Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 10:51 AM EST

PDB ID	:	2CXJ
Title	:	3D Solution Structure of S100A13
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Deposited on	:	2005-06-30

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

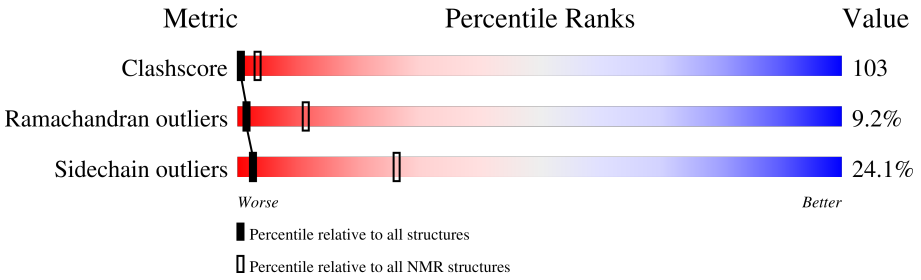
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	15% 63% 21%
1	B	98	14% 64% 21%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 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:1-A:98, B:1-B:98 (196)	0.46	7

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3184 atoms, of which 1614 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S100 calcium-binding protein A13.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	98	1592	496	807	135	152	2	0
1	B	98	1592	496	807	135	152	2	0

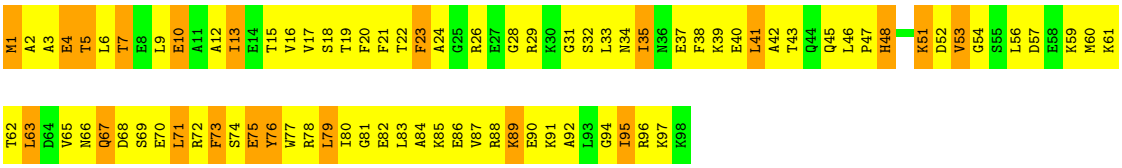
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

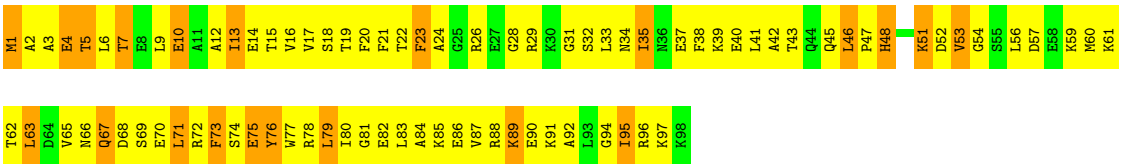
• Molecule 1: S100 calcium-binding protein A13

Chain A: 15% 63% 21%



• Molecule 1: S100 calcium-binding protein A13

Chain B: 14% 64% 21%



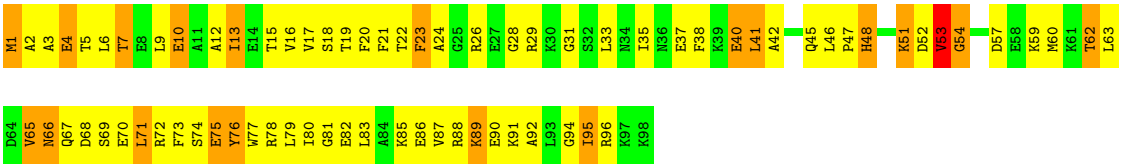
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

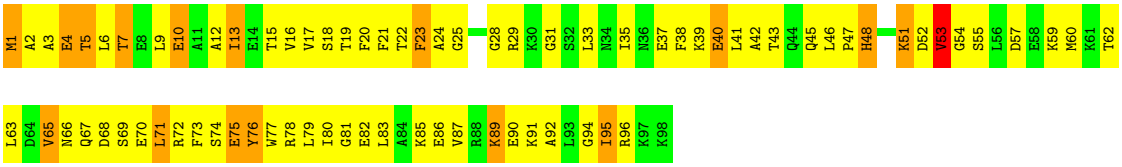
• Molecule 1: S100 calcium-binding protein A13

Chain A: 23% 56% 19%



• Molecule 1: S100 calcium-binding protein A13

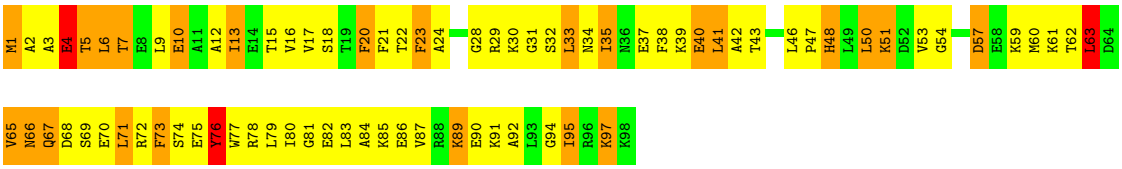
Chain B: 21% 61% 16%



4.2.2 Score per residue for model 2

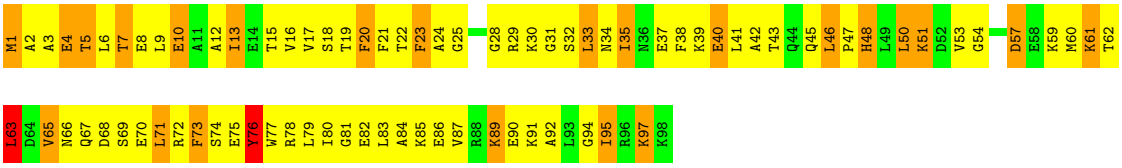
• Molecule 1: S100 calcium-binding protein A13

Chain A: 20% 52% 24%



• Molecule 1: S100 calcium-binding protein A13

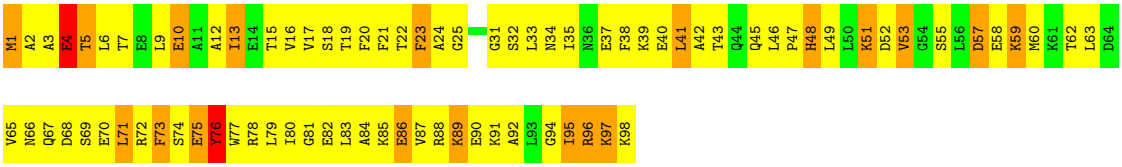
Chain B: 16% 58% 23%



4.2.3 Score per residue for model 3

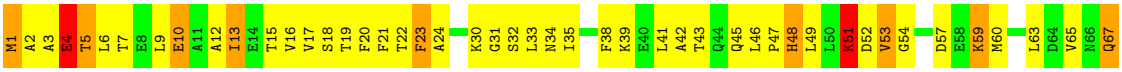
• Molecule 1: S100 calcium-binding protein A13

Chain A: 16% 62% 19%



• Molecule 1: S100 calcium-binding protein A13

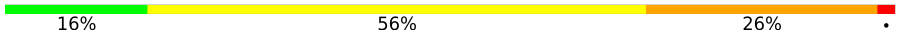
Chain B: 21% 59% 16%

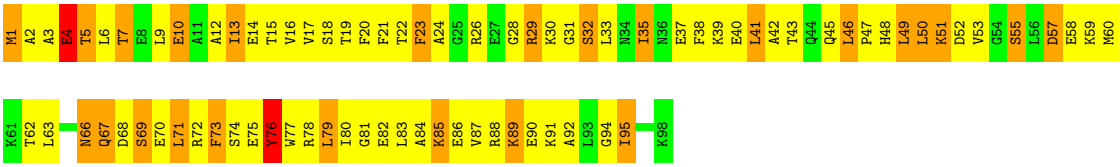


4.2.4 Score per residue for model 4

• Molecule 1: S100 calcium-binding protein A13

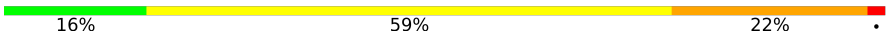
Chain A:





• Molecule 1: S100 calcium-binding protein A13

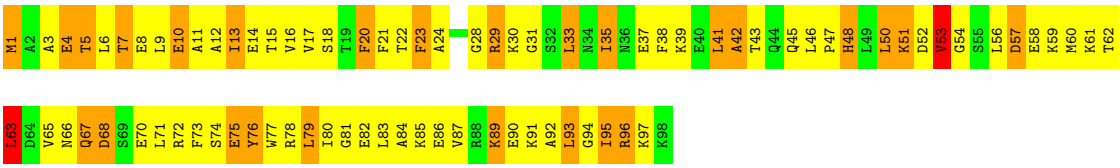
Chain B:



4.2.5 Score per residue for model 5

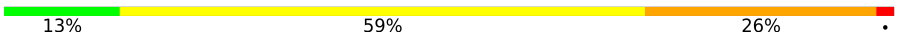
• Molecule 1: S100 calcium-binding protein A13

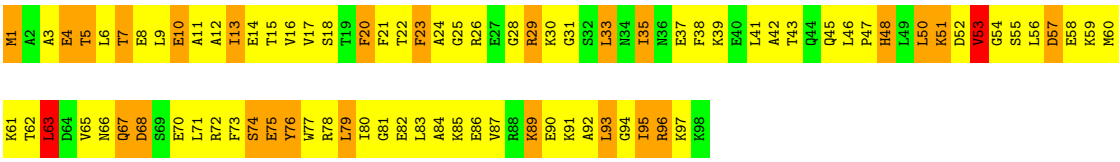
Chain A:



• Molecule 1: S100 calcium-binding protein A13

Chain B:

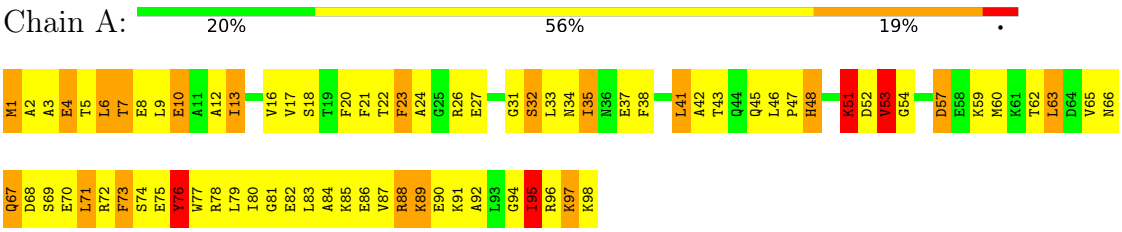




4.2.6 Score per residue for model 6

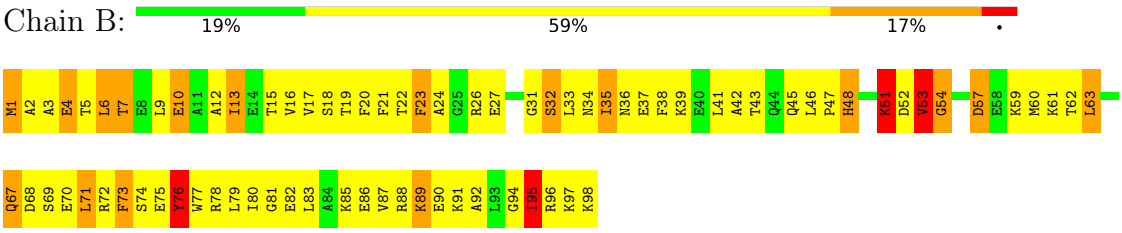
- Molecule 1: S100 calcium-binding protein A13

Chain A:



- Molecule 1: S100 calcium-binding protein A13

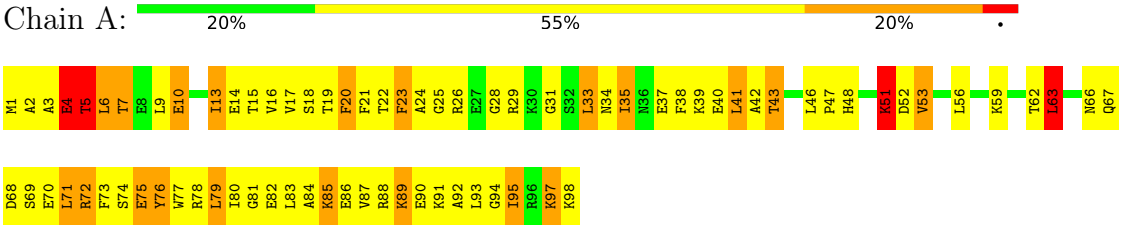
Chain B:



4.2.7 Score per residue for model 7 (medoid)

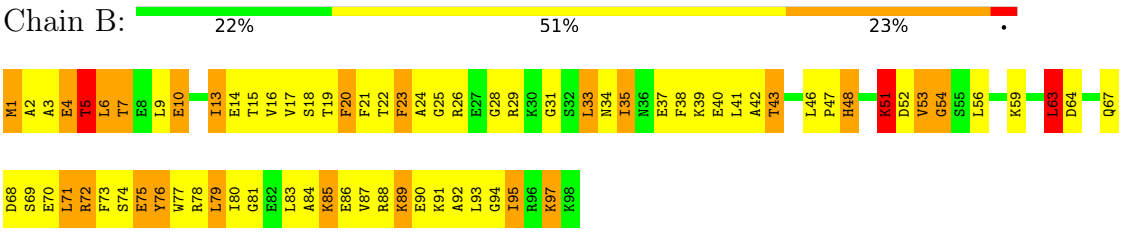
- Molecule 1: S100 calcium-binding protein A13

Chain A:



- Molecule 1: S100 calcium-binding protein A13

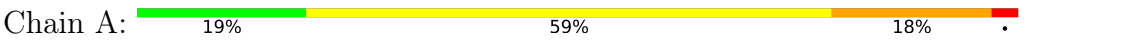
Chain B:



4.2.8 Score per residue for model 8

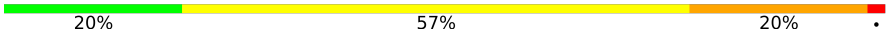
- Molecule 1: S100 calcium-binding protein A13

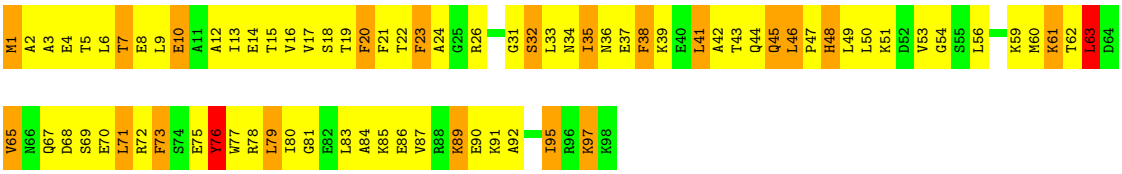
Chain A:



• Molecule 1: S100 calcium-binding protein A13

Chain B:

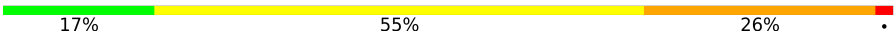




4.2.9 Score per residue for model 9

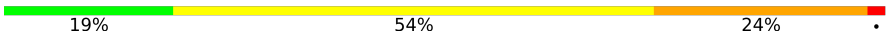
• Molecule 1: S100 calcium-binding protein A13

Chain A:



• Molecule 1: S100 calcium-binding protein A13

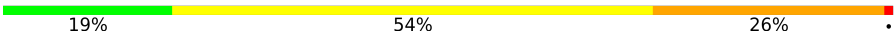
Chain B:

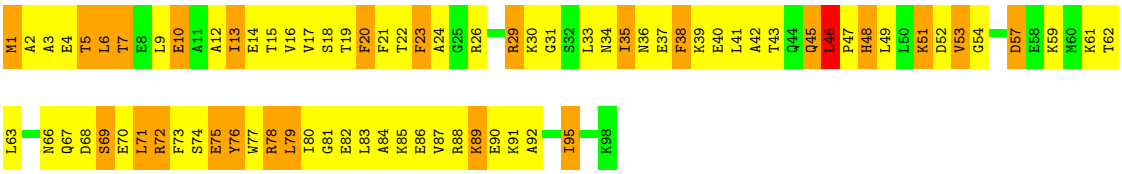


4.2.10 Score per residue for model 10

• Molecule 1: S100 calcium-binding protein A13

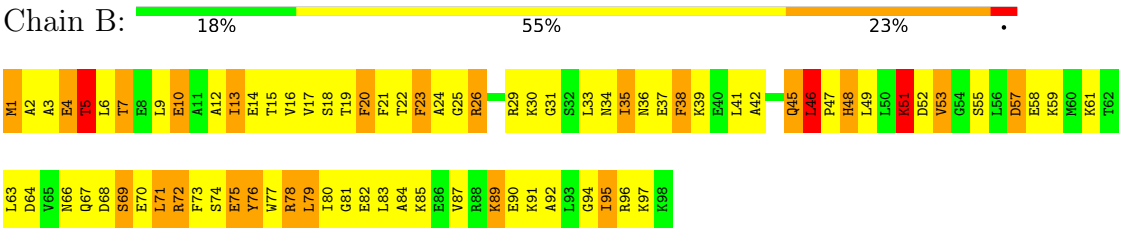
Chain A:





• Molecule 1: S100 calcium-binding protein A13

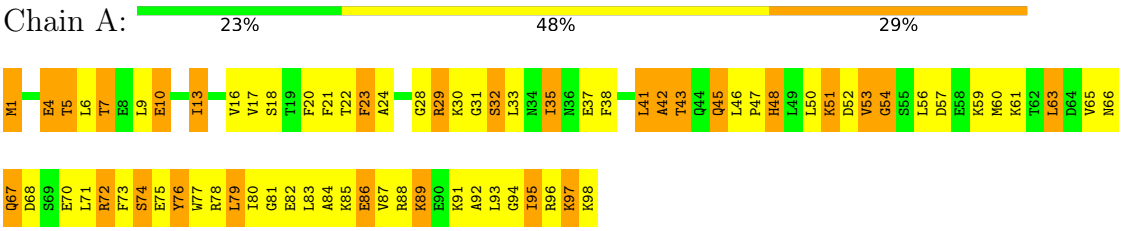
Chain B:



4.2.11 Score per residue for model 11

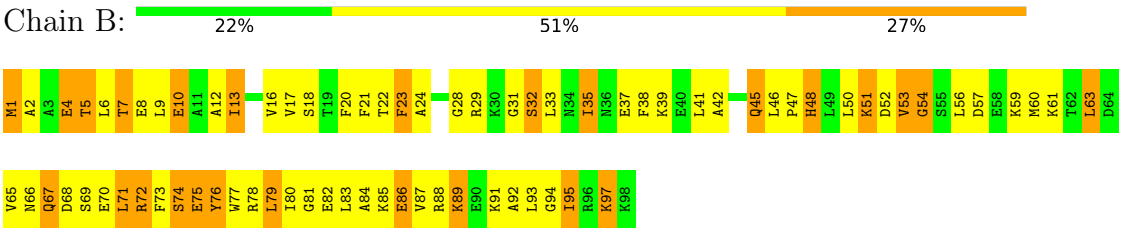
• Molecule 1: S100 calcium-binding protein A13

Chain A:



• Molecule 1: S100 calcium-binding protein A13

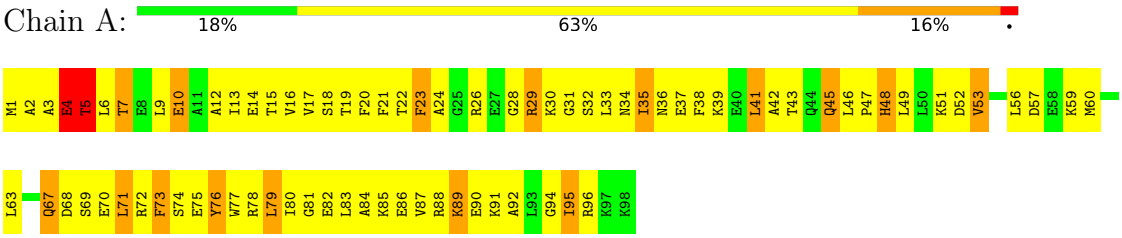
Chain B:



4.2.12 Score per residue for model 12

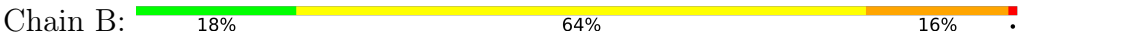
• Molecule 1: S100 calcium-binding protein A13

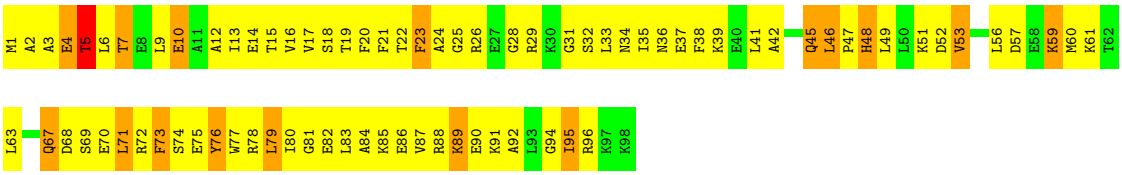
Chain A:



• Molecule 1: S100 calcium-binding protein A13

Chain B:

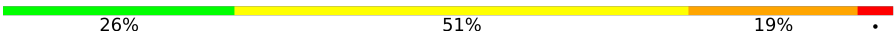


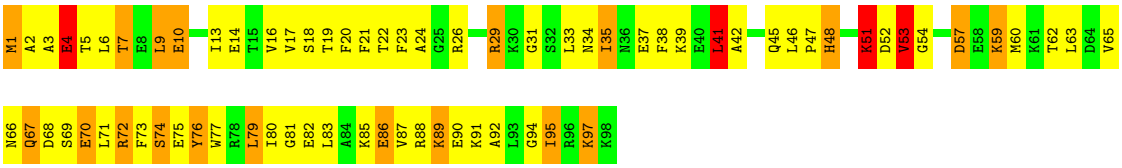


4.2.13 Score per residue for model 13

- Molecule 1: S100 calcium-binding protein A13

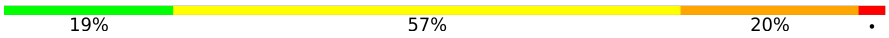
Chain A:

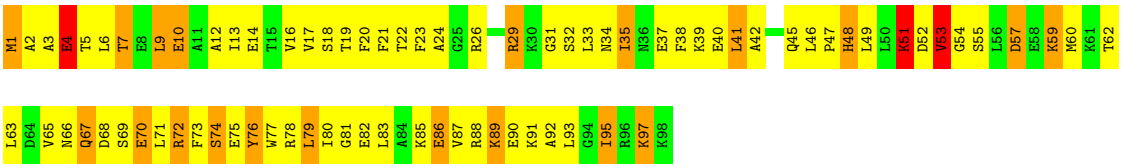




- Molecule 1: S100 calcium-binding protein A13

Chain B:

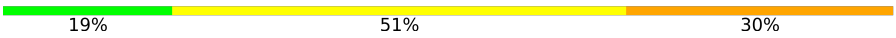




4.2.14 Score per residue for model 14

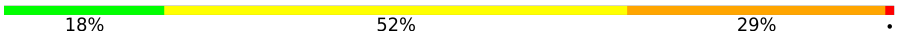
- Molecule 1: S100 calcium-binding protein A13

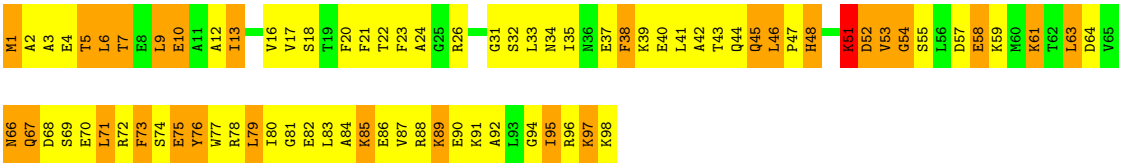
Chain A:



- Molecule 1: S100 calcium-binding protein A13

Chain B:

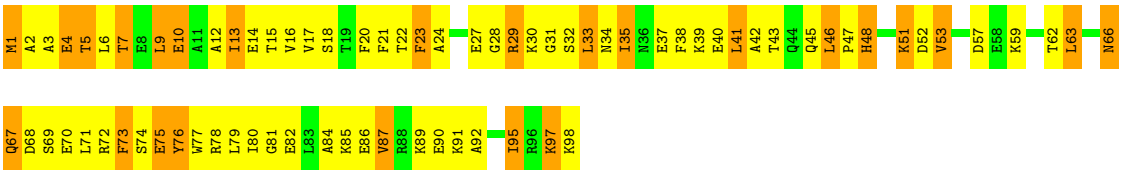




4.2.15 Score per residue for model 15

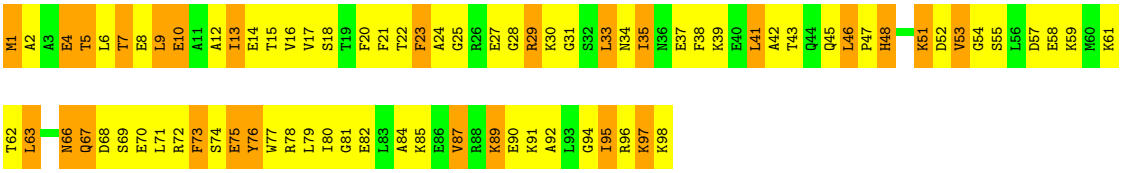
- Molecule 1: S100 calcium-binding protein A13

Chain A: 22% 52% 26%



- Molecule 1: S100 calcium-binding protein A13

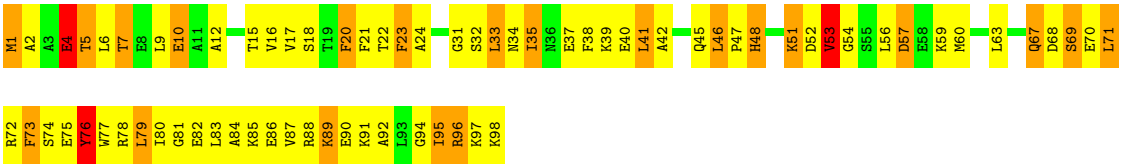
Chain B: 18% 55% 27%



4.2.16 Score per residue for model 16

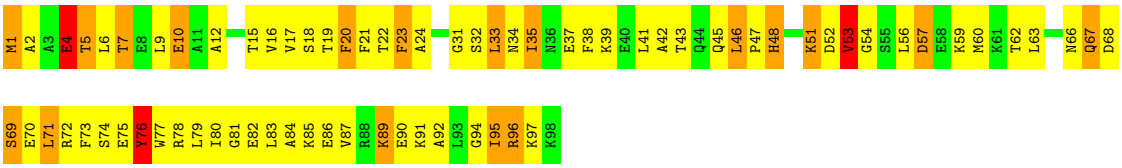
- Molecule 1: S100 calcium-binding protein A13

Chain A: 26% 50% 21% •



- Molecule 1: S100 calcium-binding protein A13

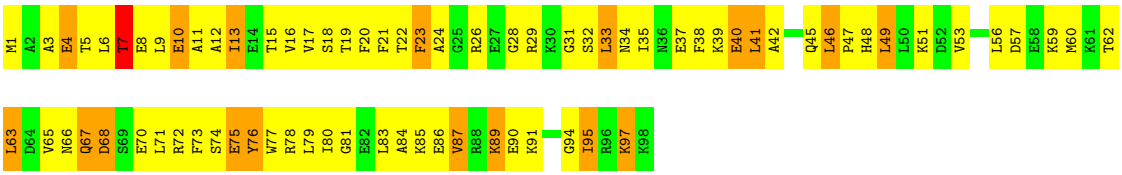
Chain B: 24% 54% 18% •



4.2.17 Score per residue for model 17

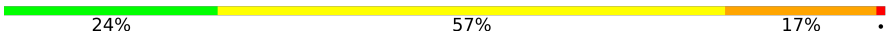
- Molecule 1: S100 calcium-binding protein A13

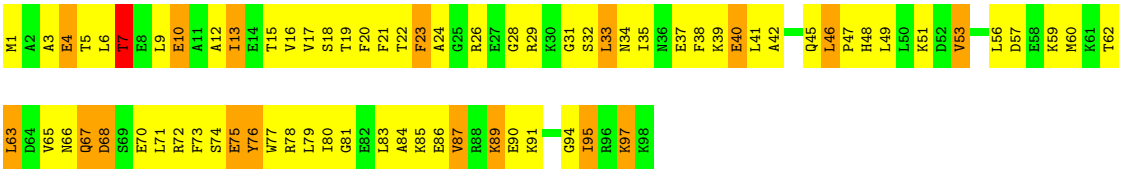
Chain A: 22% 58% 18% •



• Molecule 1: S100 calcium-binding protein A13

Chain B:

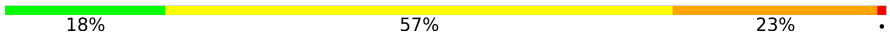


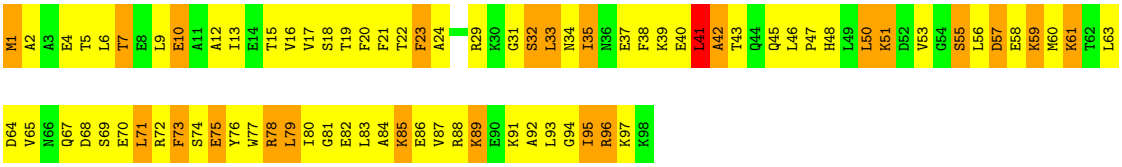


4.2.18 Score per residue for model 18

• Molecule 1: S100 calcium-binding protein A13

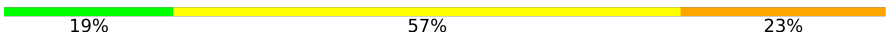
Chain A:





• Molecule 1: S100 calcium-binding protein A13

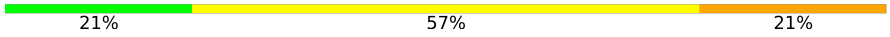
Chain B:



4.2.19 Score per residue for model 19

• Molecule 1: S100 calcium-binding protein A13

Chain A:



• Molecule 1: S100 calcium-binding protein A13

Chain B: 17% 61% 21%

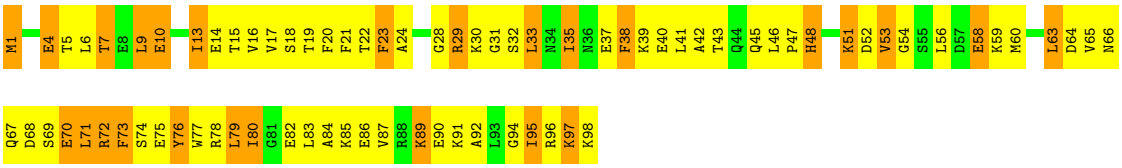
4.2.20 Score per residue for model 20

• Molecule 1: S100 calcium-binding protein A13

Chain A: 16% 55% 29%

• Molecule 1: S100 calcium-binding protein A13

Chain B: 20% 53% 27%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	785	807	806	201±13
1	B	785	807	806	199±14
All	All	31400	32280	32240	6543

