2 | 1:A:115:TYR:CE2 | 0.40 | 3.04 | 18 | 1 |
| 1:A:14:TYR:CD1 | 1:A:14:TYR:N | 0.40 | 2.89 | 10 | 1 |
| 1:A:68:LYS:CG | 1:A:79:GLU:HB2 | 0.40 | 2.46 | 3 | 1 |
| 1:A:12:LYS:HB3 | 1:A:12:LYS:NZ | 0.40 | 2.31 | 5 | 1 |
| 1:A:102:ARG:O | 1:A:109:LEU:CD2 | 0.40 | 2.69 | 12 | 1 |
| 1:A:81:ALA:O | 1:A:103:VAL:CG1 | 0.40 | 2.69 | 19 | 1 |
| 1:A:8:GLU:HB2 | 1:A:92:TYR:CD2 | 0.40 | 2.51 | 4 | 1 |
| 1:A:27:ARG:HH12 | 1:A:109:LEU:HD11 | 0.40 | 1.75 | 4 | 1 |
| 1:A:33:LYS:CG | 1:A:53:VAL:CG1 | 0.40 | 2.98 | 2 | 1 |
| 1:A:109:LEU:HD23 | 1:A:109:LEU:N | 0.40 | 2.31 | 18 | 1 |
| 1:A:24:PHE:CD2 | 1:A:27:ARG:NH2 | 0.40 | 2.89 | 11 | 1 |
| 1:A:79:GLU:HG2 | 1:A:80:GLU:N | 0.40 | 2.31 | 9 | 1 |
| 1:A:88:LEU:HD12 | 1:A:132:LEU:CD1 | 0.40 | 2.43 | 13 | 1 |
| 1:A:8:GLU:OE1 | 1:A:92:TYR:CD1 | 0.40 | 2.74 | 13 | 1 |
| 1:A:82:LYS:HG2 | 1:A:83:LYS:CE | 0.40 | 2.46 | 15 | 1 |
| 1:A:88:LEU:N | 1:A:88:LEU:CD2 | 0.40 | 2.84 | 15 | 1 |
| 1:A:15:VAL:HG13 | 1:A:35:ALA:C | 0.40 | 2.36 | 17 | 1 |
| 1:A:45:ASP:O | 1:A:45:ASP:OD1 | 0.40 | 2.39 | 17 | 1 |
| 1:A:67:LYS:HD2 | 1:A:67:LYS:C | 0.40 | 2.36 | 19 | 1 |
| 1:A:69:THR:O | 1:A:77:TYR:HB2 | 0.40 | 2.16 | 18 | 1 |
| 1:A:53:VAL:CG2 | 1:A:62:TRP:HB3 | 0.40 | 2.46 | 18 | 1 |
| 1:A:60:ARG:N | 1:A:60:ARG:HD2 | 0.40 | 2.30 | 11 | 1 |
| 1:A:43:GLY:O | 1:A:44:GLU:HG2 | 0.40 | 2.15 | 7 | 1 |
| 1:A:23:GLU:OE1 | 1:A:23:GLU:N | 0.40 | 2.54 | 14 | 1 |
| 1:A:27:ARG:CD | 1:A:31:LYS:NZ | 0.40 | 2.85 | 13 | 1 |
| 1:A:35:ALA:HA | 1:A:54:PRO:HD2 | 0.40 | 1.93 | 13 | 1 |
| 1:A:36:MET:O | 1:A:52:ALA:N | 0.40 | 2.52 | 10 | 1 |
| 1:A:30:ASP:O | 1:A:154:VAL:HG12 | 0.40 | 2.15 | 6 | 1 |
| 1:A:93:LYS:O | 1:A:94:SER:CB | 0.40 | 2.69 | 17 | 1 |
| 1:A:34:MET:HA | 1:A:146:LEU:HD21 | 0.40 | 1.93 | 5 | 1 |
| 1:A:74:GLU:CG | 1:A:88:LEU:HA | 0.40 | 2.47 | 19 | 1 |
| 1:A:120:GLU:O | 1:A:120:GLU:HG3 | 0.40 | 2.16 | 19 | 1 |
| 1:A:80:GLU:OE1 | 1:A:82:LYS:HB2 | 0.40 | 2.17 | 7 | 1 |
| 1:A:94:SER:O | 1:A:117:ARG:N | 0.40 | 2.53 | 14 | 1 |
| 1:A:8:GLU:OE1 | 1:A:92:TYR:CG | 0.40 | 2.74 | 13 | 1 |
| 1:A:22:THR:O | 1:A:23:GLU:O | 0.40 | 2.39 | 15 | 1 |
| 1:A:6:ARG:CB | 1:A:6:ARG:NH1 | 0.40 | 2.85 | 6 | 1 |
| 1:A:83:LYS:N | 1:A:83:LYS:CD | 0.40 | 2.85 | 8 | 1 |
| 1:A:102:ARG:N | 1:A:102:ARG:CD | 0.40 | 2.84 | 3 | 1 |
| 1:A:88:LEU:CD2 | 1:A:97:VAL:HG23 | 0.40 | 2.47 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:51:TYR:CD1 | 1:A:53:VAL:HG23 | 0.40 | 2.52 | 4 | 1 |
| 1:A:13:TRP:NE1 | 1:A:115:TYR:CZ | 0.40 | 2.90 | 2 | 1 |
| 1:A:91:ASP:OD2 | 1:A:95:TYR:CE2 | 0.40 | 2.74 | 14 | 1 |
| 1:A:99:TYR:CZ | 1:A:101:THR:HG22 | 0.40 | 2.51 | 13 | 1 |
| 1:A:104:LYS:HD3 | 1:A:105:ASP:N | 0.40 | 2.32 | 15 | 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 | 142/157 (90%) | 109±4 (77±3%) | 21±4 (15±2%) | 12±3 (8±2%) | 2 | 14 |
| All | All | 2840/3140 (90%) | 2180 (77%) | 429 (15%) | 231 (8%) | 2 | 14 |

All 35 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 | 137 | ASN | 19 |
| 1 | A | 22 | THR | 14 |
| 1 | A | 43 | GLY | 13 |
| 1 | A | 81 | ALA | 13 |
| 1 | A | 80 | GLU | 13 |
| 1 | A | 94 | SER | 13 |
| 1 | A | 45 | ASP | 10 |
| 1 | A | 68 | LYS | 10 |
| 1 | A | 32 | MET | 9 |
| 1 | A | 138 | TYR | 9 |
| 1 | A | 73 | GLY | 8 |
| 1 | A | 31 | LYS | 8 |
| 1 | A | 60 | ARG | 7 |
| 1 | A | 120 | GLU | 7 |
| 1 | A | 72 | ASP | 7 |
| 1 | A | 82 | LYS | 6 |
| 1 | A | 5 | ASP | 6 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 141 | GLU | 6 |
| 1 | A | 152 | CYS | 6 |
| 1 | A | 105 | ASP | 5 |
| 1 | A | 59 | CYS | 4 |
| 1 | A | 146 | LEU | 4 |
| 1 | A | 23 | GLU | 4 |
| 1 | A | 20 | SER | 4 |
| 1 | A | 44 | GLU | 4 |
| 1 | A | 147 | PRO | 4 |
| 1 | A | 16 | VAL | 4 |
| 1 | A | 21 | ASN | 3 |
| 1 | A | 90 | THR | 3 |
| 1 | A | 153 | THR | 2 |
| 1 | A | 154 | VAL | 2 |
| 1 | A | 54 | PRO | 1 |
| 1 | A | 93 | LYS | 1 |
| 1 | A | 75 | VAL | 1 |
| 1 | A | 89 | ASP | 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 | 123/137 (90%) | 112±3 (91±2%) | 11±3 (9±2%) | 16 61 |
| All | All | 2460/2740 (90%) | 2236 (91%) | 224 (9%) | 16 61 |

All 61 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 | 48 | LYS | 16 |
| 1 | A | 117 | ARG | 12 |
| 1 | A | 98 | ILE | 11 |
| 1 | A | 93 | LYS | 10 |
| 1 | A | 67 | LYS | 9 |
| 1 | A | 77 | TYR | 9 |
| 1 | A | 15 | VAL | 8 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 33 | LYS | 7 |
| 1 | A | 112 | MET | 6 |
| 1 | A | 12 | LYS | 6 |
| 1 | A | 95 | TYR | 6 |
| 1 | A | 51 | TYR | 6 |
| 1 | A | 18 | LEU | 5 |
| 1 | A | 41 | PHE | 5 |
| 1 | A | 21 | ASN | 5 |
| 1 | A | 83 | LYS | 5 |
| 1 | A | 107 | ARG | 5 |
| 1 | A | 138 | TYR | 5 |
| 1 | A | 63 | GLU | 4 |
| 1 | A | 6 | ARG | 4 |
| 1 | A | 82 | LYS | 4 |
| 1 | A | 60 | ARG | 4 |
| 1 | A | 16 | VAL | 4 |
| 1 | A | 31 | LYS | 3 |
| 1 | A | 115 | TYR | 3 |
| 1 | A | 68 | LYS | 3 |
| 1 | A | 92 | TYR | 3 |
| 1 | A | 109 | LEU | 3 |
| 1 | A | 80 | GLU | 3 |
| 1 | A | 47 | LEU | 3 |
| 1 | A | 136 | ARG | 3 |
| 1 | A | 61 | LYS | 3 |
| 1 | A | 88 | LEU | 2 |
| 1 | A | 76 | TYR | 2 |
| 1 | A | 39 | ILE | 2 |
| 1 | A | 71 | ASP | 2 |
| 1 | A | 42 | LEU | 2 |
| 1 | A | 38 | ARG | 2 |
| 1 | A | 132 | LEU | 2 |
| 1 | A | 29 | LYS | 2 |
| 1 | A | 135 | GLU | 2 |
| 1 | A | 79 | GLU | 2 |
| 1 | A | 137 | ASN | 2 |
| 1 | A | 84 | LYS | 2 |
| 1 | A | 85 | VAL | 1 |
| 1 | A | 152 | CYS | 1 |
| 1 | A | 154 | VAL | 1 |
| 1 | A | 90 | THR | 1 |
| 1 | A | 26 | LEU | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 102 | ARG | 1 |
| 1 | A | 110 | HIS | 1 |
| 1 | A | 131 | LYS | 1 |
| 1 | A | 145 | MET | 1 |
| 1 | A | 104 | LYS | 1 |
| 1 | A | 74 | GLU | 1 |
| 1 | A | 142 | MET | 1 |
| 1 | A | 27 | ARG | 1 |
| 1 | A | 46 | GLU | 1 |
| 1 | A | 111 | MET | 1 |
| 1 | A | 32 | MET | 1 |
| 1 | A | 139 | THR | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4664

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 | 1050 |
| Number of shifts mapped to atoms | 1050 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 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 |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 145 | -1.19 ± 0.15 | Should be applied |
| $^{13}\text{C}_\beta$ | 137 | -1.06 ± 0.09 | Should be applied |
| $^{13}\text{C}'$ | 137 | -0.78 ± 0.11 | Should be applied |
| ^{15}N | 138 | -0.37 ± 0.31 | 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 53%, i.e. 941 atoms were assigned a chemical shift out of a possible 1790. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 647/702 (92%) | 256/280 (91%) | 262/284 (92%) | 129/138 (93%) |
| Sidechain | 294/939 (31%) | 167/552 (30%) | 127/341 (37%) | 0/46 (0%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 0/149 (0%) | 0/77 (0%) | 0/68 (0%) | 0/4 (0%) |
| Overall | 941/1790 (53%) | 423/909 (47%) | 389/693 (56%) | 129/188 (69%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 1016 atoms were assigned a chemical shift out of a possible 1976. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 695/773 (90%) | 275/308 (89%) | 282/314 (90%) | 138/151 (91%) |
| Sidechain | 321/1054 (30%) | 184/620 (30%) | 137/382 (36%) | 0/52 (0%) |
| Aromatic | 0/149 (0%) | 0/77 (0%) | 0/68 (0%) | 0/4 (0%) |
| Overall | 1016/1976 (51%) | 459/1005 (46%) | 419/764 (55%) | 138/207 (67%) |

7.1.4 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 | 94 | SER | H | 11.29 | 11.23 – 5.33 | 5.1 |

7.1.5 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:

