Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 06:45 PM BST

PDB ID	:	1Y7Q
Title	:	Mammalian SCAN domain dimer is a domain-swapped homologue of the HIV capsid C-terminal domain
Authors	:	Ivanov, D.; Stone, J.R.; Maki, J.L.; Collins, T.; Wagner, G.
Deposited on	:	2004-12-09

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 (i) symbol.

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

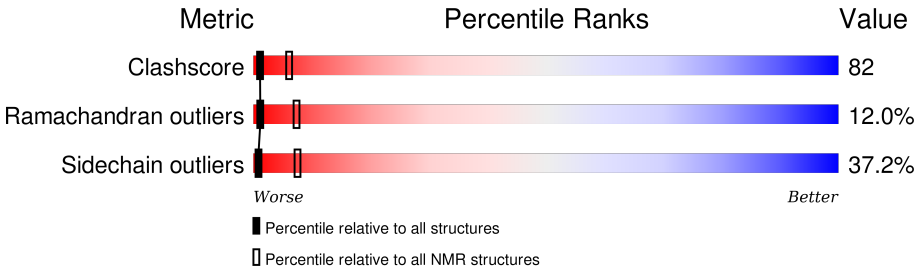
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	98	8% 57% 20% 14%
1	B	98	8% 52% 21% 18%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:44-A:127, B:47-B:126 (164)	1.27	13

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3304 atoms, of which 1682 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger protein 174.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1652	509	841	149	146	7	
1	B	98	Total	C	H	N	O	S	0
			1652	509	841	149	146	7	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLY	-	CLONING ARTIFACT	UNP Q15697
A	36	SER	-	CLONING ARTIFACT	UNP Q15697
A	100	GLU	PRO	ENGINEERED	UNP Q15697
A	111	LEU	PRO	ENGINEERED	UNP Q15697
B	35	GLY	-	CLONING ARTIFACT	UNP Q15697
B	36	SER	-	CLONING ARTIFACT	UNP Q15697
B	100	GLU	PRO	ENGINEERED	UNP Q15697
B	111	LEU	PRO	ENGINEERED	UNP Q15697

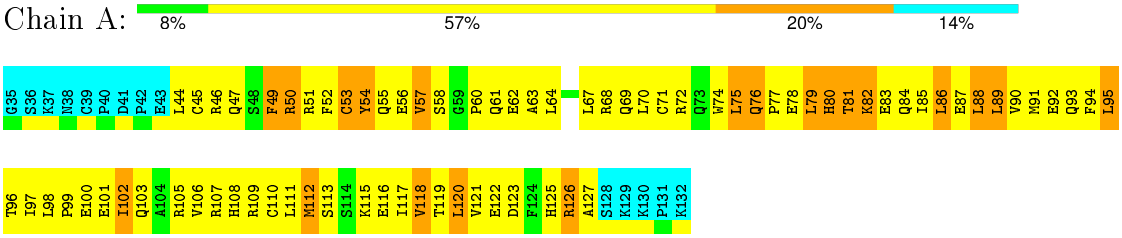
4 Residue-property plots (i)

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.

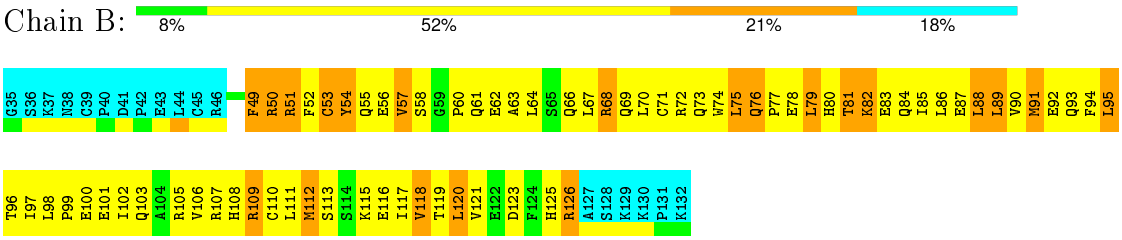
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

Chain B:



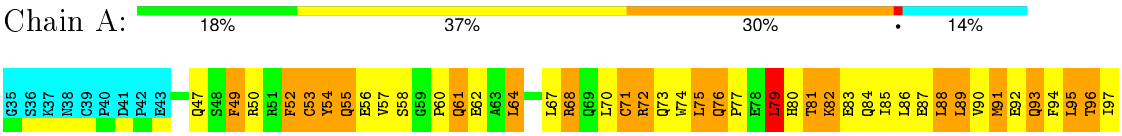
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

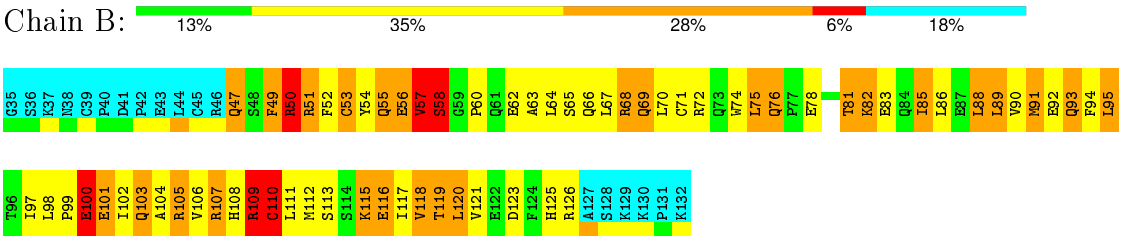
4.2.1 Score per residue for model 1

- Molecule 1: Zinc finger protein 174

Chain A:

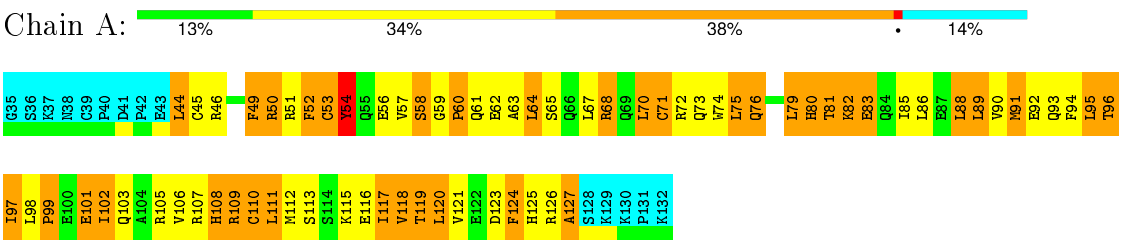


• Molecule 1: Zinc finger protein 174

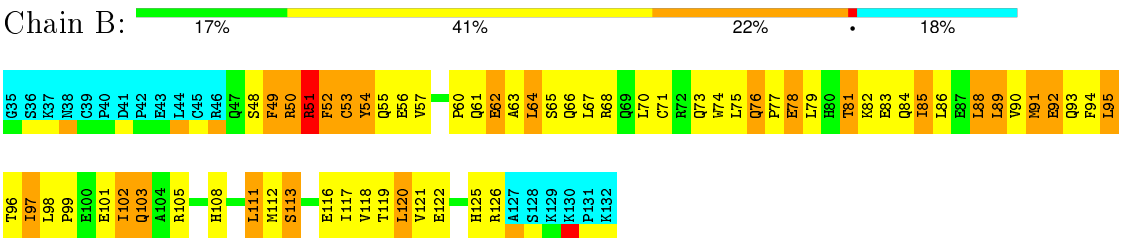


4.2.2 Score per residue for model 2

• Molecule 1: Zinc finger protein 174

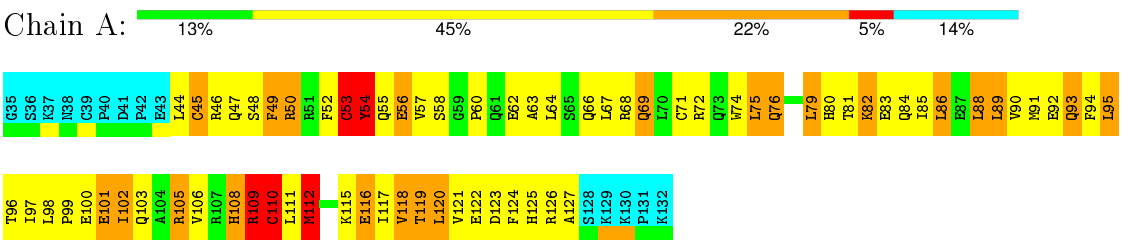


• Molecule 1: Zinc finger protein 174



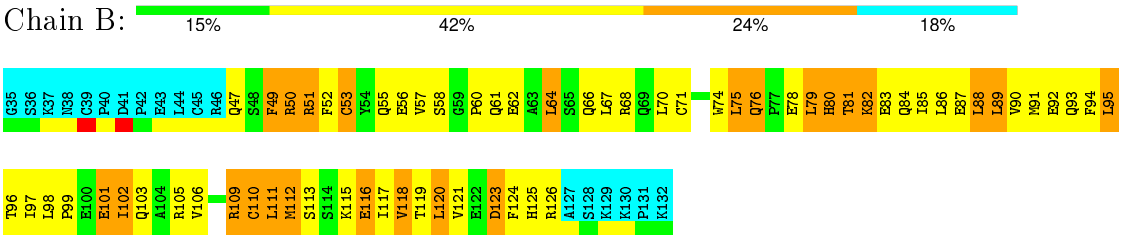
4.2.3 Score per residue for model 3

• Molecule 1: Zinc finger protein 174



• Molecule 1: Zinc finger protein 174

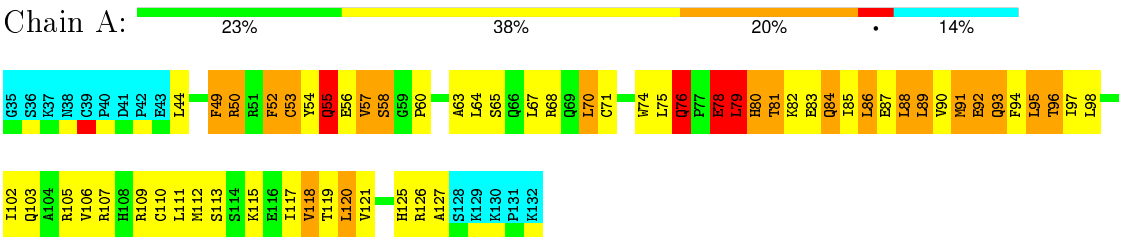
Chain B:



4.2.4 Score per residue for model 4

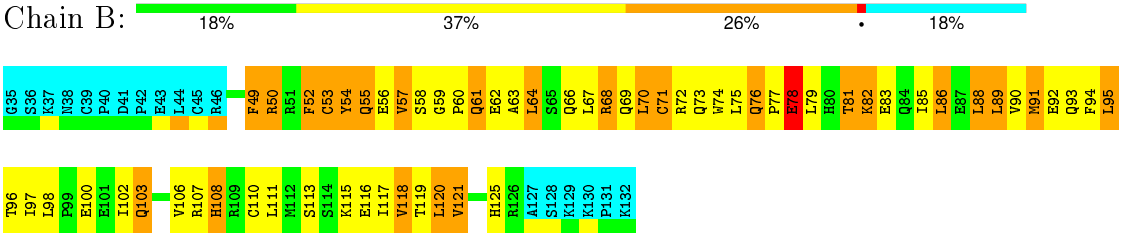
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

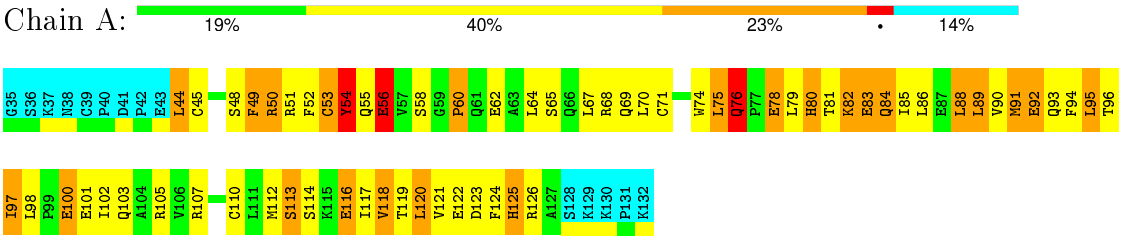
Chain B:



4.2.5 Score per residue for model 5

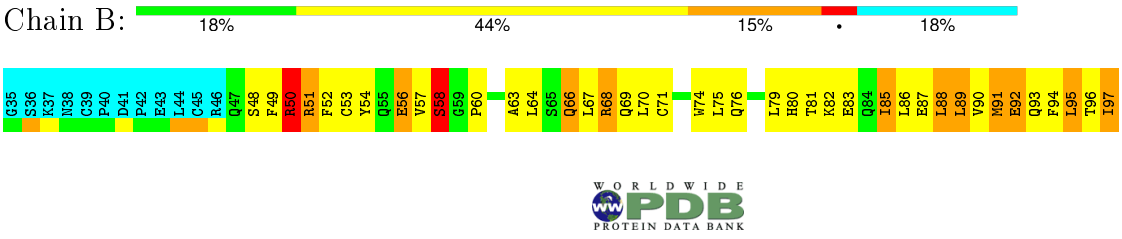
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

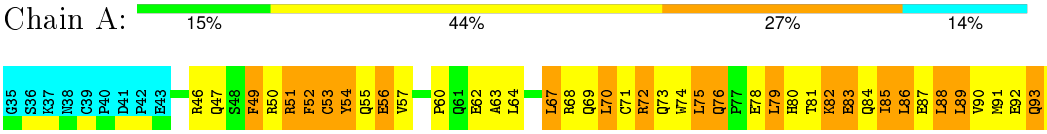
Chain B:



4.2.6 Score per residue for model 6

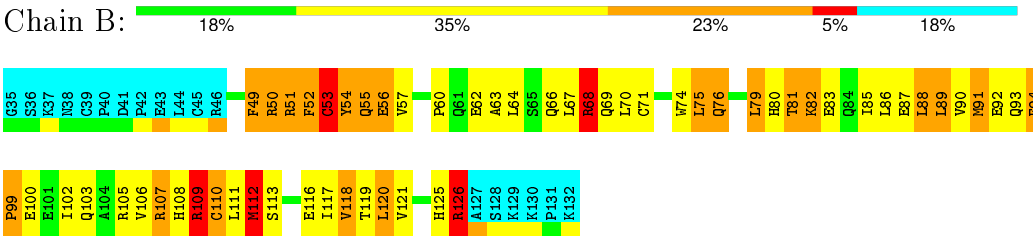
• Molecule 1: Zinc finger protein 174

Chain A:



• Molecule 1: Zinc finger protein 174

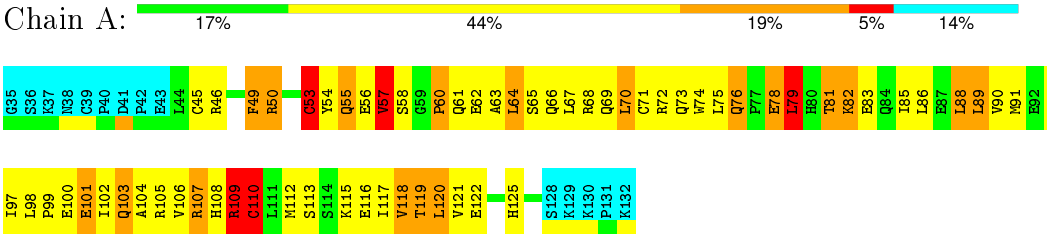
Chain B:



4.2.7 Score per residue for model 7

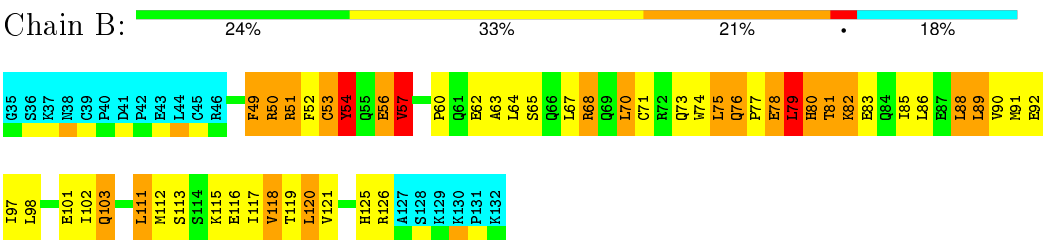
• Molecule 1: Zinc finger protein 174

Chain A:



• Molecule 1: Zinc finger protein 174

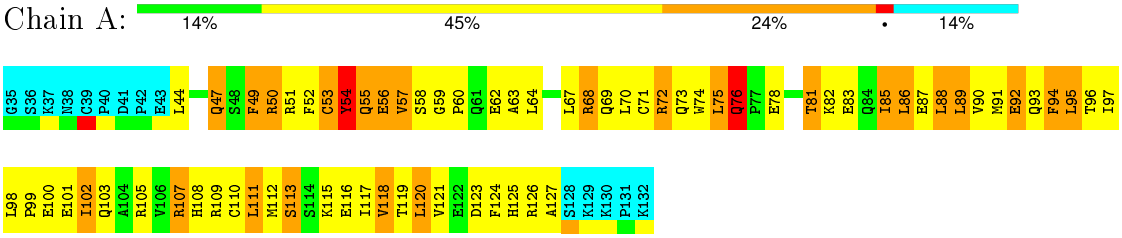
Chain B:



4.2.8 Score per residue for model 8

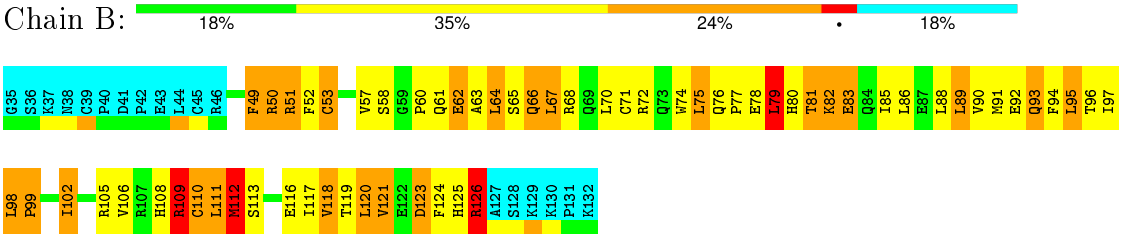
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

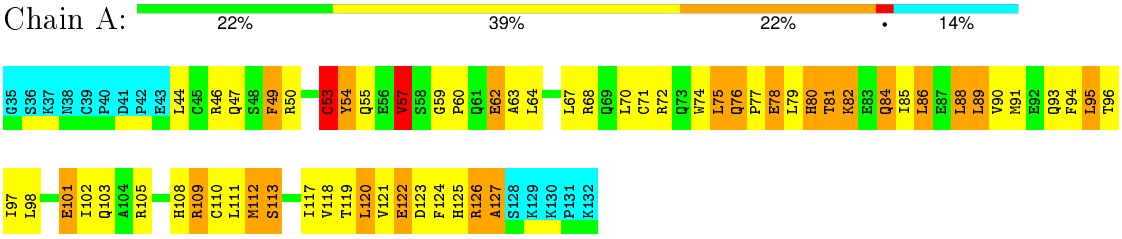
Chain B:



4.2.9 Score per residue for model 9

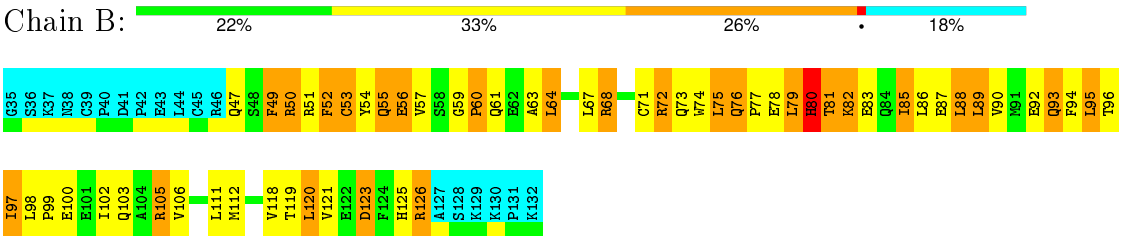
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

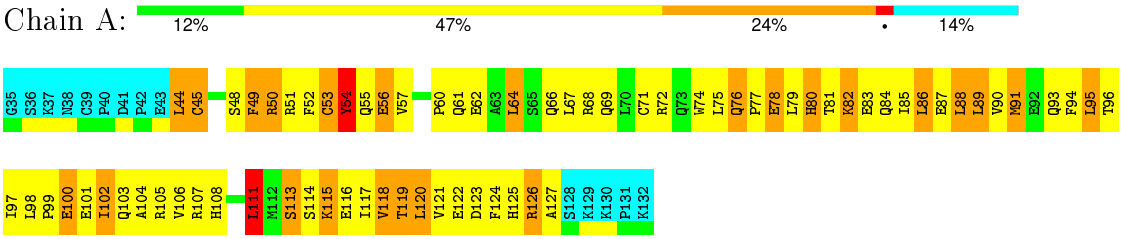
Chain B:



4.2.10 Score per residue for model 10

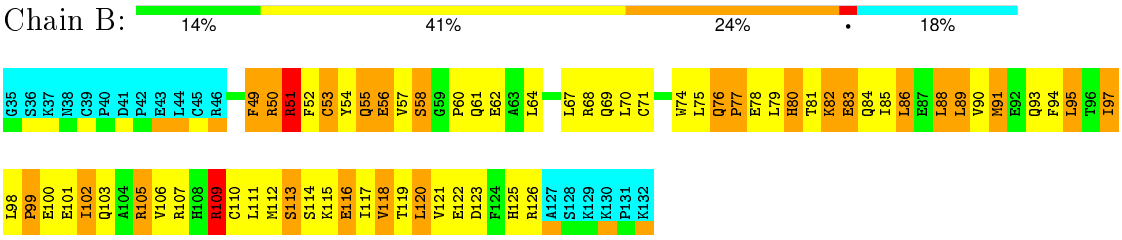
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

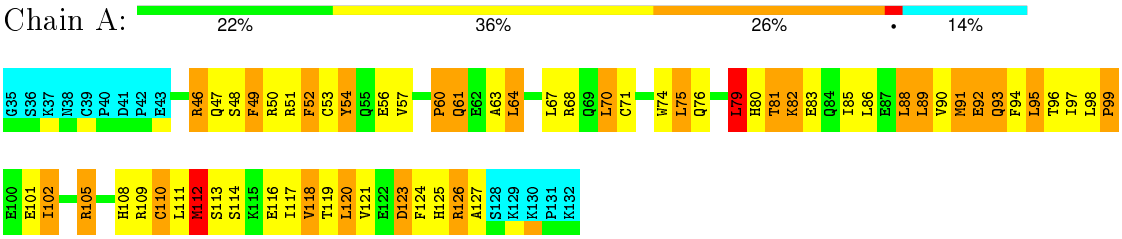
Chain B:



4.2.11 Score per residue for model 11

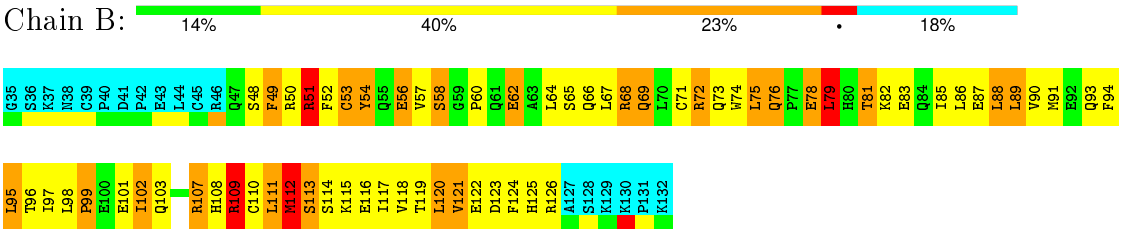
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

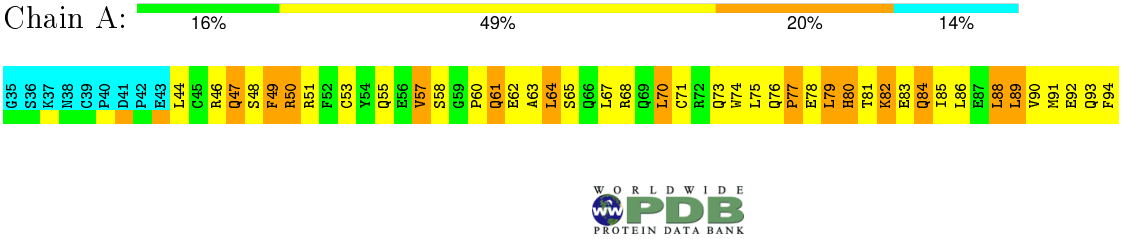
Chain B:



4.2.12 Score per residue for model 12

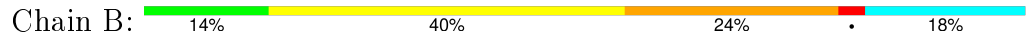
- Molecule 1: Zinc finger protein 174

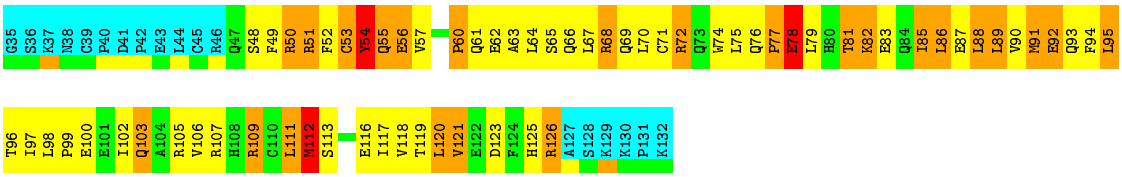
Chain A:



• Molecule 1: Zinc finger protein 174

Chain B:

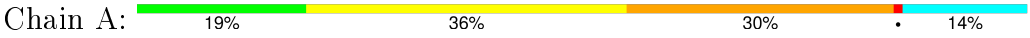


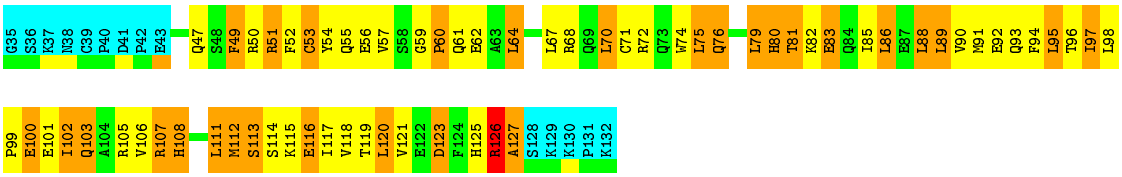


4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Zinc finger protein 174

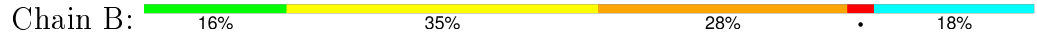
Chain A:

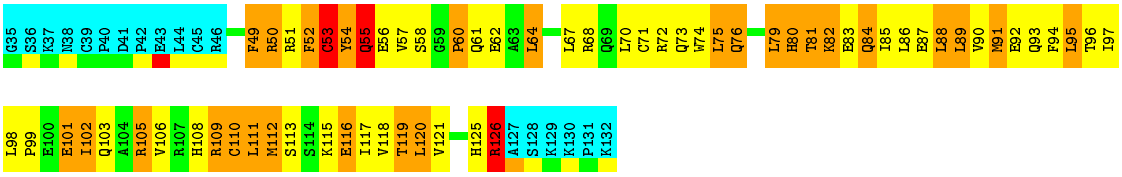




• Molecule 1: Zinc finger protein 174

Chain B:

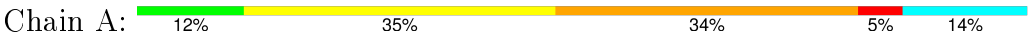


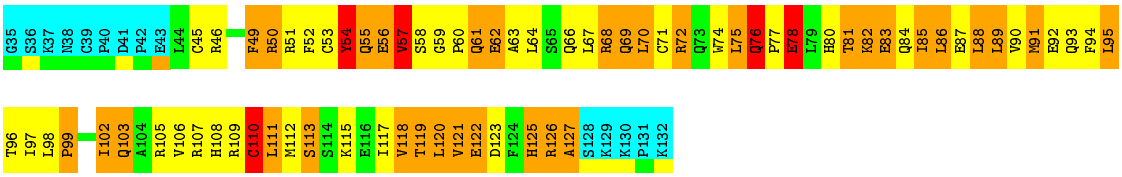


4.2.14 Score per residue for model 14

• Molecule 1: Zinc finger protein 174

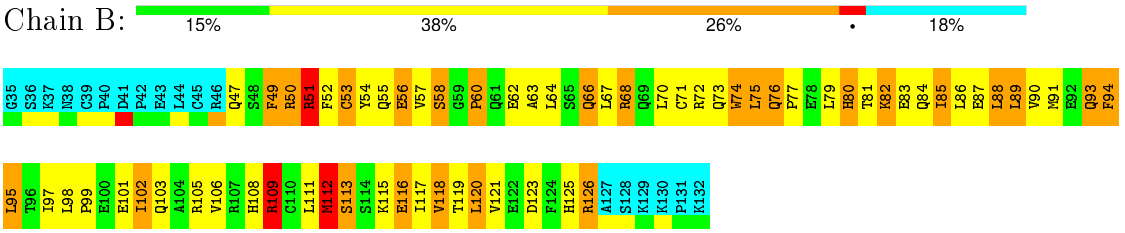
Chain A:





• Molecule 1: Zinc finger protein 174

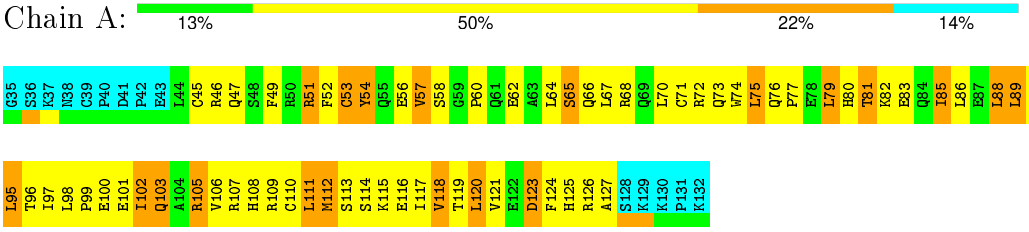
Chain B:



4.2.15 Score per residue for model 15

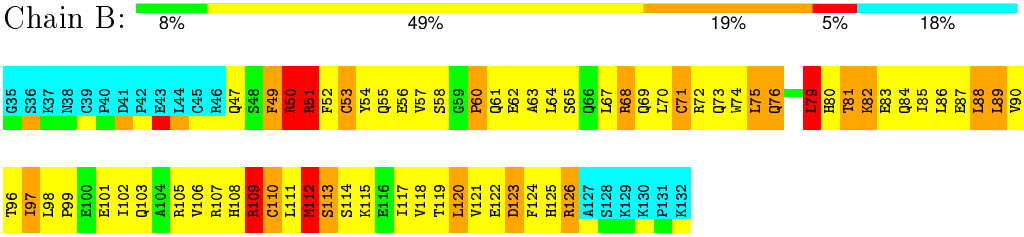
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

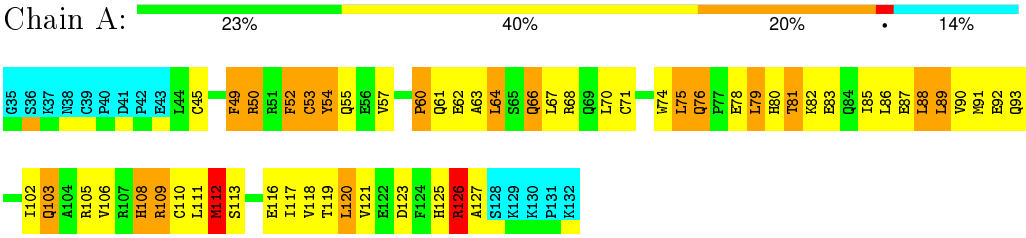
Chain B:



4.2.16 Score per residue for model 16

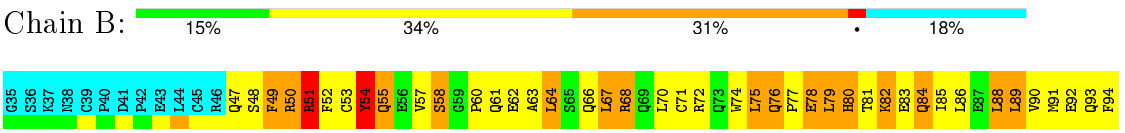
- Molecule 1: Zinc finger protein 174

Chain A:



- Molecule 1: Zinc finger protein 174

Chain B:



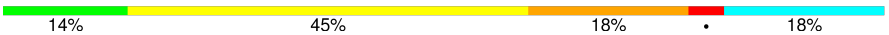
4.2.17 Score per residue for model 17

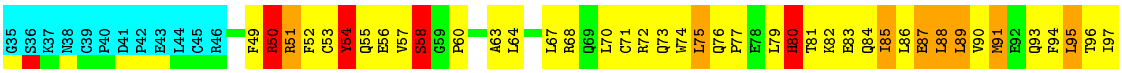
• Molecule 1: Zinc finger protein 174

Chain A:

• Molecule 1: Zinc finger protein 174

Chain B:

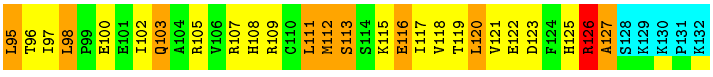




4.2.18 Score per residue for model 18

• Molecule 1: Zinc finger protein 174

Chain A:



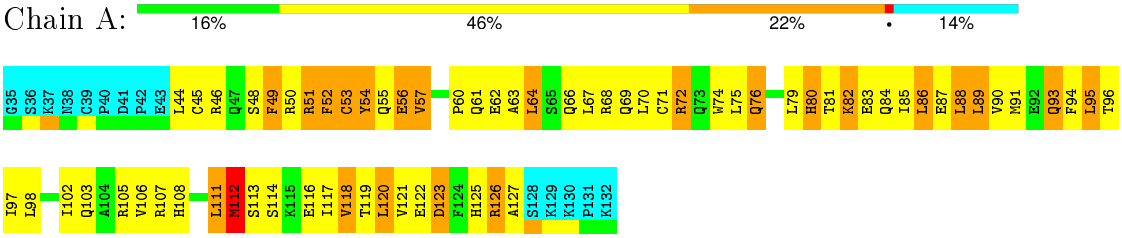
• Molecule 1: Zinc finger protein 174

Chain B:

4.2.19 Score per residue for model 19

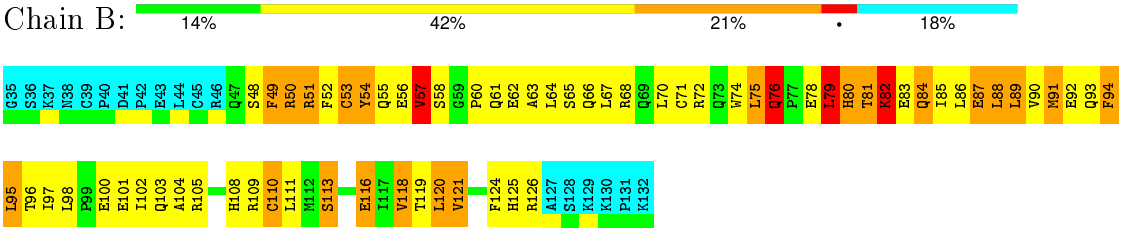
• Molecule 1: Zinc finger protein 174

Chain A:



• Molecule 1: Zinc finger protein 174

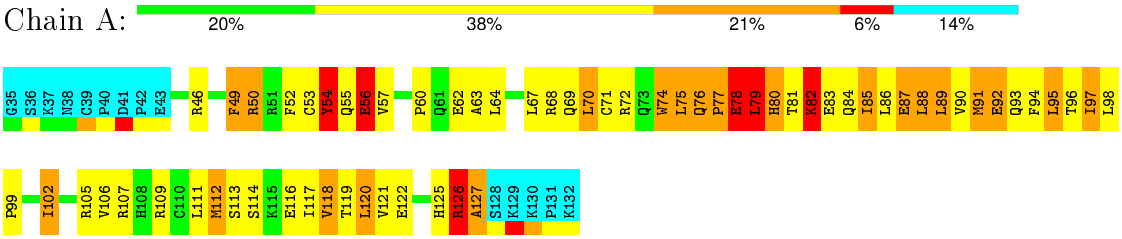
Chain B:



4.2.20 Score per residue for model 20

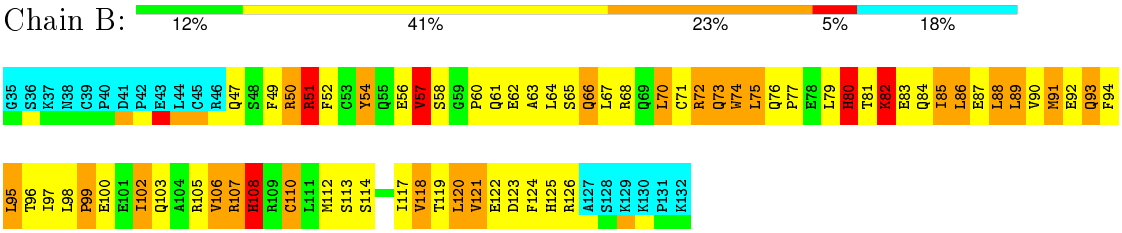
• Molecule 1: Zinc finger protein 174

Chain A:



• Molecule 1: Zinc finger protein 174

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.6
CYANA	refinement	1.0.6

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

6 Model quality

6.1 Standard geometry

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

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	707	732	718	149±13
1	B	677	698	684	142±15
All	All	27680	28600	28040	4588

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 82.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:52:PHE:CE1	1:B:67:LEU:HD22	1.14	1.78	8	1
1:A:75:LEU:HD11	1:B:89:LEU:HD21	1.11	1.18	9	20
1:B:94:PHE:CZ	1:B:118:VAL:HG23	1.11	1.79	2	20
1:A:52:PHE:CE1	1:A:67:LEU:HD11	1.10	1.80	13	1
1:A:89:LEU:HD21	1:B:75:LEU:HD11	1.09	1.19	3	20
1:B:94:PHE:CZ	1:B:98:LEU:HD11	1.07	1.83	12	13
1:A:75:LEU:HD13	1:B:85:ILE:HG23	1.06	1.14	17	6
1:A:94:PHE:CZ	1:A:98:LEU:HD11	1.06	1.84	16	8
1:A:85:ILE:HD13	1:B:85:ILE:HD13	1.05	1.26	11	6
1:A:94:PHE:CE2	1:A:98:LEU:HD11	1.05	1.85	9	1
1:A:94:PHE:CZ	1:B:64:LEU:HD11	1.03	1.87	1	1
1:A:49:PHE:CG	1:A:70:LEU:HD22	1.00	1.91	5	2
1:A:85:ILE:HG23	1:B:75:LEU:HD13	0.99	1.34	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ILE:CG2	1:B:75:LEU:HD13	0.99	1.87	17	15
1:B:94:PHE:CE1	1:B:98:LEU:HD11	0.98	1.94	1	4
1:A:75:LEU:CD2	1:A:88:LEU:HD11	0.97	1.89	18	1
1:A:95:LEU:N	1:A:95:LEU:HD13	0.97	1.75	2	8
1:B:52:PHE:CE2	1:B:67:LEU:HD22	0.97	1.95	16	1
1:A:94:PHE:CZ	1:A:118:VAL:HG23	0.96	1.95	3	18
1:A:89:LEU:HD21	1:B:75:LEU:CD1	0.96	1.90	5	20
1:A:75:LEU:HD13	1:B:85:ILE:CG2	0.96	1.90	17	16
1:A:111:LEU:HD23	1:A:111:LEU:O	0.95	1.62	18	2
1:B:98:LEU:HD13	1:B:121:VAL:HG21	0.94	1.39	5	8
1:A:89:LEU:HD13	1:B:71:CYS:HB3	0.94	1.40	10	15
1:A:53:CYS:CB	1:B:97:ILE:HG21	0.93	1.93	16	3
1:A:52:PHE:CG	1:A:67:LEU:HD21	0.93	1.98	15	3
1:A:120:LEU:O	1:A:120:LEU:HD22	0.93	1.63	7	1
1:A:120:LEU:HD22	1:A:120:LEU:O	0.93	1.63	2	1
1:B:75:LEU:CD2	1:B:88:LEU:HD11	0.91	1.94	18	1
1:A:90:VAL:HG22	1:B:68:ARG:HA	0.91	1.41	4	4
1:A:79:LEU:HD13	1:A:80:HIS:N	0.91	1.81	11	2
1:A:93:GLN:O	1:A:97:ILE:HG23	0.91	1.64	17	4
1:B:79:LEU:HD13	1:B:80:HIS:N	0.91	1.81	15	1
1:A:52:PHE:CE1	1:B:97:ILE:HG21	0.91	2.01	13	1
1:B:93:GLN:O	1:B:96:THR:HG22	0.91	1.66	12	17
1:A:52:PHE:CD1	1:A:67:LEU:HD21	0.91	2.00	13	2
1:A:98:LEU:HD13	1:A:121:VAL:HG21	0.91	1.41	13	11
1:A:85:ILE:HG21	1:B:85:ILE:HG21	0.90	1.38	10	5
1:A:89:LEU:CD2	1:B:75:LEU:HD11	0.90	1.97	20	18
1:B:78:GLU:O	1:B:79:LEU:HD22	0.90	1.67	8	2
1:A:75:LEU:CD1	1:B:89:LEU:HD21	0.90	1.97	16	19
1:A:75:LEU:HD12	1:B:86:LEU:HD12	0.89	1.40	8	3
1:A:75:LEU:HD23	1:A:88:LEU:HD11	0.88	1.41	18	1
1:A:94:PHE:CE1	1:A:118:VAL:HG23	0.88	2.03	7	15
1:A:98:LEU:HD13	1:A:121:VAL:CG2	0.88	1.99	13	5
1:A:102:ILE:O	1:A:106:VAL:HG13	0.88	1.69	13	3
1:A:95:LEU:HD13	1:A:95:LEU:N	0.87	1.84	12	12
1:A:74:TRP:CZ2	1:A:88:LEU:HD11	0.87	2.05	6	1
1:B:86:LEU:O	1:B:89:LEU:HD12	0.86	1.70	10	17
1:A:97:ILE:HD11	1:B:63:ALA:HB1	0.86	1.48	15	10
1:B:94:PHE:CE1	1:B:118:VAL:HG23	0.86	2.06	10	12
1:A:63:ALA:HB1	1:B:97:ILE:HD11	0.86	1.47	17	11
1:B:75:LEU:HD23	1:B:88:LEU:HG	0.86	1.48	1	7
1:B:49:PHE:CD1	1:B:70:LEU:HD11	0.86	2.06	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:MET:C	1:A:95:LEU:HD22	0.86	1.91	17	8
1:A:74:TRP:CE3	1:B:89:LEU:HD22	0.85	2.06	14	20
1:A:80:HIS:NE2	1:B:85:ILE:HG21	0.85	1.87	20	1
1:A:89:LEU:HD22	1:B:74:TRP:CE3	0.85	2.06	20	18
1:B:91:MET:C	1:B:95:LEU:HD22	0.85	1.93	20	9
1:A:68:ARG:HA	1:B:90:VAL:HG22	0.85	1.48	15	7
1:A:75:LEU:HD11	1:B:89:LEU:CD2	0.84	2.02	18	17
1:A:106:VAL:HG23	1:A:120:LEU:CD2	0.84	2.02	6	1
1:B:75:LEU:HD23	1:B:88:LEU:HD23	0.84	1.49	6	5
1:A:86:LEU:O	1:A:90:VAL:HG23	0.84	1.73	15	17
1:A:86:LEU:O	1:A:89:LEU:HD12	0.84	1.73	3	17
1:A:93:GLN:O	1:A:96:THR:HG22	0.84	1.72	9	19
1:A:64:LEU:HD21	1:B:118:VAL:HG21	0.84	1.49	11	1
1:B:91:MET:O	1:B:95:LEU:HD22	0.83	1.73	2	9
1:B:61:GLN:O	1:B:64:LEU:HD12	0.83	1.73	2	2
1:A:85:ILE:CG1	1:B:85:ILE:HG21	0.83	2.03	6	2
1:A:82:LYS:O	1:A:86:LEU:HD13	0.83	1.73	5	12
1:A:85:ILE:HG22	1:B:75:LEU:HD13	0.83	1.47	2	9
1:A:64:LEU:HD11	1:B:94:PHE:CE1	0.83	2.08	18	5
1:B:95:LEU:N	1:B:95:LEU:HD13	0.83	1.87	8	12
1:A:86:LEU:HD22	1:B:75:LEU:HD13	0.83	1.51	9	1
1:B:102:ILE:HG23	1:B:117:ILE:HG23	0.82	1.50	17	1
1:A:64:LEU:HD23	1:B:90:VAL:HG12	0.82	1.49	20	6
1:A:89:LEU:HD21	1:B:75:LEU:HD21	0.82	1.48	13	7
1:A:53:CYS:HB3	1:B:97:ILE:HG21	0.82	1.48	19	3
1:A:91:MET:O	1:A:95:LEU:HD22	0.82	1.74	19	15
1:B:86:LEU:O	1:B:90:VAL:HG23	0.82	1.74	6	17
1:B:75:LEU:HD22	1:B:85:ILE:HD12	0.82	1.50	19	1
1:B:82:LYS:O	1:B:86:LEU:HD13	0.82	1.74	8	14
1:A:75:LEU:HD23	1:A:88:LEU:HG	0.82	1.50	1	6
1:B:52:PHE:CZ	1:B:57:VAL:HG13	0.82	2.09	9	1
1:A:75:LEU:HD11	1:B:89:LEU:HD11	0.82	1.50	11	7
1:A:89:LEU:HD11	1:B:75:LEU:HD11	0.81	1.48	7	7
1:B:67:LEU:HD23	1:B:67:LEU:N	0.81	1.88	16	2
1:A:85:ILE:HG21	1:B:85:ILE:CG2	0.81	2.06	16	5
1:B:79:LEU:O	1:B:79:LEU:HD22	0.80	1.74	19	2
1:B:61:GLN:HA	1:B:64:LEU:HD21	0.80	1.52	18	3
1:B:93:GLN:O	1:B:97:ILE:HG23	0.80	1.76	10	6
1:B:49:PHE:CE1	1:B:70:LEU:HD11	0.80	2.11	5	1
1:B:94:PHE:CZ	1:B:118:VAL:HG22	0.79	2.12	12	4
1:A:97:ILE:HG21	1:B:52:PHE:CD1	0.79	2.13	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:LEU:CD2	1:B:88:LEU:HD23	0.79	2.08	4	4
1:A:71:CYS:HB3	1:B:89:LEU:HD13	0.78	1.53	7	14
1:A:85:ILE:HG12	1:B:85:ILE:HG21	0.78	1.54	6	6
1:B:101:GLU:HB3	1:B:120:LEU:HD11	0.78	1.54	13	1
1:A:86:LEU:HA	1:A:89:LEU:HD11	0.78	1.53	9	10
1:A:85:ILE:HD13	1:B:85:ILE:CD1	0.78	2.09	1	2
1:B:102:ILE:O	1:B:106:VAL:HG23	0.78	1.79	13	7
1:A:64:LEU:CD1	1:B:94:PHE:CD1	0.78	2.67	11	9
1:A:123:ASP:O	1:A:127:ALA:HB3	0.78	1.77	1	1
1:B:111:LEU:HD13	1:B:117:ILE:HG12	0.78	1.53	4	1
1:B:79:LEU:HD22	1:B:79:LEU:O	0.77	1.79	15	1
1:B:75:LEU:HD22	1:B:88:LEU:HD11	0.77	1.54	18	1
1:A:125:HIS:CG	1:B:54:TYR:HH	0.77	1.97	14	1
1:A:94:PHE:CZ	1:A:118:VAL:HG22	0.77	2.14	9	1
1:B:94:PHE:CE2	1:B:98:LEU:HD11	0.77	2.13	13	6
1:A:82:LYS:O	1:A:86:LEU:HD22	0.77	1.79	4	5
1:A:120:LEU:HD22	1:A:120:LEU:C	0.77	2.00	2	1
1:B:102:ILE:HD12	1:B:103:GLN:N	0.77	1.95	19	10
1:A:49:PHE:CD2	1:A:67:LEU:HD23	0.77	2.15	17	3
1:A:67:LEU:HD13	1:B:93:GLN:HG3	0.77	1.57	10	2
1:A:75:LEU:CD2	1:A:88:LEU:HD22	0.77	2.10	19	3
1:B:74:TRP:CZ2	1:B:88:LEU:HD11	0.77	2.14	7	1
1:A:49:PHE:CE2	1:A:67:LEU:HD23	0.76	2.14	11	2
1:A:86:LEU:HD23	1:A:86:LEU:N	0.76	1.94	9	1
1:A:54:TYR:CE1	1:B:98:LEU:CD2	0.76	2.67	19	5
1:A:94:PHE:CZ	1:A:118:VAL:CG2	0.76	2.69	18	18
1:A:90:VAL:HG12	1:B:64:LEU:HD23	0.76	1.55	17	6
1:A:98:LEU:HD22	1:A:121:VAL:HG11	0.76	1.57	1	2
1:A:85:ILE:HG21	1:B:85:ILE:HG12	0.76	1.56	2	5
1:B:94:PHE:CZ	1:B:118:VAL:CG2	0.76	2.68	11	18
1:A:52:PHE:CZ	1:A:67:LEU:HD11	0.76	2.16	13	1
1:A:75:LEU:HD13	1:B:85:ILE:HG22	0.76	1.57	6	8
1:A:102:ILE:HB	1:A:120:LEU:HD21	0.76	1.56	10	1
1:A:64:LEU:N	1:A:64:LEU:HD13	0.76	1.95	11	3
1:A:61:GLN:O	1:A:64:LEU:HD12	0.75	1.80	10	2
1:A:75:LEU:CD2	1:A:88:LEU:HD23	0.75	2.12	4	4
1:B:105:ARG:CB	1:B:120:LEU:HD22	0.75	2.11	17	2
1:B:85:ILE:HG22	1:B:86:LEU:HD12	0.75	1.59	17	2
1:B:102:ILE:HA	1:B:120:LEU:HD21	0.75	1.58	1	10
1:A:105:ARG:HG3	1:A:120:LEU:HD22	0.75	1.57	3	1
1:A:98:LEU:CD1	1:A:121:VAL:HG21	0.75	2.12	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:HD13	1:A:121:VAL:N	0.75	1.97	2	2
1:A:84:GLN:O	1:A:88:LEU:HD13	0.75	1.82	18	1
1:B:79:LEU:C	1:B:79:LEU:HD22	0.74	2.02	15	2
1:A:95:LEU:CD1	1:A:95:LEU:N	0.74	2.50	11	12
1:A:63:ALA:HB1	1:B:97:ILE:CD1	0.74	2.13	17	7
1:B:79:LEU:HB3	1:B:81:THR:HG22	0.74	1.57	5	1
1:A:102:ILE:CB	1:A:120:LEU:HD11	0.74	2.11	7	1
1:A:52:PHE:CE2	1:B:97:ILE:HD13	0.74	2.17	10	4
1:A:85:ILE:CD1	1:B:85:ILE:HD12	0.74	2.13	17	4
1:A:89:LEU:CD2	1:B:75:LEU:HD21	0.74	2.11	13	6
1:A:80:HIS:CE1	1:B:85:ILE:HG21	0.74	2.18	20	1
1:A:79:LEU:HD13	1:A:79:LEU:O	0.74	1.82	4	1
1:B:75:LEU:O	1:B:79:LEU:HD21	0.74	1.83	13	1
1:A:53:CYS:SG	1:B:97:ILE:HD13	0.74	2.23	19	2
1:B:98:LEU:HD13	1:B:121:VAL:CG2	0.74	2.10	5	4
1:A:95:LEU:N	1:A:95:LEU:CD1	0.73	2.51	14	8
1:A:85:ILE:HG22	1:B:75:LEU:CD1	0.73	2.14	2	6
1:A:85:ILE:CG2	1:B:85:ILE:HG21	0.73	2.13	10	6
1:A:49:PHE:CB	1:A:70:LEU:HD22	0.72	2.14	12	4
1:A:89:LEU:HD13	1:B:71:CYS:SG	0.72	2.24	11	7
1:A:79:LEU:C	1:A:79:LEU:HD22	0.72	2.03	1	2
1:A:123:ASP:HA	1:A:127:ALA:HB3	0.72	1.60	14	3
1:A:78:GLU:O	1:A:79:LEU:CB	0.72	2.37	4	1
1:A:94:PHE:CD1	1:B:64:LEU:HB3	0.72	2.20	8	1
1:B:102:ILE:N	1:B:102:ILE:HD12	0.72	2.00	17	1
1:A:57:VAL:HG11	1:A:62:GLU:O	0.72	1.84	2	3
1:A:89:LEU:HD21	1:B:75:LEU:CG	0.72	2.14	5	11
1:A:86:LEU:HD12	1:B:75:LEU:HD12	0.72	1.62	1	2
1:A:75:LEU:CD1	1:B:89:LEU:HD11	0.72	2.14	11	7
1:B:52:PHE:O	1:B:53:CYS:C	0.71	2.27	12	2
1:B:117:ILE:N	1:B:117:ILE:HD13	0.71	2.00	7	1
1:A:64:LEU:HG	1:B:94:PHE:CD1	0.71	2.20	10	12
1:B:81:THR:HG23	1:B:82:LYS:HD3	0.71	1.59	19	1
1:B:121:VAL:HG12	1:B:125:HIS:CE1	0.71	2.20	7	4
1:A:86:LEU:HD21	1:B:72:ARG:HB2	0.71	1.62	20	1
1:A:120:LEU:C	1:A:120:LEU:HD22	0.71	2.06	7	1
1:A:94:PHE:CE2	1:A:98:LEU:CD1	0.71	2.72	9	1
1:B:86:LEU:HA	1:B:89:LEU:HD11	0.71	1.63	13	8
1:A:121:VAL:O	1:A:125:HIS:CD2	0.71	2.44	5	19
1:A:74:TRP:CE3	1:B:89:LEU:CD2	0.71	2.74	17	5
1:A:102:ILE:HD13	1:A:103:GLN:H	0.71	1.46	14	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:52:PHE:CB	1:B:67:LEU:HD21	0.71	2.15	15	3
1:B:49:PHE:O	1:B:50:ARG:CB	0.71	2.38	12	4
1:A:88:LEU:HD12	1:A:88:LEU:C	0.71	2.07	8	2
1:A:118:VAL:HG21	1:B:61:GLN:HA	0.71	1.61	8	5
1:A:121:VAL:CG1	1:A:125:HIS:CE1	0.71	2.73	13	8
1:A:121:VAL:HG13	1:A:125:HIS:CE1	0.70	2.21	4	7
1:B:111:LEU:HD22	1:B:111:LEU:C	0.70	2.07	13	1
1:A:102:ILE:HA	1:A:120:LEU:HD21	0.70	1.63	4	9
1:A:94:PHE:CZ	1:B:64:LEU:CD1	0.70	2.72	1	1
1:B:95:LEU:HD13	1:B:95:LEU:N	0.70	2.01	12	4
1:A:57:VAL:HG21	1:A:63:ALA:HA	0.70	1.62	2	4
1:A:64:LEU:HD23	1:B:94:PHE:CD2	0.70	2.21	10	2
1:A:75:LEU:CD1	1:B:85:ILE:HG22	0.70	2.16	4	9
1:A:49:PHE:CD2	1:A:70:LEU:HD22	0.70	2.22	5	1
1:A:71:CYS:SG	1:B:89:LEU:HD13	0.70	2.26	3	8
1:A:79:LEU:HD22	1:A:79:LEU:O	0.70	1.85	11	2
1:A:80:HIS:CD2	1:A:80:HIS:N	0.70	2.58	4	1
1:A:57:VAL:HG22	1:A:62:GLU:HB3	0.70	1.64	17	2
1:A:97:ILE:CD1	1:B:63:ALA:HB1	0.70	2.17	15	11
1:B:75:LEU:O	1:B:76:GLN:O	0.70	2.10	13	9
1:A:106:VAL:CG2	1:A:111:LEU:HD13	0.70	2.17	1	1
1:B:95:LEU:CD1	1:B:95:LEU:N	0.69	2.55	1	8
1:A:93:GLN:HG2	1:B:67:LEU:HD22	0.69	1.64	9	4
1:A:53:CYS:HB3	1:B:97:ILE:HD13	0.69	1.65	11	3
1:B:121:VAL:HG12	1:B:125:HIS:NE2	0.69	2.02	15	6
1:B:94:PHE:O	1:B:98:LEU:HG	0.69	1.87	11	20
1:A:89:LEU:CD1	1:B:75:LEU:HD11	0.69	2.17	7	7
1:B:52:PHE:CE1	1:B:56:GLU:CB	0.69	2.75	15	4
1:A:94:PHE:CD2	1:B:64:LEU:HD23	0.69	2.21	4	2
1:B:98:LEU:CD1	1:B:102:ILE:HG21	0.69	2.18	8	5
1:A:97:ILE:HG21	1:B:67:LEU:HD11	0.69	1.65	20	4
1:A:106:VAL:CG2	1:A:111:LEU:HD12	0.69	2.18	20	1
1:B:75:LEU:CD2	1:B:88:LEU:CD1	0.69	2.70	18	1
1:A:89:LEU:HD11	1:B:75:LEU:CD1	0.69	2.17	7	9
1:A:102:ILE:HD13	1:A:103:GLN:N	0.69	2.02	14	3
1:A:50:ARG:HG3	1:B:96:THR:HG21	0.69	1.65	11	1
1:B:75:LEU:HD23	1:B:88:LEU:CD2	0.68	2.18	19	3
1:A:85:ILE:CD1	1:B:85:ILE:HD13	0.68	2.18	8	4
1:B:91:MET:O	1:B:95:LEU:CD2	0.68	2.41	18	10
1:B:71:CYS:SG	1:B:72:ARG:N	0.68	2.65	4	4
1:B:52:PHE:CD2	1:B:67:LEU:HD22	0.68	2.23	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HD21	1:A:88:LEU:HD22	0.68	1.66	19	2
1:B:79:LEU:O	1:B:79:LEU:HD13	0.68	1.89	7	1
1:A:54:TYR:CZ	1:B:98:LEU:CD2	0.68	2.76	16	3
1:A:93:GLN:CD	1:B:49:PHE:CZ	0.68	2.67	14	2
1:B:79:LEU:O	1:B:80:HIS:C	0.68	2.32	17	4
1:A:102:ILE:HG22	1:A:121:VAL:CG2	0.68	2.19	1	1
1:A:93:GLN:HG3	1:B:49:PHE:CZ	0.68	2.24	8	4
1:A:89:LEU:CD2	1:B:74:TRP:CE3	0.68	2.76	17	9
1:A:49:PHE:CE2	1:A:67:LEU:CD2	0.68	2.77	11	2
1:A:102:ILE:HD12	1:A:103:GLN:N	0.68	2.03	16	6
1:A:53:CYS:HB2	1:B:97:ILE:HG21	0.68	1.63	16	2
1:A:118:VAL:HG13	1:B:60:PRO:HB2	0.68	1.65	9	4
1:B:50:ARG:O	1:B:51:ARG:CB	0.68	2.42	20	16
1:B:80:HIS:N	1:B:80:HIS:CD2	0.68	2.60	14	1
1:A:52:PHE:CE1	1:B:97:ILE:CG2	0.68	2.77	13	1
1:A:49:PHE:O	1:A:70:LEU:HD22	0.68	1.87	6	1
1:A:93:GLN:HG3	1:B:67:LEU:HD13	0.68	1.65	16	2
1:A:80:HIS:CD2	1:A:80:HIS:C	0.67	2.68	9	1
1:B:98:LEU:HD22	1:B:121:VAL:HG21	0.67	1.65	17	3
1:A:67:LEU:HD11	1:B:97:ILE:HG21	0.67	1.66	17	6
1:B:52:PHE:CZ	1:B:67:LEU:HD22	0.67	2.23	16	1
1:B:102:ILE:HD13	1:B:103:GLN:N	0.67	2.04	20	3
1:A:49:PHE:CZ	1:A:71:CYS:SG	0.67	2.88	13	13
1:A:111:LEU:HD13	1:A:111:LEU:N	0.67	2.05	2	1
1:B:121:VAL:O	1:B:125:HIS:CD2	0.67	2.48	8	19
1:A:61:GLN:O	1:A:64:LEU:CD2	0.67	2.43	13	6
1:A:75:LEU:HD13	1:A:85:ILE:HG12	0.67	1.66	4	2
1:B:75:LEU:HD22	1:B:85:ILE:CG1	0.67	2.19	6	2
1:A:97:ILE:HD12	1:B:52:PHE:CE2	0.67	2.25	2	2
1:A:98:LEU:HD13	1:A:102:ILE:HG21	0.67	1.67	9	5
1:A:94:PHE:CD1	1:B:64:LEU:CD1	0.67	2.77	3	5
1:A:57:VAL:HG21	1:A:62:GLU:C	0.66	2.10	12	10
1:A:90:VAL:CG1	1:B:64:LEU:HD23	0.66	2.20	17	4
1:A:94:PHE:CD1	1:B:64:LEU:HG	0.66	2.25	4	10
1:A:98:LEU:CD1	1:A:102:ILE:HG21	0.66	2.20	18	4
1:B:57:VAL:HG23	1:B:59:GLY:O	0.66	1.90	4	2
1:A:89:LEU:HD21	1:B:75:LEU:CD2	0.66	2.19	13	4
1:A:75:LEU:CD1	1:B:85:ILE:HG23	0.66	2.08	17	2
1:B:95:LEU:N	1:B:95:LEU:CD1	0.66	2.58	13	8
1:B:52:PHE:CE1	1:B:53:CYS:O	0.66	2.49	18	3
1:B:60:PRO:O	1:B:63:ALA:HB3	0.66	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:CE1	1:A:67:LEU:CD1	0.66	2.71	13	1
1:B:102:ILE:HD13	1:B:103:GLN:H	0.66	1.50	20	3
1:A:118:VAL:HG21	1:B:64:LEU:HD11	0.66	1.67	16	5
1:B:98:LEU:HD13	1:B:102:ILE:HG21	0.66	1.68	15	7
1:A:89:LEU:HD13	1:B:71:CYS:HB2	0.66	1.67	18	3
1:A:81:THR:HG23	1:A:83:GLU:H	0.66	1.50	8	9
1:B:106:VAL:HG22	1:B:112:MET:HG2	0.66	1.68	14	1
1:A:64:LEU:HD11	1:B:94:PHE:CZ	0.66	2.26	9	3
1:A:123:ASP:HA	1:A:127:ALA:HB2	0.66	1.68	8	10
1:A:52:PHE:O	1:A:52:PHE:CG	0.66	2.48	11	1
1:A:74:TRP:CD1	1:A:74:TRP:C	0.66	2.68	18	9
1:A:46:ARG:O	1:A:49:PHE:CD2	0.66	2.49	6	1
1:B:52:PHE:CD1	1:B:52:PHE:C	0.66	2.68	6	2
1:A:77:PRO:HG3	1:A:80:HIS:CD2	0.66	2.26	20	1
1:B:61:GLN:O	1:B:64:LEU:CD2	0.66	2.44	3	5
1:A:102:ILE:HB	1:A:120:LEU:HD11	0.66	1.66	7	1
1:B:91:MET:O	1:B:95:LEU:HG	0.66	1.91	14	4
1:A:49:PHE:CE2	1:A:71:CYS:SG	0.66	2.89	13	9
1:A:77:PRO:CG	1:A:80:HIS:CD2	0.65	2.79	20	1
1:A:113:SER:O	1:A:117:ILE:HD13	0.65	1.92	10	2
1:A:72:ARG:HA	1:B:86:LEU:HD11	0.65	1.69	18	2
1:A:111:LEU:HD23	1:A:111:LEU:C	0.65	2.09	1	2
1:A:54:TYR:CE1	1:B:98:LEU:HD21	0.65	2.26	1	2
1:A:79:LEU:O	1:A:79:LEU:HD22	0.65	1.91	1	1
1:A:94:PHE:O	1:A:98:LEU:HG	0.65	1.90	9	20
1:A:57:VAL:CG2	1:A:63:ALA:N	0.65	2.60	14	1
1:A:49:PHE:CZ	1:B:93:GLN:HG2	0.65	2.26	19	11
1:A:79:LEU:O	1:A:80:HIS:C	0.65	2.34	18	2
1:A:54:TYR:OH	1:B:121:VAL:HG11	0.65	1.91	1	2
1:A:71:CYS:SG	1:B:90:VAL:HG22	0.65	2.32	11	6
1:A:49:PHE:CE1	1:A:71:CYS:SG	0.65	2.89	6	5
1:A:72:ARG:HB2	1:B:86:LEU:HD21	0.65	1.67	18	3
1:B:78:GLU:C	1:B:79:LEU:HD22	0.65	2.12	2	2
1:A:111:LEU:HD13	1:A:117:ILE:HG13	0.65	1.68	20	1
1:A:126:ARG:O	1:A:127:ALA:HB2	0.65	1.92	14	1
1:A:106:VAL:HG23	1:A:111:LEU:HD13	0.65	1.69	1	1
1:A:98:LEU:CD2	1:B:54:TYR:CE1	0.65	2.80	11	4
1:A:64:LEU:HD23	1:B:94:PHE:CG	0.65	2.26	10	2
1:B:52:PHE:CZ	1:B:56:GLU:CB	0.64	2.80	15	3
1:A:93:GLN:NE2	1:B:49:PHE:CE2	0.64	2.66	7	1
1:B:79:LEU:N	1:B:79:LEU:HD13	0.64	2.06	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:94:PHE:CD2	1:B:95:LEU:CD1	0.64	2.81	8	7
1:A:64:LEU:O	1:A:68:ARG:N	0.64	2.30	12	20
1:A:49:PHE:HB2	1:A:70:LEU:HD13	0.64	1.69	2	2
1:A:75:LEU:HD23	1:A:88:LEU:CG	0.64	2.22	1	4
1:A:75:LEU:CD2	1:A:88:LEU:CD1	0.64	2.72	18	1
1:A:85:ILE:HD13	1:B:85:ILE:CG1	0.64	2.21	1	2
1:A:102:ILE:CB	1:A:120:LEU:HD21	0.64	2.22	10	1
1:B:95:LEU:HB3	1:B:102:ILE:HD13	0.64	1.69	6	1
1:A:49:PHE:CD1	1:A:50:ARG:N	0.64	2.66	17	14
1:A:94:PHE:CD2	1:A:95:LEU:CD1	0.64	2.81	2	8
1:B:64:LEU:H	1:B:64:LEU:HD13	0.64	1.52	16	4
1:A:75:LEU:HD11	1:B:89:LEU:CD1	0.64	2.22	1	7
1:A:54:TYR:CE1	1:B:98:LEU:HD23	0.64	2.27	11	3
1:B:52:PHE:O	1:B:53:CYS:CB	0.64	2.45	8	7
1:A:85:ILE:HG12	1:B:85:ILE:HD13	0.64	1.70	8	1
1:B:78:GLU:O	1:B:79:LEU:CB	0.64	2.46	7	2
1:A:52:PHE:CD1	1:A:52:PHE:C	0.64	2.70	11	3
1:A:107:ARG:O	1:A:108:HIS:CB	0.64	2.46	6	3
1:A:64:LEU:O	1:A:68:ARG:CB	0.64	2.46	15	17
1:A:52:PHE:CD2	1:B:97:ILE:HD13	0.64	2.28	8	3
1:B:64:LEU:O	1:B:68:ARG:CB	0.64	2.46	20	12
1:A:75:LEU:HD21	1:B:89:LEU:HD21	0.64	1.69	2	4
1:A:121:VAL:HG12	1:B:54:TYR:CZ	0.64	2.28	1	1
1:A:98:LEU:HD23	1:B:54:TYR:CD1	0.64	2.28	1	3
1:A:93:GLN:OE1	1:B:49:PHE:CZ	0.64	2.51	4	3
1:A:85:ILE:HG22	1:A:86:LEU:HD12	0.64	1.69	14	1
1:B:102:ILE:HG22	1:B:120:LEU:HD21	0.63	1.69	5	6
1:A:94:PHE:CZ	1:A:98:LEU:CD1	0.63	2.75	16	5
1:B:82:LYS:HA	1:B:85:ILE:HD12	0.63	1.70	15	2
1:A:80:HIS:CG	1:B:85:ILE:HD13	0.63	2.28	20	1
1:A:117:ILE:HA	1:A:120:LEU:HD23	0.63	1.70	15	5
1:B:81:THR:HG23	1:B:83:GLU:HB2	0.63	1.69	5	2
1:A:75:LEU:CD2	1:A:88:LEU:CD2	0.63	2.76	7	4
1:B:57:VAL:HG21	1:B:62:GLU:O	0.63	1.94	18	1
1:B:64:LEU:HD13	1:B:64:LEU:H	0.63	1.53	9	1
1:B:67:LEU:N	1:B:67:LEU:CD2	0.63	2.61	16	1
1:A:123:ASP:CA	1:A:127:ALA:HB2	0.63	2.24	19	6
1:B:49:PHE:CD1	1:B:50:ARG:N	0.63	2.66	7	12
1:A:64:LEU:CD1	1:B:94:PHE:CE1	0.63	2.79	18	7
1:A:64:LEU:HD11	1:B:118:VAL:CG2	0.63	2.23	17	3
1:A:94:PHE:HB3	1:A:95:LEU:HD13	0.63	1.69	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:105:ARG:HB3	1:B:120:LEU:HD22	0.63	1.71	17	1
1:B:76:GLN:O	1:B:80:HIS:CD2	0.63	2.50	19	2
1:B:53:CYS:O	1:B:54:TYR:C	0.63	2.37	12	6
1:A:97:ILE:HG21	1:B:52:PHE:CD2	0.63	2.29	18	1
1:A:53:CYS:HB2	1:A:67:LEU:HD11	0.63	1.70	19	2
1:A:53:CYS:HB3	1:B:97:ILE:CG2	0.63	2.24	19	2
1:B:52:PHE:HE1	1:B:67:LEU:HD22	0.62	1.48	8	1
1:A:91:MET:O	1:A:94:PHE:N	0.62	2.31	1	6
1:A:52:PHE:HB2	1:A:67:LEU:HD21	0.62	1.69	10	3
1:A:49:PHE:CZ	1:B:93:GLN:HG3	0.62	2.29	16	4
1:B:94:PHE:CE2	1:B:117:ILE:CG2	0.62	2.82	1	2
1:A:54:TYR:O	1:A:55:GLN:CB	0.62	2.46	14	2
1:A:75:LEU:HD22	1:A:88:LEU:HD21	0.62	1.70	18	1
1:B:94:PHE:CE1	1:B:98:LEU:CD1	0.62	2.80	1	1
1:A:67:LEU:HD13	1:B:93:GLN:HB3	0.62	1.69	1	5
1:B:94:PHE:CZ	1:B:98:LEU:CD1	0.62	2.78	5	5
1:A:122:GLU:O	1:A:126:ARG:CB	0.62	2.48	1	2
1:A:71:CYS:SG	1:A:72:ARG:N	0.62	2.72	1	3
1:B:85:ILE:HG22	1:B:86:LEU:CD1	0.62	2.24	17	1
1:A:49:PHE:C	1:A:49:PHE:CD1	0.62	2.73	6	1
1:A:57:VAL:HG21	1:A:63:ALA:CA	0.62	2.25	17	3
1:B:94:PHE:CE2	1:B:98:LEU:CD1	0.62	2.82	13	4
1:A:86:LEU:HD23	1:B:68:ARG:CG	0.62	2.24	20	1
1:A:121:VAL:HG12	1:B:54:TYR:CE2	0.62	2.29	1	1
1:B:75:LEU:HD23	1:B:88:LEU:CG	0.62	2.23	1	7
1:A:52:PHE:CB	1:A:67:LEU:HD21	0.62	2.24	10	4
1:A:67:LEU:HD22	1:B:93:GLN:HB3	0.62	1.71	17	1
1:A:93:GLN:OE1	1:B:49:PHE:CD1	0.62	2.52	17	2
1:A:64:LEU:H	1:A:64:LEU:HD13	0.62	1.55	1	5
1:B:80:HIS:H	1:B:80:HIS:CD2	0.62	2.12	19	1
1:A:49:PHE:CD1	1:A:49:PHE:C	0.62	2.73	2	3
1:B:49:PHE:CE2	1:B:71:CYS:SG	0.62	2.92	10	7
1:A:76:GLN:O	1:A:76:GLN:CG	0.62	2.47	3	1
1:A:106:VAL:HG13	1:A:107:ARG:N	0.62	2.10	10	2
1:A:64:LEU:HD13	1:A:64:LEU:H	0.62	1.55	16	2
1:A:67:LEU:HD12	1:B:94:PHE:HA	0.62	1.70	15	1
1:A:118:VAL:CG2	1:B:64:LEU:HD11	0.62	2.24	16	5
1:A:61:GLN:HA	1:B:118:VAL:HG21	0.62	1.72	10	2
1:B:102:ILE:CG2	1:B:121:VAL:CG2	0.62	2.78	18	1
1:A:52:PHE:CZ	1:A:54:TYR:HA	0.62	2.29	8	4
1:B:86:LEU:O	1:B:90:VAL:CG2	0.61	2.47	6	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:74:TRP:CD1	1:B:74:TRP:C	0.61	2.72	14	8
1:B:81:THR:O	1:B:83:GLU:N	0.61	2.33	19	4
1:A:117:ILE:O	1:A:121:VAL:HG23	0.61	1.95	6	3
1:B:66:GLN:O	1:B:70:LEU:HD12	0.61	1.93	2	1
1:A:111:LEU:O	1:A:111:LEU:HD23	0.61	1.94	15	1
1:A:85:ILE:CG1	1:B:85:ILE:HD13	0.61	2.26	8	1
1:A:86:LEU:HD23	1:B:68:ARG:HG3	0.61	1.71	20	1
1:B:75:LEU:HD13	1:B:85:ILE:HG12	0.61	1.71	3	3
1:A:93:GLN:OE1	1:B:49:PHE:CE2	0.61	2.53	4	1
1:B:98:LEU:HD12	1:B:102:ILE:CG2	0.61	2.25	10	1
1:B:102:ILE:HD12	1:B:102:ILE:C	0.61	2.15	12	4
1:A:64:LEU:HD12	1:B:94:PHE:CD1	0.61	2.30	1	1
1:B:81:THR:HG23	1:B:83:GLU:H	0.61	1.55	4	12
1:A:49:PHE:CD2	1:A:67:LEU:HD22	0.61	2.31	12	4
1:A:119:THR:HG22	1:A:120:LEU:N	0.61	2.11	14	3
1:A:49:PHE:HB3	1:A:70:LEU:HD22	0.61	1.71	2	1
1:A:52:PHE:CD1	1:A:52:PHE:O	0.61	2.52	11	1
1:B:79:LEU:C	1:B:80:HIS:CD2	0.61	2.74	5	2
1:A:61:GLN:HA	1:A:64:LEU:HD21	0.61	1.71	13	3
1:A:79:LEU:O	1:A:81:THR:N	0.61	2.34	18	1
1:A:74:TRP:HZ2	1:A:88:LEU:HD11	0.61	1.55	6	1
1:A:79:LEU:HD12	1:A:80:HIS:N	0.61	2.09	6	7
1:A:75:LEU:O	1:A:76:GLN:O	0.61	2.18	9	7
1:A:85:ILE:HD13	1:B:85:ILE:HG12	0.61	1.71	1	3
1:B:122:GLU:O	1:B:126:ARG:CB	0.61	2.49	18	2
1:B:102:ILE:CA	1:B:120:LEU:HD21	0.61	2.25	1	1
1:B:74:TRP:C	1:B:74:TRP:CD1	0.61	2.72	20	10
1:A:53:CYS:O	1:A:54:TYR:C	0.61	2.39	5	9
1:A:75:LEU:O	1:A:76:GLN:C	0.61	2.39	10	10
1:B:75:LEU:HD22	1:B:85:ILE:HG13	0.61	1.73	6	1
1:A:90:VAL:CG2	1:B:71:CYS:CB	0.61	2.79	11	11
1:B:114:SER:HA	1:B:117:ILE:HD12	0.61	1.73	11	2
1:A:121:VAL:HG12	1:A:125:HIS:CE1	0.60	2.31	20	6
1:A:86:LEU:HD12	1:B:75:LEU:CD1	0.60	2.25	1	1
1:B:49:PHE:CE2	1:B:74:TRP:CZ3	0.60	2.89	16	1
1:A:89:LEU:HD13	1:B:71:CYS:CB	0.60	2.27	18	13
1:A:86:LEU:O	1:A:90:VAL:CG2	0.60	2.50	15	9
1:A:101:GLU:HB3	1:A:120:LEU:HD11	0.60	1.72	15	3
1:B:52:PHE:CD1	1:B:53:CYS:O	0.60	2.54	18	2
1:A:101:GLU:OE2	1:A:124:PHE:CE1	0.60	2.55	1	1
1:B:54:TYR:CE2	1:B:58:SER:O	0.60	2.54	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:77:PRO:O	1:B:78:GLU:CB	0.60	2.49	10	6
1:A:71:CYS:HB2	1:B:89:LEU:HD13	0.60	1.73	2	3
1:A:49:PHE:CG	1:A:50:ARG:N	0.60	2.69	8	11
1:A:86:LEU:O	1:A:89:LEU:CD1	0.60	2.49	16	9
1:B:79:LEU:O	1:B:80:HIS:CG	0.60	2.54	13	2
1:A:45:CYS:SG	1:A:70:LEU:HD11	0.60	2.35	14	1
1:B:49:PHE:O	1:B:52:PHE:CE2	0.60	2.54	16	1
1:A:90:VAL:HG22	1:B:71:CYS:SG	0.60	2.36	17	6
1:A:106:VAL:HG13	1:A:111:LEU:HD21	0.60	1.73	19	1
1:A:77:PRO:CD	1:A:80:HIS:CE1	0.60	2.84	20	1
1:A:99:PRO:O	1:A:102:ILE:HG23	0.60	1.96	10	2
1:B:74:TRP:HZ2	1:B:88:LEU:HD11	0.60	1.57	7	1
1:B:102:ILE:HD13	1:B:117:ILE:CG2	0.60	2.26	1	1
1:A:49:PHE:CD2	1:B:93:GLN:HG3	0.60	2.30	15	1
1:A:84:GLN:O	1:A:88:LEU:HD22	0.60	1.97	9	1
1:A:64:LEU:HD22	1:A:64:LEU:N	0.60	2.12	2	3
1:A:53:CYS:H	1:B:97:ILE:HG22	0.60	1.57	1	2
1:A:92:GLU:O	1:A:95:LEU:HD22	0.60	1.97	1	1
1:A:94:PHE:CE2	1:A:117:ILE:CG2	0.60	2.84	7	2
1:A:81:THR:HG22	1:A:84:GLN:OE1	0.60	1.96	20	1
1:B:49:PHE:O	1:B:50:ARG:CG	0.60	2.50	17	3
1:A:111:LEU:O	1:A:112:MET:CB	0.60	2.50	15	4
1:A:64:LEU:N	1:A:64:LEU:HD22	0.60	2.12	16	3
1:A:101:GLU:CG	1:A:124:PHE:CD1	0.60	2.84	2	1
1:B:61:GLN:O	1:B:64:LEU:HD22	0.60	1.96	3	5
1:A:111:LEU:HD12	1:A:117:ILE:CD1	0.60	2.27	12	1
1:A:49:PHE:CD1	1:B:93:GLN:HB3	0.60	2.32	15	1
1:B:102:ILE:HG23	1:B:117:ILE:CG2	0.59	2.26	17	1
1:A:64:LEU:CD1	1:B:118:VAL:CG2	0.59	2.79	5	4
1:B:85:ILE:N	1:B:85:ILE:HD13	0.59	2.12	19	1
1:A:121:VAL:HG13	1:A:125:HIS:NE2	0.59	2.11	13	7
1:A:106:VAL:HG12	1:A:107:ARG:N	0.59	2.11	6	2
1:A:50:ARG:CG	1:B:96:THR:HG21	0.59	2.26	11	1
1:B:121:VAL:HG13	1:B:125:HIS:NE2	0.59	2.13	3	2
1:A:71:CYS:SG	1:B:90:VAL:HG23	0.59	2.36	10	2
1:B:55:GLN:O	1:B:56:GLU:CB	0.59	2.49	10	1
1:A:49:PHE:CE2	1:B:93:GLN:HG3	0.59	2.31	15	2
1:A:80:HIS:CB	1:B:85:ILE:HD13	0.59	2.27	20	1
1:B:49:PHE:CE1	1:B:74:TRP:CZ3	0.59	2.91	7	3
1:B:80:HIS:CD2	1:B:80:HIS:O	0.59	2.56	20	2
1:B:57:VAL:HG23	1:B:63:ALA:HA	0.59	1.75	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:PHE:CG	1:B:50:ARG:N	0.59	2.70	16	1
1:A:71:CYS:SG	1:B:90:VAL:CG2	0.59	2.90	10	9
1:A:74:TRP:HE1	1:A:88:LEU:HD11	0.59	1.57	3	2
1:B:52:PHE:CZ	1:B:56:GLU:HB2	0.59	2.32	14	3
1:A:93:GLN:HG2	1:B:49:PHE:CD1	0.59	2.33	5	1
1:A:78:GLU:O	1:A:79:LEU:HD22	0.59	1.98	20	2
1:A:109:ARG:O	1:A:110:CYS:CB	0.59	2.51	11	4
1:B:98:LEU:CD1	1:B:121:VAL:HG21	0.59	2.22	5	3
1:A:64:LEU:HD11	1:B:94:PHE:CD1	0.59	2.33	11	3
1:A:80:HIS:N	1:A:80:HIS:CD2	0.59	2.70	19	1
1:A:53:CYS:CB	1:B:97:ILE:HD13	0.59	2.28	11	2
1:B:52:PHE:HD2	1:B:67:LEU:HD21	0.59	1.56	18	1
1:A:121:VAL:O	1:A:125:HIS:CG	0.58	2.56	10	6
1:B:52:PHE:CE1	1:B:66:GLN:CB	0.58	2.86	14	4
1:A:52:PHE:C	1:A:52:PHE:CD1	0.58	2.76	19	2
1:B:50:ARG:O	1:B:51:ARG:HB3	0.58	1.96	20	2
1:A:81:THR:C	1:A:85:ILE:HD12	0.58	2.17	4	1
1:A:93:GLN:OE1	1:B:49:PHE:CE1	0.58	2.56	4	3
1:A:106:VAL:HG13	1:A:112:MET:SD	0.58	2.37	6	1
1:A:95:LEU:O	1:A:98:LEU:N	0.58	2.35	2	4
1:A:99:PRO:O	1:A:102:ILE:HD12	0.58	1.97	3	2
1:A:75:LEU:HD22	1:A:88:LEU:HD23	0.58	1.74	7	1
1:B:89:LEU:O	1:B:93:GLN:CG	0.58	2.51	12	1
1:B:93:GLN:OE1	1:B:96:THR:HG21	0.58	1.98	18	3
1:B:49:PHE:CE2	1:B:67:LEU:HD22	0.58	2.34	6	2
1:A:44:LEU:HD13	1:A:45:CYS:N	0.58	2.14	5	5
1:B:114:SER:HA	1:B:117:ILE:HD13	0.58	1.76	18	2
1:A:94:PHE:CG	1:B:64:LEU:HD23	0.58	2.34	4	2
1:B:81:THR:OG1	1:B:82:LYS:N	0.58	2.36	19	13
1:A:64:LEU:HD23	1:B:90:VAL:CG1	0.58	2.27	20	1
1:A:86:LEU:N	1:A:86:LEU:CD2	0.58	2.67	9	1
1:A:97:ILE:HD11	1:B:63:ALA:CB	0.58	2.29	5	4
1:A:64:LEU:CD1	1:A:64:LEU:N	0.58	2.67	11	1
1:A:106:VAL:HG23	1:A:111:LEU:HD12	0.58	1.76	20	1
1:B:75:LEU:O	1:B:88:LEU:HD21	0.58	1.99	5	1
1:B:117:ILE:HA	1:B:120:LEU:HD23	0.58	1.73	10	5
1:A:80:HIS:CD2	1:A:84:GLN:CD	0.58	2.76	3	1
1:B:64:LEU:N	1:B:64:LEU:HD13	0.58	2.14	9	3
1:A:99:PRO:O	1:A:101:GLU:N	0.58	2.36	10	3
1:A:50:ARG:HA	1:A:50:ARG:NE	0.58	2.13	6	1
1:B:67:LEU:O	1:B:70:LEU:N	0.58	2.36	15	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LEU:HD21	1:B:54:TYR:CE1	0.58	2.33	19	1
1:A:79:LEU:C	1:A:79:LEU:HD13	0.58	2.20	4	1
1:A:121:VAL:O	1:A:125:HIS:N	0.58	2.37	14	1
1:B:49:PHE:C	1:B:49:PHE:CD1	0.58	2.77	8	7
1:A:94:PHE:C	1:A:95:LEU:HD13	0.58	2.17	11	3
1:B:49:PHE:CD2	1:B:50:ARG:N	0.58	2.72	16	1
1:A:91:MET:O	1:A:95:LEU:CD2	0.57	2.52	11	13
1:A:71:CYS:O	1:A:74:TRP:N	0.57	2.37	7	14
1:B:90:VAL:O	1:B:94:PHE:CB	0.57	2.52	20	10
1:B:97:ILE:HG13	1:B:98:LEU:N	0.57	2.14	12	12
1:A:71:CYS:CB	1:B:90:VAL:CG2	0.57	2.83	9	11
1:B:80:HIS:CD2	1:B:80:HIS:N	0.57	2.71	7	3
1:B:101:GLU:HG3	1:B:120:LEU:HD11	0.57	1.75	5	1
1:A:80:HIS:C	1:A:80:HIS:CD2	0.57	2.77	12	2
1:B:75:LEU:O	1:B:76:GLN:CG	0.57	2.52	13	1
1:B:79:LEU:HD22	1:B:84:GLN:HE21	0.57	1.57	13	1
1:A:80:HIS:CG	1:A:84:GLN:CD	0.57	2.78	14	1
1:B:87:GLU:O	1:B:91:MET:CB	0.57	2.52	14	5
1:A:98:LEU:HD22	1:A:121:VAL:HG21	0.57	1.77	2	2
1:A:102:ILE:CG2	1:A:121:VAL:CG2	0.57	2.82	1	4
1:A:57:VAL:O	1:A:58:SER:CB	0.57	2.52	7	3
1:A:111:LEU:HD13	1:A:116:GLU:HB3	0.57	1.75	12	1
1:B:106:VAL:HG22	1:B:111:LEU:HD11	0.57	1.75	9	1
1:A:121:VAL:CG1	1:B:54:TYR:CE2	0.57	2.88	1	1
1:A:102:ILE:HG22	1:A:120:LEU:HD11	0.57	1.74	2	1
1:B:111:LEU:HD12	1:B:116:GLU:HG2	0.57	1.77	17	1
1:A:53:CYS:SG	1:A:63:ALA:O	0.57	2.62	19	3
1:B:94:PHE:CZ	1:B:117:ILE:HG22	0.57	2.35	1	1
1:A:94:PHE:HE1	1:A:118:VAL:HG23	0.57	1.58	7	11
1:A:57:VAL:HG21	1:A:62:GLU:O	0.57	2.00	3	4
1:A:49:PHE:CB	1:A:70:LEU:HD13	0.57	2.29	5	1
1:A:57:VAL:CG1	1:A:58:SER:N	0.57	2.68	12	1
1:B:106:VAL:HG23	1:B:107:ARG:N	0.57	2.15	1	1
1:A:86:LEU:HD23	1:A:86:LEU:H	0.57	1.58	9	1
1:B:91:MET:CE	1:B:95:LEU:HD11	0.57	2.30	1	3
1:A:54:TYR:CE2	1:B:121:VAL:HG11	0.57	2.33	15	1
1:A:92:GLU:O	1:A:95:LEU:CD2	0.57	2.53	1	1
1:A:111:LEU:O	1:A:112:MET:CG	0.57	2.52	15	1
1:A:103:GLN:HB2	1:A:111:LEU:HD23	0.57	1.76	6	1
1:A:71:CYS:HB3	1:B:89:LEU:CD1	0.57	2.30	3	2
1:A:79:LEU:HD13	1:A:80:HIS:H	0.57	1.56	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:61:GLN:CA	1:B:64:LEU:HD21	0.57	2.29	18	1
1:A:106:VAL:HA	1:A:111:LEU:HD21	0.57	1.76	16	1
1:B:64:LEU:O	1:B:68:ARG:N	0.56	2.38	16	17
1:A:72:ARG:HG2	1:B:86:LEU:HD23	0.56	1.77	8	2
1:B:71:CYS:O	1:B:74:TRP:N	0.56	2.37	10	13
1:B:113:SER:O	1:B:116:GLU:N	0.56	2.38	10	8
1:B:49:PHE:HD1	1:B:70:LEU:HD21	0.56	1.60	5	1
1:A:98:LEU:HD12	1:A:117:ILE:HG22	0.56	1.76	13	1
1:B:86:LEU:O	1:B:89:LEU:CD1	0.56	2.53	6	10
1:B:87:GLU:O	1:B:91:MET:CG	0.56	2.53	18	3
1:B:79:LEU:O	1:B:81:THR:N	0.56	2.39	20	2
1:B:64:LEU:HD22	1:B:64:LEU:N	0.56	2.14	18	4
1:A:93:GLN:HB3	1:B:67:LEU:HD13	0.56	1.75	4	7
1:A:102:ILE:CA	1:A:120:LEU:HD11	0.56	2.30	7	1
1:B:106:VAL:O	1:B:111:LEU:HD13	0.56	2.01	18	1
1:A:106:VAL:HG23	1:A:120:LEU:HD22	0.56	1.76	6	1
1:A:71:CYS:CB	1:B:89:LEU:HD13	0.56	2.31	14	13
1:B:57:VAL:O	1:B:58:SER:CB	0.56	2.53	19	9
1:A:64:LEU:CD1	1:B:118:VAL:HG21	0.56	2.31	17	3
1:A:61:GLN:O	1:A:64:LEU:HD22	0.56	1.99	16	6
1:A:50:ARG:O	1:B:96:THR:CG2	0.56	2.53	11	4
1:B:56:GLU:O	1:B:57:VAL:C	0.56	2.43	20	2
1:A:91:MET:HG3	1:A:95:LEU:HD11	0.56	1.77	4	1
1:B:57:VAL:HG21	1:B:62:GLU:C	0.56	2.21	18	6
1:A:106:VAL:HG23	1:A:120:LEU:HD23	0.56	1.75	6	1
1:B:106:VAL:HA	1:B:111:LEU:HD21	0.56	1.76	3	1
1:A:44:LEU:C	1:A:44:LEU:HD13	0.56	2.21	18	5
1:A:80:HIS:CG	1:B:81:THR:HG1	0.56	2.18	18	1
1:B:78:GLU:O	1:B:79:LEU:CD2	0.56	2.53	11	2
1:B:111:LEU:O	1:B:111:LEU:HD22	0.56	2.01	13	3
1:A:64:LEU:HD11	1:B:118:VAL:HG21	0.56	1.78	12	3
1:B:79:LEU:CD1	1:B:79:LEU:O	0.56	2.54	7	1
1:A:94:PHE:CG	1:B:64:LEU:HB3	0.56	2.35	8	1
1:B:99:PRO:O	1:B:102:ILE:CD1	0.56	2.54	20	7
1:A:81:THR:OG1	1:B:80:HIS:CG	0.56	2.59	17	1
1:A:86:LEU:HD11	1:B:72:ARG:HA	0.56	1.77	20	1
1:B:52:PHE:CE1	1:B:66:GLN:HB3	0.56	2.36	5	4
1:A:75:LEU:HD23	1:A:88:LEU:HD23	0.56	1.76	4	2
1:A:114:SER:HA	1:A:117:ILE:HD12	0.56	1.77	13	1
1:A:52:PHE:HE2	1:B:97:ILE:HD13	0.56	1.58	10	2
1:B:94:PHE:CE1	1:B:98:LEU:HD21	0.56	2.36	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ILE:HG13	1:B:85:ILE:HG21	0.56	1.78	6	1
1:A:87:GLU:O	1:A:91:MET:CB	0.56	2.54	14	6
1:B:102:ILE:N	1:B:102:ILE:CD1	0.56	2.68	17	1
1:A:75:LEU:CG	1:B:89:LEU:HD21	0.56	2.30	16	6
1:A:52:PHE:O	1:A:55:GLN:CB	0.56	2.54	10	4
1:A:96:THR:HG23	1:B:51:ARG:HG3	0.55	1.78	8	2
1:B:71:CYS:O	1:B:74:TRP:HB3	0.55	2.01	1	15
1:A:90:VAL:CG2	1:B:71:CYS:SG	0.55	2.94	20	12
1:B:117:ILE:O	1:B:121:VAL:HG23	0.55	2.01	7	3
1:A:94:PHE:CZ	1:A:117:ILE:HG22	0.55	2.36	7	1
1:A:57:VAL:HG22	1:A:62:GLU:CB	0.55	2.31	14	1
1:A:49:PHE:CG	1:B:93:GLN:HB3	0.55	2.36	15	1
1:A:98:LEU:HB2	1:A:102:ILE:HD12	0.55	1.78	11	1
1:A:85:ILE:HG23	1:B:85:ILE:CG2	0.55	2.32	19	1
1:B:121:VAL:CG1	1:B:125:HIS:NE2	0.55	2.69	13	6
1:B:70:LEU:O	1:B:74:TRP:N	0.55	2.39	7	6
1:A:94:PHE:CE1	1:B:64:LEU:HG	0.55	2.35	4	2
1:A:93:GLN:NE2	1:A:96:THR:HG21	0.55	2.16	2	2
1:A:54:TYR:CA	1:B:97:ILE:HD12	0.55	2.30	15	1
1:B:102:ILE:C	1:B:102:ILE:HD12	0.55	2.22	5	3
1:B:102:ILE:O	1:B:106:VAL:HG22	0.55	2.01	1	2
1:A:102:ILE:HA	1:A:120:LEU:HD11	0.55	1.77	7	1
1:A:49:PHE:CZ	1:B:93:GLN:CD	0.55	2.79	12	1
1:B:101:GLU:OE1	1:B:121:VAL:HG13	0.55	2.01	10	1
1:B:52:PHE:HB3	1:B:67:LEU:HD21	0.55	1.78	2	3
1:A:49:PHE:CZ	1:B:93:GLN:CG	0.55	2.89	16	1
1:A:85:ILE:CG2	1:B:75:LEU:CD1	0.55	2.84	4	4
1:B:52:PHE:CZ	1:B:56:GLU:HB3	0.55	2.35	15	3
1:A:97:ILE:CD1	1:B:63:ALA:CB	0.55	2.84	20	1
1:A:68:ARG:HA	1:B:90:VAL:HG21	0.55	1.77	6	3
1:A:94:PHE:CE1	1:B:64:LEU:CD1	0.55	2.89	1	2
1:B:64:LEU:N	1:B:64:LEU:HD22	0.55	2.16	13	1
1:A:86:LEU:CD2	1:B:75:LEU:HD13	0.55	2.30	9	1
1:A:72:ARG:O	1:A:76:GLN:CB	0.55	2.55	17	7
1:A:54:TYR:CD1	1:B:97:ILE:HD12	0.55	2.37	19	2
1:A:102:ILE:HD12	1:A:102:ILE:C	0.55	2.21	16	2
1:A:93:GLN:CD	1:B:49:PHE:CG	0.55	2.80	17	1
1:B:94:PHE:O	1:B:98:LEU:CD1	0.55	2.55	17	1
1:B:121:VAL:CG1	1:B:125:HIS:CE1	0.55	2.90	3	5
1:B:121:VAL:HG13	1:B:125:HIS:CE1	0.55	2.37	12	4
1:A:52:PHE:CZ	1:A:56:GLU:HB2	0.55	2.36	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:79:LEU:N	1:B:79:LEU:HD22	0.55	2.16	18	1
1:A:75:LEU:HD22	1:A:84:GLN:OE1	0.55	2.02	17	1
1:B:109:ARG:O	1:B:110:CYS:CB	0.55	2.54	3	3
1:A:112:MET:CE	1:A:117:ILE:HD11	0.55	2.30	13	1
1:A:77:PRO:O	1:A:78:GLU:CB	0.55	2.55	9	4
1:A:82:LYS:HA	1:A:85:ILE:HD12	0.55	1.79	2	1
1:B:111:LEU:C	1:B:111:LEU:CD2	0.55	2.75	13	2
1:A:94:PHE:CE1	1:A:98:LEU:HD11	0.54	2.37	20	8
1:A:47:GLN:O	1:A:51:ARG:CB	0.54	2.56	6	6
1:A:94:PHE:CE1	1:B:64:LEU:HD11	0.54	2.37	11	3
1:B:49:PHE:CE2	1:B:67:LEU:CD2	0.54	2.90	19	2
1:A:64:LEU:HD13	1:B:94:PHE:CD1	0.54	2.36	16	6
1:A:81:THR:HG23	1:A:83:GLU:HB2	0.54	1.78	19	1
1:B:50:ARG:O	1:B:51:ARG:CG	0.54	2.56	13	2
1:B:64:LEU:HD13	1:B:65:SER:N	0.54	2.18	8	1
1:A:74:TRP:C	1:A:74:TRP:CD1	0.54	2.80	17	8
1:A:95:LEU:HD13	1:A:95:LEU:H	0.54	1.58	4	3
1:B:49:PHE:O	1:B:52:PHE:CZ	0.54	2.60	16	1
1:B:121:VAL:O	1:B:125:HIS:CG	0.54	2.60	17	2
1:A:85:ILE:CG2	1:B:85:ILE:CG2	0.54	2.85	7	5
1:A:52:PHE:CD2	1:A:67:LEU:HD11	0.54	2.38	10	1
1:A:91:MET:HG3	1:A:95:LEU:HD21	0.54	1.79	6	2
1:A:88:LEU:HG	1:A:89:LEU:HG	0.54	1.80	8	1
1:B:113:SER:O	1:B:117:ILE:CD1	0.54	2.55	5	5
1:A:72:ARG:O	1:A:76:GLN:CA	0.54	2.56	17	4
1:A:93:GLN:CG	1:B:67:LEU:HD13	0.54	2.32	17	3
1:B:105:ARG:O	1:B:111:LEU:HD21	0.54	2.01	9	1
1:B:92:GLU:HA	1:B:95:LEU:HD22	0.54	1.78	13	3
1:A:80:HIS:HB3	1:B:85:ILE:HD13	0.54	1.80	20	1
1:B:103:GLN:O	1:B:107:ARG:CD	0.54	2.55	5	1
1:A:67:LEU:CD1	1:B:97:ILE:HG21	0.54	2.32	10	1
1:B:94:PHE:CE1	1:B:118:VAL:CG2	0.54	2.90	2	2
1:A:85:ILE:HG22	1:A:86:LEU:CD1	0.54	2.31	14	1
1:A:67:LEU:HD21	1:B:93:GLN:HB3	0.54	1.78	6	1
1:A:99:PRO:O	1:A:102:ILE:CD1	0.54	2.55	3	10
1:A:97:ILE:HG13	1:A:98:LEU:N	0.54	2.15	16	8
1:A:93:GLN:HG3	1:B:49:PHE:CD1	0.54	2.37	20	2
1:A:82:LYS:O	1:A:86:LEU:CD2	0.54	2.55	4	2
1:B:82:LYS:O	1:B:86:LEU:HD22	0.54	2.03	10	1
1:A:52:PHE:CE1	1:A:66:GLN:HB3	0.54	2.38	18	1
1:A:47:GLN:O	1:A:51:ARG:CG	0.54	2.56	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:CE1	1:A:56:GLU:CB	0.54	2.90	6	1
1:B:98:LEU:HD12	1:B:102:ILE:HG21	0.54	1.79	9	3
1:B:94:PHE:O	1:B:97:ILE:HG12	0.54	2.02	11	2
1:B:50:ARG:O	1:B:51:ARG:CZ	0.54	2.56	20	1
1:A:112:MET:SD	1:A:112:MET:N	0.54	2.81	20	1
1:A:114:SER:HA	1:A:117:ILE:HD13	0.54	1.79	11	5
1:A:121:VAL:CG1	1:B:54:TYR:CZ	0.54	2.90	1	1
1:A:80:HIS:CE1	1:A:84:GLN:HB3	0.54	2.38	9	1
1:B:98:LEU:HD22	1:B:121:VAL:HG11	0.54	1.78	18	2
1:A:97:ILE:HD12	1:B:54:TYR:HD1	0.54	1.63	10	3
1:A:121:VAL:HG12	1:A:122:GLU:N	0.54	2.18	14	1
1:A:102:ILE:HG22	1:A:120:LEU:HD21	0.54	1.80	16	3
1:B:57:VAL:HG11	1:B:62:GLU:O	0.53	2.03	16	4
1:B:112:MET:CE	1:B:117:ILE:HD11	0.53	2.33	17	2
1:A:52:PHE:CZ	1:B:97:ILE:HG21	0.53	2.37	13	1
1:A:111:LEU:O	1:A:112:MET:HG2	0.53	2.03	15	1
1:A:93:GLN:OE1	1:A:96:THR:HG21	0.53	2.04	16	2
1:B:75:LEU:O	1:B:76:GLN:C	0.53	2.45	5	12
1:A:57:VAL:HG21	1:A:63:ALA:N	0.53	2.18	17	2
1:A:89:LEU:HD23	1:B:74:TRP:CZ3	0.53	2.38	17	2
1:A:61:GLN:HA	1:A:64:LEU:CD2	0.53	2.32	11	1
1:B:104:ALA:O	1:B:108:HIS:CD2	0.53	2.61	19	1
1:A:111:LEU:CD2	1:A:111:LEU:N	0.53	2.71	10	1
1:A:44:LEU:O	1:A:48:SER:CB	0.53	2.57	12	1
1:B:49:PHE:CD2	1:B:67:LEU:HD22	0.53	2.38	12	2
1:B:52:PHE:CD1	1:B:67:LEU:HD21	0.53	2.39	3	1
1:A:80:HIS:CD2	1:A:84:GLN:CG	0.53	2.91	3	1
1:A:57:VAL:HG22	1:A:62:GLU:CG	0.53	2.34	12	1
1:A:86:LEU:HA	1:A:89:LEU:HD12	0.53	1.80	18	1
1:A:101:GLU:CG	1:A:124:PHE:CG	0.53	2.91	2	1
1:A:87:GLU:O	1:A:91:MET:CG	0.53	2.56	19	2
1:A:75:LEU:CD2	1:A:88:LEU:HD21	0.53	2.32	18	1
1:B:78:GLU:C	1:B:79:LEU:CD2	0.53	2.77	18	2
1:B:103:GLN:HB2	1:B:111:LEU:HD23	0.53	1.81	1	1
1:A:53:CYS:O	1:A:55:GLN:N	0.53	2.42	9	9
1:A:93:GLN:HG2	1:B:49:PHE:CE2	0.53	2.39	9	4
1:A:111:LEU:O	1:A:111:LEU:CD2	0.53	2.57	2	1
1:A:80:HIS:ND1	1:A:84:GLN:CB	0.53	2.72	9	1
1:B:61:GLN:O	1:B:64:LEU:HD13	0.53	2.03	8	1
1:A:90:VAL:O	1:A:94:PHE:CB	0.53	2.56	17	6
1:B:52:PHE:CE1	1:B:56:GLU:HB3	0.53	2.38	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:CD2	1:B:97:ILE:HG21	0.53	2.38	4	2
1:B:108:HIS:O	1:B:109:ARG:CB	0.53	2.56	15	4
1:B:66:GLN:O	1:B:70:LEU:HD23	0.53	2.04	18	1
1:B:60:PRO:O	1:B:63:ALA:CB	0.53	2.56	9	1
1:A:105:ARG:C	1:A:105:ARG:CD	0.53	2.77	11	1
1:B:75:LEU:CD2	1:B:88:LEU:HD22	0.53	2.34	20	2
1:A:57:VAL:HG21	1:A:62:GLU:HB3	0.53	1.80	20	2
1:A:93:GLN:OE1	1:B:49:PHE:CD2	0.53	2.62	4	1
1:A:53:CYS:HA	1:B:97:ILE:HG22	0.53	1.80	13	1
1:B:49:PHE:CD1	1:B:49:PHE:C	0.53	2.80	9	5
1:A:111:LEU:HD13	1:A:111:LEU:H	0.53	1.63	2	2
1:A:53:CYS:HB3	1:B:97:ILE:CD1	0.53	2.34	11	1
1:A:71:CYS:SG	1:B:89:LEU:CD1	0.53	2.97	3	1
1:A:94:PHE:O	1:A:97:ILE:CG1	0.53	2.56	9	7
1:A:111:LEU:O	1:A:111:LEU:HD22	0.53	2.04	14	1
1:A:95:LEU:HD22	1:A:95:LEU:H	0.53	1.64	1	1
1:A:98:LEU:CD2	1:B:54:TYR:CD1	0.53	2.91	1	1
1:B:63:ALA:O	1:B:67:LEU:HG	0.53	2.04	8	2
1:B:98:LEU:HD22	1:B:121:VAL:CG2	0.53	2.34	17	1
1:A:93:GLN:HG3	1:B:49:PHE:CG	0.53	2.39	20	2
1:B:111:LEU:HB3	1:B:117:ILE:HD11	0.53	1.81	4	1
1:B:52:PHE:HZ	1:B:57:VAL:HG22	0.53	1.64	12	1
1:B:49:PHE:HB2	1:B:70:LEU:HD13	0.53	1.80	2	2
1:A:94:PHE:CD2	1:B:64:LEU:HD21	0.53	2.39	1	1
1:B:72:ARG:O	1:B:76:GLN:CB	0.53	2.57	11	6
1:A:93:GLN:OE1	1:B:67:LEU:HD21	0.53	2.04	11	2
1:A:105:ARG:CZ	1:A:112:MET:SD	0.53	2.96	11	1
1:A:97:ILE:HG22	1:B:53:CYS:H	0.52	1.64	15	4
1:A:90:VAL:HG23	1:B:71:CYS:SG	0.52	2.43	15	3
1:A:93:GLN:HG3	1:B:49:PHE:CE1	0.52	2.39	20	1
1:A:74:TRP:NE1	1:A:88:LEU:HD11	0.52	2.19	3	1
1:A:49:PHE:CD1	1:A:70:LEU:HD22	0.52	2.37	5	1
1:A:82:LYS:O	1:A:86:LEU:CD1	0.52	2.55	12	3
1:B:111:LEU:O	1:B:111:LEU:HD23	0.52	2.04	16	2
1:B:98:LEU:CB	1:B:99:PRO:CD	0.52	2.87	6	1
1:A:89:LEU:HD23	1:B:74:TRP:CE3	0.52	2.40	17	1
1:A:125:HIS:O	1:A:126:ARG:CB	0.52	2.57	13	5
1:A:91:MET:HE2	1:A:91:MET:HA	0.52	1.78	17	1
1:A:79:LEU:C	1:A:79:LEU:CD2	0.52	2.77	12	2
1:B:80:HIS:O	1:B:80:HIS:CD2	0.52	2.62	10	1
1:B:68:ARG:O	1:B:72:ARG:CB	0.52	2.58	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:O	1:A:53:CYS:CB	0.52	2.57	6	2
1:A:55:GLN:O	1:A:56:GLU:C	0.52	2.48	1	7
1:B:93:GLN:O	1:B:96:THR:N	0.52	2.42	15	10
1:A:86:LEU:HA	1:A:89:LEU:CD1	0.52	2.35	18	8
1:A:91:MET:HE2	1:A:95:LEU:HD11	0.52	1.81	16	3
1:A:49:PHE:CD1	1:A:67:LEU:HD22	0.52	2.38	3	1
1:A:79:LEU:HD12	1:A:80:HIS:CE1	0.52	2.39	4	1
1:A:101:GLU:HG2	1:A:124:PHE:CD1	0.52	2.39	2	1
1:B:50:ARG:CG	1:B:50:ARG:O	0.52	2.55	8	2
1:A:89:LEU:CD1	1:B:71:CYS:HB3	0.52	2.34	11	4
1:A:64:LEU:HG	1:B:94:PHE:CG	0.52	2.39	15	2
1:B:52:PHE:CE1	1:B:57:VAL:HG13	0.52	2.38	9	1
1:B:64:LEU:HD22	1:B:64:LEU:C	0.52	2.24	8	1
1:B:52:PHE:HZ	1:B:57:VAL:HG13	0.52	1.60	9	3
1:A:54:TYR:OH	1:B:125:HIS:CE1	0.52	2.63	11	2
1:A:54:TYR:CZ	1:A:57:VAL:HG11	0.52	2.40	14	1
1:A:52:PHE:CZ	1:A:56:GLU:CB	0.52	2.93	18	1
1:B:50:ARG:O	1:B:50:ARG:CD	0.52	2.58	8	2
1:B:61:GLN:O	1:B:64:LEU:CD1	0.52	2.58	8	2
1:A:60:PRO:HB2	1:B:118:VAL:HG13	0.52	1.79	7	4
1:B:81:THR:C	1:B:83:GLU:N	0.52	2.62	20	6
1:A:52:PHE:O	1:A:53:CYS:C	0.52	2.48	3	6
1:A:86:LEU:O	1:A:90:VAL:N	0.52	2.37	20	2
1:A:77:PRO:HB3	1:A:80:HIS:CD2	0.52	2.40	12	1
1:B:94:PHE:CE2	1:B:117:ILE:HG22	0.52	2.39	1	2
1:A:94:PHE:CZ	1:A:118:VAL:HG21	0.52	2.39	1	1
1:B:106:VAL:HG22	1:B:111:LEU:CD1	0.52	2.33	9	1
1:B:85:ILE:O	1:B:88:LEU:N	0.52	2.42	19	6
1:A:49:PHE:CG	1:A:70:LEU:CD2	0.52	2.83	5	1
1:B:76:GLN:N	1:B:77:PRO:HD3	0.52	2.20	20	5
1:A:78:GLU:O	1:A:79:LEU:CD2	0.52	2.58	20	2
1:A:93:GLN:HG3	1:B:49:PHE:CD2	0.52	2.40	20	2
1:B:57:VAL:CG2	1:B:58:SER:N	0.52	2.73	3	2
1:B:106:VAL:HG23	1:B:111:LEU:HG	0.52	1.82	4	1
1:A:49:PHE:O	1:A:67:LEU:HD22	0.52	2.05	1	2
1:A:121:VAL:CG1	1:A:122:GLU:N	0.52	2.73	14	1
1:A:76:GLN:N	1:A:77:PRO:HD3	0.52	2.20	18	3
1:A:53:CYS:SG	1:A:63:ALA:HA	0.52	2.45	19	3
1:A:121:VAL:CG1	1:A:125:HIS:NE2	0.52	2.73	19	5
1:B:79:LEU:C	1:B:79:LEU:HD13	0.52	2.25	19	1
1:B:93:GLN:OE1	1:B:93:GLN:N	0.52	2.43	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HB3	1:B:74:TRP:CZ3	0.52	2.39	3	5
1:A:49:PHE:O	1:B:93:GLN:NE2	0.52	2.43	10	1
1:B:54:TYR:CD2	1:B:57:VAL:HG11	0.52	2.39	7	1
1:A:126:ARG:O	1:A:127:ALA:CB	0.52	2.58	14	1
1:A:71:CYS:HB2	1:B:90:VAL:CG2	0.51	2.35	6	8
1:A:101:GLU:OE1	1:A:124:PHE:CE1	0.51	2.62	11	1
1:A:93:GLN:HG2	1:B:49:PHE:CZ	0.51	2.41	1	4
1:A:106:VAL:CG1	1:A:107:ARG:N	0.51	2.73	10	2
1:A:50:ARG:CG	1:B:93:GLN:OE1	0.51	2.58	7	2
1:A:61:GLN:HA	1:A:64:LEU:HD11	0.51	1.83	12	1
1:A:46:ARG:HD2	1:A:74:TRP:CZ2	0.51	2.40	14	1
1:B:52:PHE:CE2	1:B:57:VAL:HG22	0.51	2.40	14	1
1:A:74:TRP:CZ3	1:B:89:LEU:HB3	0.51	2.39	16	2
1:B:107:ARG:O	1:B:108:HIS:CB	0.51	2.58	1	1
1:A:125:HIS:ND1	1:B:54:TYR:CE2	0.51	2.78	1	1
1:A:85:ILE:HD13	1:B:82:LYS:HD2	0.51	1.82	6	1
1:B:57:VAL:CG2	1:B:63:ALA:N	0.51	2.72	20	2
1:A:75:LEU:HD21	1:B:89:LEU:CD2	0.51	2.35	16	5
1:A:57:VAL:O	1:A:62:GLU:CB	0.51	2.58	7	1
1:A:57:VAL:HG22	1:A:62:GLU:C	0.51	2.26	14	1
1:B:74:TRP:CZ2	1:B:92:GLU:HG2	0.51	2.41	2	1
1:B:78:GLU:C	1:B:79:LEU:HD13	0.51	2.24	16	1
1:B:81:THR:HG23	1:B:83:GLU:HB3	0.51	1.82	17	1
1:B:102:ILE:HB	1:B:117:ILE:HG23	0.51	1.81	11	1
1:A:78:GLU:O	1:A:79:LEU:HB3	0.51	2.05	4	1
1:A:112:MET:N	1:A:112:MET:SD	0.51	2.83	9	2
1:A:94:PHE:CG	1:B:64:LEU:HD12	0.51	2.40	9	3
1:A:85:ILE:HD11	1:B:84:GLN:HB2	0.51	1.82	20	1
1:B:91:MET:O	1:B:95:LEU:CG	0.51	2.58	14	4
1:A:67:LEU:HD13	1:B:93:GLN:CB	0.51	2.35	16	1
1:A:67:LEU:O	1:A:70:LEU:N	0.51	2.44	8	7
1:B:75:LEU:O	1:B:79:LEU:CD2	0.51	2.57	13	1
1:B:112:MET:N	1:B:112:MET:SD	0.51	2.84	15	2
1:A:90:VAL:CG2	1:B:71:CYS:HB2	0.51	2.36	16	8
1:A:81:THR:HG23	1:A:82:LYS:N	0.51	2.19	17	4
1:A:53:CYS:SG	1:A:67:LEU:CD1	0.51	2.99	11	1
1:B:72:ARG:O	1:B:76:GLN:CA	0.51	2.59	19	1
1:B:102:ILE:O	1:B:106:VAL:CG2	0.51	2.58	6	5
1:B:48:SER:OG	1:B:49:PHE:CD2	0.51	2.63	5	1
1:A:113:SER:O	1:A:117:ILE:CD1	0.51	2.59	14	6
1:B:80:HIS:CD2	1:B:84:GLN:HB3	0.51	2.40	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:CD2	1:A:120:LEU:C	0.51	2.73	2	1
1:A:111:LEU:H	1:A:111:LEU:HD13	0.51	1.65	8	1
1:A:126:ARG:O	1:A:127:ALA:C	0.51	2.49	20	4
1:A:85:ILE:O	1:A:88:LEU:HB2	0.51	2.06	18	2
1:B:49:PHE:CE1	1:B:71:CYS:SG	0.51	2.99	14	2
1:A:92:GLU:O	1:A:96:THR:HB	0.51	2.06	1	2
1:A:113:SER:O	1:A:116:GLU:CB	0.51	2.58	13	1
1:B:117:ILE:CD1	1:B:117:ILE:N	0.51	2.71	7	1
1:A:48:SER:O	1:A:52:PHE:CB	0.51	2.59	19	1
1:A:54:TYR:CE2	1:B:125:HIS:CE1	0.51	2.99	5	4
1:A:74:TRP:CZ3	1:B:89:LEU:HD23	0.51	2.41	20	3
1:A:64:LEU:HD12	1:B:94:PHE:CG	0.51	2.39	1	3
1:A:77:PRO:HG2	1:B:82:LYS:CG	0.51	2.36	15	1
1:B:107:ARG:O	1:B:108:HIS:C	0.51	2.49	6	1
1:A:90:VAL:HG23	1:B:71:CYS:CB	0.51	2.36	8	8
1:A:72:ARG:CD	1:B:86:LEU:HD23	0.51	2.36	8	1
1:A:87:GLU:O	1:A:91:MET:HB2	0.51	2.06	14	4
1:A:89:LEU:O	1:A:93:GLN:HB2	0.51	2.04	2	4
1:A:99:PRO:C	1:A:101:GLU:N	0.51	2.64	10	2
1:B:79:LEU:C	1:B:79:LEU:CD2	0.51	2.75	15	1
1:B:106:VAL:HG22	1:B:112:MET:SD	0.50	2.46	17	1
1:B:86:LEU:HA	1:B:89:LEU:CD1	0.50	2.35	10	8
1:A:89:LEU:HD23	1:B:88:LEU:HD11	0.50	1.83	20	1
1:A:49:PHE:CD2	1:A:50:ARG:N	0.50	2.79	3	2
1:B:79:LEU:O	1:B:80:HIS:CB	0.50	2.58	13	3
1:B:106:VAL:HB	1:B:111:LEU:HD11	0.50	1.82	4	1
1:A:93:GLN:NE2	1:B:49:PHE:CZ	0.50	2.79	7	1
1:A:74:TRP:CZ3	1:B:89:LEU:CB	0.50	2.94	16	1
1:A:81:THR:OG1	1:A:82:LYS:N	0.50	2.44	1	12
1:B:103:GLN:O	1:B:107:ARG:CG	0.50	2.59	17	1
1:A:77:PRO:HD3	1:A:80:HIS:CE1	0.50	2.40	20	1
1:A:80:HIS:O	1:B:80:HIS:O	0.50	2.29	20	1
1:B:113:SER:O	1:B:117:ILE:HD12	0.50	2.06	5	3
1:A:76:GLN:O	1:A:80:HIS:CD2	0.50	2.65	4	1
1:B:91:MET:HE3	1:B:95:LEU:HD21	0.50	1.82	14	1
1:A:75:LEU:CD1	1:B:86:LEU:HD12	0.50	2.27	8	1
1:B:52:PHE:CZ	1:B:54:TYR:HA	0.50	2.41	6	4
1:B:54:TYR:CD1	1:B:57:VAL:HG11	0.50	2.42	20	1
1:B:94:PHE:O	1:B:97:ILE:CG1	0.50	2.59	7	3
1:A:117:ILE:HG22	1:A:118:VAL:N	0.50	2.20	10	1
1:B:125:HIS:O	1:B:126:ARG:CB	0.50	2.59	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:72:ARG:O	1:B:76:GLN:CG	0.50	2.59	11	1
1:B:49:PHE:CD1	1:B:67:LEU:CD2	0.50	2.94	5	1
1:A:100:GLU:O	1:A:103:GLN:N	0.50	2.44	13	6
1:B:106:VAL:HG23	1:B:107:ARG:H	0.50	1.65	1	1
1:A:113:SER:O	1:A:116:GLU:N	0.50	2.44	15	7
1:A:57:VAL:CG2	1:A:62:GLU:C	0.50	2.79	14	3
1:A:111:LEU:C	1:A:112:MET:CG	0.50	2.80	3	3
1:A:102:ILE:HG22	1:A:121:VAL:HG23	0.50	1.83	2	1
1:A:52:PHE:CD2	1:A:67:LEU:HD21	0.50	2.40	15	1
1:A:75:LEU:HD12	1:B:86:LEU:CD1	0.50	2.27	8	1
1:B:94:PHE:C	1:B:95:LEU:HD13	0.50	2.26	1	2
1:B:85:ILE:HG22	1:B:86:LEU:N	0.50	2.22	14	2
1:B:76:GLN:O	1:B:80:HIS:NE2	0.50	2.45	19	1
1:B:81:THR:O	1:B:82:LYS:C	0.50	2.50	19	3
1:B:52:PHE:CZ	1:B:55:GLN:HB2	0.50	2.42	10	1
1:A:50:ARG:CD	1:A:50:ARG:O	0.50	2.59	2	1
1:A:52:PHE:CE1	1:A:53:CYS:O	0.50	2.65	1	1
1:B:100:GLU:O	1:B:103:GLN:N	0.50	2.45	17	4
1:B:49:PHE:CZ	1:B:71:CYS:SG	0.50	3.05	1	3
1:B:71:CYS:O	1:B:75:LEU:HD12	0.50	2.07	20	2
1:A:93:GLN:HG3	1:B:49:PHE:CE2	0.50	2.42	20	1
1:A:71:CYS:O	1:A:74:TRP:HB3	0.50	2.07	8	16
1:B:77:PRO:CB	1:B:84:GLN:CD	0.50	2.80	17	1
1:A:121:VAL:HG12	1:A:125:HIS:NE2	0.50	2.22	20	4
1:A:98:LEU:CD1	1:A:117:ILE:HG22	0.50	2.36	13	2
1:B:111:LEU:N	1:B:111:LEU:HD23	0.50	2.21	10	1
1:B:89:LEU:CB	1:B:93:GLN:OE1	0.50	2.60	14	1
1:A:49:PHE:CE1	1:A:50:ARG:HB2	0.50	2.42	6	1
1:A:64:LEU:CD1	1:A:64:LEU:H	0.50	2.19	16	1
1:B:113:SER:O	1:B:116:GLU:CB	0.50	2.60	11	3
1:A:71:CYS:CB	1:B:90:VAL:HG23	0.50	2.37	9	3
1:A:68:ARG:O	1:A:72:ARG:CB	0.50	2.60	6	1
1:B:91:MET:O	1:B:92:GLU:C	0.49	2.50	6	11
1:B:102:ILE:CD1	1:B:103:GLN:N	0.49	2.72	12	7
1:B:93:GLN:O	1:B:95:LEU:N	0.49	2.45	14	3
1:B:57:VAL:HG23	1:B:62:GLU:CB	0.49	2.37	1	2
1:B:91:MET:HE3	1:B:91:MET:HA	0.49	1.82	10	2
1:A:104:ALA:O	1:A:108:HIS:HA	0.49	2.06	10	3
1:B:62:GLU:OE2	1:B:65:SER:CB	0.49	2.59	2	1
1:B:108:HIS:O	1:B:109:ARG:C	0.49	2.50	13	3
1:B:52:PHE:O	1:B:55:GLN:N	0.49	2.45	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:HG	1:A:89:LEU:N	0.49	2.22	19	1
1:B:85:ILE:O	1:B:88:LEU:CB	0.49	2.61	7	6
1:B:87:GLU:O	1:B:91:MET:HB2	0.49	2.07	18	4
1:A:57:VAL:CG2	1:A:63:ALA:CA	0.49	2.90	14	1
1:B:67:LEU:CD2	1:B:67:LEU:N	0.49	2.72	8	1
1:A:44:LEU:HD13	1:A:44:LEU:C	0.49	2.27	3	4
1:B:102:ILE:CG2	1:B:117:ILE:HG23	0.49	2.33	17	1
1:B:55:GLN:O	1:B:56:GLU:C	0.49	2.51	13	4
1:A:102:ILE:O	1:A:106:VAL:HG12	0.49	2.07	10	1
1:B:111:LEU:HD22	1:B:111:LEU:O	0.49	2.06	7	1
1:B:57:VAL:HG21	1:B:63:ALA:HA	0.49	1.83	9	3
1:B:102:ILE:HD13	1:B:117:ILE:HG23	0.49	1.83	1	1
1:A:50:ARG:HG2	1:A:67:LEU:HD21	0.49	1.85	6	1
1:B:102:ILE:CG2	1:B:117:ILE:CG2	0.49	2.90	17	1
1:A:108:HIS:O	1:A:109:ARG:CB	0.49	2.61	16	2
1:B:79:LEU:CD1	1:B:79:LEU:N	0.49	2.76	3	1
1:A:75:LEU:HD22	1:A:85:ILE:HG23	0.49	1.84	2	1
1:B:99:PRO:O	1:B:101:GLU:N	0.49	2.45	1	1
1:A:77:PRO:HG2	1:B:82:LYS:CB	0.49	2.37	15	1
1:A:98:LEU:CD2	1:B:54:TYR:CZ	0.49	2.95	19	2
1:A:93:GLN:NE2	1:B:49:PHE:O	0.49	2.45	7	2
1:A:112:MET:SD	1:A:112:MET:O	0.49	2.71	11	1
1:A:52:PHE:HD2	1:B:97:ILE:HG21	0.49	1.67	4	1
1:B:95:LEU:N	1:B:95:LEU:HD23	0.49	2.23	7	4
1:B:57:VAL:HG22	1:B:62:GLU:HG2	0.49	1.85	18	1
1:B:124:PHE:O	1:B:124:PHE:CD1	0.49	2.66	17	1
1:A:75:LEU:CD2	1:B:89:LEU:HD21	0.49	2.37	2	3
1:B:94:PHE:O	1:B:97:ILE:HG13	0.49	2.06	5	4
1:A:67:LEU:O	1:A:71:CYS:SG	0.49	2.69	7	1
1:A:64:LEU:CD2	1:B:94:PHE:CD2	0.49	2.95	12	1
1:A:88:LEU:HD11	1:B:89:LEU:HD23	0.49	1.84	14	1
1:A:85:ILE:O	1:A:89:LEU:CD1	0.49	2.61	15	1
1:B:49:PHE:CE2	1:B:50:ARG:HB3	0.49	2.43	16	1
1:B:67:LEU:O	1:B:71:CYS:SG	0.49	2.71	17	3
1:B:99:PRO:HD2	1:B:102:ILE:HD13	0.49	1.83	17	1
1:B:94:PHE:O	1:B:98:LEU:CG	0.49	2.61	17	2
1:A:81:THR:O	1:A:84:GLN:N	0.49	2.46	20	1
1:A:64:LEU:HD22	1:A:64:LEU:H	0.49	1.68	16	2
1:A:97:ILE:HG21	1:B:52:PHE:HD1	0.49	1.62	3	1
1:A:89:LEU:HD21	1:B:75:LEU:HG	0.49	1.81	2	3
1:B:117:ILE:H	1:B:117:ILE:HD12	0.49	1.66	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:LEU:N	1:A:111:LEU:HD13	0.49	2.23	8	2
1:A:75:LEU:CD2	1:A:84:GLN:OE1	0.49	2.61	17	1
1:A:125:HIS:CE1	1:B:54:TYR:CE2	0.49	3.00	1	5
1:A:57:VAL:HG21	1:A:62:GLU:CB	0.49	2.37	20	1
1:B:106:VAL:HG13	1:B:107:ARG:N	0.49	2.22	4	1
1:A:52:PHE:CD1	1:A:67:LEU:CD2	0.49	2.89	13	1
1:A:64:LEU:H	1:A:64:LEU:HD22	0.49	1.67	13	2
1:A:94:PHE:CD2	1:B:64:LEU:CD2	0.49	2.95	2	1
1:B:94:PHE:HE1	1:B:118:VAL:HG23	0.49	1.61	18	7
1:B:89:LEU:O	1:B:93:GLN:NE2	0.49	2.45	11	3
1:A:46:ARG:O	1:A:50:ARG:CB	0.49	2.61	18	4
1:B:64:LEU:HD22	1:B:64:LEU:H	0.49	1.68	9	2
1:A:54:TYR:CZ	1:B:98:LEU:HD22	0.49	2.42	16	1
1:A:120:LEU:HG	1:A:121:VAL:N	0.48	2.23	9	14
1:A:90:VAL:HG22	1:B:71:CYS:CB	0.48	2.38	11	2
1:A:79:LEU:CD1	1:A:79:LEU:O	0.48	2.59	4	1
1:A:104:ALA:O	1:A:108:HIS:CA	0.48	2.60	10	3
1:B:57:VAL:CG2	1:B:62:GLU:O	0.48	2.61	18	1
1:B:104:ALA:O	1:B:108:HIS:HA	0.48	2.08	1	1
1:A:49:PHE:HZ	1:A:71:CYS:HG	0.48	1.37	15	1
1:A:49:PHE:CE1	1:A:74:TRP:CZ3	0.48	3.01	16	1
1:B:75:LEU:CD2	1:B:88:LEU:HG	0.48	2.38	5	1
1:A:64:LEU:HG	1:B:94:PHE:CE1	0.48	2.43	10	1
1:B:75:LEU:HD22	1:B:88:LEU:CD1	0.48	2.32	18	1
1:B:104:ALA:O	1:B:108:HIS:CA	0.48	2.61	1	1
1:A:90:VAL:HG23	1:B:71:CYS:HG	0.48	1.68	15	1
1:B:108:HIS:CD2	1:B:109:ARG:N	0.48	2.81	6	1
1:B:67:LEU:O	1:B:69:GLN:N	0.48	2.46	6	4
1:B:53:CYS:O	1:B:55:GLN:N	0.48	2.46	4	5
1:A:75:LEU:HD22	1:A:85:ILE:CG1	0.48	2.38	5	1
1:A:85:ILE:HG21	1:B:85:ILE:CG1	0.48	2.37	1	1
1:A:75:LEU:HD22	1:A:88:LEU:HD22	0.48	1.83	8	2
1:A:97:ILE:CG2	1:B:52:PHE:HB3	0.48	2.38	20	2
1:A:75:LEU:CD1	1:B:85:ILE:CG2	0.48	2.90	4	3
1:A:100:GLU:O	1:A:103:GLN:CG	0.48	2.61	7	1
1:A:57:VAL:HG13	1:A:59:GLY:O	0.48	2.08	14	1
1:B:93:GLN:N	1:B:93:GLN:NE2	0.48	2.61	14	1
1:B:89:LEU:CA	1:B:93:GLN:OE1	0.48	2.61	14	1
1:A:49:PHE:CE1	1:B:93:GLN:HG2	0.48	2.42	1	1
1:A:85:ILE:HD12	1:B:85:ILE:CD1	0.48	2.39	14	3
1:A:49:PHE:CD2	1:A:67:LEU:CD2	0.48	2.96	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:C	1:A:120:LEU:CD2	0.48	2.79	7	1
1:A:108:HIS:O	1:A:110:CYS:N	0.48	2.47	14	1
1:A:106:VAL:CG1	1:A:112:MET:CG	0.48	2.92	6	1
1:A:86:LEU:HD13	1:B:72:ARG:HA	0.48	1.85	9	1
1:B:52:PHE:CZ	1:B:57:VAL:CG1	0.48	2.92	9	1
1:A:94:PHE:CE2	1:A:117:ILE:HG22	0.48	2.43	8	3
1:B:49:PHE:O	1:B:51:ARG:N	0.48	2.46	2	6
1:A:53:CYS:O	1:A:54:TYR:O	0.48	2.32	8	3
1:A:91:MET:O	1:A:92:GLU:C	0.48	2.51	4	7
1:A:85:ILE:O	1:A:88:LEU:N	0.48	2.45	9	2
1:A:90:VAL:O	1:A:94:PHE:HB2	0.48	2.08	14	3
1:B:91:MET:HG3	1:B:95:LEU:HD21	0.48	1.85	5	1
1:A:64:LEU:HD13	1:A:64:LEU:N	0.48	2.24	13	1
1:A:101:GLU:OE1	1:A:124:PHE:CD1	0.48	2.67	15	1
1:A:72:ARG:CG	1:B:86:LEU:HD23	0.48	2.39	19	2
1:A:49:PHE:HB2	1:A:70:LEU:HD22	0.48	1.85	7	3
1:A:98:LEU:CD1	1:A:117:ILE:CG2	0.48	2.92	15	2
1:B:101:GLU:CD	1:B:121:VAL:HG13	0.48	2.28	10	1
1:B:55:GLN:O	1:B:56:GLU:O	0.48	2.32	1	1
1:B:54:TYR:O	1:B:55:GLN:CB	0.48	2.61	6	1
1:A:93:GLN:HG2	1:B:49:PHE:CE1	0.48	2.44	16	1
1:A:82:LYS:CD	1:A:82:LYS:N	0.48	2.76	8	1
1:A:68:ARG:HA	1:B:90:VAL:CG2	0.48	2.38	12	14
1:A:53:CYS:SG	1:A:63:ALA:CA	0.48	3.01	16	3
1:B:64:LEU:HD13	1:B:64:LEU:N	0.48	2.21	3	1
1:A:104:ALA:O	1:A:108:HIS:N	0.48	2.47	7	3
1:A:61:GLN:O	1:A:64:LEU:CD1	0.48	2.61	12	1
1:A:56:GLU:O	1:A:57:VAL:C	0.48	2.51	14	1
1:B:64:LEU:CD1	1:B:64:LEU:H	0.48	2.16	9	1
1:A:97:ILE:HD12	1:A:98:LEU:CD2	0.48	2.39	8	1
1:B:49:PHE:HB2	1:B:52:PHE:CZ	0.48	2.44	8	1
1:A:64:LEU:O	1:A:68:ARG:HB2	0.48	2.07	2	6
1:B:91:MET:O	1:B:95:LEU:HD13	0.48	2.08	11	6
1:A:121:VAL:CG1	1:B:54:TYR:OH	0.48	2.62	9	3
1:A:46:ARG:HD3	1:A:74:TRP:CZ2	0.48	2.44	19	1
1:A:94:PHE:CE1	1:A:118:VAL:CG2	0.48	2.97	3	2
1:B:49:PHE:CD1	1:B:67:LEU:HD22	0.48	2.44	5	1
1:A:111:LEU:N	1:A:111:LEU:CD2	0.48	2.76	13	1
1:B:57:VAL:HG21	1:B:62:GLU:CB	0.48	2.39	10	1
1:A:86:LEU:CA	1:A:89:LEU:HD11	0.48	2.32	9	1
1:B:80:HIS:CD2	1:B:80:HIS:C	0.48	2.87	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:GLN:HG2	1:B:49:PHE:CD2	0.48	2.44	17	1
1:B:106:VAL:CG2	1:B:112:MET:SD	0.48	3.02	17	1
1:B:49:PHE:O	1:B:50:ARG:HB2	0.48	2.09	12	3
1:A:52:PHE:CZ	1:A:66:GLN:HB3	0.48	2.43	17	1
1:A:89:LEU:CD1	1:B:71:CYS:SG	0.48	2.99	11	2
1:A:64:LEU:H	1:A:64:LEU:CD1	0.48	2.19	1	3
1:A:106:VAL:CG1	1:A:107:ARG:H	0.48	2.22	10	1
1:A:49:PHE:CE1	1:B:93:GLN:CD	0.48	2.88	12	1
1:A:52:PHE:CE2	1:A:56:GLU:HB2	0.48	2.43	18	1
1:A:52:PHE:CZ	1:A:56:GLU:HB3	0.48	2.44	2	2
1:A:94:PHE:CG	1:B:64:LEU:CD2	0.48	2.97	2	1
1:B:52:PHE:CB	1:B:67:LEU:CD2	0.48	2.91	15	1
1:A:64:LEU:HD21	1:B:94:PHE:CD2	0.47	2.44	8	2
1:A:126:ARG:O	1:A:127:ALA:O	0.47	2.32	17	2
1:B:52:PHE:HD1	1:B:67:LEU:HD21	0.47	1.67	3	1
1:A:93:GLN:NE2	1:B:67:LEU:HD22	0.47	2.24	4	1
1:A:57:VAL:CG2	1:A:58:SER:N	0.47	2.76	4	1
1:A:101:GLU:OE1	1:A:101:GLU:N	0.47	2.47	2	1
1:B:57:VAL:CG1	1:B:62:GLU:OE1	0.47	2.62	2	1
1:A:97:ILE:HD13	1:B:63:ALA:HB1	0.47	1.85	8	1
1:B:52:PHE:CD1	1:B:67:LEU:HD22	0.47	2.39	8	1
1:A:54:TYR:HD1	1:B:97:ILE:HD12	0.47	1.69	19	4
1:A:111:LEU:HD22	1:A:111:LEU:O	0.47	2.07	2	2
1:A:85:ILE:CG1	1:B:85:ILE:HD12	0.47	2.39	17	1
1:B:75:LEU:HD21	1:B:88:LEU:CD2	0.47	2.38	20	1
1:A:102:ILE:O	1:A:106:VAL:HG23	0.47	2.09	16	3
1:A:94:PHE:CD1	1:B:64:LEU:HD12	0.47	2.44	3	1
1:A:98:LEU:HD12	1:A:117:ILE:CG2	0.47	2.39	13	3
1:A:112:MET:CE	1:A:117:ILE:HG13	0.47	2.39	18	1
1:B:52:PHE:CD2	1:B:67:LEU:HD21	0.47	2.43	18	1
1:A:54:TYR:OH	1:B:121:VAL:CG1	0.47	2.60	1	2
1:A:47:GLN:O	1:A:51:ARG:N	0.47	2.47	6	1
1:B:57:VAL:HG11	1:B:66:GLN:HB2	0.47	1.86	8	1
1:B:81:THR:O	1:B:84:GLN:N	0.47	2.47	20	1
1:A:106:VAL:HG22	1:A:111:LEU:HD12	0.47	1.86	20	1
1:B:64:LEU:H	1:B:64:LEU:CD1	0.47	2.18	3	4
1:A:93:GLN:NE2	1:B:49:PHE:CD2	0.47	2.82	7	2
1:A:52:PHE:O	1:A:53:CYS:O	0.47	2.32	15	3
1:B:54:TYR:O	1:B:56:GLU:N	0.47	2.47	18	4
1:A:52:PHE:CZ	1:A:57:VAL:HG22	0.47	2.44	10	1
1:A:106:VAL:HG13	1:A:107:ARG:H	0.47	1.66	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:57:VAL:CG2	1:B:62:GLU:CB	0.47	2.92	10	1
1:B:57:VAL:HG21	1:B:62:GLU:HB3	0.47	1.85	12	1
1:A:50:ARG:NH2	1:B:96:THR:CB	0.47	2.77	12	1
1:A:103:GLN:HA	1:A:106:VAL:HG12	0.47	1.85	1	2
1:A:85:ILE:O	1:A:88:LEU:HB3	0.47	2.10	19	1
1:A:97:ILE:CG2	1:B:67:LEU:HD11	0.47	2.38	20	1
1:A:75:LEU:HD21	1:A:88:LEU:HG	0.47	1.85	10	1
1:B:80:HIS:CG	1:B:84:GLN:HB2	0.47	2.44	16	2
1:A:80:HIS:CG	1:A:84:GLN:HB2	0.47	2.44	10	2
1:A:81:THR:HG23	1:A:83:GLU:HB3	0.47	1.86	18	1
1:A:81:THR:HG23	1:A:83:GLU:CB	0.47	2.39	18	1
1:A:52:PHE:HB3	1:A:67:LEU:HD21	0.47	1.85	1	1
1:A:54:TYR:CE2	1:B:121:VAL:CG1	0.47	2.98	15	1
1:B:57:VAL:HG23	1:B:58:SER:N	0.47	2.25	16	3
1:A:52:PHE:CE1	1:A:55:GLN:N	0.47	2.82	3	1
1:B:49:PHE:CD1	1:B:70:LEU:HD21	0.47	2.43	5	1
1:B:94:PHE:CE2	1:B:118:VAL:HG23	0.47	2.43	13	1
1:B:108:HIS:O	1:B:109:ARG:CG	0.47	2.63	14	3
1:B:93:GLN:OE1	1:B:96:THR:CG2	0.47	2.63	2	1
1:A:111:LEU:C	1:A:111:LEU:CD2	0.47	2.81	1	1
1:A:46:ARG:HG2	1:A:74:TRP:CE2	0.47	2.45	9	1
1:B:125:HIS:C	1:B:126:ARG:CG	0.47	2.81	8	1
1:A:75:LEU:C	1:A:76:GLN:CG	0.47	2.82	17	1
1:A:81:THR:C	1:A:83:GLU:N	0.47	2.68	17	11
1:B:72:ARG:HG3	1:B:73:GLN:N	0.47	2.25	9	2
1:A:79:LEU:HD12	1:A:80:HIS:CD2	0.47	2.43	3	1
1:A:79:LEU:CD1	1:A:80:HIS:CD2	0.47	2.97	3	1
1:A:52:PHE:CG	1:A:53:CYS:N	0.47	2.82	13	1
1:B:79:LEU:HD12	1:B:80:HIS:N	0.47	2.24	13	3
1:B:80:HIS:C	1:B:80:HIS:CD2	0.47	2.88	10	1
1:B:78:GLU:O	1:B:79:LEU:HB2	0.47	2.09	2	3
1:A:80:HIS:CE1	1:A:84:GLN:CB	0.47	2.98	9	1
1:B:75:LEU:HD21	1:B:88:LEU:CD1	0.47	2.39	17	3
1:A:91:MET:O	1:A:95:LEU:HD13	0.47	2.09	17	4
1:B:67:LEU:O	1:B:68:ARG:C	0.47	2.53	6	6
1:B:57:VAL:CG2	1:B:62:GLU:HB3	0.47	2.40	12	3
1:A:111:LEU:O	1:A:112:MET:HB3	0.47	2.09	11	2
1:B:93:GLN:C	1:B:95:LEU:N	0.47	2.67	14	6
1:A:52:PHE:O	1:A:55:GLN:N	0.47	2.47	10	2
1:A:122:GLU:O	1:A:127:ALA:N	0.47	2.47	18	2
1:A:97:ILE:CG2	1:B:52:PHE:CD1	0.47	2.94	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:LEU:CG	1:B:94:PHE:CD1	0.47	2.98	18	2
1:B:105:ARG:CB	1:B:120:LEU:HD13	0.47	2.40	1	1
1:B:52:PHE:CZ	1:B:66:GLN:HG2	0.47	2.44	1	1
1:B:115:LYS:O	1:B:119:THR:CB	0.47	2.62	16	2
1:A:49:PHE:CE1	1:A:67:LEU:HD23	0.47	2.45	6	1
1:B:125:HIS:CD2	1:B:126:ARG:HB2	0.47	2.45	16	1
1:A:81:THR:O	1:A:83:GLU:N	0.47	2.48	20	5
1:A:53:CYS:SG	1:A:67:LEU:HD12	0.47	2.50	11	1
1:A:82:LYS:O	1:A:86:LEU:HB2	0.47	2.10	19	3
1:A:123:ASP:CB	1:A:127:ALA:HB2	0.47	2.40	19	1
1:A:74:TRP:CE3	1:B:89:LEU:HD23	0.47	2.44	20	1
1:B:50:ARG:O	1:B:50:ARG:CG	0.47	2.62	4	1
1:B:64:LEU:H	1:B:64:LEU:HD22	0.47	1.70	13	1
1:B:54:TYR:C	1:B:56:GLU:N	0.47	2.68	10	3
1:A:91:MET:CE	1:A:95:LEU:HD11	0.47	2.40	10	1
1:B:125:HIS:N	1:B:125:HIS:CD2	0.47	2.83	7	1
1:A:125:HIS:CE1	1:B:58:SER:O	0.47	2.67	14	1
1:B:85:ILE:HA	1:B:88:LEU:HD22	0.47	1.86	2	1
1:A:121:VAL:HG12	1:B:54:TYR:OH	0.47	2.09	1	1
1:A:114:SER:O	1:A:117:ILE:N	0.47	2.48	15	1
1:A:93:GLN:O	1:A:95:LEU:N	0.47	2.48	8	1
1:A:101:GLU:OE1	1:A:124:PHE:CZ	0.47	2.68	11	1
1:A:50:ARG:CG	1:A:51:ARG:N	0.47	2.78	19	1
1:A:86:LEU:CD1	1:A:86:LEU:N	0.47	2.78	19	2
1:A:75:LEU:HB2	1:A:80:HIS:HE2	0.47	1.70	20	1
1:A:93:GLN:CD	1:B:49:PHE:CD2	0.47	2.88	5	1
1:B:49:PHE:C	1:B:50:ARG:CG	0.47	2.82	5	1
1:A:49:PHE:CE2	1:A:67:LEU:HD22	0.47	2.44	4	1
1:B:82:LYS:O	1:B:86:LEU:CD1	0.47	2.62	13	2
1:B:52:PHE:HB2	1:B:67:LEU:CD2	0.47	2.40	15	2
1:A:101:GLU:HG3	1:A:124:PHE:CD1	0.47	2.45	2	1
1:A:49:PHE:CD2	1:A:70:LEU:CB	0.47	2.98	11	1
1:A:72:ARG:O	1:A:76:GLN:HB2	0.47	2.10	10	2
1:B:49:PHE:O	1:B:50:ARG:HB3	0.47	2.10	12	1
1:A:54:TYR:OH	1:B:121:VAL:HG12	0.47	2.10	18	1
1:A:64:LEU:CD2	1:B:90:VAL:HG12	0.47	2.35	15	1
1:A:85:ILE:HD11	1:B:85:ILE:HD12	0.46	1.87	17	1
1:A:81:THR:CG2	1:A:84:GLN:OE1	0.46	2.63	20	1
1:B:61:GLN:O	1:B:61:GLN:CG	0.46	2.63	18	1
1:A:94:PHE:CE2	1:A:118:VAL:HG23	0.46	2.45	9	2
1:B:112:MET:SD	1:B:113:SER:CB	0.46	3.03	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:SER:O	1:A:117:ILE:HD12	0.46	2.10	1	2
1:A:62:GLU:O	1:A:65:SER:CB	0.46	2.64	15	1
1:A:85:ILE:HD11	1:B:82:LYS:CD	0.46	2.40	8	1
1:A:96:THR:HG23	1:B:51:ARG:CG	0.46	2.39	8	1
1:B:112:MET:C	1:B:112:MET:CE	0.46	2.83	11	1
1:A:105:ARG:NH1	1:A:112:MET:SD	0.46	2.88	11	1
1:A:50:ARG:O	1:A:50:ARG:CD	0.46	2.63	10	1
1:B:52:PHE:CE1	1:B:56:GLU:HB2	0.46	2.44	15	2
1:A:98:LEU:HD12	1:A:102:ILE:HG21	0.46	1.84	18	1
1:B:77:PRO:O	1:B:78:GLU:CG	0.46	2.62	18	2
1:A:97:ILE:HD12	1:B:52:PHE:HE2	0.46	1.67	2	1
1:B:106:VAL:HG13	1:B:120:LEU:CD2	0.46	2.40	1	1
1:B:93:GLN:N	1:B:93:GLN:CD	0.46	2.68	8	1
1:B:120:LEU:HG	1:B:121:VAL:N	0.46	2.25	18	18
1:A:94:PHE:CD1	1:B:64:LEU:HD13	0.46	2.43	3	3
1:A:95:LEU:H	1:A:95:LEU:HD22	0.46	1.70	4	1
1:A:102:ILE:CA	1:A:120:LEU:HD21	0.46	2.39	6	2
1:B:85:ILE:O	1:B:88:LEU:HB2	0.46	2.11	12	5
1:A:98:LEU:HB3	1:A:102:ILE:HG21	0.46	1.87	7	1
1:A:93:GLN:O	1:A:96:THR:N	0.46	2.49	7	6
1:B:52:PHE:C	1:B:53:CYS:HG	0.46	2.13	17	1
1:A:52:PHE:CE2	1:A:54:TYR:HA	0.46	2.46	20	1
1:B:75:LEU:HD22	1:B:88:LEU:HD22	0.46	1.88	20	2
1:A:101:GLU:HG3	1:A:124:PHE:CE1	0.46	2.46	2	3
1:B:80:HIS:CG	1:B:84:GLN:CB	0.46	2.98	10	1
1:A:46:ARG:CG	1:A:47:GLN:N	0.46	2.78	12	1
1:A:88:LEU:CD1	1:A:88:LEU:C	0.46	2.79	8	1
1:A:90:VAL:CG2	1:B:68:ARG:HA	0.46	2.41	14	14
1:A:79:LEU:C	1:A:81:THR:N	0.46	2.69	19	1
1:A:79:LEU:O	1:A:80:HIS:O	0.46	2.33	20	1
1:B:49:PHE:CD1	1:B:49:PHE:N	0.46	2.84	20	1
1:A:119:THR:CG2	1:A:120:LEU:N	0.46	2.77	7	2
1:A:91:MET:HA	1:A:91:MET:HE2	0.46	1.88	7	1
1:A:64:LEU:O	1:A:65:SER:C	0.46	2.54	12	1
1:A:121:VAL:O	1:A:125:HIS:HB3	0.46	2.11	14	1
1:A:118:VAL:HG21	1:B:60:PRO:O	0.46	2.11	15	1
1:B:57:VAL:HG21	1:B:63:ALA:CA	0.46	2.40	9	1
1:B:78:GLU:CB	1:B:79:LEU:HD13	0.46	2.41	16	1
1:A:93:GLN:OE1	1:B:49:PHE:CG	0.46	2.68	4	1
1:B:116:GLU:O	1:B:119:THR:N	0.46	2.48	13	1
1:A:77:PRO:O	1:A:79:LEU:HD13	0.46	2.11	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:80:HIS:O	1:B:85:ILE:CD1	0.46	2.64	5	1
1:B:111:LEU:CD2	1:B:111:LEU:O	0.46	2.64	7	1
1:A:93:GLN:HA	1:A:96:THR:CG2	0.46	2.41	1	1
1:A:117:ILE:HD12	1:A:117:ILE:H	0.46	1.71	16	1
1:B:93:GLN:N	1:B:93:GLN:OE1	0.46	2.49	8	1
1:A:52:PHE:HB3	1:B:97:ILE:CG2	0.46	2.41	14	2
1:B:57:VAL:CG2	1:B:63:ALA:CA	0.46	2.94	20	2
1:A:70:LEU:O	1:A:74:TRP:N	0.46	2.49	1	4
1:A:82:LYS:NZ	1:B:72:ARG:NH1	0.46	2.64	4	1
1:A:122:GLU:O	1:A:126:ARG:C	0.46	2.54	10	1
1:B:81:THR:HG23	1:B:82:LYS:N	0.46	2.26	16	3
1:B:92:GLU:CA	1:B:95:LEU:HD22	0.46	2.40	13	2
1:B:50:ARG:C	1:B:51:ARG:HG2	0.46	2.32	20	1
1:A:89:LEU:CG	1:B:75:LEU:HD11	0.46	2.40	5	1
1:A:110:CYS:C	1:A:112:MET:HE2	0.46	2.31	2	1
1:B:60:PRO:O	1:B:63:ALA:N	0.46	2.46	9	1
1:B:111:LEU:O	1:B:112:MET:HB3	0.46	2.10	16	1
1:B:111:LEU:H	1:B:111:LEU:HD13	0.46	1.71	7	2
1:A:89:LEU:HD22	1:B:74:TRP:CD2	0.46	2.43	20	2
1:A:67:LEU:O	1:A:69:GLN:N	0.46	2.49	14	3
1:B:52:PHE:O	1:B:53:CYS:O	0.46	2.34	15	2
1:A:55:GLN:CG	1:A:56:GLU:N	0.46	2.75	5	1
1:A:85:ILE:HG12	1:B:85:ILE:CD1	0.45	2.40	8	1
1:A:121:VAL:HG11	1:B:54:TYR:OH	0.45	2.11	9	3
1:A:89:LEU:CB	1:B:74:TRP:CZ3	0.45	3.00	3	1
1:A:71:CYS:CB	1:B:89:LEU:CD1	0.45	2.94	3	1
1:B:70:LEU:O	1:B:73:GLN:N	0.45	2.49	14	1
1:A:80:HIS:ND1	1:B:81:THR:OG1	0.45	2.44	18	1
1:B:54:TYR:O	1:B:55:GLN:C	0.45	2.54	18	2
1:B:93:GLN:NE2	1:B:93:GLN:HA	0.45	2.26	2	1
1:B:86:LEU:C	1:B:89:LEU:HD12	0.45	2.29	10	1
1:A:77:PRO:C	1:A:78:GLU:CG	0.45	2.85	14	1
1:B:75:LEU:HD23	1:B:88:LEU:HD11	0.45	1.80	18	1
1:A:102:ILE:HG22	1:A:120:LEU:CD1	0.45	2.41	2	1
1:A:84:GLN:NE2	1:A:88:LEU:CD2	0.45	2.79	6	1
1:B:91:MET:C	1:B:95:LEU:HD21	0.45	2.31	6	1
1:A:52:PHE:CZ	1:A:57:VAL:HG13	0.45	2.45	8	1
1:A:81:THR:OG1	1:B:80:HIS:ND1	0.45	2.49	17	1
1:A:93:GLN:OE1	1:B:49:PHE:O	0.45	2.35	4	1
1:B:102:ILE:H	1:B:102:ILE:HD13	0.45	1.72	10	1
1:B:52:PHE:CZ	1:B:70:LEU:HD22	0.45	2.46	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ILE:O	1:A:88:LEU:CB	0.45	2.65	8	4
1:B:57:VAL:CG1	1:B:66:GLN:HB2	0.45	2.42	8	1
1:B:57:VAL:HG12	1:B:66:GLN:HG3	0.45	1.88	3	1
1:A:125:HIS:CE1	1:B:54:TYR:OH	0.45	2.69	5	1
1:A:119:THR:O	1:A:122:GLU:CG	0.45	2.65	7	1
1:B:89:LEU:O	1:B:93:GLN:HB2	0.45	2.11	9	2
1:A:50:ARG:HA	1:B:93:GLN:NE2	0.45	2.26	2	1
1:A:50:ARG:NE	1:A:50:ARG:O	0.45	2.50	2	1
1:A:52:PHE:CE2	1:A:56:GLU:HB3	0.45	2.45	2	1
1:B:98:LEU:HD13	1:B:102:ILE:HG12	0.45	1.88	17	1
1:A:93:GLN:CD	1:B:67:LEU:HD21	0.45	2.32	11	1
1:A:77:PRO:HD3	1:A:80:HIS:NE2	0.45	2.26	20	1
1:A:71:CYS:CB	1:B:90:VAL:HG22	0.45	2.42	3	2
1:A:80:HIS:CD2	1:A:84:GLN:HG3	0.45	2.46	3	1
1:B:103:GLN:HA	1:B:106:VAL:HG12	0.45	1.87	4	1
1:B:91:MET:O	1:B:93:GLN:N	0.45	2.49	18	4
1:B:99:PRO:O	1:B:100:GLU:C	0.45	2.55	1	1
1:B:82:LYS:N	1:B:82:LYS:HE3	0.45	2.26	10	1
1:A:121:VAL:O	1:A:123:ASP:N	0.45	2.50	14	1
1:A:57:VAL:C	1:A:59:GLY:N	0.45	2.69	2	2
1:A:72:ARG:O	1:A:76:GLN:N	0.45	2.49	14	2
1:A:80:HIS:NE2	1:A:84:GLN:CD	0.45	2.69	3	1
1:B:52:PHE:O	1:B:56:GLU:CG	0.45	2.64	5	1
1:B:91:MET:HE1	1:B:95:LEU:HD11	0.45	1.89	1	1
1:A:45:CYS:O	1:A:49:PHE:CD2	0.45	2.70	15	1
1:A:85:ILE:HD13	1:B:82:LYS:CD	0.45	2.42	6	1
1:B:49:PHE:C	1:B:51:ARG:N	0.45	2.70	9	1
1:A:92:GLU:CA	1:A:95:LEU:HD22	0.45	2.42	12	5
1:B:112:MET:CE	1:B:116:GLU:HB2	0.45	2.42	3	4
1:B:52:PHE:C	1:B:52:PHE:CD1	0.45	2.89	13	2
1:B:91:MET:C	1:B:93:GLN:N	0.45	2.69	7	3
1:A:46:ARG:HD2	1:A:74:TRP:CE2	0.45	2.47	14	1
1:A:125:HIS:CE1	1:B:54:TYR:HH	0.45	2.27	14	1
1:B:91:MET:CE	1:B:95:LEU:HD21	0.45	2.42	14	1
1:A:94:PHE:CE2	1:B:64:LEU:HD21	0.45	2.47	2	1
1:A:94:PHE:CE2	1:B:64:LEU:HD11	0.45	2.42	1	1
1:B:111:LEU:CD2	1:B:111:LEU:C	0.45	2.85	11	2
1:B:81:THR:O	1:B:85:ILE:HG12	0.45	2.12	19	1
1:A:90:VAL:N	1:B:71:CYS:SG	0.45	2.90	20	1
1:A:52:PHE:CZ	1:B:97:ILE:HG12	0.45	2.47	13	1
1:A:89:LEU:CD1	1:B:71:CYS:HB2	0.45	2.42	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:HD2	1:A:67:LEU:HD11	0.45	1.71	10	2
1:B:67:LEU:O	1:B:71:CYS:N	0.45	2.50	7	1
1:A:123:ASP:O	1:A:127:ALA:O	0.45	2.35	14	1
1:A:118:VAL:HG13	1:B:60:PRO:CB	0.45	2.42	18	1
1:B:84:GLN:O	1:B:88:LEU:HD13	0.45	2.12	2	1
1:A:49:PHE:CD1	1:B:93:GLN:CB	0.45	3.00	15	1
1:A:93:GLN:NE2	1:B:49:PHE:CE1	0.45	2.85	9	1
1:B:49:PHE:CE2	1:B:67:LEU:HD23	0.45	2.45	19	1
1:B:57:VAL:HG23	1:B:63:ALA:CA	0.45	2.40	20	2
1:A:93:GLN:HG2	1:B:49:PHE:CG	0.45	2.47	5	1
1:B:82:LYS:O	1:B:86:LEU:HB2	0.45	2.12	5	2
1:A:75:LEU:HD21	1:A:88:LEU:CG	0.45	2.42	18	1
1:A:49:PHE:O	1:A:67:LEU:CD2	0.45	2.64	1	1
1:A:67:LEU:HB3	1:B:90:VAL:HG13	0.45	1.88	6	1
1:A:106:VAL:CG1	1:A:112:MET:HG2	0.45	2.42	6	1
1:A:56:GLU:OE1	1:A:66:GLN:NE2	0.44	2.50	19	1
1:A:72:ARG:HA	1:B:86:LEU:CD2	0.44	2.43	3	3
1:A:99:PRO:O	1:A:100:GLU:C	0.44	2.55	10	2
1:B:70:LEU:O	1:B:71:CYS:C	0.44	2.55	7	2
1:A:62:GLU:N	1:A:62:GLU:OE1	0.44	2.50	14	1
1:B:53:CYS:C	1:B:55:GLN:N	0.44	2.70	18	1
1:B:85:ILE:O	1:B:89:LEU:CD1	0.44	2.66	2	1
1:A:110:CYS:H	1:A:111:LEU:HD13	0.44	1.72	2	1
1:B:106:VAL:CG2	1:B:107:ARG:N	0.44	2.80	1	1
1:A:64:LEU:CB	1:B:90:VAL:CG1	0.44	2.96	1	1
1:A:71:CYS:HB2	1:B:90:VAL:HG22	0.44	1.89	6	1
1:B:67:LEU:C	1:B:69:GLN:N	0.44	2.71	11	4
1:B:57:VAL:HB	1:B:62:GLU:CG	0.44	2.42	13	3
1:B:72:ARG:O	1:B:76:GLN:HB2	0.44	2.13	4	1
1:A:57:VAL:O	1:A:59:GLY:N	0.44	2.51	2	1
1:A:86:LEU:HD22	1:B:75:LEU:CD1	0.44	2.34	9	1
1:A:77:PRO:O	1:A:78:GLU:CG	0.44	2.64	9	1
1:B:111:LEU:O	1:B:112:MET:CB	0.44	2.65	16	1
1:A:98:LEU:HD23	1:B:54:TYR:CE1	0.44	2.47	11	1
1:A:49:PHE:CD2	1:A:70:LEU:HB3	0.44	2.48	11	1
1:B:54:TYR:CE2	1:B:57:VAL:HG11	0.44	2.46	7	1
1:B:86:LEU:O	1:B:90:VAL:N	0.44	2.45	14	2
1:A:80:HIS:ND1	1:A:84:GLN:CD	0.44	2.71	6	1
1:A:106:VAL:CG2	1:A:120:LEU:HD23	0.44	2.42	6	1
1:A:105:ARG:CB	1:A:120:LEU:HD22	0.44	2.42	8	1
1:A:85:ILE:HG13	1:B:85:ILE:CD1	0.44	2.43	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:52:PHE:O	1:B:55:GLN:CB	0.44	2.66	17	1
1:B:49:PHE:CD2	1:B:67:LEU:HD23	0.44	2.47	19	1
1:A:75:LEU:CD2	1:A:88:LEU:HG	0.44	2.42	12	3
1:A:50:ARG:NH2	1:B:96:THR:OG1	0.44	2.50	12	1
1:B:95:LEU:O	1:B:98:LEU:N	0.44	2.50	18	1
1:A:123:ASP:O	1:A:127:ALA:CB	0.44	2.58	1	1
1:B:125:HIS:O	1:B:126:ARG:CG	0.44	2.65	8	1
1:A:50:ARG:HA	1:B:93:GLN:CG	0.44	2.43	11	4
1:B:101:GLU:OE2	1:B:124:PHE:CE1	0.44	2.70	3	2
1:A:80:HIS:O	1:A:80:HIS:CD2	0.44	2.70	12	2
1:B:112:MET:HG2	1:B:113:SER:N	0.44	2.26	12	2
1:A:52:PHE:CE1	1:A:56:GLU:HB2	0.44	2.48	14	1
1:A:101:GLU:HG3	1:A:124:PHE:CG	0.44	2.47	2	1
1:B:47:GLN:NE2	1:B:47:GLN:O	0.44	2.51	1	1
1:A:63:ALA:CB	1:B:97:ILE:HD11	0.44	2.41	8	2
1:A:53:CYS:CB	1:A:67:LEU:HD11	0.44	2.41	19	1
1:A:54:TYR:O	1:A:57:VAL:O	0.44	2.35	13	1
1:A:115:LYS:O	1:A:119:THR:CB	0.44	2.65	10	2
1:B:106:VAL:HG11	1:B:117:ILE:HA	0.44	1.90	1	1
1:B:51:ARG:CG	1:B:51:ARG:O	0.44	2.66	16	1
1:A:93:GLN:C	1:A:95:LEU:N	0.44	2.70	8	3
1:A:74:TRP:O	1:A:74:TRP:HD1	0.44	1.95	18	2
1:A:82:LYS:CD	1:A:86:LEU:HD21	0.44	2.43	3	1
1:A:65:SER:O	1:A:68:ARG:HB3	0.44	2.12	2	2
1:B:75:LEU:HA	1:B:88:LEU:CD2	0.44	2.42	12	1
1:B:103:GLN:O	1:B:110:CYS:O	0.44	2.36	1	1
1:B:99:PRO:C	1:B:101:GLU:N	0.44	2.71	1	1
1:B:84:GLN:O	1:B:88:LEU:HD22	0.44	2.12	15	1
1:B:52:PHE:CE1	1:B:67:LEU:CD2	0.44	2.74	8	1
1:A:123:ASP:HA	1:A:127:ALA:CB	0.44	2.42	6	6
1:A:52:PHE:CZ	1:A:56:GLU:HG3	0.44	2.47	19	1
1:A:68:ARG:CA	1:B:90:VAL:HG22	0.44	2.41	20	1
1:A:82:LYS:C	1:A:86:LEU:HD22	0.44	2.33	4	2
1:B:75:LEU:HA	1:B:88:LEU:HD11	0.44	1.89	5	1
1:A:101:GLU:HG3	1:A:124:PHE:CZ	0.44	2.48	5	2
1:A:125:HIS:CG	1:B:54:TYR:OH	0.44	2.67	14	1
1:A:57:VAL:HG23	1:A:63:ALA:HA	0.44	1.88	14	1
1:A:52:PHE:CZ	1:A:66:GLN:CB	0.44	3.00	18	1
1:A:90:VAL:CG1	1:B:64:LEU:CB	0.44	2.95	18	1
1:B:52:PHE:CE2	1:B:57:VAL:HG11	0.44	2.48	1	1
1:A:72:ARG:NE	1:B:86:LEU:HD23	0.44	2.27	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:PHE:HB2	1:B:70:LEU:HD23	0.44	1.88	16	1
1:B:125:HIS:CD2	1:B:125:HIS:C	0.44	2.90	16	1
1:B:79:LEU:O	1:B:80:HIS:CD2	0.44	2.70	3	1
1:A:80:HIS:CD2	1:A:84:GLN:NE2	0.44	2.86	14	2
1:B:112:MET:CE	1:B:116:GLU:CB	0.44	2.95	3	1
1:A:78:GLU:O	1:A:79:LEU:HD12	0.44	2.13	5	1
1:A:75:LEU:HD12	1:B:89:LEU:HD11	0.44	1.90	12	1
1:A:53:CYS:CB	1:B:97:ILE:CG2	0.44	2.83	16	1
1:A:50:ARG:CD	1:A:50:ARG:C	0.43	2.87	5	3
1:A:112:MET:CE	1:A:116:GLU:HB2	0.43	2.42	7	4
1:A:67:LEU:C	1:A:69:GLN:N	0.43	2.71	3	3
1:B:83:GLU:CG	1:B:84:GLN:N	0.43	2.81	3	1
1:A:102:ILE:CD1	1:A:103:GLN:N	0.43	2.78	14	2
1:A:91:MET:O	1:A:94:PHE:HB3	0.43	2.13	1	1
1:B:74:TRP:HD1	1:B:74:TRP:O	0.43	1.95	18	4
1:A:105:ARG:NE	1:A:105:ARG:O	0.43	2.52	11	1
1:A:77:PRO:CD	1:A:80:HIS:NE2	0.43	2.81	20	1
1:A:81:THR:O	1:A:82:LYS:C	0.43	2.57	20	1
1:A:92:GLU:HA	1:A:95:LEU:CD2	0.43	2.44	3	3
1:A:74:TRP:CD2	1:B:89:LEU:HD22	0.43	2.48	3	1
1:A:122:GLU:O	1:A:126:ARG:HB2	0.43	2.11	1	2
1:A:72:ARG:O	1:A:76:GLN:CG	0.43	2.67	14	2
1:B:49:PHE:N	1:B:49:PHE:CD1	0.43	2.86	12	1
1:A:76:GLN:N	1:A:77:PRO:CD	0.43	2.81	18	1
1:B:87:GLU:O	1:B:91:MET:HG3	0.43	2.12	18	1
1:B:91:MET:HE2	1:B:95:LEU:HD11	0.43	1.90	15	1
1:A:93:GLN:OE1	1:A:96:THR:CG2	0.43	2.66	16	1
1:A:64:LEU:N	1:A:64:LEU:CD2	0.43	2.80	16	1
1:B:89:LEU:O	1:B:93:GLN:OE1	0.43	2.37	17	2
1:A:80:HIS:CD2	1:B:85:ILE:HD13	0.43	2.48	20	1
1:B:54:TYR:CG	1:B:57:VAL:HG11	0.43	2.48	20	1
1:A:104:ALA:HA	1:A:108:HIS:CA	0.43	2.43	10	2
1:B:91:MET:O	1:B:95:LEU:HD21	0.43	2.14	18	1
1:A:54:TYR:CZ	1:B:121:VAL:HG11	0.43	2.48	15	1
1:B:81:THR:HG23	1:B:83:GLU:CB	0.43	2.44	17	1
1:A:125:HIS:N	1:A:125:HIS:CD2	0.43	2.87	20	1
1:A:112:MET:HG2	1:A:113:SER:N	0.43	2.28	20	2
1:A:46:ARG:CD	1:A:74:TRP:CZ2	0.43	3.01	3	1
1:A:52:PHE:CE1	1:B:97:ILE:HG12	0.43	2.48	13	1
1:A:57:VAL:CG2	1:A:62:GLU:HG2	0.43	2.43	12	1
1:A:85:ILE:HG22	1:A:86:LEU:N	0.43	2.28	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:PHE:O	1:A:97:ILE:HG13	0.43	2.13	9	2
1:B:122:GLU:O	1:B:126:ARG:HB2	0.43	2.13	18	1
1:B:49:PHE:HB2	1:B:70:LEU:CB	0.43	2.43	2	1
1:B:52:PHE:O	1:B:52:PHE:CD1	0.43	2.72	2	1
1:A:101:GLU:HG3	1:A:124:PHE:CD2	0.43	2.48	2	1
1:A:101:GLU:HG2	1:A:124:PHE:CG	0.43	2.49	2	1
1:A:85:ILE:CD1	1:B:85:ILE:HG12	0.43	2.42	1	1
1:A:101:GLU:OE1	1:A:124:PHE:CG	0.43	2.71	15	1
1:A:80:HIS:ND1	1:A:84:GLN:HB2	0.43	2.27	9	1
1:A:108:HIS:O	1:A:109:ARG:C	0.43	2.55	9	1
1:A:93:GLN:HE22	1:B:50:ARG:NH1	0.43	2.12	16	1
1:B:91:MET:CE	1:B:91:MET:HA	0.43	2.42	20	2
1:A:108:HIS:O	1:A:109:ARG:CD	0.43	2.67	3	1
1:A:91:MET:CE	1:A:114:SER:HB2	0.43	2.43	5	1
1:A:57:VAL:HG22	1:A:62:GLU:HG2	0.43	1.91	12	1
1:B:54:TYR:O	1:B:55:GLN:CG	0.43	2.67	6	1
1:A:53:CYS:HB3	1:B:97:ILE:CB	0.43	2.43	16	1
1:B:75:LEU:CD2	1:B:88:LEU:CD2	0.43	2.96	20	2
1:B:76:GLN:N	1:B:77:PRO:CD	0.43	2.81	20	1
1:A:86:LEU:O	1:B:71:CYS:SG	0.43	2.76	4	1
1:A:46:ARG:HG3	1:A:74:TRP:CZ2	0.43	2.49	7	1
1:A:118:VAL:CG1	1:B:60:PRO:HB2	0.43	2.43	18	1
1:B:98:LEU:CB	1:B:99:PRO:HD2	0.43	2.43	6	1
1:B:106:VAL:CG2	1:B:111:LEU:HD11	0.43	2.43	9	1
1:A:74:TRP:HD1	1:A:74:TRP:C	0.43	2.14	20	1
1:A:75:LEU:HD22	1:A:85:ILE:HG13	0.43	1.90	5	1
1:A:95:LEU:C	1:A:97:ILE:N	0.43	2.71	2	2
1:A:52:PHE:CE1	1:A:67:LEU:HD21	0.43	2.46	13	1
1:A:71:CYS:HB2	1:B:89:LEU:CD1	0.43	2.43	1	1
1:A:47:GLN:O	1:A:51:ARG:HB2	0.43	2.14	15	1
1:A:102:ILE:CG1	1:A:103:GLN:N	0.43	2.82	6	1
1:A:102:ILE:CG2	1:A:121:VAL:HG22	0.43	2.43	9	1
1:A:91:MET:HE3	1:A:91:MET:HA	0.43	1.89	9	1
1:A:67:LEU:O	1:A:68:ARG:C	0.43	2.57	14	5
1:A:102:ILE:HD13	1:A:102:ILE:H	0.43	1.74	11	1
1:A:85:ILE:HG23	1:B:85:ILE:HG21	0.43	1.90	3	2
1:B:73:GLN:O	1:B:76:GLN:NE2	0.43	2.52	20	1
1:A:75:LEU:O	1:A:80:HIS:CG	0.43	2.72	4	1
1:B:89:LEU:O	1:B:93:GLN:HG2	0.43	2.13	15	2
1:A:94:PHE:CE1	1:A:118:VAL:HG21	0.43	2.48	1	1
1:B:104:ALA:O	1:B:108:HIS:N	0.43	2.51	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:91:MET:O	1:B:94:PHE:N	0.43	2.51	1	1
1:A:124:PHE:O	1:A:127:ALA:O	0.43	2.37	1	1
1:A:94:PHE:O	1:A:97:ILE:HG12	0.43	2.13	15	2
1:A:75:LEU:HD21	1:A:88:LEU:CD2	0.43	2.43	17	2
1:B:52:PHE:C	1:B:53:CYS:SG	0.43	2.98	17	1
1:A:102:ILE:C	1:A:102:ILE:HD12	0.43	2.34	19	1
1:B:75:LEU:C	1:B:76:GLN:CG	0.43	2.87	20	1
1:B:49:PHE:HB2	1:B:70:LEU:HD12	0.43	1.91	14	1
1:A:74:TRP:C	1:A:74:TRP:HD1	0.43	2.12	18	1
1:A:54:TYR:CD1	1:B:98:LEU:HD23	0.43	2.49	18	1
1:A:49:PHE:CB	1:A:70:LEU:HB3	0.43	2.44	1	1
1:A:50:ARG:NE	1:A:50:ARG:CA	0.43	2.78	6	1
1:B:99:PRO:HD2	1:B:102:ILE:CD1	0.43	2.43	17	1
1:B:52:PHE:CZ	1:B:66:GLN:CB	0.43	3.01	20	1
1:B:106:VAL:CA	1:B:111:LEU:HD21	0.43	2.44	4	1
1:A:85:ILE:CD1	1:B:82:LYS:HD2	0.43	2.43	10	1
1:A:94:PHE:CE2	1:A:117:ILE:HG21	0.43	2.47	7	1
1:A:110:CYS:N	1:A:111:LEU:HD13	0.43	2.29	2	1
1:B:112:MET:CE	1:B:112:MET:C	0.43	2.88	6	1
1:A:97:ILE:HG21	1:B:52:PHE:HB3	0.42	1.91	11	1
1:A:52:PHE:HD2	1:B:97:ILE:HD13	0.42	1.74	20	1
1:A:102:ILE:HB	1:A:117:ILE:HG23	0.42	1.91	20	1
1:B:92:GLU:OE1	1:B:93:GLN:NE2	0.42	2.52	5	1
1:A:103:GLN:HA	1:A:106:VAL:HG22	0.42	1.89	14	1
1:A:121:VAL:C	1:A:123:ASP:N	0.42	2.71	14	1
1:A:93:GLN:OE1	1:B:51:ARG:N	0.42	2.52	6	2
1:A:112:MET:CE	1:A:116:GLU:CB	0.42	2.97	6	1
1:A:95:LEU:O	1:A:98:LEU:O	0.42	2.37	8	1
1:A:53:CYS:C	1:A:55:GLN:N	0.42	2.72	17	1
1:B:57:VAL:O	1:B:57:VAL:CG1	0.42	2.66	20	1
1:A:106:VAL:HG12	1:A:111:LEU:HD21	0.42	1.92	3	1
1:A:50:ARG:HG3	1:A:51:ARG:N	0.42	2.28	5	1
1:B:105:ARG:O	1:B:108:HIS:O	0.42	2.37	13	1
1:B:105:ARG:HG3	1:B:106:VAL:HG13	0.42	1.91	10	1
1:B:125:HIS:CD2	1:B:125:HIS:N	0.42	2.87	12	1
1:A:97:ILE:HD12	1:A:98:LEU:HD23	0.42	1.91	18	1
1:A:112:MET:SD	1:A:116:GLU:CG	0.42	3.06	15	1
1:A:89:LEU:CD2	1:B:74:TRP:CZ3	0.42	3.02	20	1
1:A:49:PHE:O	1:A:52:PHE:N	0.42	2.52	4	3
1:B:106:VAL:N	1:B:111:LEU:HD21	0.42	2.29	4	1
1:B:49:PHE:CD2	1:B:70:LEU:HB3	0.42	2.49	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:GLN:O	1:A:76:GLN:NE2	0.42	2.52	12	1
1:A:57:VAL:CG2	1:A:62:GLU:HB3	0.42	2.44	9	1
1:B:52:PHE:HZ	1:B:70:LEU:HD12	0.42	1.75	8	1
1:B:80:HIS:HB2	1:B:84:GLN:HB2	0.42	1.92	19	1
1:B:75:LEU:HA	1:B:88:LEU:CD1	0.42	2.43	5	1
1:A:80:HIS:CA	1:A:84:GLN:HB3	0.42	2.44	4	1
1:B:79:LEU:HD12	1:B:80:HIS:H	0.42	1.74	13	1
1:A:64:LEU:HD22	1:A:65:SER:N	0.42	2.30	7	1
1:A:46:ARG:HG3	1:A:47:GLN:N	0.42	2.29	12	1
1:A:45:CYS:SG	1:A:70:LEU:CD1	0.42	3.08	14	1
1:B:98:LEU:CD1	1:B:117:ILE:CG2	0.42	2.98	15	1
1:A:50:ARG:NE	1:A:67:LEU:HG	0.42	2.28	6	1
1:A:112:MET:HE2	1:A:116:GLU:CB	0.42	2.43	6	1
1:A:54:TYR:CE2	1:A:58:SER:O	0.42	2.73	8	1
1:B:75:LEU:O	1:B:76:GLN:HG2	0.42	2.15	13	1
1:A:111:LEU:CD2	1:A:111:LEU:C	0.42	2.87	14	1
1:A:49:PHE:HB2	1:A:70:LEU:CB	0.42	2.45	1	1
1:A:80:HIS:CE1	1:B:85:ILE:CG2	0.42	3.00	20	1
1:A:86:LEU:HD11	1:B:72:ARG:CA	0.42	2.44	20	1
1:A:101:GLU:N	1:A:101:GLU:CD	0.42	2.73	3	1
1:A:75:LEU:HD23	1:A:88:LEU:CD2	0.42	2.44	4	1
1:B:69:GLN:HG2	1:B:70:LEU:N	0.42	2.30	4	1
1:A:50:ARG:O	1:A:50:ARG:HG2	0.42	2.14	13	1
1:A:93:GLN:HE21	1:A:96:THR:HG21	0.42	1.74	13	1
1:A:95:LEU:H	1:A:95:LEU:HD13	0.42	1.62	2	1
1:A:113:SER:C	1:A:115:LYS:N	0.42	2.71	2	1
1:B:106:VAL:CG2	1:B:107:ARG:H	0.42	2.28	1	1
1:A:111:LEU:O	1:A:112:MET:HB2	0.42	2.14	15	1
1:A:75:LEU:C	1:B:82:LYS:HZ3	0.42	2.18	8	1
1:A:89:LEU:CD1	1:B:71:CYS:CB	0.42	2.98	11	1
1:A:112:MET:HB2	1:A:116:GLU:CB	0.42	2.44	11	1
1:B:107:ARG:C	1:B:107:ARG:CD	0.42	2.87	20	1
1:B:107:ARG:O	1:B:108:HIS:O	0.42	2.38	20	1
1:A:82:LYS:O	1:A:86:LEU:CB	0.42	2.68	4	1
1:B:74:TRP:CZ2	1:B:88:LEU:CD1	0.42	2.98	7	1
1:A:88:LEU:HD13	1:A:88:LEU:HA	0.42	1.73	2	2
1:A:86:LEU:HD21	1:B:72:ARG:CG	0.42	2.45	12	1
1:B:113:SER:O	1:B:117:ILE:HD13	0.42	2.15	1	1
1:B:98:LEU:HB3	1:B:99:PRO:CD	0.42	2.44	6	1
1:B:79:LEU:HD12	1:B:80:HIS:CD2	0.42	2.49	6	1
1:A:93:GLN:OE1	1:B:50:ARG:O	0.42	2.38	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ARG:HA	1:B:93:GLN:OE1	0.42	2.14	16	1
1:A:82:LYS:CD	1:A:86:LEU:CD2	0.42	2.98	3	1
1:B:93:GLN:NE2	1:B:97:ILE:HG22	0.42	2.30	10	1
1:B:101:GLU:CB	1:B:120:LEU:HD11	0.42	2.45	10	1
1:B:75:LEU:HD22	1:B:88:LEU:HD23	0.42	1.91	2	1
1:B:81:THR:HG21	1:B:83:GLU:OE2	0.42	2.15	2	1
1:B:52:PHE:CZ	1:B:57:VAL:HG11	0.42	2.49	1	1
1:B:105:ARG:HG3	1:B:120:LEU:HD22	0.42	1.91	16	2
1:A:87:GLU:O	1:A:91:MET:N	0.42	2.53	17	1
1:B:108:HIS:O	1:B:110:CYS:N	0.42	2.53	5	1
1:A:78:GLU:O	1:A:79:LEU:HB2	0.42	2.10	4	2
1:A:93:GLN:CG	1:B:49:PHE:CZ	0.42	3.02	4	1
1:A:98:LEU:HB3	1:A:102:ILE:CG2	0.42	2.45	13	1
1:A:80:HIS:CG	1:A:84:GLN:CB	0.42	3.03	12	1
1:A:52:PHE:CE1	1:A:66:GLN:CB	0.42	3.02	18	1
1:A:93:GLN:CG	1:B:67:LEU:HD22	0.42	2.45	18	1
1:A:91:MET:CE	1:A:91:MET:HA	0.42	2.45	9	1
1:A:85:ILE:HG21	1:B:85:ILE:HG23	0.42	1.87	16	1
1:A:54:TYR:CE1	1:A:63:ALA:HB2	0.42	2.50	17	1
1:A:73:GLN:O	1:A:76:GLN:CD	0.42	2.58	17	2
1:A:75:LEU:HD21	1:A:88:LEU:CD1	0.42	2.45	17	2
1:A:71:CYS:SG	1:B:89:LEU:HB2	0.42	2.55	17	1
1:A:49:PHE:HB3	1:A:70:LEU:HD13	0.42	1.91	5	1
1:A:91:MET:O	1:A:93:GLN:N	0.42	2.53	6	2
1:A:85:ILE:HG21	1:B:85:ILE:CD1	0.42	2.45	13	1
1:B:108:HIS:CD2	1:B:108:HIS:C	0.42	2.93	18	1
1:A:82:LYS:HB2	1:A:86:LEU:HD21	0.42	1.92	9	1
1:A:111:LEU:C	1:A:112:MET:SD	0.42	2.99	9	1
1:A:126:ARG:O	1:A:126:ARG:CG	0.41	2.65	17	1
1:B:80:HIS:HB2	1:B:84:GLN:CB	0.41	2.45	19	1
1:A:79:LEU:HD13	1:A:79:LEU:HA	0.41	1.77	20	1
1:A:108:HIS:O	1:A:109:ARG:NE	0.41	2.52	3	1
1:B:79:LEU:C	1:B:80:HIS:CG	0.41	2.91	5	1
1:B:113:SER:C	1:B:115:LYS:N	0.41	2.73	4	1
1:B:111:LEU:HD13	1:B:111:LEU:N	0.41	2.30	13	1
1:B:60:PRO:C	1:B:62:GLU:N	0.41	2.73	14	2
1:B:51:ARG:O	1:B:53:CYS:N	0.41	2.53	14	1
1:B:74:TRP:HD1	1:B:74:TRP:C	0.41	2.15	14	1
1:A:68:ARG:O	1:A:71:CYS:SG	0.41	2.64	1	1
1:A:49:PHE:CE1	1:A:74:TRP:CE3	0.41	3.08	1	1
1:B:112:MET:SD	1:B:113:SER:N	0.41	2.93	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:98:LEU:HB3	1:B:102:ILE:CD1	0.41	2.45	17	1
1:B:75:LEU:HD22	1:B:85:ILE:CD1	0.41	2.36	19	1
1:B:64:LEU:O	1:B:68:ARG:HB3	0.41	2.14	20	1
1:A:82:LYS:CE	1:B:77:PRO:HG2	0.41	2.45	10	1
1:B:88:LEU:HD13	1:B:88:LEU:HA	0.41	1.75	10	2
1:B:100:GLU:O	1:B:101:GLU:C	0.41	2.57	10	1
1:A:64:LEU:CD2	1:A:65:SER:N	0.41	2.83	7	1
1:B:111:LEU:C	1:B:112:MET:SD	0.41	2.99	12	1
1:A:55:GLN:O	1:A:55:GLN:CG	0.41	2.69	12	1
1:B:57:VAL:HG11	1:B:62:GLU:OE1	0.41	2.14	2	1
1:A:91:MET:O	1:A:94:PHE:CB	0.41	2.68	1	1
1:B:106:VAL:HG21	1:B:117:ILE:HD11	0.41	1.92	1	1
1:B:57:VAL:HG23	1:B:62:GLU:HB3	0.41	1.92	1	1
1:A:85:ILE:HG13	1:B:85:ILE:HD12	0.41	1.90	17	1
1:A:57:VAL:CG1	1:A:66:GLN:CG	0.41	2.99	19	1
1:A:76:GLN:HG3	1:A:76:GLN:O	0.41	2.14	3	1
1:A:60:PRO:HB2	1:B:118:VAL:CG1	0.41	2.45	5	1
1:B:120:LEU:HD12	1:B:120:LEU:C	0.41	2.35	5	1
1:B:57:VAL:HG21	1:B:63:ALA:N	0.41	2.31	4	1
1:A:90:VAL:HG22	1:B:71:CYS:HB2	0.41	1.92	2	1
1:A:101:GLU:HG3	1:A:124:PHE:CE2	0.41	2.49	2	1
1:B:117:ILE:HD12	1:B:117:ILE:H	0.41	1.75	15	1
1:A:54:TYR:N	1:B:97:ILE:HD12	0.41	2.30	15	1
1:B:79:LEU:HD13	1:B:80:HIS:H	0.41	1.67	15	1
1:B:110:CYS:O	1:B:112:MET:SD	0.41	2.79	15	1
1:A:88:LEU:HA	1:A:88:LEU:HD13	0.41	1.73	9	1
1:B:49:PHE:O	1:B:49:PHE:CG	0.41	2.72	8	1
1:A:82:LYS:O	1:A:85:ILE:N	0.41	2.52	17	1
1:A:86:LEU:O	1:A:90:VAL:CB	0.41	2.69	19	2
1:A:117:ILE:C	1:A:119:THR:N	0.41	2.73	2	2
1:A:95:LEU:O	1:A:97:ILE:N	0.41	2.52	2	1
1:A:122:GLU:O	1:A:122:GLU:OE2	0.41	2.39	9	1
1:A:107:ARG:C	1:A:109:ARG:N	0.41	2.74	8	1
1:B:114:SER:CA	1:B:117:ILE:HD12	0.41	2.45	11	1
1:B:74:TRP:C	1:B:74:TRP:HD1	0.41	2.18	20	1
1:B:103:GLN:HA	1:B:106:VAL:CG1	0.41	2.45	4	1
1:B:52:PHE:CZ	1:B:57:VAL:HG22	0.41	2.50	14	1
1:A:71:CYS:SG	1:B:86:LEU:O	0.41	2.78	2	1
1:A:70:LEU:O	1:A:73:GLN:N	0.41	2.53	6	1
1:B:93:GLN:CD	1:B:93:GLN:N	0.41	2.73	9	1
1:B:52:PHE:HB2	1:B:67:LEU:HD21	0.41	1.92	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:GLN:NE2	1:B:50:ARG:HB3	0.41	2.31	16	1
1:A:54:TYR:O	1:A:55:GLN:HB2	0.41	2.16	8	1
1:A:125:HIS:O	1:A:126:ARG:HB2	0.41	2.14	17	1
1:A:125:HIS:O	1:A:126:ARG:CG	0.41	2.69	13	1
1:A:54:TYR:OH	1:A:59:GLY:C	0.41	2.58	13	1
1:B:74:TRP:NE1	1:B:88:LEU:HD21	0.41	2.30	7	1
1:B:90:VAL:O	1:B:94:PHE:HB3	0.41	2.15	12	1
1:B:124:PHE:CD2	1:B:125:HIS:N	0.41	2.89	18	1
1:A:57:VAL:HB	1:A:62:GLU:CB	0.41	2.46	18	2
1:A:95:LEU:CD1	1:A:95:LEU:H	0.41	2.27	1	1
1:A:49:PHE:HE1	1:A:67:LEU:HD23	0.41	1.76	6	1
1:A:50:ARG:NH2	1:A:70:LEU:HB2	0.41	2.30	6	1
1:A:80:HIS:CE1	1:A:84:GLN:HG3	0.41	2.51	6	1
1:B:67:LEU:O	1:B:71:CYS:CB	0.41	2.68	8	1
1:A:107:ARG:O	1:A:108:HIS:C	0.41	2.59	8	1
1:B:72:ARG:O	1:B:76:GLN:N	0.41	2.54	19	1
1:A:80:HIS:HB3	1:A:84:GLN:CB	0.41	2.46	4	1
1:A:64:LEU:H	1:A:64:LEU:CD2	0.41	2.28	16	2
1:A:54:TYR:O	1:A:55:GLN:C	0.41	2.59	13	1
1:B:49:PHE:O	1:B:50:ARG:C	0.41	2.59	10	3
1:A:106:VAL:HG23	1:A:116:GLU:HB3	0.41	1.91	10	1
1:A:123:ASP:OD1	1:A:127:ALA:HB2	0.41	2.16	15	1
1:A:105:ARG:HG3	1:A:106:VAL:N	0.41	2.29	15	1
1:A:52:PHE:CE2	1:A:57:VAL:HG22	0.41	2.49	6	1
1:A:60:PRO:C	1:A:62:GLU:N	0.41	2.74	16	1
1:A:48:SER:O	1:A:52:PHE:HB3	0.41	2.16	11	2
1:A:80:HIS:ND1	1:A:84:GLN:OE1	0.41	2.53	5	1
1:B:120:LEU:C	1:B:120:LEU:HD12	0.41	2.36	13	2
1:B:113:SER:O	1:B:114:SER:C	0.41	2.59	10	1
1:A:103:GLN:HB2	1:A:111:LEU:CD2	0.41	2.44	6	1
1:A:102:ILE:HG12	1:A:103:GLN:N	0.41	2.30	6	1
1:A:123:ASP:OD1	1:A:123:ASP:C	0.41	2.59	16	1
1:B:91:MET:HE3	1:B:95:LEU:HD11	0.41	1.91	8	1
1:A:56:GLU:O	1:A:57:VAL:O	0.41	2.39	17	1
1:A:93:GLN:CD	1:B:67:LEU:CD2	0.41	2.88	11	1
1:A:97:ILE:HD12	1:B:54:TYR:CD1	0.41	2.51	11	1
1:B:78:GLU:O	1:B:79:LEU:HD13	0.41	2.16	11	1
1:A:85:ILE:HG12	1:B:85:ILE:HG13	0.41	1.93	19	1
1:A:72:ARG:CG	1:B:86:LEU:CD2	0.41	2.98	19	1
1:B:50:ARG:O	1:B:51:ARG:HB2	0.41	2.15	19	1
1:A:93:GLN:OE1	1:A:97:ILE:CG2	0.41	2.69	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:106:VAL:CG1	1:B:107:ARG:N	0.41	2.83	20	2
1:B:64:LEU:O	1:B:68:ARG:HB2	0.41	2.16	5	1
1:A:93:GLN:HB3	1:B:67:LEU:HD22	0.41	1.93	10	1
1:A:93:GLN:HG2	1:B:67:LEU:HD13	0.41	1.92	7	1
1:B:91:MET:HA	1:B:91:MET:HE2	0.41	1.92	7	1
1:A:49:PHE:CE1	1:B:93:GLN:OE1	0.41	2.74	12	1
1:B:52:PHE:CZ	1:B:70:LEU:HD12	0.41	2.51	8	1
1:B:112:MET:HE1	1:B:117:ILE:HD11	0.41	1.92	17	1
1:B:107:ARG:O	1:B:109:ARG:N	0.41	2.54	11	1
1:A:53:CYS:SG	1:A:67:LEU:HG	0.41	2.55	19	1
1:A:49:PHE:CD1	1:A:70:LEU:CD2	0.41	3.04	5	1
1:A:106:VAL:CG2	1:A:107:ARG:N	0.41	2.85	13	1
1:B:61:GLN:O	1:B:61:GLN:CD	0.41	2.59	18	1
1:A:97:ILE:HD12	1:B:52:PHE:CD2	0.41	2.51	2	1
1:B:116:GLU:O	1:B:116:GLU:OE1	0.41	2.39	1	1
1:B:111:LEU:HD13	1:B:117:ILE:HG13	0.41	1.93	15	1
1:A:103:GLN:CB	1:A:111:LEU:HD23	0.41	2.45	6	1
1:A:53:CYS:HB3	1:B:97:ILE:CG1	0.41	2.46	16	1
1:B:67:LEU:C	1:B:71:CYS:SG	0.40	2.99	17	1
1:A:89:LEU:HB2	1:B:71:CYS:SG	0.40	2.56	20	1
1:B:93:GLN:OE1	1:B:93:GLN:HA	0.40	2.15	10	1
1:B:77:PRO:O	1:B:78:GLU:HB2	0.40	2.16	7	2
1:A:57:VAL:CG2	1:A:63:ALA:HA	0.40	2.45	14	1
1:A:92:GLU:HA	1:A:95:LEU:HD22	0.40	1.94	16	2
1:A:103:GLN:CB	1:A:111:LEU:CD2	0.40	2.98	6	1
1:A:53:CYS:SG	1:A:63:ALA:C	0.40	2.99	16	1
1:B:52:PHE:CD2	1:B:67:LEU:CD2	0.40	3.00	16	1
1:A:57:VAL:HG11	1:A:66:GLN:HB2	0.40	1.92	16	1
1:A:88:LEU:HD12	1:A:89:LEU:N	0.40	2.31	8	1
1:A:52:PHE:O	1:A:55:GLN:HB2	0.40	2.17	5	1
1:A:85:ILE:HG12	1:B:85:ILE:CG2	0.40	2.47	5	1
1:A:122:GLU:O	1:A:126:ARG:HB3	0.40	2.16	5	1
1:A:80:HIS:CB	1:A:84:GLN:HB3	0.40	2.46	4	1
1:B:92:GLU:CG	1:B:93:GLN:NE2	0.40	2.84	4	1
1:A:106:VAL:HB	1:A:111:LEU:CD2	0.40	2.46	4	1
1:B:99:PRO:O	1:B:103:GLN:OE1	0.40	2.39	10	1
1:B:90:VAL:O	1:B:94:PHE:HB2	0.40	2.17	14	1
1:A:94:PHE:O	1:A:98:LEU:CG	0.40	2.70	18	1
1:B:86:LEU:O	1:B:88:LEU:N	0.40	2.54	18	1
1:B:122:GLU:O	1:B:126:ARG:HB3	0.40	2.15	18	1
1:A:52:PHE:CE1	1:A:54:TYR:O	0.40	2.74	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:124:PHE:C	1:B:124:PHE:CD1	0.40	2.93	8	1
1:A:75:LEU:CB	1:A:80:HIS:HE2	0.40	2.30	20	1
1:A:76:GLN:O	1:A:76:GLN:HG2	0.40	2.16	3	1
1:A:79:LEU:O	1:A:80:HIS:HB3	0.40	2.16	10	1
1:A:120:LEU:C	1:A:120:LEU:HD13	0.40	2.37	7	1
1:B:47:GLN:O	1:B:50:ARG:CG	0.40	2.69	14	1
1:A:92:GLU:OE1	1:A:93:GLN:OE1	0.40	2.39	8	1
1:A:85:ILE:HG23	1:B:88:LEU:CD2	0.40	2.45	17	1
1:B:52:PHE:O	1:B:53:CYS:SG	0.40	2.76	17	1
1:B:78:GLU:O	1:B:79:LEU:CG	0.40	2.69	11	1
1:B:116:GLU:C	1:B:116:GLU:OE1	0.40	2.59	13	1
1:A:91:MET:CE	1:A:114:SER:HB3	0.40	2.46	10	1
1:A:52:PHE:CD1	1:A:53:CYS:O	0.40	2.75	1	1
1:A:77:PRO:CG	1:B:82:LYS:HG2	0.40	2.46	15	1
1:A:77:PRO:O	1:A:78:GLU:HB2	0.40	2.16	9	1
1:A:53:CYS:SG	1:A:67:LEU:HD11	0.40	2.57	16	1
1:B:109:ARG:C	1:B:110:CYS:SG	0.40	2.99	19	1
1:B:49:PHE:CD1	1:B:70:LEU:CD1	0.40	2.95	5	1
1:B:49:PHE:CB	1:B:70:LEU:HD12	0.40	2.46	4	1
1:B:56:GLU:O	1:B:57:VAL:O	0.40	2.40	4	1
1:A:86:LEU:O	1:A:87:GLU:C	0.40	2.60	14	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	84/98 (86%)	60±3 (71±4%)	15±3 (18±3%)	9±2 (11±2%)	1 9
1	B	80/98 (82%)	55±3 (69±4%)	14±3 (18±4%)	11±2 (13±3%)	1 6
All	All	3280/3920 (84%)	2298 (70%)	589 (18%)	393 (12%)	1 7