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 103.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:HD22	1:B:16:VAL:HG23	1.10	1.18	8	18
1:A:16:VAL:HG23	1:B:9:LEU:HD22	1.07	1.16	11	18
1:A:76:TYR:CD1	1:A:79:LEU:HD11	1.04	1.87	13	16
1:B:76:TYR:CD1	1:B:79:LEU:HD11	1.03	1.88	13	16
1:A:23:PHE:CD2	1:A:33:LEU:HD11	1.01	1.91	12	13
1:B:23:PHE:CD2	1:B:33:LEU:HD11	1.00	1.90	11	12
1:B:21:PHE:CE2	1:B:79:LEU:HD13	0.99	1.93	13	5
1:A:38:PHE:CE1	1:A:41:LEU:HD12	0.97	1.94	3	16
1:A:20:PHE:CZ	1:A:41:LEU:HD11	0.97	1.93	2	16
1:A:21:PHE:CE2	1:A:79:LEU:HD13	0.97	1.95	13	5
1:A:41:LEU:HD13	1:B:7:THR:HG21	0.96	1.37	16	6
1:B:20:PHE:CE2	1:B:41:LEU:HD11	0.96	1.95	3	7
1:B:38:PHE:CE1	1:B:41:LEU:HD12	0.96	1.95	3	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PHE:CE2	1:A:41:LEU:HD11	0.96	1.95	3	7
1:B:21:PHE:CE2	1:B:79:LEU:HD23	0.96	1.95	15	1
1:B:20:PHE:CZ	1:B:41:LEU:HD11	0.96	1.95	2	16
1:A:21:PHE:CE2	1:A:79:LEU:HD22	0.95	1.95	1	14
1:B:71:LEU:HD12	1:B:76:TYR:CG	0.94	1.97	13	11
1:B:20:PHE:CE1	1:B:41:LEU:HD11	0.94	1.97	11	13
1:A:21:PHE:CE2	1:A:79:LEU:HD23	0.94	1.95	15	2
1:B:21:PHE:CE2	1:B:79:LEU:HD22	0.94	1.96	1	14
1:B:5:THR:HG22	1:B:6:LEU:HD12	0.93	1.40	3	11
1:A:20:PHE:CE1	1:A:41:LEU:HD11	0.92	1.98	11	13
1:A:21:PHE:CZ	1:A:79:LEU:HD22	0.92	1.99	2	4
1:B:21:PHE:CZ	1:B:79:LEU:HD22	0.92	1.99	2	4
1:A:7:THR:HG21	1:B:41:LEU:HD13	0.92	1.39	16	10
1:A:5:THR:HG22	1:A:6:LEU:HD12	0.92	1.39	3	11
1:A:87:VAL:HG13	1:B:79:LEU:HD12	0.91	1.40	19	8
1:A:6:LEU:HD21	1:B:90:GLU:CG	0.91	1.95	12	10
1:A:79:LEU:HD12	1:B:87:VAL:HG13	0.91	1.42	19	8
1:B:20:PHE:CE1	1:B:41:LEU:HD21	0.91	2.01	12	8
1:A:16:VAL:HG21	1:B:9:LEU:HD23	0.90	1.43	20	1
1:B:35:ILE:CG1	1:B:63:LEU:HD23	0.90	1.96	5	5
1:A:71:LEU:HD12	1:A:76:TYR:CG	0.90	2.01	13	11
1:A:9:LEU:HD23	1:B:16:VAL:HG21	0.90	1.41	20	1
1:B:71:LEU:HD12	1:B:76:TYR:CD2	0.90	2.01	17	11
1:A:90:GLU:CG	1:B:6:LEU:HD21	0.90	1.96	12	8
1:A:16:VAL:CG2	1:B:9:LEU:HD22	0.89	1.97	2	15
1:A:35:ILE:CG1	1:A:63:LEU:HD23	0.89	1.96	5	5
1:B:69:SER:O	1:B:79:LEU:HD22	0.89	1.67	18	1
1:A:9:LEU:HD23	1:B:16:VAL:CG2	0.89	1.97	20	1
1:B:71:LEU:HD11	1:B:76:TYR:HA	0.89	1.45	4	8
1:A:38:PHE:CD1	1:A:41:LEU:HD12	0.89	2.03	14	6
1:B:38:PHE:CD1	1:B:41:LEU:HD12	0.88	2.04	14	6
1:A:9:LEU:CD2	1:B:16:VAL:HG23	0.88	1.98	2	13
1:A:71:LEU:HD12	1:A:76:TYR:CD2	0.88	2.03	17	11
1:A:9:LEU:HD22	1:B:16:VAL:CG2	0.88	1.97	2	15
1:A:69:SER:O	1:A:79:LEU:HD22	0.88	1.69	18	1
1:A:71:LEU:HD11	1:A:76:TYR:HA	0.87	1.46	4	8
1:A:16:VAL:CG2	1:B:9:LEU:HD23	0.87	1.99	20	1
1:B:35:ILE:HG21	1:B:63:LEU:O	0.87	1.70	5	8
1:A:45:GLN:NE2	1:B:7:THR:HG23	0.87	1.84	17	10
1:B:24:ALA:N	1:B:33:LEU:HD12	0.86	1.85	2	12
1:A:35:ILE:HG21	1:A:63:LEU:O	0.86	1.70	5	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:VAL:HG23	1:B:9:LEU:CD2	0.86	1.98	2	14
1:A:80:ILE:CG1	1:B:84:ALA:HB1	0.86	1.99	18	13
1:A:84:ALA:HB1	1:B:80:ILE:CG1	0.86	2.00	18	13
1:A:7:THR:HG23	1:B:45:GLN:NE2	0.85	1.86	15	11
1:A:71:LEU:HD11	1:A:73:PHE:O	0.85	1.70	12	11
1:A:5:THR:HG21	1:B:48:HIS:CG	0.85	2.06	9	2
1:A:24:ALA:N	1:A:33:LEU:HD12	0.85	1.85	2	12
1:B:71:LEU:HD11	1:B:73:PHE:O	0.85	1.70	12	11
1:B:69:SER:O	1:B:79:LEU:HD23	0.84	1.72	14	16
1:B:71:LEU:HD13	1:B:71:LEU:N	0.84	1.86	8	8
1:A:23:PHE:CE2	1:A:33:LEU:HD11	0.84	2.06	11	13
1:A:71:LEU:N	1:A:71:LEU:HD13	0.84	1.88	8	8
1:A:69:SER:O	1:A:79:LEU:HD23	0.84	1.73	3	15
1:A:20:PHE:CE1	1:A:41:LEU:HD21	0.83	2.08	12	9
1:A:90:GLU:HG2	1:B:6:LEU:HD21	0.83	1.50	12	7
1:A:71:LEU:HD21	1:A:76:TYR:CD1	0.83	2.08	14	8
1:A:41:LEU:HD13	1:B:7:THR:HG22	0.83	1.50	6	4
1:B:59:LYS:O	1:B:63:LEU:HD12	0.83	1.73	5	11
1:A:48:HIS:CG	1:B:5:THR:HG21	0.83	2.09	9	2
1:A:1:MET:HG3	1:B:42:ALA:HB3	0.82	1.51	10	10
1:A:23:PHE:CZ	1:A:33:LEU:HD21	0.82	2.08	2	4
1:A:59:LYS:O	1:A:63:LEU:HD12	0.82	1.75	8	10
1:A:41:LEU:HD13	1:B:7:THR:CG2	0.82	2.04	6	8
1:A:7:THR:CG2	1:B:41:LEU:HD13	0.82	2.04	6	7
1:A:80:ILE:HG12	1:B:84:ALA:HB1	0.82	1.50	17	9
1:A:35:ILE:HG23	1:A:67:GLN:HA	0.81	1.52	14	5
1:B:23:PHE:CE2	1:B:33:LEU:HD11	0.81	2.09	11	11
1:B:16:VAL:HG22	1:B:21:PHE:CE2	0.81	2.11	2	14
1:A:79:LEU:HB2	1:B:87:VAL:HG11	0.81	1.52	16	9
1:A:6:LEU:HD23	1:A:10:GLU:OE2	0.81	1.76	17	1
1:B:35:ILE:HG23	1:B:67:GLN:HA	0.81	1.51	14	6
1:B:6:LEU:HD23	1:B:10:GLU:OE2	0.81	1.75	17	1
1:A:24:ALA:HB2	1:A:33:LEU:CD2	0.81	2.05	20	1
1:B:24:ALA:HB2	1:B:33:LEU:CD2	0.81	2.06	20	1
1:A:42:ALA:HB3	1:B:1:MET:HG3	0.80	1.53	9	13
1:B:71:LEU:HD21	1:B:76:TYR:CD1	0.80	2.10	14	8
1:A:4:GLU:OE2	1:B:42:ALA:HB1	0.80	1.76	9	1
1:B:24:ALA:HA	1:B:33:LEU:HD12	0.80	1.54	18	2
1:A:87:VAL:HG11	1:B:79:LEU:HB2	0.80	1.54	4	10
1:A:24:ALA:CA	1:A:33:LEU:HD12	0.79	2.07	18	2
1:A:71:LEU:HD12	1:A:76:TYR:CD1	0.79	2.12	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:23:PHE:CE2	1:B:33:LEU:HD21	0.79	2.12	1	8
1:A:89:LYS:CE	1:B:6:LEU:HD11	0.79	2.08	19	1
1:A:76:TYR:HA	1:A:79:LEU:HD13	0.79	1.52	15	2
1:B:76:TYR:HA	1:B:79:LEU:HD13	0.79	1.53	15	2
1:A:39:LYS:HD3	1:A:63:LEU:HD11	0.79	1.52	20	1
1:A:84:ALA:HB1	1:B:80:ILE:HG12	0.79	1.54	17	10
1:B:24:ALA:CA	1:B:33:LEU:HD12	0.78	2.08	18	2
1:A:6:LEU:HD11	1:B:89:LYS:CE	0.78	2.08	19	1
1:A:76:TYR:O	1:B:87:VAL:HG12	0.78	1.79	18	3
1:B:20:PHE:CE2	1:B:41:LEU:HD21	0.78	2.14	19	1
1:A:23:PHE:CD2	1:A:33:LEU:HD12	0.78	2.13	20	5
1:A:23:PHE:CE2	1:A:33:LEU:HD21	0.77	2.14	1	8
1:A:24:ALA:HA	1:A:33:LEU:HD12	0.77	1.54	18	2
1:A:33:LEU:O	1:A:33:LEU:HD23	0.77	1.80	15	2
1:B:33:LEU:HD23	1:B:33:LEU:O	0.76	1.81	15	3
1:A:42:ALA:HB1	1:B:4:GLU:OE2	0.76	1.79	9	1
1:A:20:PHE:CE2	1:A:41:LEU:HD21	0.76	2.15	19	1
1:B:24:ALA:HB2	1:B:70:GLU:CD	0.76	2.01	16	6
1:A:76:TYR:CE1	1:A:79:LEU:HD11	0.76	2.15	4	10
1:A:24:ALA:HB2	1:A:70:GLU:CD	0.76	2.01	16	6
1:A:16:VAL:HG22	1:A:21:PHE:CE2	0.76	2.15	2	13
1:B:20:PHE:CD1	1:B:41:LEU:HD21	0.76	2.15	12	11
1:B:23:PHE:CZ	1:B:33:LEU:HD21	0.76	2.15	2	4
1:A:20:PHE:CD1	1:A:41:LEU:HD21	0.76	2.15	12	12
1:A:85:LYS:HG2	1:B:3:ALA:HB1	0.76	1.57	3	3
1:A:33:LEU:HD22	1:A:70:GLU:N	0.75	1.96	15	4
1:A:90:GLU:HG3	1:B:6:LEU:HD21	0.75	1.57	16	3
1:A:38:PHE:CZ	1:A:41:LEU:HD12	0.75	2.16	3	13
1:B:39:LYS:HD3	1:B:63:LEU:HD11	0.75	1.54	20	1
1:B:38:PHE:CZ	1:B:41:LEU:HD12	0.75	2.17	13	12
1:B:16:VAL:HG21	1:B:83:LEU:HG	0.75	1.58	2	12
1:B:23:PHE:CD2	1:B:33:LEU:HD12	0.75	2.16	20	5
1:B:35:ILE:HD12	1:B:67:GLN:HA	0.75	1.58	6	3
1:B:33:LEU:HD22	1:B:70:GLU:N	0.74	1.97	15	4
1:A:7:THR:HG22	1:B:41:LEU:HD13	0.74	1.58	6	2
1:A:6:LEU:HD13	1:B:90:GLU:CD	0.74	2.03	2	1
1:B:24:ALA:HB2	1:B:33:LEU:HD22	0.74	1.60	20	1
1:B:71:LEU:HD12	1:B:76:TYR:CD1	0.74	2.17	13	4
1:A:16:VAL:HG21	1:A:83:LEU:HG	0.74	1.59	2	12
1:A:87:VAL:CG1	1:B:79:LEU:HD12	0.74	2.13	19	8
1:A:71:LEU:HD21	1:A:76:TYR:CG	0.73	2.17	2	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:71:LEU:HD21	1:B:76:TYR:CG	0.73	2.17	2	8
1:A:24:ALA:HB2	1:A:33:LEU:HD22	0.73	1.58	20	1
1:B:35:ILE:HD13	1:B:63:LEU:HD23	0.73	1.61	7	4
1:A:33:LEU:HD13	1:A:70:GLU:OE1	0.73	1.84	2	1
1:A:6:LEU:HD21	1:B:90:GLU:HG2	0.73	1.60	12	5
1:B:33:LEU:HD13	1:B:70:GLU:OE1	0.73	1.84	2	1
1:B:35:ILE:N	1:B:35:ILE:HD13	0.73	1.99	5	5
1:B:71:LEU:HD11	1:B:73:PHE:C	0.72	2.05	15	11
1:A:95:ILE:HG23	1:B:74:SER:OG	0.72	1.84	18	2
1:A:7:THR:CG2	1:B:41:LEU:HD22	0.72	2.14	1	3
1:A:33:LEU:HD23	1:A:67:GLN:O	0.72	1.85	12	2
1:B:71:LEU:HD21	1:B:76:TYR:CD2	0.72	2.20	18	1
1:A:6:LEU:HD23	1:A:10:GLU:HB3	0.72	1.61	4	4
1:A:35:ILE:HD12	1:A:67:GLN:HA	0.72	1.59	6	3
1:B:33:LEU:HD23	1:B:67:GLN:O	0.71	1.85	12	2
1:A:16:VAL:HG23	1:B:9:LEU:HB3	0.71	1.59	14	3
1:A:74:SER:OG	1:B:95:ILE:HG23	0.71	1.85	18	2
1:A:35:ILE:HD13	1:A:35:ILE:N	0.71	2.00	5	5
1:A:79:LEU:N	1:A:79:LEU:HD23	0.71	2.00	18	1
1:B:79:LEU:HD23	1:B:79:LEU:N	0.71	2.00	18	1
1:A:35:ILE:HD13	1:A:63:LEU:HD23	0.71	1.61	7	5
1:A:76:TYR:CD1	1:A:79:LEU:HD12	0.71	2.20	2	1
1:B:76:TYR:CE1	1:B:79:LEU:HD11	0.71	2.21	4	7
1:A:23:PHE:CE2	1:A:41:LEU:HD21	0.71	2.20	14	2
1:B:6:LEU:HD23	1:B:10:GLU:HB3	0.70	1.60	4	4
1:B:76:TYR:CD1	1:B:79:LEU:HD12	0.70	2.21	2	1
1:A:16:VAL:HG21	1:A:83:LEU:CD1	0.70	2.15	17	1
1:A:3:ALA:HB1	1:B:85:LYS:HG2	0.70	1.61	3	2
1:A:6:LEU:HD12	1:B:89:LYS:HD2	0.70	1.62	17	2
1:B:15:THR:O	1:B:19:THR:HG23	0.70	1.87	9	10
1:B:6:LEU:HD12	1:B:6:LEU:O	0.70	1.87	9	1
1:A:21:PHE:CD2	1:A:79:LEU:HD22	0.70	2.22	14	10
1:A:24:ALA:N	1:A:33:LEU:HD22	0.70	2.01	3	2
1:B:24:ALA:N	1:B:33:LEU:HD22	0.70	2.02	3	2
1:A:87:VAL:HG12	1:B:76:TYR:O	0.70	1.86	18	2
1:A:84:ALA:HA	1:A:87:VAL:HG12	0.70	1.63	20	1
1:A:6:LEU:HD12	1:A:6:LEU:O	0.70	1.87	9	1
1:A:15:THR:O	1:A:19:THR:HG23	0.70	1.87	9	8
1:B:10:GLU:O	1:B:13:ILE:HG22	0.70	1.87	9	15
1:A:84:ALA:HB1	1:B:80:ILE:CD1	0.70	2.16	19	2
1:A:9:LEU:HB3	1:B:16:VAL:HG23	0.70	1.61	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD12	1:A:47:PRO:CD	0.70	2.17	20	1
1:B:35:ILE:HG13	1:B:63:LEU:HD23	0.69	1.63	5	2
1:A:71:LEU:HD21	1:A:76:TYR:CD2	0.69	2.21	18	1
1:A:71:LEU:HD11	1:A:73:PHE:C	0.69	2.06	15	11
1:A:87:VAL:CG2	1:B:13:ILE:HD11	0.69	2.16	19	1
1:B:20:PHE:CZ	1:B:41:LEU:HD21	0.69	2.22	19	5
1:A:33:LEU:HD22	1:A:70:GLU:HB3	0.69	1.64	15	11
1:A:71:LEU:HD13	1:A:79:LEU:HD21	0.69	1.64	20	1
1:A:71:LEU:HG	1:A:76:TYR:N	0.69	2.03	17	19
1:A:71:LEU:HG	1:A:75:GLU:N	0.69	2.03	15	11
1:A:24:ALA:HA	1:A:33:LEU:HD13	0.69	1.65	14	2
1:A:5:THR:CG2	1:A:6:LEU:HD12	0.69	2.17	8	7
1:A:45:GLN:HE21	1:B:7:THR:HG23	0.69	1.47	10	3
1:B:35:ILE:HG21	1:B:63:LEU:HA	0.68	1.65	7	8
1:A:2:ALA:O	1:B:42:ALA:HB2	0.68	1.89	13	6
1:A:92:ALA:O	1:A:95:ILE:HG22	0.68	1.88	15	4
1:A:90:GLU:CD	1:B:6:LEU:HD13	0.68	2.08	2	1
1:A:23:PHE:HB3	1:A:33:LEU:HD23	0.68	1.63	13	1
1:A:39:LYS:CD	1:A:63:LEU:HD11	0.68	2.17	20	3
1:B:39:LYS:CD	1:B:63:LEU:HD11	0.68	2.18	20	3
1:A:10:GLU:O	1:A:13:ILE:HG22	0.68	1.88	9	15
1:A:23:PHE:CD2	1:A:33:LEU:HD21	0.68	2.24	3	1
1:B:33:LEU:HD22	1:B:70:GLU:HB3	0.68	1.64	15	11
1:A:6:LEU:HD11	1:B:89:LYS:HE2	0.68	1.64	5	2
1:A:35:ILE:HG21	1:A:63:LEU:HA	0.68	1.66	1	6
1:A:35:ILE:HG13	1:A:63:LEU:HD23	0.68	1.63	5	2
1:A:5:THR:HG21	1:B:48:HIS:ND1	0.68	2.02	9	1
1:A:9:LEU:N	1:A:9:LEU:HD23	0.67	2.04	13	10
1:B:23:PHE:CE2	1:B:41:LEU:HD21	0.67	2.24	14	2
1:B:16:VAL:HG21	1:B:83:LEU:CD1	0.67	2.20	17	1
1:A:41:LEU:HD22	1:B:7:THR:CG2	0.67	2.20	12	3
1:A:71:LEU:CD2	1:A:73:PHE:CD1	0.67	2.78	5	11
1:B:71:LEU:HG	1:B:75:GLU:N	0.67	2.04	15	10
1:A:95:ILE:HG23	1:B:74:SER:CB	0.67	2.19	18	6
1:A:71:LEU:C	1:A:71:LEU:HD13	0.66	2.10	12	11
1:A:74:SER:CB	1:B:95:ILE:HG23	0.66	2.20	18	6
1:A:90:GLU:HG3	1:B:6:LEU:HD23	0.66	1.66	7	2
1:A:33:LEU:HD13	1:A:70:GLU:HB3	0.66	1.66	12	16
1:A:89:LYS:HD2	1:B:6:LEU:HD12	0.66	1.65	17	2
1:B:71:LEU:CD2	1:B:73:PHE:CD1	0.66	2.78	5	11
1:B:23:PHE:CD2	1:B:33:LEU:HD21	0.66	2.25	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD23	1:B:90:GLU:HG3	0.66	1.65	7	2
1:B:9:LEU:HD23	1:B:9:LEU:N	0.66	2.04	13	13
1:A:79:LEU:HD12	1:B:87:VAL:CG1	0.66	2.20	13	8
1:B:23:PHE:HB3	1:B:33:LEU:HD23	0.66	1.66	13	1
1:A:71:LEU:HD12	1:A:79:LEU:HD21	0.66	1.67	18	1
1:A:71:LEU:HD13	1:A:71:LEU:N	0.66	2.04	20	1
1:A:35:ILE:HG22	1:A:38:PHE:CD2	0.66	2.26	14	2
1:A:23:PHE:C	1:A:33:LEU:HD22	0.66	2.11	14	1
1:A:5:THR:HG23	1:A:6:LEU:N	0.66	2.06	14	1
1:B:46:LEU:HD12	1:B:47:PRO:CD	0.66	2.21	20	1
1:B:5:THR:HG23	1:B:6:LEU:N	0.66	2.05	14	1
1:A:48:HIS:CD2	1:B:6:LEU:HD11	0.66	2.26	9	1
1:B:35:ILE:HG22	1:B:38:PHE:CD2	0.66	2.26	14	2
1:A:80:ILE:HD11	1:B:84:ALA:HB1	0.66	1.69	19	1
1:A:80:ILE:CD1	1:B:84:ALA:HB1	0.65	2.20	19	2
1:B:6:LEU:HD13	1:B:10:GLU:OE1	0.65	1.91	9	1
1:B:23:PHE:C	1:B:33:LEU:HD22	0.65	2.12	14	1
1:A:52:ASP:O	1:A:53:VAL:HG12	0.65	1.92	5	8
1:A:33:LEU:HD23	1:A:33:LEU:C	0.65	2.12	15	2
1:A:7:THR:HG23	1:B:45:GLN:HE21	0.65	1.52	10	3
1:B:71:LEU:HG	1:B:76:TYR:N	0.65	2.07	12	18
1:A:89:LYS:CD	1:B:5:THR:HG22	0.65	2.22	10	3
1:B:24:ALA:HA	1:B:33:LEU:HD13	0.65	1.68	14	2
1:A:6:LEU:HD21	1:B:90:GLU:HG3	0.65	1.68	1	6
1:B:52:ASP:O	1:B:53:VAL:HG12	0.65	1.92	5	8
1:B:69:SER:C	1:B:79:LEU:HD22	0.65	2.11	18	1
1:B:71:LEU:HD13	1:B:71:LEU:C	0.65	2.12	12	11
1:B:42:ALA:HB3	1:B:59:LYS:HG2	0.65	1.67	16	2
1:A:89:LYS:HE2	1:B:6:LEU:HD11	0.64	1.68	5	2
1:B:95:ILE:HG23	1:B:98:LYS:HE2	0.64	1.69	14	1
1:A:84:ALA:HB1	1:B:80:ILE:HD11	0.64	1.69	19	1
1:B:84:ALA:HA	1:B:87:VAL:HG12	0.64	1.70	20	1
1:B:21:PHE:CD2	1:B:79:LEU:HD22	0.64	2.27	14	9
1:B:33:LEU:HD23	1:B:33:LEU:C	0.64	2.12	15	6
1:B:92:ALA:O	1:B:95:ILE:HG22	0.64	1.91	15	5
1:B:71:LEU:HD11	1:B:76:TYR:CA	0.64	2.22	8	8
1:B:33:LEU:HD13	1:B:70:GLU:HB3	0.64	1.69	4	15
1:B:33:LEU:HD21	1:B:37:GLU:H	0.64	1.51	13	1
1:B:46:LEU:O	1:B:51:LYS:HG3	0.64	1.92	17	2
1:B:71:LEU:N	1:B:71:LEU:CD1	0.64	2.60	4	8
1:B:24:ALA:CA	1:B:33:LEU:HD22	0.64	2.22	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ILE:HD11	1:B:86:GLU:CB	0.64	2.22	12	1
1:B:53:VAL:O	1:B:53:VAL:HG13	0.64	1.92	1	6
1:A:84:ALA:HB1	1:B:80:ILE:HG13	0.64	1.68	5	7
1:A:39:LYS:CE	1:A:63:LEU:HD11	0.64	2.23	10	3
1:A:42:ALA:HB2	1:B:2:ALA:O	0.64	1.92	13	5
1:A:58:GLU:O	1:B:2:ALA:HB2	0.64	1.93	14	2
1:B:71:LEU:HD12	1:B:79:LEU:HD21	0.64	1.70	18	1
1:B:24:ALA:HB1	1:B:72:ARG:HD3	0.64	1.69	6	5
1:A:5:THR:HG22	1:A:6:LEU:CD1	0.64	2.23	13	7
1:B:71:LEU:O	1:B:76:TYR:CE1	0.63	2.51	7	11
1:A:2:ALA:HB3	1:B:59:LYS:HE3	0.63	1.70	3	1
1:A:6:LEU:HD13	1:A:10:GLU:OE1	0.63	1.92	9	1
1:A:50:LEU:HD22	1:A:93:LEU:HD13	0.63	1.70	11	2
1:B:20:PHE:CZ	1:B:23:PHE:CE2	0.63	2.86	3	3
1:B:71:LEU:HD13	1:B:79:LEU:HD21	0.63	1.68	20	1
1:A:83:LEU:HD13	1:B:83:LEU:HD22	0.63	1.70	18	2
1:A:48:HIS:ND1	1:B:5:THR:HG21	0.63	2.08	9	1
1:A:24:ALA:CA	1:A:33:LEU:HD22	0.63	2.22	3	1
1:B:5:THR:CG2	1:B:6:LEU:HD12	0.63	2.24	8	7
1:A:7:THR:HG23	1:B:45:GLN:CD	0.63	2.14	16	2
1:A:35:ILE:HD12	1:A:35:ILE:H	0.63	1.53	13	2
1:A:23:PHE:CZ	1:A:41:LEU:HD21	0.63	2.28	14	2
1:A:13:ILE:O	1:A:17:VAL:HG12	0.63	1.94	8	17
1:A:71:LEU:N	1:A:71:LEU:CD1	0.63	2.61	2	8
1:A:59:LYS:HE3	1:B:2:ALA:HB3	0.63	1.69	3	1
1:A:85:LYS:HD2	1:B:3:ALA:HB3	0.63	1.71	10	1
1:A:2:ALA:HB2	1:B:58:GLU:O	0.63	1.94	14	2
1:B:71:LEU:HD11	1:B:76:TYR:CG	0.63	2.29	18	1
1:A:20:PHE:CZ	1:A:41:LEU:HD21	0.62	2.29	19	5
1:A:41:LEU:HD22	1:B:7:THR:HG22	0.62	1.71	1	3
1:A:71:LEU:HD22	1:A:72:ARG:H	0.62	1.52	11	10
1:B:16:VAL:HG22	1:B:21:PHE:CZ	0.62	2.30	12	8
1:A:20:PHE:CZ	1:A:23:PHE:CZ	0.62	2.87	18	2
1:A:95:ILE:HG23	1:A:98:LYS:HE2	0.62	1.71	14	1
1:B:13:ILE:O	1:B:17:VAL:HG12	0.62	1.94	19	17
1:B:21:PHE:CE1	1:B:79:LEU:HD22	0.62	2.29	2	2
1:A:80:ILE:HG13	1:B:84:ALA:HB1	0.62	1.69	5	6
1:B:71:LEU:HD22	1:B:72:ARG:H	0.62	1.54	11	10
1:A:24:ALA:HB1	1:A:72:ARG:HD3	0.62	1.70	8	5
1:A:20:PHE:CZ	1:A:23:PHE:CE2	0.62	2.88	3	3
1:A:76:TYR:CD1	1:A:79:LEU:HD22	0.62	2.29	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:PHE:CZ	1:B:23:PHE:CZ	0.62	2.87	18	2
1:A:71:LEU:O	1:A:76:TYR:CE1	0.62	2.52	7	11
1:B:35:ILE:HD12	1:B:35:ILE:H	0.62	1.54	13	3
1:A:33:LEU:HD21	1:A:37:GLU:H	0.62	1.53	13	1
1:A:53:VAL:HG13	1:A:53:VAL:O	0.61	1.94	5	4
1:A:77:TRP:O	1:A:80:ILE:HG22	0.61	1.95	18	6
1:B:39:LYS:CE	1:B:63:LEU:HD11	0.61	2.25	10	2
1:A:3:ALA:HB3	1:B:85:LYS:HD2	0.61	1.70	10	1
1:A:42:ALA:HB3	1:A:59:LYS:HG2	0.61	1.72	16	2
1:A:50:LEU:HD11	1:A:89:LYS:CD	0.61	2.26	5	1
1:A:21:PHE:CE1	1:A:79:LEU:HD22	0.61	2.30	2	2
1:A:21:PHE:HE2	1:A:79:LEU:HD13	0.61	1.54	20	2
1:B:21:PHE:HE2	1:B:79:LEU:HD13	0.61	1.54	20	2
1:B:33:LEU:HD21	1:B:69:SER:HB3	0.61	1.73	15	1
1:A:16:VAL:HG22	1:A:21:PHE:CZ	0.61	2.31	12	6
1:A:48:HIS:CB	1:B:5:THR:HG21	0.61	2.26	3	3
1:B:5:THR:HG22	1:B:6:LEU:CD1	0.61	2.26	13	7
1:A:24:ALA:HA	1:A:33:LEU:HB2	0.61	1.73	13	3
1:A:69:SER:C	1:A:79:LEU:HD22	0.61	2.14	18	1
1:A:13:ILE:HD11	1:B:87:VAL:CG2	0.61	2.25	19	1
1:A:6:LEU:HD11	1:B:48:HIS:CD2	0.61	2.30	9	1
1:A:33:LEU:C	1:A:33:LEU:HD23	0.61	2.15	17	4
1:A:71:LEU:HD11	1:A:76:TYR:CA	0.61	2.22	4	8
1:A:83:LEU:HD22	1:B:83:LEU:HD13	0.61	1.73	18	2
1:A:71:LEU:HD22	1:A:72:ARG:N	0.61	2.11	12	11
1:A:73:PHE:C	1:B:95:ILE:HG23	0.61	2.16	19	3
1:B:50:LEU:HD22	1:B:93:LEU:HD13	0.61	1.71	11	2
1:B:6:LEU:HD23	1:B:10:GLU:CB	0.60	2.26	4	1
1:A:5:THR:HG22	1:B:89:LYS:CD	0.60	2.25	9	3
1:B:76:TYR:CD1	1:B:79:LEU:HD22	0.60	2.30	15	2
1:A:85:LYS:HE3	1:B:3:ALA:HB2	0.60	1.71	5	2
1:B:95:ILE:HG23	1:B:95:ILE:O	0.60	1.95	3	4
1:A:6:LEU:HD23	1:A:10:GLU:CB	0.60	2.26	4	1
1:B:23:PHE:CZ	1:B:41:LEU:HD21	0.60	2.31	14	2
1:A:86:GLU:CB	1:B:13:ILE:HD11	0.60	2.26	12	1
1:A:95:ILE:O	1:A:95:ILE:HG23	0.60	1.97	3	3
1:A:95:ILE:HG23	1:B:73:PHE:C	0.60	2.17	19	3
1:A:33:LEU:HD21	1:A:69:SER:HB3	0.60	1.72	15	1
1:A:9:LEU:HD21	1:B:21:PHE:CE1	0.60	2.32	19	1
1:A:21:PHE:CE1	1:B:9:LEU:HD21	0.60	2.32	19	1
1:B:71:LEU:HD22	1:B:72:ARG:N	0.60	2.12	12	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD11	1:B:89:LYS:HE3	0.60	1.73	19	1
1:B:23:PHE:CD2	1:B:37:GLU:HB2	0.60	2.32	13	2
1:A:9:LEU:CB	1:B:16:VAL:HG23	0.60	2.26	14	2
1:B:39:LYS:HD3	1:B:63:LEU:HD21	0.59	1.72	8	2
1:B:71:LEU:HD21	1:B:74:SER:N	0.59	2.12	1	9
1:B:76:TYR:CD1	1:B:79:LEU:CD1	0.59	2.85	6	10
1:B:71:LEU:HD22	1:B:71:LEU:C	0.59	2.17	4	9
1:A:13:ILE:HD13	1:A:13:ILE:O	0.59	1.96	14	3
1:A:45:GLN:CD	1:B:7:THR:HG23	0.59	2.16	16	2
1:A:5:THR:HG21	1:B:89:LYS:HB3	0.59	1.72	19	1
1:A:76:TYR:CD1	1:A:79:LEU:CD1	0.59	2.83	6	9
1:A:39:LYS:HE2	1:A:63:LEU:HD11	0.59	1.73	14	3
1:A:70:GLU:HB2	1:A:79:LEU:HD21	0.59	1.73	2	1
1:B:6:LEU:HD12	1:B:10:GLU:CB	0.59	2.27	2	1
1:A:5:THR:HG23	1:B:89:LYS:HE3	0.59	1.73	8	1
1:B:24:ALA:HA	1:B:33:LEU:HB2	0.59	1.73	13	4
1:A:21:PHE:CZ	1:A:79:LEU:HD23	0.59	2.31	15	1
1:A:24:ALA:HB3	1:A:72:ARG:HD3	0.59	1.74	13	1
1:A:71:LEU:C	1:A:71:LEU:HD22	0.59	2.18	4	5
1:B:77:TRP:O	1:B:80:ILE:HG22	0.59	1.98	18	7
1:A:95:ILE:HG23	1:A:95:ILE:O	0.59	1.98	14	1
1:A:74:SER:HB3	1:B:95:ILE:HG23	0.59	1.75	6	4
1:B:13:ILE:HD13	1:B:13:ILE:O	0.59	1.97	14	5
1:A:6:LEU:HD21	1:B:90:GLU:CD	0.59	2.18	16	2
1:A:24:ALA:HB3	1:A:72:ARG:CD	0.59	2.27	13	1
1:B:24:ALA:HB3	1:B:72:ARG:CD	0.59	2.28	13	1
1:A:6:LEU:HD12	1:A:10:GLU:CB	0.59	2.28	2	1
1:A:24:ALA:HB2	1:A:70:GLU:HG2	0.59	1.74	10	5
1:A:20:PHE:HD2	1:B:9:LEU:HD21	0.58	1.58	13	6
1:A:39:LYS:HD3	1:A:63:LEU:HD21	0.58	1.73	8	2
1:A:89:LYS:CD	1:B:6:LEU:HD12	0.58	2.28	17	1
1:A:71:LEU:CD2	1:A:76:TYR:CD1	0.58	2.85	6	8
1:B:71:LEU:CD2	1:B:76:TYR:CD1	0.58	2.86	6	8
1:B:50:LEU:HD13	1:B:93:LEU:HD13	0.58	1.75	5	2
1:A:46:LEU:O	1:A:51:LYS:HG3	0.58	1.98	10	2
1:A:85:LYS:HE3	1:B:3:ALA:HB3	0.58	1.73	19	1
1:A:71:LEU:N	1:A:79:LEU:HD11	0.58	2.13	17	1
1:B:31:GLY:O	1:B:72:ARG:N	0.58	2.37	3	18
1:A:35:ILE:HG12	1:A:63:LEU:HD23	0.58	1.75	5	3
1:A:23:PHE:CG	1:A:33:LEU:HD21	0.58	2.34	3	1
1:A:48:HIS:HB3	1:B:5:THR:HG21	0.58	1.74	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:GLU:HG2	1:B:6:LEU:HD11	0.58	1.75	6	2
1:A:24:ALA:HB2	1:A:70:GLU:OE1	0.58	1.98	16	2
1:B:21:PHE:CZ	1:B:79:LEU:HD23	0.58	2.32	15	1
1:A:6:LEU:HD12	1:B:89:LYS:CD	0.58	2.28	17	1
1:A:9:LEU:HD21	1:B:20:PHE:HD2	0.58	1.59	13	6
1:B:24:ALA:HB2	1:B:70:GLU:HG2	0.58	1.74	12	5
1:B:13:ILE:HD12	1:B:83:LEU:HD21	0.58	1.75	19	1
1:B:24:ALA:HA	1:B:33:LEU:HD22	0.58	1.75	3	1
1:A:35:ILE:CD1	1:A:63:LEU:HD23	0.58	2.29	1	3
1:A:42:ALA:CB	1:A:59:LYS:HG2	0.58	2.29	9	18
1:A:89:LYS:HE3	1:B:5:THR:HG23	0.58	1.76	8	1
1:A:33:LEU:HD13	1:A:70:GLU:CB	0.58	2.28	12	12
1:B:21:PHE:N	1:B:21:PHE:CD1	0.58	2.70	13	9
1:A:33:LEU:HD23	1:A:70:GLU:HB3	0.58	1.76	14	2
1:B:50:LEU:HD11	1:B:89:LYS:CD	0.58	2.28	5	1
1:A:21:PHE:N	1:A:21:PHE:CD1	0.57	2.69	13	10
1:A:33:LEU:HD23	1:A:33:LEU:O	0.57	1.98	17	1
1:A:24:ALA:CB	1:A:33:LEU:HD22	0.57	2.29	20	1
1:B:35:ILE:HD13	1:B:35:ILE:H	0.57	1.59	11	1
1:A:79:LEU:CB	1:B:87:VAL:HG11	0.57	2.30	17	2
1:A:35:ILE:HD12	1:A:35:ILE:N	0.57	2.13	13	3
1:B:24:ALA:HB3	1:B:72:ARG:HD3	0.57	1.75	13	1
1:A:46:LEU:HD12	1:A:47:PRO:CG	0.57	2.29	20	1
1:A:20:PHE:CE1	1:A:23:PHE:CE2	0.57	2.93	18	6
1:A:59:LYS:CE	1:B:2:ALA:HB3	0.57	2.29	3	1
1:A:45:GLN:HE22	1:B:7:THR:HG23	0.57	1.59	15	3
1:B:35:ILE:HD12	1:B:35:ILE:N	0.57	2.14	13	3
1:A:23:PHE:CD2	1:A:37:GLU:HB2	0.57	2.33	13	2
1:B:63:LEU:HD23	1:B:64:ASP:N	0.57	2.14	14	2
1:A:35:ILE:CD1	1:A:63:LEU:HD21	0.57	2.29	18	1
1:A:3:ALA:HB2	1:B:85:LYS:HE3	0.57	1.75	5	2
1:A:7:THR:HG22	1:B:41:LEU:HD22	0.57	1.76	12	3
1:A:20:PHE:CD2	1:B:9:LEU:HD21	0.57	2.35	15	3
1:A:16:VAL:HG23	1:B:9:LEU:CB	0.57	2.29	14	2
1:A:3:ALA:HB3	1:B:85:LYS:HE3	0.57	1.75	19	1
1:A:71:LEU:O	1:A:71:LEU:HD22	0.57	1.99	14	4
1:A:50:LEU:HD13	1:A:93:LEU:HD13	0.57	1.74	5	2
1:B:24:ALA:HB2	1:B:70:GLU:OE1	0.57	2.00	16	2
1:B:35:ILE:HG21	1:B:63:LEU:CA	0.57	2.29	1	3
1:B:35:ILE:CD1	1:B:63:LEU:HD23	0.57	2.30	1	3
1:B:70:GLU:CG	1:B:71:LEU:N	0.57	2.67	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD11	1:A:76:TYR:CG	0.57	2.34	18	1
1:A:23:PHE:CG	1:A:37:GLU:HB2	0.56	2.35	7	15
1:A:9:LEU:HD21	1:B:20:PHE:CD2	0.56	2.35	15	3
1:A:87:VAL:HG11	1:B:79:LEU:CB	0.56	2.30	17	2
1:B:85:LYS:O	1:B:89:LYS:CE	0.56	2.53	6	9
1:B:76:TYR:HD1	1:B:79:LEU:HD12	0.56	1.60	2	1
1:A:2:ALA:HB3	1:B:59:LYS:CE	0.56	2.30	3	1
1:A:31:GLY:O	1:A:72:ARG:N	0.56	2.38	3	18
1:A:51:LYS:HA	1:B:5:THR:HG21	0.56	1.77	4	2
1:A:91:LYS:HA	1:B:76:TYR:HB2	0.56	1.78	18	18
1:B:71:LEU:HD22	1:B:71:LEU:O	0.56	1.99	14	7
1:A:5:THR:HG21	1:B:51:LYS:HA	0.56	1.76	4	1
1:A:89:LYS:HB3	1:B:5:THR:HG21	0.56	1.77	19	1
1:A:35:ILE:HG21	1:A:63:LEU:CA	0.56	2.31	1	3
1:A:89:LYS:HD2	1:B:5:THR:HG22	0.56	1.76	6	3
1:B:76:TYR:CG	1:B:79:LEU:HD11	0.56	2.35	10	5
1:A:16:VAL:HG11	1:A:83:LEU:HD11	0.56	1.75	18	3
1:A:23:PHE:CE2	1:A:33:LEU:HD12	0.56	2.34	20	1
1:B:33:LEU:HD23	1:B:70:GLU:HB3	0.56	1.77	3	2
1:B:46:LEU:HD12	1:B:47:PRO:CG	0.56	2.31	20	1
1:A:23:PHE:CD1	1:A:37:GLU:HB2	0.56	2.36	2	11
1:B:20:PHE:CE1	1:B:23:PHE:CE2	0.56	2.94	18	3
1:A:31:GLY:HA3	1:A:73:PHE:CE2	0.56	2.35	12	1
1:A:13:ILE:HD12	1:A:83:LEU:HD21	0.56	1.77	19	1
1:A:46:LEU:HD12	1:A:47:PRO:HG3	0.56	1.77	20	1
1:A:23:PHE:CZ	1:A:33:LEU:CD2	0.56	2.88	1	2
1:A:5:THR:HG22	1:A:6:LEU:N	0.56	2.15	19	10
1:A:13:ILE:O	1:A:13:ILE:HD13	0.56	2.00	9	9
1:B:23:PHE:CG	1:B:33:LEU:HD11	0.56	2.35	19	4
1:B:71:LEU:HD21	1:B:73:PHE:CD1	0.56	2.36	7	10
1:A:76:TYR:CE1	1:A:79:LEU:HD22	0.56	2.35	15	2
1:B:35:ILE:CD1	1:B:63:LEU:HD21	0.56	2.30	18	1
1:A:87:VAL:HG22	1:B:13:ILE:HD11	0.56	1.75	19	1
1:A:50:LEU:HD11	1:A:89:LYS:O	0.56	1.99	2	1
1:B:23:PHE:CG	1:B:33:LEU:HD21	0.56	2.36	3	1
1:A:35:ILE:HD13	1:A:35:ILE:H	0.56	1.60	11	1
1:A:24:ALA:HA	1:A:33:LEU:HD22	0.56	1.75	3	1
1:A:76:TYR:CG	1:A:79:LEU:HD11	0.56	2.36	8	6
1:A:21:PHE:HA	1:A:70:GLU:OE1	0.55	2.01	2	5
1:A:23:PHE:CE2	1:A:33:LEU:CD1	0.55	2.89	5	6
1:B:23:PHE:CD2	1:B:33:LEU:CD1	0.55	2.89	17	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LYS:HD3	1:B:5:THR:HG23	0.55	1.78	20	2
1:A:5:THR:CG2	1:B:48:HIS:CD2	0.55	2.88	14	1
1:B:42:ALA:CB	1:B:59:LYS:HG2	0.55	2.31	19	18
1:A:63:LEU:HD23	1:A:64:ASP:N	0.55	2.17	18	2
1:B:56:LEU:N	1:B:56:LEU:HD22	0.55	2.17	18	1
1:A:20:PHE:CZ	1:A:41:LEU:CD1	0.55	2.88	12	7
1:A:6:LEU:HD12	1:A:10:GLU:HB3	0.55	1.79	2	1
1:A:56:LEU:N	1:A:56:LEU:HD22	0.55	2.16	18	1
1:A:20:PHE:CE1	1:A:23:PHE:CD2	0.55	2.94	12	10
1:B:23:PHE:CG	1:B:37:GLU:HB2	0.55	2.36	10	16
1:B:70:GLU:C	1:B:71:LEU:HD13	0.55	2.20	8	2
1:B:60:MET:HA	1:B:63:LEU:HD13	0.55	1.79	3	1
1:A:23:PHE:CD2	1:A:33:LEU:CD1	0.55	2.89	17	11
1:A:79:LEU:HD12	1:A:79:LEU:N	0.55	2.17	15	1
1:B:71:LEU:CD1	1:B:71:LEU:N	0.55	2.70	18	1
1:A:70:GLU:CG	1:A:71:LEU:N	0.55	2.69	15	9
1:A:49:LEU:C	1:A:49:LEU:HD23	0.55	2.21	4	2
1:B:49:LEU:C	1:B:49:LEU:HD23	0.55	2.22	4	2
1:A:95:ILE:N	1:B:73:PHE:O	0.55	2.40	10	12
1:B:33:LEU:HD13	1:B:70:GLU:CB	0.55	2.31	12	11
1:A:31:GLY:CA	1:A:73:PHE:CE2	0.55	2.90	12	1
1:B:31:GLY:HA3	1:B:73:PHE:CE2	0.55	2.36	12	1
1:B:21:PHE:HA	1:B:33:LEU:HD11	0.55	1.78	20	1
1:A:59:LYS:HA	1:B:2:ALA:HB2	0.55	1.79	12	7
1:A:33:LEU:HD22	1:A:70:GLU:H	0.55	1.61	5	4
1:A:6:LEU:HD11	1:B:90:GLU:HG2	0.55	1.76	6	2
1:A:21:PHE:CD2	1:A:79:LEU:HD23	0.55	2.36	15	1
1:A:21:PHE:HA	1:A:33:LEU:HD11	0.55	1.79	20	1
1:B:31:GLY:CA	1:B:73:PHE:CD2	0.55	2.90	12	1
1:A:23:PHE:CD2	1:A:37:GLU:CB	0.55	2.90	14	2
1:B:20:PHE:CZ	1:B:41:LEU:CD2	0.55	2.90	19	1
1:B:46:LEU:HD12	1:B:47:PRO:HG3	0.55	1.79	20	1
1:A:71:LEU:HD21	1:A:73:PHE:CD1	0.55	2.37	11	10
1:A:95:ILE:HG23	1:B:74:SER:HB3	0.54	1.79	2	4
1:A:6:LEU:HD23	1:B:90:GLU:CG	0.54	2.31	7	2
1:B:16:VAL:HG11	1:B:83:LEU:HD11	0.54	1.77	18	3
1:A:85:LYS:HZ3	1:B:7:THR:CB	0.54	2.15	1	1
1:B:70:GLU:HB2	1:B:79:LEU:HD21	0.54	1.77	2	1
1:A:33:LEU:N	1:A:33:LEU:HD23	0.54	2.17	20	1
1:B:50:LEU:HD11	1:B:89:LYS:O	0.54	2.01	2	1
1:A:87:VAL:HG11	1:B:79:LEU:HD12	0.54	1.80	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:TYR:CE1	1:A:79:LEU:CD1	0.54	2.91	18	1
1:A:53:VAL:O	1:A:53:VAL:CG1	0.54	2.56	5	4
1:A:85:LYS:O	1:A:89:LYS:CE	0.54	2.55	6	8
1:B:53:VAL:O	1:B:53:VAL:CG1	0.54	2.55	6	6
1:B:71:LEU:N	1:B:79:LEU:HD11	0.54	2.17	17	1
1:A:71:LEU:CD1	1:A:71:LEU:N	0.54	2.71	18	1
1:B:51:LYS:HG2	1:B:52:ASP:N	0.54	2.18	6	12
1:A:71:LEU:HD22	1:A:71:LEU:C	0.54	2.23	14	4
1:B:23:PHE:CE2	1:B:33:LEU:CD1	0.54	2.91	16	5
1:A:21:PHE:CE2	1:A:79:LEU:CD2	0.54	2.91	9	6
1:A:83:LEU:HD22	1:B:83:LEU:HD22	0.54	1.80	1	4
1:B:33:LEU:HB3	1:B:70:GLU:HB3	0.54	1.80	5	9
1:B:79:LEU:N	1:B:79:LEU:CD2	0.54	2.70	18	1
1:B:46:LEU:CB	1:B:47:PRO:CD	0.54	2.86	15	14
1:B:20:PHE:CZ	1:B:41:LEU:CD1	0.54	2.90	9	6
1:B:6:LEU:HD12	1:B:10:GLU:HB3	0.54	1.79	2	1
1:A:71:LEU:HD22	1:A:71:LEU:O	0.54	2.03	3	3
1:B:71:LEU:HD23	1:B:73:PHE:C	0.54	2.23	18	1
1:A:23:PHE:CG	1:A:33:LEU:HD11	0.54	2.38	18	4
1:B:95:ILE:HG21	1:B:98:LYS:HE2	0.54	1.80	20	2
1:B:33:LEU:HD22	1:B:70:GLU:H	0.54	1.62	5	3
1:B:35:ILE:N	1:B:35:ILE:CD1	0.54	2.70	5	4
1:A:46:LEU:CB	1:A:47:PRO:CD	0.53	2.86	16	14
1:A:71:LEU:HD21	1:A:74:SER:N	0.53	2.18	1	8
1:A:21:PHE:O	1:A:33:LEU:HD21	0.53	2.03	20	1
1:B:16:VAL:CG2	1:B:21:PHE:CZ	0.53	2.91	13	3
1:A:6:LEU:CD2	1:B:48:HIS:CD2	0.53	2.91	2	1
1:B:20:PHE:O	1:B:23:PHE:CD1	0.53	2.62	13	3
1:B:23:PHE:CZ	1:B:33:LEU:CD2	0.53	2.91	1	1
1:A:48:HIS:CD2	1:B:6:LEU:CD1	0.53	2.91	9	1
1:A:48:HIS:CD2	1:B:5:THR:CG2	0.53	2.91	14	1
1:A:82:GLU:O	1:B:9:LEU:HD13	0.53	2.03	14	1
1:B:71:LEU:HB3	1:B:76:TYR:CD1	0.53	2.38	12	10
1:B:39:LYS:HE2	1:B:63:LEU:HD11	0.53	1.79	14	3
1:A:20:PHE:HA	1:A:23:PHE:CE1	0.53	2.39	13	2
1:B:33:LEU:HD23	1:B:33:LEU:N	0.53	2.18	20	1
1:A:31:GLY:O	1:A:73:PHE:CD1	0.53	2.61	2	3
1:A:1:MET:HG2	1:B:39:LYS:HA	0.53	1.80	12	4
1:A:48:HIS:NE2	1:B:6:LEU:HD21	0.53	2.18	9	1
1:A:71:LEU:O	1:A:76:TYR:CZ	0.53	2.61	17	8
1:A:38:PHE:O	1:A:41:LEU:HG	0.53	2.03	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LYS:HA	1:B:1:MET:HB2	0.53	1.81	10	6
1:A:48:HIS:CD2	1:B:6:LEU:HD21	0.53	2.38	2	1
1:A:83:LEU:HD22	1:B:87:VAL:CG2	0.53	2.32	17	2
1:A:86:GLU:HA	1:B:6:LEU:HD23	0.53	1.80	6	1
1:B:24:ALA:CB	1:B:33:LEU:HD22	0.53	2.31	20	1
1:B:73:PHE:CZ	1:B:75:GLU:CG	0.53	2.92	20	5
1:A:32:SER:HB3	1:A:73:PHE:CE1	0.53	2.38	12	8
1:A:71:LEU:HG	1:A:75:GLU:CB	0.53	2.33	20	8
1:B:21:PHE:CD2	1:B:79:LEU:HD23	0.53	2.37	15	1
1:A:71:LEU:HB3	1:A:76:TYR:CD1	0.53	2.37	10	10
1:A:48:HIS:CD2	1:B:6:LEU:CD2	0.53	2.91	2	1
1:A:2:ALA:HB2	1:B:59:LYS:HA	0.53	1.80	12	6
1:B:21:PHE:O	1:B:33:LEU:HD21	0.53	2.04	20	1
1:A:16:VAL:N	1:B:12:ALA:HB2	0.53	2.19	15	10
1:A:33:LEU:CB	1:A:70:GLU:CG	0.53	2.86	19	6
1:A:70:GLU:HA	1:A:79:LEU:HD21	0.53	1.81	15	2
1:B:46:LEU:CB	1:B:47:PRO:HD3	0.53	2.34	10	18
1:A:70:GLU:C	1:A:71:LEU:HD13	0.53	2.22	8	2
1:A:32:SER:CB	1:A:73:PHE:CE1	0.53	2.92	18	3
1:A:39:LYS:HA	1:B:1:MET:HG2	0.53	1.80	12	2
1:A:9:LEU:HD13	1:B:82:GLU:O	0.53	2.04	14	1
1:B:33:LEU:CD2	1:B:72:ARG:CD	0.53	2.87	20	1
1:B:33:LEU:CD1	1:B:70:GLU:HB2	0.53	2.34	20	1
1:A:20:PHE:CE1	1:A:41:LEU:CD2	0.53	2.87	12	4
1:A:41:LEU:CD1	1:B:7:THR:HG21	0.53	2.25	1	3
1:B:16:VAL:HB	1:B:83:LEU:HD21	0.53	1.81	12	3
1:A:60:MET:HA	1:A:63:LEU:HD13	0.53	1.79	3	1
1:B:89:LYS:HG3	1:B:90:GLU:N	0.53	2.19	19	4
1:B:21:PHE:CE2	1:B:79:LEU:CD2	0.53	2.91	10	6
1:B:24:ALA:CB	1:B:72:ARG:CG	0.53	2.86	13	1
1:A:87:VAL:HG23	1:B:79:LEU:HD12	0.53	1.81	20	1
1:B:31:GLY:O	1:B:73:PHE:CD1	0.52	2.62	2	3
1:B:32:SER:CB	1:B:73:PHE:CE1	0.52	2.92	18	3
1:A:33:LEU:CD1	1:A:70:GLU:HB2	0.52	2.32	20	1
1:A:16:VAL:CG2	1:A:21:PHE:CZ	0.52	2.92	13	3
1:A:20:PHE:O	1:A:23:PHE:CD1	0.52	2.62	18	4
1:A:87:VAL:CG2	1:B:83:LEU:HD22	0.52	2.34	17	2
1:B:71:LEU:C	1:B:71:LEU:CD2	0.52	2.77	4	3
1:B:48:HIS:CG	1:B:49:LEU:N	0.52	2.78	9	3
1:A:24:ALA:CB	1:A:72:ARG:CG	0.52	2.87	13	1
1:A:83:LEU:N	1:B:9:LEU:HD12	0.52	2.19	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:PHE:CZ	1:A:75:GLU:CG	0.52	2.92	20	6
1:B:23:PHE:CD1	1:B:37:GLU:HB2	0.52	2.39	11	10
1:A:85:LYS:CD	1:B:3:ALA:CB	0.52	2.88	7	1
1:A:18:SER:O	1:A:22:THR:CG2	0.52	2.58	17	20
1:B:71:LEU:O	1:B:76:TYR:CZ	0.52	2.62	17	8
1:A:71:LEU:HG	1:A:75:GLU:CA	0.52	2.35	16	7
1:A:71:LEU:C	1:A:71:LEU:CD2	0.52	2.78	4	3
1:A:67:GLN:NE2	1:A:68:ASP:CA	0.52	2.72	5	3
1:B:41:LEU:HD23	1:B:41:LEU:N	0.52	2.19	8	2
1:B:31:GLY:CA	1:B:73:PHE:CE2	0.52	2.91	12	1
1:A:33:LEU:CD2	1:A:72:ARG:CD	0.52	2.87	20	1
1:A:12:ALA:HB2	1:B:16:VAL:N	0.52	2.20	16	9
1:A:24:ALA:CB	1:A:33:LEU:HB2	0.52	2.35	4	10
1:A:71:LEU:HG	1:A:75:GLU:C	0.52	2.25	2	11
1:B:20:PHE:CE1	1:B:41:LEU:CD2	0.52	2.86	12	4
1:B:38:PHE:O	1:B:41:LEU:HG	0.52	2.04	2	15
1:A:31:GLY:CA	1:A:73:PHE:CD2	0.52	2.92	12	1
1:A:33:LEU:HB3	1:A:70:GLU:HB3	0.52	1.82	5	8
1:A:71:LEU:CB	1:A:75:GLU:HB2	0.52	2.35	6	7
1:A:6:LEU:CD1	1:B:48:HIS:CD2	0.52	2.92	9	1
1:A:7:THR:HG23	1:B:45:GLN:HG3	0.52	1.81	14	1
1:B:23:PHE:CD2	1:B:37:GLU:CB	0.52	2.92	14	1
1:A:16:VAL:HB	1:A:83:LEU:HD21	0.52	1.82	12	3
1:A:46:LEU:CB	1:A:47:PRO:HD3	0.52	2.33	10	18
1:A:21:PHE:O	1:A:70:GLU:OE2	0.52	2.27	5	8
1:A:33:LEU:HG	1:A:34:ASN:N	0.52	2.20	14	4
1:A:82:GLU:HB3	1:B:9:LEU:HD11	0.52	1.82	6	7
1:B:21:PHE:HA	1:B:70:GLU:OE1	0.52	2.05	2	5
1:A:82:GLU:C	1:B:9:LEU:HD12	0.52	2.25	3	4
1:A:24:ALA:CB	1:A:72:ARG:CD	0.52	2.88	13	1
1:A:72:ARG:CD	1:A:72:ARG:N	0.52	2.72	20	2
1:A:70:GLU:HG2	1:A:71:LEU:N	0.52	2.20	16	1
1:A:20:PHE:CZ	1:A:41:LEU:CD2	0.52	2.92	19	1
1:A:76:TYR:O	1:B:87:VAL:CG1	0.52	2.58	5	15
1:A:23:PHE:CZ	1:A:33:LEU:HG	0.52	2.40	17	3
1:A:86:GLU:HB2	1:B:13:ILE:HD11	0.52	1.81	12	1
1:B:24:ALA:CB	1:B:72:ARG:CD	0.52	2.88	13	1
1:A:20:PHE:CE2	1:A:41:LEU:CD2	0.52	2.92	19	1
1:B:45:GLN:O	1:B:51:LYS:CE	0.52	2.58	19	1
1:A:84:ALA:CA	1:A:87:VAL:HG12	0.52	2.32	20	1
1:B:24:ALA:HB2	1:B:33:LEU:HD23	0.52	1.79	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:PHE:O	1:B:95:ILE:N	0.51	2.43	10	11
1:B:18:SER:O	1:B:22:THR:CG2	0.51	2.58	18	20
1:A:21:PHE:CG	1:A:70:GLU:OE1	0.51	2.63	4	2
1:B:21:PHE:CG	1:B:70:GLU:OE1	0.51	2.63	4	2
1:B:23:PHE:CZ	1:B:33:LEU:HG	0.51	2.40	17	3
1:A:70:GLU:HA	1:A:79:LEU:HD23	0.51	1.81	19	5
1:A:42:ALA:O	1:A:46:LEU:CG	0.51	2.58	20	2
1:A:5:THR:HG23	1:B:89:LYS:HD3	0.51	1.81	20	2
1:A:1:MET:HE2	1:B:59:LYS:HE3	0.51	1.80	16	1
1:A:7:THR:HG21	1:B:41:LEU:CD1	0.51	2.34	9	3
1:A:68:ASP:O	1:A:78:ARG:CB	0.51	2.59	5	8
1:A:42:ALA:HA	1:A:45:GLN:HB2	0.51	1.82	9	3
1:A:5:THR:HG22	1:B:89:LYS:HD2	0.51	1.81	6	3
1:A:79:LEU:HD12	1:B:87:VAL:HG11	0.51	1.81	13	1
1:B:79:LEU:N	1:B:79:LEU:HD12	0.51	2.19	15	1
1:A:71:LEU:HD23	1:A:73:PHE:C	0.51	2.26	18	1
1:B:33:LEU:CB	1:B:70:GLU:CG	0.51	2.89	1	6
1:B:16:VAL:HG21	1:B:83:LEU:CG	0.51	2.35	3	4
1:B:75:GLU:OE1	1:B:77:TRP:CE2	0.51	2.64	14	4
1:B:33:LEU:HB3	1:B:70:GLU:CB	0.51	2.36	1	8
1:A:42:ALA:O	1:A:46:LEU:HG	0.51	2.06	12	20
1:A:76:TYR:HD1	1:A:79:LEU:HD12	0.51	1.60	2	1
1:B:21:PHE:O	1:B:70:GLU:OE2	0.51	2.29	5	8
1:A:5:THR:HG21	1:B:48:HIS:HB3	0.51	1.83	3	1
1:A:45:GLN:NE2	1:B:7:THR:CG2	0.51	2.74	16	6
1:A:52:ASP:O	1:A:53:VAL:HG23	0.51	2.06	14	1
1:A:1:MET:CE	1:B:43:THR:HG23	0.51	2.35	19	7
1:B:73:PHE:CZ	1:B:75:GLU:HG2	0.51	2.41	1	11
1:B:70:GLU:HG2	1:B:71:LEU:N	0.51	2.19	16	2
1:B:31:GLY:HA2	1:B:73:PHE:CD2	0.51	2.41	12	3
1:B:34:ASN:HA	1:B:67:GLN:HB2	0.51	1.81	12	2
1:A:42:ALA:CB	1:A:59:LYS:CG	0.51	2.89	16	2
1:B:72:ARG:CD	1:B:72:ARG:N	0.51	2.72	20	2
1:B:23:PHE:CE2	1:B:33:LEU:HD12	0.51	2.41	20	1
1:A:73:PHE:CZ	1:A:75:GLU:HG2	0.51	2.41	10	11
1:A:5:THR:CG2	1:B:50:LEU:HD23	0.51	2.36	2	1
1:A:17:VAL:HA	1:A:21:PHE:HB2	0.51	1.82	4	6
1:B:71:LEU:HD21	1:B:76:TYR:CA	0.51	2.36	2	1
1:B:32:SER:HB2	1:B:73:PHE:CE1	0.51	2.41	4	2
1:A:6:LEU:HD23	1:B:86:GLU:HA	0.51	1.81	6	1
1:A:41:LEU:N	1:A:41:LEU:HD23	0.51	2.21	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:PHE:O	1:B:20:PHE:CD1	0.51	2.64	14	2
1:B:20:PHE:HA	1:B:23:PHE:CE1	0.51	2.40	13	1
1:B:77:TRP:CD1	1:B:78:ARG:N	0.51	2.79	1	4
1:A:1:MET:O	1:B:38:PHE:CE1	0.51	2.64	17	18
1:B:23:PHE:CD1	1:B:70:GLU:OE1	0.51	2.63	3	1
1:A:13:ILE:HD11	1:B:86:GLU:HB2	0.51	1.80	12	1
1:A:9:LEU:CD2	1:B:20:PHE:HB3	0.51	2.35	13	3
1:A:20:PHE:O	1:A:20:PHE:CD1	0.51	2.64	14	2
1:A:33:LEU:CD2	1:A:37:GLU:CG	0.51	2.88	13	1
1:A:33:LEU:HB3	1:A:70:GLU:CB	0.51	2.36	1	8
1:B:24:ALA:CB	1:B:33:LEU:HB2	0.51	2.36	4	9
1:B:52:ASP:O	1:B:53:VAL:CG1	0.51	2.59	12	9
1:B:35:ILE:HG12	1:B:63:LEU:HD23	0.51	1.76	5	3
1:B:71:LEU:HD21	1:B:73:PHE:HD1	0.51	1.66	12	1
1:A:85:LYS:CE	1:B:3:ALA:CB	0.51	2.89	7	3
1:A:49:LEU:C	1:A:49:LEU:HD13	0.51	2.26	8	1
1:A:89:LYS:HD3	1:B:5:THR:CG2	0.51	2.36	20	4
1:B:23:PHE:HB3	1:B:33:LEU:HD21	0.51	1.82	14	1
1:A:76:TYR:HD1	1:A:79:LEU:HD13	0.51	1.66	17	1
1:A:38:PHE:CE1	1:B:1:MET:O	0.50	2.64	17	18
1:B:32:SER:HB3	1:B:73:PHE:CE1	0.50	2.41	12	8
1:A:54:GLY:CA	1:B:4:GLU:CG	0.50	2.89	8	2
1:B:41:LEU:C	1:B:45:GLN:CG	0.50	2.80	12	2
1:A:53:VAL:CG1	1:A:53:VAL:O	0.50	2.59	16	2
1:A:46:LEU:HD12	1:A:47:PRO:HD3	0.50	1.82	20	1
1:A:48:HIS:CE1	1:B:6:LEU:O	0.50	2.65	10	11
1:B:42:ALA:CB	1:B:59:LYS:HG3	0.50	2.36	18	2
1:B:71:LEU:N	1:B:71:LEU:HD13	0.50	2.21	18	1
1:B:16:VAL:CG2	1:B:21:PHE:CE2	0.50	2.92	2	1
1:B:71:LEU:CB	1:B:75:GLU:HB2	0.50	2.35	18	7
1:A:6:LEU:HD12	1:A:6:LEU:H	0.50	1.66	3	2
1:B:71:LEU:HD13	1:B:71:LEU:H	0.50	1.66	20	6
1:A:48:HIS:CG	1:A:49:LEU:N	0.50	2.79	9	3
1:B:89:LYS:CG	1:B:90:GLU:N	0.50	2.75	19	1
1:A:71:LEU:HD23	1:A:75:GLU:HB2	0.50	1.84	1	8
1:B:9:LEU:O	1:B:12:ALA:HB3	0.50	2.06	17	12
1:B:47:PRO:HA	1:B:51:LYS:HE2	0.50	1.84	11	4
1:B:71:LEU:HG	1:B:75:GLU:CB	0.50	2.36	4	8
1:A:86:GLU:HG3	1:A:87:VAL:HG23	0.50	1.82	4	1
1:B:86:GLU:HG3	1:B:87:VAL:HG23	0.50	1.82	4	1
1:A:75:GLU:OE1	1:A:77:TRP:CE2	0.50	2.64	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD11	1:B:89:LYS:NZ	0.50	2.22	18	1
1:A:24:ALA:HB2	1:A:33:LEU:HD23	0.50	1.79	20	1
1:A:91:LYS:HB2	1:B:77:TRP:HB3	0.50	1.84	20	1
1:A:9:LEU:O	1:A:12:ALA:HB3	0.50	2.06	17	11
1:A:71:LEU:CG	1:A:76:TYR:N	0.50	2.75	2	6
1:A:23:PHE:CD1	1:A:70:GLU:OE1	0.50	2.64	3	1
1:B:32:SER:OG	1:B:33:LEU:N	0.50	2.45	18	5
1:A:56:LEU:HD13	1:A:56:LEU:C	0.50	2.27	5	2
1:B:42:ALA:HA	1:B:45:GLN:HB2	0.50	1.83	9	4
1:A:71:LEU:HD23	1:A:73:PHE:O	0.50	2.06	18	2
1:A:89:LYS:HG3	1:A:90:GLU:N	0.50	2.21	19	1
1:A:76:TYR:O	1:B:87:VAL:CG2	0.50	2.60	20	1
1:A:73:PHE:CE1	1:A:75:GLU:CG	0.50	2.94	19	8
1:B:42:ALA:O	1:B:46:LEU:HG	0.50	2.06	12	17
1:A:76:TYR:CE1	1:A:79:LEU:HD12	0.50	2.41	2	2
1:A:77:TRP:HB3	1:B:91:LYS:HB2	0.50	1.83	20	2
1:A:41:LEU:C	1:A:45:GLN:CG	0.50	2.80	12	2
1:B:49:LEU:HD13	1:B:49:LEU:C	0.50	2.26	8	1
1:A:56:LEU:N	1:A:56:LEU:HD23	0.50	2.21	17	1
1:B:23:PHE:CZ	1:B:34:ASN:O	0.50	2.64	2	1
1:A:6:LEU:O	1:B:48:HIS:CE1	0.50	2.64	6	11
1:A:85:LYS:CG	1:B:3:ALA:HB1	0.50	2.36	9	1
1:A:31:GLY:O	1:A:73:PHE:N	0.50	2.45	7	12
1:A:23:PHE:CE1	1:A:34:ASN:O	0.50	2.65	2	1
1:A:35:ILE:N	1:A:35:ILE:CD1	0.50	2.74	11	4
1:B:24:ALA:CA	1:B:33:LEU:HB2	0.50	2.37	13	4
1:A:3:ALA:CB	1:B:85:LYS:CD	0.50	2.90	7	1
1:A:89:LYS:CD	1:B:6:LEU:N	0.50	2.75	9	1
1:A:23:PHE:HB3	1:A:33:LEU:HD21	0.50	1.83	14	1
1:B:20:PHE:CE1	1:B:23:PHE:CD2	0.50	3.00	2	9
1:B:31:GLY:O	1:B:72:ARG:CB	0.50	2.60	17	12
1:A:3:ALA:CB	1:B:85:LYS:CE	0.50	2.90	7	3
1:A:76:TYR:HB2	1:B:91:LYS:HA	0.50	1.82	17	14
1:B:83:LEU:O	1:B:86:GLU:CG	0.50	2.60	2	6
1:A:9:LEU:HD11	1:B:82:GLU:HB3	0.50	1.84	6	5
1:B:76:TYR:HD1	1:B:79:LEU:HD11	0.50	1.54	14	3
1:A:67:GLN:NE2	1:A:68:ASP:N	0.50	2.60	5	5
1:A:7:THR:CG2	1:B:45:GLN:NE2	0.50	2.74	5	3
1:A:68:ASP:O	1:A:78:ARG:HB2	0.50	2.07	20	7
1:A:79:LEU:HD12	1:B:87:VAL:HG23	0.50	1.82	20	1
1:A:42:ALA:O	1:A:46:LEU:N	0.49	2.45	14	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ASP:O	1:A:53:VAL:CG1	0.49	2.59	12	9
1:B:39:LYS:HE2	1:B:63:LEU:HD21	0.49	1.84	2	1
1:A:9:LEU:HD12	1:B:82:GLU:C	0.49	2.27	3	4
1:A:84:ALA:O	1:A:88:ARG:N	0.49	2.44	14	11
1:B:75:GLU:OE1	1:B:77:TRP:NE1	0.49	2.45	18	5
1:B:56:LEU:C	1:B:56:LEU:HD13	0.49	2.27	5	2
1:A:38:PHE:O	1:B:1:MET:HB2	0.49	2.06	10	7
1:B:73:PHE:CE1	1:B:75:GLU:HG2	0.49	2.41	19	5
1:A:6:LEU:N	1:B:89:LYS:CD	0.49	2.75	9	1
1:A:26:ARG:CG	1:A:37:GLU:CG	0.49	2.90	14	2
1:B:52:ASP:O	1:B:53:VAL:HG23	0.49	2.07	14	1
1:A:24:ALA:HB2	1:A:33:LEU:HB2	0.49	1.83	6	9
1:B:42:ALA:O	1:B:46:LEU:N	0.49	2.45	14	18
1:A:16:VAL:HG21	1:A:83:LEU:CG	0.49	2.35	3	4
1:A:74:SER:O	1:A:77:TRP:CZ3	0.49	2.65	18	10
1:A:32:SER:HB2	1:A:73:PHE:CE1	0.49	2.42	4	2
1:B:50:LEU:HD23	1:B:50:LEU:H	0.49	1.67	11	1
1:A:87:VAL:HG11	1:B:80:ILE:HA	0.49	1.82	20	1
1:A:7:THR:O	1:A:10:GLU:CG	0.49	2.60	10	20
1:B:31:GLY:O	1:B:73:PHE:N	0.49	2.45	19	11
1:B:61:LYS:O	1:B:65:VAL:HG23	0.49	2.06	2	2
1:A:20:PHE:CE1	1:A:23:PHE:CG	0.49	3.00	3	1
1:B:24:ALA:HA	1:B:33:LEU:CB	0.49	2.36	13	1
1:A:97:LYS:CD	1:B:30:LYS:CB	0.49	2.90	15	1
1:A:46:LEU:O	1:A:51:LYS:CE	0.49	2.61	17	8
1:A:73:PHE:CE1	1:A:75:GLU:HG2	0.49	2.41	19	5
1:A:90:GLU:CG	1:B:6:LEU:HD23	0.49	2.38	14	2
1:A:73:PHE:HB2	1:B:95:ILE:HG22	0.49	1.83	18	1
1:B:24:ALA:HA	1:B:33:LEU:HB3	0.49	1.84	20	1
1:A:51:LYS:HG2	1:A:52:ASP:N	0.49	2.23	13	12
1:A:52:ASP:O	1:A:53:VAL:CB	0.49	2.61	14	8
1:A:95:ILE:HG22	1:B:73:PHE:HB2	0.49	1.83	18	2
1:A:71:LEU:HD13	1:A:71:LEU:H	0.49	1.67	18	6
1:A:72:ARG:N	1:A:72:ARG:CD	0.49	2.75	10	4
1:B:26:ARG:CD	1:B:37:GLU:CG	0.49	2.91	17	1
1:A:6:LEU:HD12	1:B:89:LYS:HG3	0.49	1.83	4	1
1:A:24:ALA:CA	1:A:33:LEU:HB2	0.49	2.36	13	5
1:A:4:GLU:CG	1:B:54:GLY:CA	0.49	2.91	8	2
1:A:71:LEU:HD21	1:A:76:TYR:CE1	0.49	2.42	14	1
1:A:1:MET:O	1:B:38:PHE:CD1	0.49	2.65	3	14
1:B:71:LEU:CG	1:B:76:TYR:N	0.49	2.76	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:GLY:HA3	1:B:76:TYR:CD2	0.49	2.43	3	9
1:B:74:SER:O	1:B:77:TRP:CZ3	0.49	2.65	18	7
1:A:32:SER:OG	1:A:33:LEU:N	0.49	2.45	9	5
1:A:56:LEU:HD12	1:A:57:ASP:N	0.49	2.23	16	2
1:B:9:LEU:N	1:B:9:LEU:CD2	0.49	2.75	13	2
1:B:68:ASP:O	1:B:78:ARG:HB2	0.49	2.08	20	5
1:A:13:ILE:HA	1:A:16:VAL:HG12	0.49	1.84	13	3
1:A:24:ALA:HA	1:A:33:LEU:CB	0.49	2.37	13	1
1:A:6:LEU:CD1	1:B:48:HIS:CE1	0.49	2.96	14	1
1:B:56:LEU:HD12	1:B:57:ASP:N	0.49	2.23	16	1
1:B:52:ASP:O	1:B:53:VAL:CB	0.49	2.61	14	8
1:A:6:LEU:HD21	1:B:48:HIS:CD2	0.49	2.41	2	1
1:A:23:PHE:CZ	1:A:34:ASN:O	0.49	2.66	2	1
1:A:89:LYS:HD2	1:B:6:LEU:N	0.49	2.22	9	3
1:A:3:ALA:HB1	1:B:85:LYS:CG	0.49	2.37	9	1
1:B:33:LEU:CD2	1:B:37:GLU:CG	0.49	2.90	13	1
1:A:31:GLY:O	1:A:72:ARG:CB	0.49	2.61	10	14
1:B:68:ASP:O	1:B:78:ARG:CB	0.49	2.61	5	8
1:B:17:VAL:HA	1:B:21:PHE:HB2	0.49	1.85	4	3
1:B:70:GLU:HA	1:B:79:LEU:HD23	0.49	1.85	19	5
1:A:33:LEU:HD22	1:A:37:GLU:HG3	0.49	1.84	13	1
1:A:13:ILE:HD11	1:B:87:VAL:HG22	0.49	1.84	19	1
1:A:5:THR:HB	1:B:48:HIS:CG	0.49	2.43	16	3
1:A:76:TYR:HD1	1:A:79:LEU:HD11	0.49	1.58	14	3
1:B:6:LEU:HD12	1:B:6:LEU:H	0.49	1.67	3	1
1:B:33:LEU:HG	1:B:34:ASN:N	0.49	2.23	14	4
1:A:53:VAL:O	1:A:53:VAL:HG13	0.49	2.08	16	2
1:A:50:LEU:HD23	1:A:50:LEU:H	0.49	1.67	11	1
1:B:26:ARG:CG	1:B:37:GLU:CG	0.49	2.91	14	2
1:A:16:VAL:CB	1:A:83:LEU:HD21	0.48	2.38	12	3
1:B:13:ILE:O	1:B:13:ILE:HD13	0.48	2.08	5	7
1:A:33:LEU:CD2	1:A:70:GLU:HB3	0.48	2.35	15	5
1:B:20:PHE:CE1	1:B:23:PHE:CG	0.48	3.01	3	1
1:B:46:LEU:O	1:B:51:LYS:CE	0.48	2.61	10	8
1:B:67:GLN:HG2	1:B:68:ASP:N	0.48	2.23	8	5
1:B:35:ILE:HG22	1:B:38:PHE:CG	0.48	2.43	14	1
1:A:80:ILE:CG2	1:A:81:GLY:N	0.48	2.77	19	20
1:B:73:PHE:CE1	1:B:75:GLU:CG	0.48	2.96	19	8
1:A:38:PHE:CD1	1:B:1:MET:O	0.48	2.66	3	13
1:A:5:THR:N	1:B:45:GLN:OE1	0.48	2.46	17	3
1:A:30:LYS:CB	1:B:97:LYS:CD	0.48	2.91	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ARG:CD	1:A:37:GLU:CG	0.48	2.91	17	1
1:B:24:ALA:HB2	1:B:33:LEU:HB2	0.48	1.84	6	9
1:A:37:GLU:O	1:A:40:GLU:HG2	0.48	2.07	3	6
1:A:74:SER:O	1:A:77:TRP:CE3	0.48	2.67	6	8
1:A:94:GLY:CA	1:B:76:TYR:CD2	0.48	2.97	4	2
1:B:72:ARG:CA	1:B:72:ARG:NE	0.48	2.76	13	4
1:A:31:GLY:HA2	1:A:73:PHE:CD2	0.48	2.43	12	2
1:A:9:LEU:HD12	1:B:83:LEU:N	0.48	2.23	13	1
1:A:20:PHE:HB3	1:B:9:LEU:CD2	0.48	2.38	13	1
1:B:13:ILE:HA	1:B:16:VAL:HG12	0.48	1.85	13	3
1:A:83:LEU:HD11	1:B:86:GLU:OE1	0.48	2.09	14	1
1:A:87:VAL:CG1	1:B:76:TYR:O	0.48	2.62	5	13
1:B:71:LEU:HD23	1:B:75:GLU:HB2	0.48	1.85	5	8
1:B:23:PHE:CE1	1:B:34:ASN:O	0.48	2.66	2	1
1:A:24:ALA:HB2	1:A:70:GLU:CG	0.48	2.37	10	7
1:A:73:PHE:CZ	1:A:75:GLU:CD	0.48	2.87	3	1
1:B:62:THR:HG22	1:B:66:ASN:HB2	0.48	1.83	4	1
1:A:39:LYS:CE	1:A:63:LEU:CD1	0.48	2.92	10	1
1:A:1:MET:HE2	1:B:43:THR:HG23	0.48	1.86	20	1
1:B:23:PHE:CD1	1:B:37:GLU:HG3	0.48	2.44	17	7
1:A:7:THR:HG22	1:A:8:GLU:OE1	0.48	2.09	8	1
1:A:85:LYS:CE	1:B:3:ALA:HB3	0.48	2.38	8	1
1:A:45:GLN:O	1:A:51:LYS:CE	0.48	2.61	19	1
1:A:89:LYS:HE3	1:B:6:LEU:HD11	0.48	1.83	19	1
1:A:24:ALA:HA	1:A:33:LEU:HB3	0.48	1.85	20	1
1:A:80:ILE:HA	1:B:87:VAL:HG11	0.48	1.86	20	1
1:A:33:LEU:CD1	1:A:70:GLU:HB3	0.48	2.38	12	10
1:B:16:VAL:CB	1:B:83:LEU:HD21	0.48	2.39	12	3
1:A:5:THR:HB	1:B:48:HIS:CD2	0.48	2.43	7	1
1:A:16:VAL:HG13	1:A:17:VAL:N	0.48	2.22	8	6
1:A:5:THR:CG2	1:B:89:LYS:HD3	0.48	2.38	17	4
1:A:5:THR:HG21	1:B:48:HIS:CD2	0.48	2.43	14	1
1:B:56:LEU:HD23	1:B:56:LEU:N	0.48	2.22	17	1
1:B:70:GLU:HA	1:B:79:LEU:HD21	0.48	1.85	15	2
1:B:89:LYS:NZ	1:B:89:LYS:HB3	0.48	2.24	7	4
1:A:79:LEU:HA	1:A:82:GLU:CG	0.48	2.39	15	3
1:A:39:LYS:O	1:B:1:MET:HG2	0.48	2.09	7	4
1:B:21:PHE:CD2	1:B:70:GLU:OE1	0.48	2.67	6	2
1:B:72:ARG:N	1:B:72:ARG:CD	0.48	2.75	7	4
1:B:50:LEU:HD11	1:B:89:LYS:HB2	0.48	1.86	11	1
1:A:6:LEU:CD1	1:B:89:LYS:CE	0.48	2.89	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HB2	1:B:48:HIS:CE1	0.48	2.43	19	3
1:A:46:LEU:O	1:A:51:LYS:CD	0.48	2.62	16	11
1:B:80:ILE:CG2	1:B:81:GLY:N	0.48	2.77	8	19
1:B:62:THR:CG2	1:B:66:ASN:ND2	0.48	2.77	9	2
1:A:14:GLU:HA	1:A:17:VAL:HG12	0.48	1.85	20	7
1:A:21:PHE:CD2	1:A:79:LEU:CD2	0.48	2.96	19	6
1:A:1:MET:HB2	1:B:39:LYS:HA	0.48	1.84	10	4
1:A:39:LYS:HE3	1:A:63:LEU:HD11	0.48	1.85	10	1
1:A:71:LEU:HD21	1:A:73:PHE:HD1	0.48	1.68	12	1
1:B:24:ALA:CB	1:B:72:ARG:HG2	0.48	2.38	13	1
1:A:6:LEU:HD12	1:B:48:HIS:CE1	0.48	2.44	14	1
1:A:42:ALA:N	1:A:45:GLN:OE1	0.48	2.47	16	2
1:A:57:ASP:O	1:A:60:MET:N	0.48	2.47	12	14
1:B:87:VAL:HG12	1:B:87:VAL:O	0.48	2.09	19	7
1:B:73:PHE:CZ	1:B:75:GLU:CD	0.48	2.87	3	1
1:A:23:PHE:CD1	1:A:23:PHE:C	0.48	2.87	11	4
1:B:14:GLU:HA	1:B:17:VAL:HG12	0.48	1.84	20	8
1:B:82:GLU:O	1:B:85:LYS:N	0.48	2.47	20	11
1:A:6:LEU:N	1:B:89:LYS:HD2	0.48	2.24	9	3
1:A:71:LEU:CD2	1:A:71:LEU:C	0.48	2.82	6	5
1:A:72:ARG:O	1:B:97:LYS:CE	0.48	2.62	9	9
1:A:59:LYS:NZ	1:B:2:ALA:HB3	0.48	2.24	3	1
1:B:24:ALA:HB2	1:B:70:GLU:CG	0.48	2.39	10	6
1:A:49:LEU:CD1	1:A:50:LEU:N	0.48	2.77	8	1
1:B:16:VAL:HG13	1:B:17:VAL:N	0.48	2.23	8	6
1:B:49:LEU:CD1	1:B:50:LEU:N	0.48	2.77	8	1
1:A:48:HIS:CG	1:B:5:THR:CG2	0.48	2.90	9	1
1:A:46:LEU:O	1:A:48:HIS:N	0.48	2.47	10	2
1:B:31:GLY:O	1:B:72:ARG:HG2	0.48	2.09	13	2
1:B:6:LEU:HD23	1:B:10:GLU:CD	0.48	2.28	17	1
1:A:23:PHE:CE1	1:A:33:LEU:HG	0.48	2.44	19	1
1:A:54:GLY:HA2	1:B:4:GLU:HG3	0.48	1.86	20	1
1:A:54:GLY:CA	1:B:4:GLU:HG3	0.47	2.39	8	2
1:A:46:LEU:O	1:A:51:LYS:CG	0.47	2.62	10	2
1:B:42:ALA:O	1:B:46:LEU:CG	0.47	2.62	20	2
1:A:31:GLY:O	1:A:72:ARG:HG2	0.47	2.09	13	2
1:A:71:LEU:HD11	1:A:76:TYR:CD2	0.47	2.44	18	1
1:B:84:ALA:CA	1:B:87:VAL:HG12	0.47	2.38	20	1
1:A:1:MET:CE	1:B:43:THR:CG2	0.47	2.92	1	3
1:A:2:ALA:HA	1:B:62:THR:HG21	0.47	1.85	4	4
1:A:42:ALA:HA	1:A:45:GLN:HG2	0.47	1.86	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:PHE:CG	1:B:74:SER:N	0.47	2.81	11	6
1:A:61:LYS:O	1:A:65:VAL:HG23	0.47	2.09	2	2
1:A:23:PHE:CG	1:A:33:LEU:CD2	0.47	2.96	3	1
1:A:83:LEU:O	1:A:86:GLU:HG2	0.47	2.10	4	5
1:B:26:ARG:CZ	1:B:36:ASN:ND2	0.47	2.77	8	1
1:B:39:LYS:CE	1:B:63:LEU:CD1	0.47	2.92	10	1
1:A:75:GLU:OE2	1:A:77:TRP:CH2	0.47	2.67	13	2
1:A:90:GLU:CD	1:B:6:LEU:HD21	0.47	2.28	16	1
1:A:55:SER:O	1:A:59:LYS:CD	0.47	2.63	18	1
1:A:71:LEU:C	1:A:71:LEU:CD1	0.47	2.83	12	7
1:A:82:GLU:O	1:A:85:LYS:N	0.47	2.46	20	16
1:B:7:THR:O	1:B:10:GLU:CG	0.47	2.62	8	20
1:A:87:VAL:HG12	1:A:87:VAL:O	0.47	2.09	19	8
1:B:71:LEU:HG	1:B:75:GLU:CA	0.47	2.40	16	7
1:B:71:LEU:CD2	1:B:71:LEU:C	0.47	2.82	6	5
1:A:9:LEU:HD13	1:B:16:VAL:CG2	0.47	2.39	5	4
1:A:75:GLU:OE2	1:A:77:TRP:CZ2	0.47	2.67	5	4
1:B:75:GLU:OE2	1:B:77:TRP:CZ2	0.47	2.67	17	5
1:A:26:ARG:CZ	1:A:36:ASN:ND2	0.47	2.77	8	1
1:A:56:LEU:C	1:A:56:LEU:HD23	0.47	2.29	12	1
1:B:56:LEU:HD23	1:B:56:LEU:C	0.47	2.29	12	1
1:A:48:HIS:CD2	1:B:5:THR:HG21	0.47	2.44	14	1
1:A:48:HIS:CE1	1:B:6:LEU:CD1	0.47	2.97	14	1
1:A:70:GLU:HA	1:A:79:LEU:HD11	0.47	1.87	15	1
1:A:33:LEU:CD1	1:A:70:GLU:OE1	0.47	2.63	16	1
1:A:1:MET:HG2	1:B:39:LYS:O	0.47	2.08	7	7
1:A:33:LEU:HB3	1:A:70:GLU:CG	0.47	2.40	1	5
1:A:95:ILE:HG22	1:B:73:PHE:C	0.47	2.29	10	2
1:A:91:LYS:HA	1:B:76:TYR:CB	0.47	2.40	2	5
1:A:97:LYS:CE	1:B:72:ARG:O	0.47	2.62	9	9
1:B:21:PHE:O	1:B:70:GLU:OE1	0.47	2.33	18	6
1:B:32:SER:HA	1:B:71:LEU:HA	0.47	1.86	2	2
1:B:23:PHE:CD1	1:B:23:PHE:C	0.47	2.87	4	7
1:B:33:LEU:CD1	1:B:70:GLU:HB3	0.47	2.39	12	9
1:A:72:ARG:NE	1:A:72:ARG:CA	0.47	2.77	13	5
1:A:85:LYS:HD3	1:B:9:LEU:HD12	0.47	1.86	12	1
1:B:33:LEU:HD22	1:B:70:GLU:CB	0.47	2.37	15	1
1:A:94:GLY:O	1:A:96:ARG:N	0.47	2.47	3	11
1:B:46:LEU:O	1:B:51:LYS:CD	0.47	2.63	17	10
1:A:83:LEU:O	1:A:86:GLU:CG	0.47	2.63	5	4
1:A:2:ALA:HB3	1:B:59:LYS:NZ	0.47	2.24	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:SER:CB	1:A:71:LEU:HA	0.47	2.39	16	3
1:B:71:LEU:HD11	1:B:76:TYR:CD2	0.47	2.44	18	1
1:B:69:SER:HA	1:B:78:ARG:HB3	0.47	1.86	20	1
1:A:91:LYS:CG	1:A:92:ALA:N	0.47	2.78	18	18
1:B:86:GLU:O	1:B:90:GLU:CG	0.47	2.62	20	8
1:A:21:PHE:O	1:A:70:GLU:OE1	0.47	2.32	18	6
1:A:62:THR:CG2	1:A:66:ASN:ND2	0.47	2.78	9	2
1:A:7:THR:HG22	1:B:45:GLN:OE1	0.47	2.08	3	1
1:B:46:LEU:O	1:B:51:LYS:CG	0.47	2.62	17	2
1:A:24:ALA:HB2	1:A:72:ARG:NH1	0.47	2.25	14	1
1:A:24:ALA:N	1:A:33:LEU:CD1	0.47	2.76	18	1
1:A:47:PRO:HA	1:A:51:LYS:HE2	0.47	1.85	3	4
1:A:65:VAL:HG12	1:A:66:ASN:ND2	0.47	2.24	1	1
1:A:32:SER:HA	1:A:71:LEU:HA	0.47	1.87	4	2
1:A:71:LEU:HD21	1:A:76:TYR:CA	0.47	2.39	2	1
1:A:83:LEU:O	1:A:86:GLU:HG3	0.47	2.10	3	3
1:B:71:LEU:HG	1:B:75:GLU:HB2	0.47	1.86	2	6
1:B:76:TYR:CE1	1:B:79:LEU:HD12	0.47	2.43	2	1
1:B:70:GLU:HG3	1:B:71:LEU:N	0.47	2.25	3	1
1:A:6:LEU:CD1	1:B:89:LYS:CG	0.47	2.93	4	1
1:A:70:GLU:HA	1:A:79:LEU:CD2	0.47	2.40	16	4
1:B:84:ALA:O	1:B:88:ARG:N	0.47	2.47	14	6
1:B:20:PHE:CZ	1:B:33:LEU:HD11	0.47	2.45	15	2
1:A:45:GLN:OE1	1:B:5:THR:N	0.47	2.47	17	3
1:A:4:GLU:CG	1:B:42:ALA:CB	0.47	2.92	11	1
1:B:41:LEU:HB3	1:B:45:GLN:OE1	0.47	2.10	13	1
1:B:75:GLU:OE2	1:B:77:TRP:CH2	0.47	2.67	13	1
1:A:46:LEU:HD23	1:A:54:GLY:H	0.47	1.69	14	1
1:B:76:TYR:CE1	1:B:79:LEU:HD22	0.47	2.44	15	1
1:B:33:LEU:CD1	1:B:70:GLU:OE1	0.47	2.62	16	1
1:A:79:LEU:N	1:A:79:LEU:CD2	0.47	2.71	18	1
1:A:7:THR:HB	1:A:9:LEU:CD1	0.47	2.39	20	1
1:B:18:SER:O	1:B:22:THR:HG21	0.47	2.09	20	8
1:B:42:ALA:N	1:B:45:GLN:OE1	0.47	2.48	16	2
1:B:91:LYS:CG	1:B:92:ALA:N	0.47	2.78	20	18
1:B:94:GLY:O	1:B:96:ARG:N	0.47	2.48	12	13
1:A:5:THR:HG22	1:A:6:LEU:H	0.47	1.70	3	4
1:A:50:LEU:HD23	1:B:5:THR:CG2	0.47	2.40	2	1
1:A:76:TYR:CB	1:B:91:LYS:HA	0.47	2.39	2	2
1:A:45:GLN:OE1	1:B:7:THR:HG22	0.47	2.09	3	1
1:B:23:PHE:CG	1:B:33:LEU:CD2	0.47	2.98	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HG21	1:A:63:LEU:C	0.47	2.30	5	1
1:A:80:ILE:N	1:B:87:VAL:HG11	0.47	2.25	7	5
1:A:4:GLU:HG3	1:B:54:GLY:CA	0.47	2.40	8	2
1:A:26:ARG:NE	1:A:36:ASN:ND2	0.47	2.63	8	1
1:A:5:THR:CG2	1:B:48:HIS:CG	0.47	2.90	9	1
1:A:85:LYS:NZ	1:B:3:ALA:CB	0.47	2.78	10	1
1:B:53:VAL:HG12	1:B:53:VAL:O	0.47	2.10	10	2
1:A:71:LEU:HD13	1:A:72:ARG:N	0.47	2.24	11	3
1:A:21:PHE:CZ	1:A:79:LEU:HB3	0.47	2.45	14	2
1:A:20:PHE:CZ	1:A:70:GLU:OE1	0.47	2.67	20	1
1:A:48:HIS:NE2	1:B:6:LEU:O	0.47	2.48	11	12
1:B:33:LEU:CD2	1:B:70:GLU:HB3	0.47	2.35	15	4
1:A:5:THR:HG21	1:B:48:HIS:CB	0.47	2.40	6	2
1:A:70:GLU:HG3	1:A:71:LEU:N	0.47	2.23	3	2
1:B:51:LYS:CG	1:B:52:ASP:N	0.47	2.78	14	4
1:B:5:THR:HG22	1:B:6:LEU:N	0.47	2.25	19	6
1:A:16:VAL:CG2	1:B:9:LEU:HD13	0.47	2.40	5	3
1:A:27:GLU:CG	1:A:34:ASN:ND2	0.47	2.78	6	2
1:A:23:PHE:CE2	1:A:70:GLU:HG3	0.47	2.45	20	1
1:A:26:ARG:CG	1:A:37:GLU:HG3	0.47	2.40	14	4
1:A:62:THR:HG21	1:B:2:ALA:HA	0.47	1.85	4	4
1:B:33:LEU:CB	1:B:70:GLU:HB3	0.47	2.40	11	7
1:A:94:GLY:C	1:B:73:PHE:O	0.47	2.54	17	13
1:A:42:ALA:CB	1:A:59:LYS:HG3	0.47	2.40	3	2
1:B:50:LEU:HD11	1:B:89:LYS:HD2	0.47	1.87	5	1
1:A:89:LYS:HD2	1:B:5:THR:CG2	0.47	2.40	6	1
1:A:34:ASN:O	1:A:67:GLN:O	0.47	2.34	13	6
1:A:23:PHE:CE2	1:A:41:LEU:CD2	0.47	2.95	14	2
1:B:24:ALA:HB3	1:B:72:ARG:CG	0.47	2.40	13	1
1:B:76:TYR:CE1	1:B:79:LEU:CD1	0.47	2.98	18	1
1:A:87:VAL:CG2	1:B:76:TYR:O	0.47	2.63	20	1
1:A:83:LEU:HB3	1:B:83:LEU:HD13	0.46	1.87	1	1
1:B:70:GLU:HA	1:B:79:LEU:CD2	0.46	2.40	16	3
1:A:50:LEU:HD11	1:A:89:LYS:HD3	0.46	1.87	5	1
1:B:75:GLU:OE1	1:B:78:ARG:CG	0.46	2.63	18	5
1:A:6:LEU:O	1:B:48:HIS:NE2	0.46	2.49	11	12
1:B:69:SER:O	1:B:79:LEU:CD2	0.46	2.62	13	3
1:B:5:THR:HG22	1:B:6:LEU:H	0.46	1.71	3	3
1:B:57:ASP:O	1:B:60:MET:N	0.46	2.48	12	11
1:B:42:ALA:O	1:B:46:LEU:CB	0.46	2.64	17	6
1:A:20:PHE:CZ	1:A:33:LEU:HD11	0.46	2.45	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:HG23	1:B:1:MET:HE3	0.46	1.87	8	4
1:A:41:LEU:N	1:A:41:LEU:CD2	0.46	2.78	8	2
1:A:35:ILE:HG22	1:A:38:PHE:CG	0.46	2.45	14	2
1:A:33:LEU:O	1:A:70:GLU:CG	0.46	2.64	13	1
1:A:23:PHE:HB3	1:A:37:GLU:HB2	0.46	1.86	14	1
1:A:14:GLU:CG	1:A:15:THR:N	0.46	2.78	15	1
1:A:54:GLY:N	1:B:4:GLU:CG	0.46	2.79	16	1
1:A:7:THR:CB	1:A:9:LEU:CD1	0.46	2.94	20	1
1:B:15:THR:O	1:B:19:THR:N	0.46	2.49	3	10
1:B:71:LEU:C	1:B:71:LEU:CD1	0.46	2.84	10	7
1:B:21:PHE:CA	1:B:70:GLU:OE1	0.46	2.64	2	1
1:B:23:PHE:CZ	1:B:38:PHE:HB2	0.46	2.46	11	7
1:A:23:PHE:CE1	1:A:70:GLU:HB2	0.46	2.45	3	1
1:A:85:LYS:O	1:A:89:LYS:HE3	0.46	2.10	6	3
1:B:79:LEU:O	1:B:82:GLU:N	0.46	2.48	20	3
1:A:74:SER:N	1:B:95:ILE:HG23	0.46	2.25	16	3
1:B:49:LEU:HD23	1:B:50:LEU:N	0.46	2.25	4	1
1:A:68:ASP:CB	1:A:78:ARG:HG3	0.46	2.40	11	4
1:A:6:LEU:HD23	1:B:86:GLU:CA	0.46	2.41	6	1
1:B:71:LEU:C	1:B:72:ARG:HD2	0.46	2.31	20	5
1:B:71:LEU:CD1	1:B:76:TYR:CD2	0.46	2.96	11	2
1:A:24:ALA:N	1:A:70:GLU:OE2	0.46	2.45	14	1
1:A:89:LYS:CE	1:B:6:LEU:CD1	0.46	2.90	19	1
1:B:20:PHE:CZ	1:B:70:GLU:OE1	0.46	2.69	20	1
1:A:75:GLU:O	1:A:77:TRP:N	0.46	2.49	2	5
1:A:49:LEU:HD23	1:A:50:LEU:N	0.46	2.25	4	1
1:B:74:SER:O	1:B:77:TRP:CE3	0.46	2.68	16	6
1:A:21:PHE:CD1	1:A:79:LEU:HD22	0.46	2.45	13	1
1:A:86:GLU:OE1	1:B:83:LEU:HD11	0.46	2.10	14	1
1:B:90:GLU:O	1:B:94:GLY:N	0.46	2.49	20	2
1:A:45:GLN:O	1:A:51:LYS:HE2	0.46	2.10	19	1
1:A:1:MET:SD	1:B:39:LYS:HA	0.46	2.50	5	9
1:A:9:LEU:HD12	1:B:82:GLU:O	0.46	2.11	5	2
1:B:35:ILE:HG21	1:B:63:LEU:C	0.46	2.30	5	2
1:A:85:LYS:HZ2	1:B:3:ALA:HB1	0.46	1.71	4	1
1:B:29:ARG:HG2	1:B:30:LYS:N	0.46	2.25	5	4
1:A:74:SER:CB	1:B:91:LYS:O	0.46	2.63	18	2
1:B:79:LEU:HD23	1:B:79:LEU:H	0.46	1.67	18	1
1:A:7:THR:CB	1:B:85:LYS:HZ1	0.46	2.23	1	1
1:A:41:LEU:O	1:A:43:THR:N	0.46	2.49	19	10
1:A:24:ALA:CB	1:A:72:ARG:HG2	0.46	2.40	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:70:GLU:CA	1:B:79:LEU:HD11	0.46	2.41	15	1
1:A:79:LEU:HD23	1:A:79:LEU:H	0.46	1.65	18	1
1:B:42:ALA:HB3	1:B:59:LYS:HG3	0.46	1.88	18	1
1:A:33:LEU:CB	1:A:70:GLU:HB3	0.46	2.41	11	7
1:B:33:LEU:HB3	1:B:70:GLU:CG	0.46	2.41	1	2
1:B:30:LYS:C	1:B:72:ARG:HB2	0.46	2.31	2	1
1:A:62:THR:HG22	1:A:66:ASN:HB2	0.46	1.86	4	1
1:A:76:TYR:CD2	1:B:94:GLY:CA	0.46	2.98	4	2
1:A:85:LYS:O	1:A:89:LYS:NZ	0.46	2.48	10	5
1:A:86:GLU:CA	1:B:6:LEU:HD23	0.46	2.41	6	1
1:B:34:ASN:O	1:B:67:GLN:O	0.46	2.34	13	6
1:A:16:VAL:HG11	1:A:83:LEU:HD21	0.46	1.88	11	2
1:B:37:GLU:O	1:B:40:GLU:HG2	0.46	2.11	13	2
1:B:24:ALA:N	1:B:70:GLU:OE2	0.46	2.45	14	1
1:A:7:THR:CB	1:A:9:LEU:HD12	0.46	2.40	20	1
1:B:65:VAL:HG12	1:B:66:ASN:ND2	0.46	2.26	1	1
1:B:71:LEU:HG	1:B:75:GLU:C	0.46	2.31	16	9
1:A:95:ILE:CG2	1:B:74:SER:CB	0.46	2.94	2	3
1:A:9:LEU:CG	1:B:16:VAL:HG23	0.46	2.41	6	5
1:A:89:LYS:CG	1:B:6:LEU:HD12	0.46	2.41	4	1
1:B:64:ASP:O	1:B:67:GLN:OE1	0.46	2.34	20	4
1:B:41:LEU:N	1:B:41:LEU:CD2	0.46	2.78	8	1
1:A:86:GLU:CB	1:B:10:GLU:HA	0.46	2.40	9	1
1:B:26:ARG:CG	1:B:37:GLU:HG3	0.46	2.41	14	3
1:B:33:LEU:O	1:B:70:GLU:CG	0.46	2.63	13	1
1:B:70:GLU:O	1:B:70:GLU:HG2	0.46	2.11	13	1
1:B:24:ALA:HB2	1:B:72:ARG:NH1	0.46	2.26	14	1
1:B:70:GLU:HA	1:B:79:LEU:HD11	0.46	1.87	15	1
1:A:79:LEU:HD12	1:A:79:LEU:H	0.46	1.70	17	1
1:A:35:ILE:CD1	1:A:63:LEU:CD2	0.46	2.94	18	1
1:A:48:HIS:CB	1:A:51:LYS:HB2	0.46	2.41	20	3
1:B:20:PHE:CE2	1:B:41:LEU:CD2	0.46	2.96	19	1
1:B:59:LYS:O	1:B:63:LEU:CD1	0.46	2.63	1	7
1:A:9:LEU:O	1:A:12:ALA:N	0.46	2.49	18	11
1:A:16:VAL:CG2	1:A:21:PHE:CE2	0.46	2.95	2	2
1:A:21:PHE:CA	1:A:70:GLU:OE1	0.46	2.63	2	1
1:A:1:MET:HB2	1:B:38:PHE:O	0.46	2.11	16	6
1:A:21:PHE:CD2	1:A:70:GLU:OE1	0.46	2.69	6	2
1:A:50:LEU:O	1:B:5:THR:HG21	0.46	2.11	8	1
1:B:24:ALA:CB	1:B:72:ARG:HD3	0.46	2.41	11	1
1:B:14:GLU:O	1:B:17:VAL:HG12	0.46	2.11	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:CD2	1:A:76:TYR:CE1	0.46	2.99	14	1
1:B:23:PHE:CE2	1:B:41:LEU:CD2	0.46	2.97	14	1
1:A:70:GLU:CA	1:A:79:LEU:HD11	0.46	2.41	15	1
1:A:5:THR:HG23	1:B:89:LYS:CB	0.46	2.41	18	1
1:A:46:LEU:CD1	1:A:47:PRO:HD3	0.46	2.41	20	1
1:A:79:LEU:O	1:A:82:GLU:N	0.46	2.49	20	3
1:B:32:SER:HB3	1:B:71:LEU:CB	0.46	2.40	14	3
1:A:5:THR:CG2	1:B:51:LYS:HA	0.46	2.41	4	2
1:B:23:PHE:CE1	1:B:33:LEU:HG	0.46	2.46	19	3
1:B:4:GLU:CA	1:B:4:GLU:OE1	0.46	2.64	17	2
1:A:14:GLU:O	1:A:17:VAL:HG12	0.46	2.10	15	2
1:B:55:SER:O	1:B:59:LYS:CD	0.46	2.64	18	1
1:B:32:SER:HB3	1:B:73:PHE:CZ	0.45	2.46	2	2
1:A:48:HIS:CG	1:B:5:THR:HB	0.45	2.46	3	2
1:A:86:GLU:HB2	1:B:10:GLU:HA	0.45	1.87	5	2
1:A:3:ALA:HB1	1:A:7:THR:OG1	0.45	2.12	8	2
1:B:46:LEU:O	1:B:48:HIS:N	0.45	2.49	10	2
1:B:49:LEU:HD12	1:B:49:LEU:N	0.45	2.27	10	2
1:A:42:ALA:HB3	1:B:1:MET:HB3	0.45	1.87	14	1
1:A:66:ASN:OD1	1:A:66:ASN:N	0.45	2.49	14	2
1:A:71:LEU:HD21	1:A:76:TYR:CE2	0.45	2.45	18	1
1:B:6:LEU:HD22	1:B:10:GLU:HB3	0.45	1.88	19	1
1:A:23:PHE:CE1	1:A:33:LEU:HB2	0.45	2.47	20	1
1:A:48:HIS:CE1	1:B:6:LEU:HB2	0.45	2.46	19	3
1:B:17:VAL:HA	1:B:21:PHE:CD2	0.45	2.46	13	12
1:A:6:LEU:HD12	1:A:6:LEU:N	0.45	2.25	3	1
1:A:73:PHE:O	1:B:94:GLY:C	0.45	2.55	11	7
1:A:73:PHE:HB3	1:B:97:LYS:CE	0.45	2.41	5	1
1:B:27:GLU:CG	1:B:34:ASN:ND2	0.45	2.79	15	2
1:B:49:LEU:HD13	1:B:50:LEU:N	0.45	2.26	8	1
1:A:1:MET:CG	1:B:42:ALA:HB3	0.45	2.35	10	1
1:A:50:LEU:HD11	1:A:89:LYS:HB2	0.45	1.88	11	1
1:B:71:LEU:HD13	1:B:72:ARG:N	0.45	2.26	11	2
1:A:20:PHE:CZ	1:A:38:PHE:CD2	0.45	3.05	13	1
1:B:33:LEU:HD22	1:B:37:GLU:HG3	0.45	1.87	13	1
1:A:75:GLU:OE1	1:A:77:TRP:NE1	0.45	2.49	18	3
1:B:71:LEU:HD23	1:B:73:PHE:O	0.45	2.10	18	1
1:A:69:SER:O	1:A:79:LEU:CD2	0.45	2.65	13	4
1:A:39:LYS:HE2	1:A:63:LEU:HD21	0.45	1.87	2	1
1:B:77:TRP:O	1:B:80:ILE:CG2	0.45	2.65	20	13
1:A:32:SER:HB3	1:A:71:LEU:CB	0.45	2.41	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:TYR:CD2	1:B:94:GLY:HA3	0.45	2.46	16	6
1:B:51:LYS:HG2	1:B:53:VAL:N	0.45	2.26	6	7
1:B:32:SER:OG	1:B:73:PHE:CZ	0.45	2.66	6	1
1:B:89:LYS:HG2	1:B:90:GLU:N	0.45	2.26	9	4
1:A:1:MET:CG	1:B:39:LYS:O	0.45	2.64	17	3
1:B:50:LEU:HD13	1:B:93:LEU:HB2	0.45	1.88	11	1
1:A:83:LEU:HD12	1:B:87:VAL:CG2	0.45	2.42	14	1
1:B:42:ALA:CB	1:B:59:LYS:CG	0.45	2.95	16	1
1:A:71:LEU:HB3	1:A:75:GLU:HB2	0.45	1.88	18	1
1:A:42:ALA:O	1:A:46:LEU:CB	0.45	2.64	17	4
1:A:23:PHE:CZ	1:A:38:PHE:HB2	0.45	2.46	11	6
1:A:5:THR:CG2	1:B:89:LYS:HD2	0.45	2.42	6	1
1:A:34:ASN:C	1:A:35:ILE:HD13	0.45	2.31	16	2
1:A:6:LEU:HD23	1:A:10:GLU:CD	0.45	2.30	17	1
1:A:26:ARG:HG3	1:A:37:GLU:HG3	0.45	1.88	19	1
1:B:23:PHE:CE1	1:B:33:LEU:HB2	0.45	2.46	20	1
1:B:33:LEU:CD2	1:B:72:ARG:HD3	0.45	2.42	20	1
1:A:16:VAL:CG1	1:A:83:LEU:HD21	0.45	2.42	12	2
1:A:77:TRP:CD1	1:A:77:TRP:C	0.45	2.90	7	15
1:B:46:LEU:HB3	1:B:47:PRO:HD3	0.45	1.88	6	6
1:A:5:THR:OG1	1:B:51:LYS:HA	0.45	2.12	7	5
1:B:23:PHE:CE1	1:B:70:GLU:HB2	0.45	2.47	3	1
1:B:52:ASP:O	1:B:53:VAL:HB	0.45	2.11	11	6
1:B:75:GLU:CA	1:B:75:GLU:OE1	0.45	2.65	3	1
1:A:80:ILE:HG23	1:A:81:GLY:N	0.45	2.27	18	5
1:A:92:ALA:O	1:A:95:ILE:CG2	0.45	2.65	8	1
1:B:26:ARG:NE	1:B:36:ASN:ND2	0.45	2.63	8	1
1:A:7:THR:OG1	1:B:45:GLN:NE2	0.45	2.50	16	3
1:A:49:LEU:N	1:A:49:LEU:HD12	0.45	2.25	10	1
1:B:33:LEU:CG	1:B:70:GLU:OE2	0.45	2.65	13	1
1:A:82:GLU:HA	1:A:85:LYS:CD	0.45	2.42	1	3
1:A:71:LEU:HG	1:A:75:GLU:HB2	0.45	1.89	4	4
1:A:89:LYS:CG	1:B:6:LEU:CD1	0.45	2.95	4	1
1:A:62:THR:OG1	1:B:2:ALA:CB	0.45	2.65	6	2
1:A:71:LEU:C	1:A:72:ARG:HD2	0.45	2.32	20	5
1:B:34:ASN:OD1	1:B:35:ILE:CD1	0.45	2.65	7	5
1:A:49:LEU:HD13	1:A:50:LEU:N	0.45	2.26	8	1
1:A:51:LYS:CD	1:B:5:THR:HB	0.45	2.42	18	3
1:A:54:GLY:HA2	1:B:4:GLU:CG	0.45	2.42	8	3
1:B:85:LYS:O	1:B:89:LYS:NZ	0.45	2.49	17	5
1:A:46:LEU:HD21	1:A:54:GLY:O	0.45	2.11	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:GLN:HG3	1:B:7:THR:HG23	0.45	1.87	14	1
1:B:48:HIS:CB	1:B:51:LYS:HB2	0.45	2.40	20	3
1:A:80:ILE:HD12	1:B:87:VAL:HB	0.45	1.87	19	1
1:A:6:LEU:CD2	1:B:90:GLU:CG	0.45	2.95	15	3
1:A:52:ASP:O	1:A:53:VAL:HB	0.45	2.11	11	6
1:A:73:PHE:CE1	1:A:75:GLU:HB2	0.45	2.47	20	3
1:B:67:GLN:NE2	1:B:68:ASP:CA	0.45	2.80	5	1
1:A:50:LEU:HD21	1:B:6:LEU:HD11	0.45	1.88	11	1
1:B:45:GLN:HA	1:B:48:HIS:CE1	0.45	2.47	13	3
1:A:23:PHE:CZ	1:A:41:LEU:CD2	0.45	3.00	13	2
1:A:48:HIS:CD2	1:B:6:LEU:HB2	0.45	2.47	17	1
1:B:20:PHE:CE2	1:B:23:PHE:CD2	0.45	3.05	19	1
1:B:16:VAL:CG1	1:B:83:LEU:HD21	0.45	2.42	1	2
1:A:92:ALA:O	1:A:95:ILE:HG12	0.45	2.12	4	6
1:A:29:ARG:CG	1:A:30:LYS:N	0.45	2.79	5	3
1:A:47:PRO:HA	1:A:51:LYS:CE	0.45	2.42	4	4
1:A:89:LYS:NZ	1:A:89:LYS:HB3	0.45	2.27	7	3
1:B:3:ALA:HB1	1:B:7:THR:OG1	0.45	2.12	8	1
1:A:39:LYS:O	1:B:1:MET:CG	0.45	2.65	17	2
1:B:73:PHE:CE2	1:B:75:GLU:HG2	0.45	2.46	15	1
1:A:20:PHE:CE1	1:A:23:PHE:CZ	0.45	3.04	18	1
1:B:75:GLU:OE1	1:B:77:TRP:CZ2	0.45	2.70	19	1
1:A:23:PHE:CD1	1:A:37:GLU:HG3	0.45	2.47	17	7
1:A:37:GLU:O	1:A:40:GLU:CG	0.45	2.65	17	6
1:A:59:LYS:O	1:A:63:LEU:CD1	0.45	2.65	3	8
1:B:37:GLU:O	1:B:40:GLU:CG	0.45	2.65	17	7
1:A:12:ALA:HA	1:B:15:THR:HG21	0.45	1.89	2	1
1:B:75:GLU:O	1:B:77:TRP:N	0.45	2.50	2	5
1:A:43:THR:HG23	1:B:1:MET:CE	0.45	2.42	19	4
1:B:32:SER:CB	1:B:71:LEU:HA	0.45	2.41	16	3
1:B:35:ILE:O	1:B:39:LYS:HG2	0.45	2.12	10	6
1:A:27:GLU:HG2	1:A:34:ASN:ND2	0.45	2.27	15	2
1:A:47:PRO:HA	1:A:51:LYS:HE3	0.45	1.89	7	2
1:B:45:GLN:OE1	1:B:51:LYS:CE	0.45	2.65	8	1
1:B:26:ARG:NE	1:B:36:ASN:CB	0.45	2.80	12	1
1:A:82:GLU:O	1:B:9:LEU:CD1	0.45	2.65	14	1
1:A:91:LYS:O	1:B:74:SER:CB	0.45	2.65	18	2
1:A:5:THR:CG2	1:B:89:LYS:HB3	0.45	2.40	19	1
1:A:45:GLN:O	1:A:46:LEU:C	0.45	2.55	19	2
1:A:7:THR:HG23	1:B:45:GLN:HE22	0.45	1.71	20	1
1:A:33:LEU:CD2	1:A:72:ARG:HD2	0.45	2.42	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:77:TRP:CD1	1:B:77:TRP:C	0.45	2.90	2	17
1:B:77:TRP:O	1:B:80:ILE:HB	0.45	2.12	1	4
1:B:49:LEU:N	1:B:49:LEU:HD22	0.45	2.27	3	1
1:A:33:LEU:C	1:A:33:LEU:CD2	0.45	2.83	5	3
1:B:58:GLU:O	1:B:62:THR:CB	0.45	2.65	5	1
1:A:89:LYS:CD	1:B:5:THR:CG2	0.45	2.95	17	2
1:A:95:ILE:HD13	1:A:95:ILE:O	0.45	2.12	6	1
1:A:42:ALA:HB1	1:A:59:LYS:CD	0.45	2.42	7	1
1:A:85:LYS:HE2	1:B:7:THR:CG2	0.45	2.42	7	1
1:A:45:GLN:OE1	1:A:51:LYS:CE	0.45	2.65	8	1
1:A:45:GLN:HA	1:A:48:HIS:CE1	0.45	2.47	13	2
1:A:70:GLU:C	1:A:79:LEU:HD11	0.45	2.32	17	2
1:A:6:LEU:HD11	1:B:90:GLU:CG	0.45	2.42	17	1
1:A:89:LYS:NZ	1:B:6:LEU:HD11	0.45	2.26	18	1
1:A:91:LYS:CB	1:B:76:TYR:HB2	0.44	2.42	2	1
1:B:95:ILE:HD13	1:B:95:ILE:O	0.44	2.12	6	1
1:A:67:GLN:HG2	1:A:68:ASP:N	0.44	2.26	9	3
1:A:95:ILE:O	1:A:98:LYS:CG	0.44	2.65	14	5
1:A:75:GLU:OE1	1:A:77:TRP:CZ2	0.44	2.70	19	2
1:A:85:LYS:HE3	1:B:3:ALA:CB	0.44	2.42	13	2
1:A:9:LEU:CD1	1:B:82:GLU:O	0.44	2.65	14	1
1:A:75:GLU:OE1	1:A:78:ARG:CG	0.44	2.65	18	4
1:B:95:ILE:O	1:B:98:LYS:CG	0.44	2.66	14	3
1:A:73:PHE:CE2	1:A:75:GLU:HG2	0.44	2.46	15	1
1:B:33:LEU:C	1:B:33:LEU:CD2	0.44	2.85	18	3
1:A:21:PHE:CZ	1:B:9:LEU:CD1	0.44	3.00	17	2
1:A:84:ALA:HB2	1:B:80:ILE:O	0.44	2.11	17	1
1:A:46:LEU:N	1:A:47:PRO:CD	0.44	2.80	20	2
1:B:20:PHE:CE1	1:B:23:PHE:CZ	0.44	3.05	18	1
1:B:42:ALA:HA	1:B:45:GLN:HG2	0.44	1.89	1	1
1:A:49:LEU:HD22	1:A:49:LEU:N	0.44	2.27	3	2
1:B:6:LEU:HD12	1:B:6:LEU:N	0.44	2.26	3	1
1:A:85:LYS:CE	1:B:7:THR:HG21	0.44	2.42	5	2
1:B:41:LEU:O	1:B:43:THR:N	0.44	2.50	19	5
1:B:67:GLN:NE2	1:B:68:ASP:N	0.44	2.66	17	3
1:B:85:LYS:O	1:B:89:LYS:HE3	0.44	2.12	6	3
1:A:33:LEU:HB2	1:A:70:GLU:CG	0.44	2.41	19	4
1:B:33:LEU:HB2	1:B:70:GLU:CG	0.44	2.42	7	3
1:A:5:THR:CG2	1:A:6:LEU:CD1	0.44	2.93	18	2
1:A:26:ARG:HG2	1:A:37:GLU:CG	0.44	2.42	14	1
1:A:6:LEU:HB2	1:B:48:HIS:CD2	0.44	2.46	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:ARG:HG3	1:B:37:GLU:HG3	0.44	1.89	19	1
1:A:86:GLU:O	1:A:90:GLU:CG	0.44	2.65	9	7
1:B:9:LEU:O	1:B:12:ALA:N	0.44	2.50	18	11
1:A:39:LYS:HA	1:B:1:MET:CG	0.44	2.42	16	5
1:A:3:ALA:HB1	1:B:85:LYS:HZ2	0.44	1.71	4	1
1:A:29:ARG:HG2	1:A:30:LYS:N	0.44	2.27	5	6
1:A:67:GLN:NE2	1:A:68:ASP:HA	0.44	2.27	5	1
1:B:46:LEU:O	1:B:51:LYS:HG2	0.44	2.12	20	2
1:A:24:ALA:CB	1:A:72:ARG:HD3	0.44	2.43	11	1
1:B:46:LEU:HD21	1:B:54:GLY:O	0.44	2.12	11	2
1:A:53:VAL:N	1:B:4:GLU:OE2	0.44	2.50	13	1
1:B:24:ALA:HB2	1:B:70:GLU:OE2	0.44	2.13	14	1
1:B:21:PHE:HB3	1:B:70:GLU:OE2	0.44	2.12	16	1
1:B:85:LYS:O	1:B:89:LYS:HE2	0.44	2.12	17	1
1:A:73:PHE:CB	1:B:97:LYS:HE2	0.44	2.42	19	1
1:A:10:GLU:O	1:A:13:ILE:CG2	0.44	2.65	3	13
1:B:6:LEU:CD1	1:B:10:GLU:CB	0.44	2.95	2	1
1:B:79:LEU:HA	1:B:82:GLU:CG	0.44	2.42	15	2
1:B:49:LEU:CD2	1:B:50:LEU:N	0.44	2.80	4	1
1:A:58:GLU:O	1:A:62:THR:CB	0.44	2.66	5	1
1:B:33:LEU:CB	1:B:70:GLU:OE1	0.44	2.66	5	2
1:A:1:MET:HE3	1:B:43:THR:HG23	0.44	1.90	6	1
1:A:86:GLU:CG	1:B:9:LEU:HB2	0.44	2.43	6	6
1:B:92:ALA:O	1:B:95:ILE:CG2	0.44	2.66	8	1
1:A:9:LEU:N	1:A:9:LEU:CD2	0.44	2.74	13	2
1:A:1:MET:HB3	1:B:42:ALA:HB3	0.44	1.89	14	1
1:B:21:PHE:CZ	1:B:79:LEU:HB3	0.44	2.47	14	1
1:A:33:LEU:CD2	1:A:72:ARG:HD3	0.44	2.43	20	1
1:A:18:SER:O	1:A:22:THR:HG21	0.44	2.12	20	8
1:B:10:GLU:O	1:B:13:ILE:CG2	0.44	2.66	3	12
1:A:33:LEU:O	1:A:67:GLN:O	0.44	2.36	12	5
1:A:4:GLU:HB3	1:B:54:GLY:CA	0.44	2.42	6	2
1:A:62:THR:CB	1:B:2:ALA:CB	0.44	2.95	6	1
1:B:27:GLU:HG2	1:B:34:ASN:ND2	0.44	2.26	15	2
1:A:5:THR:HG22	1:B:89:LYS:HD3	0.44	1.90	9	1
1:A:4:GLU:CA	1:A:4:GLU:OE1	0.44	2.65	17	2
1:B:20:PHE:CZ	1:B:38:PHE:CD2	0.44	3.06	13	1
1:A:6:LEU:CB	1:A:10:GLU:HB3	0.44	2.43	14	1
1:B:71:LEU:HD21	1:B:76:TYR:CE1	0.44	2.48	14	1
1:A:33:LEU:HD22	1:A:70:GLU:CB	0.44	2.38	15	1
1:A:69:SER:HA	1:A:78:ARG:HB3	0.44	1.89	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:SER:HB2	1:B:71:LEU:CB	0.44	2.43	20	1
1:A:59:LYS:HA	1:B:2:ALA:N	0.44	2.28	6	3
1:A:77:TRP:O	1:A:80:ILE:CG2	0.44	2.66	13	12
1:B:24:ALA:CB	1:B:72:ARG:NH1	0.44	2.81	3	2
1:A:67:GLN:NE2	1:A:68:ASP:OD1	0.44	2.51	4	2
1:A:85:LYS:HE2	1:B:7:THR:HG21	0.44	1.89	5	1
1:B:29:ARG:CG	1:B:30:LYS:N	0.44	2.81	20	2
1:B:67:GLN:CG	1:B:68:ASP:N	0.44	2.80	8	5
1:B:39:LYS:HD2	1:B:63:LEU:HD11	0.44	1.88	8	1
1:A:6:LEU:HD21	1:B:48:HIS:NE2	0.44	2.27	9	1
1:A:45:GLN:NE2	1:A:45:GLN:N	0.44	2.65	14	2
1:B:16:VAL:HG11	1:B:83:LEU:HD21	0.44	1.89	11	2
1:A:4:GLU:OE1	1:A:4:GLU:N	0.44	2.50	17	1
1:A:9:LEU:CD1	1:B:21:PHE:CZ	0.44	3.01	17	2
1:B:33:LEU:CD2	1:B:72:ARG:HD2	0.44	2.43	20	1
1:A:75:GLU:CD	1:A:77:TRP:CZ2	0.44	2.91	2	4
1:A:2:ALA:CB	1:B:62:THR:OG1	0.44	2.66	6	2
1:A:71:LEU:HB3	1:A:75:GLU:CB	0.44	2.43	18	1
1:A:85:LYS:CG	1:B:5:THR:O	0.44	2.66	19	1
1:A:46:LEU:O	1:A:51:LYS:HG2	0.44	2.13	20	1
1:B:46:LEU:HD12	1:B:47:PRO:HD3	0.44	1.89	20	1
1:A:70:GLU:CB	1:A:79:LEU:HD21	0.44	2.42	2	1
1:A:75:GLU:CA	1:A:75:GLU:OE1	0.44	2.65	3	1
1:A:55:SER:CB	1:A:58:GLU:CB	0.44	2.96	4	1
1:B:33:LEU:CD2	1:B:34:ASN:O	0.44	2.66	10	3
1:A:7:THR:O	1:A:10:GLU:HG2	0.44	2.13	12	6
1:B:33:LEU:O	1:B:67:GLN:O	0.44	2.35	12	6
1:A:2:ALA:CB	1:B:62:THR:CB	0.44	2.96	6	1
1:A:33:LEU:CB	1:A:70:GLU:HG3	0.44	2.43	19	5
1:B:21:PHE:O	1:B:72:ARG:CD	0.44	2.66	13	1
1:A:86:GLU:HB3	1:B:10:GLU:HA	0.44	1.90	17	1
1:B:24:ALA:N	1:B:33:LEU:CD1	0.44	2.77	18	1
1:A:5:THR:O	1:B:85:LYS:CG	0.44	2.66	19	1
1:B:62:THR:CG2	1:B:66:ASN:OD1	0.44	2.66	17	5
1:A:50:LEU:HD11	1:A:89:LYS:C	0.44	2.34	2	1
1:B:75:GLU:CD	1:B:77:TRP:CZ2	0.44	2.92	2	2
1:A:84:ALA:CB	1:B:80:ILE:CG1	0.44	2.95	5	1
1:A:4:GLU:CG	1:B:54:GLY:HA2	0.44	2.43	14	3
1:B:72:ARG:NE	1:B:72:ARG:HA	0.44	2.27	13	2
1