All 56 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	60	PRO	20
1	B	60	PRO	20
1	A	126	ARG	17
1	B	51	ARG	17
1	B	53	CYS	15
1	B	81	THR	14
1	A	79	LEU	12
1	A	54	TYR	12
1	B	112	MET	12
1	A	109	ARG	11
1	B	126	ARG	11
1	A	110	CYS	11
1	B	110	CYS	11
1	A	81	THR	11
1	B	109	ARG	11
1	A	53	CYS	11
1	B	50	ARG	11
1	B	99	PRO	10
1	A	112	MET	10
1	B	76	GLN	9
1	A	76	GLN	9
1	A	127	ALA	8
1	B	55	GLN	8
1	B	79	LEU	8
1	B	78	GLU	8
1	B	56	GLU	8
1	A	108	HIS	7
1	B	54	TYR	7
1	A	78	GLU	6
1	A	55	GLN	6
1	A	56	GLU	5
1	B	80	HIS	5
1	B	57	VAL	5
1	A	57	VAL	4
1	B	108	HIS	4
1	B	77	PRO	4
1	B	58	SER	4
1	A	99	PRO	3
1	B	82	LYS	3
1	B	68	ARG	3
1	B	94	PHE	3
1	A	100	GLU	2
1	B	92	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	80	HIS	2
1	A	77	PRO	2
1	A	117	ILE	1
1	A	68	ARG	1
1	A	59	GLY	1
1	A	82	LYS	1
1	A	122	GLU	1
1	A	52	PHE	1
1	B	111	LEU	1
1	A	94	PHE	1
1	B	100	GLU	1
1	A	111	LEU	1
1	A	58	SER	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	80/93 (86%)	50±4 (63±5%)	30±4 (37±5%)	1 7
1	B	77/93 (83%)	49±4 (63±6%)	28±4 (37±6%)	1 8
All	All	3140/3720 (84%)	1972 (63%)	1168 (37%)	1 7

All 142 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	89	LEU	20
1	B	88	LEU	20
1	A	95	LEU	20
1	A	88	LEU	20
1	B	89	LEU	20
1	A	119	THR	20
1	B	120	LEU	20
1	B	95	LEU	20
1	A	49	PHE	19
1	A	120	LEU	19
1	B	119	THR	19

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Mol	Chain	Res	Type	Models (Total)
1	A	105	ARG	17
1	B	82	LYS	16
1	A	118	VAL	16
1	B	49	PHE	16
1	A	75	LEU	15
1	B	75	LEU	15
1	A	82	LYS	14
1	A	54	TYR	14
1	A	70	LEU	14
1	B	113	SER	14
1	B	91	MET	13
1	A	50	ARG	13
1	B	50	ARG	13
1	B	118	VAL	12
1	B	109	ARG	12
1	A	102	ILE	12
1	B	110	CYS	12
1	B	116	GLU	12
1	B	126	ARG	12
1	B	112	MET	12
1	B	105	ARG	12
1	A	76	GLN	11
1	A	112	MET	11
1	B	111	LEU	11
1	A	113	SER	11
1	A	107	ARG	11
1	B	80	HIS	10
1	A	80	HIS	10
1	A	111	LEU	10
1	A	69	GLN	10
1	B	79	LEU	10
1	A	110	CYS	10
1	B	58	SER	10
1	B	115	LYS	10
1	A	86	LEU	10
1	A	115	LYS	10
1	A	51	ARG	10
1	A	57	VAL	9
1	B	68	ARG	9
1	A	56	GLU	9
1	B	103	GLN	9
1	A	91	MET	9

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Mol	Chain	Res	Type	Models (Total)
1	A	109	ARG	9
1	B	87	GLU	9
1	B	102	ILE	9
1	B	101	GLU	9
1	B	85	ILE	9
1	A	64	LEU	9
1	A	78	GLU	8
1	B	66	GLN	8
1	B	64	LEU	8
1	A	52	PHE	8
1	B	54	TYR	8
1	A	93	GLN	8
1	A	58	SER	8
1	A	72	ARG	8
1	A	103	GLN	8
1	A	126	ARG	8
1	B	107	ARG	8
1	B	76	GLN	7
1	B	121	VAL	7
1	A	92	GLU	7
1	A	53	CYS	7
1	B	122	GLU	7
1	B	65	SER	7
1	B	51	ARG	7
1	A	123	ASP	7
1	A	84	GLN	7
1	B	73	GLN	7
1	A	47	GLN	6
1	B	72	ARG	6
1	A	85	ILE	6
1	B	123	ASP	6
1	A	79	LEU	6
1	A	87	GLU	6
1	A	116	GLU	6
1	A	101	GLU	6
1	B	93	GLN	6
1	B	97	ILE	6
1	B	55	GLN	6
1	A	66	GLN	6
1	A	108	HIS	5
1	B	52	PHE	5
1	A	83	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	B	78	GLU	5
1	B	57	VAL	5
1	B	69	GLN	5
1	A	73	GLN	5
1	B	100	GLU	5
1	A	97	ILE	5
1	B	92	GLU	5
1	A	61	GLN	5
1	A	45	CYS	5
1	B	62	GLU	5
1	B	47	GLN	5
1	B	61	GLN	4
1	A	55	GLN	4
1	B	56	GLU	4
1	B	106	VAL	4
1	B	84	GLN	4
1	B	108	HIS	4
1	B	86	LEU	4
1	A	44	LEU	4
1	A	122	GLU	4
1	B	124	PHE	4
1	A	62	GLU	4
1	A	124	PHE	4
1	A	48	SER	4
1	A	68	ARG	4
1	A	125	HIS	3
1	A	65	SER	3
1	A	96	THR	3
1	B	53	CYS	3
1	A	100	GLU	3
1	B	70	LEU	3
1	B	48	SER	3
1	A	46	ARG	2
1	B	125	HIS	2
1	A	71	CYS	2
1	B	98	LEU	2
1	A	74	TRP	2
1	B	74	TRP	2
1	B	67	LEU	2
1	B	83	GLU	2
1	B	71	CYS	2
1	A	81	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	98	LEU	1
1	A	67	LEU	1
1	B	114	SER	1
1	A	114	SER	1
1	A	121	VAL	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided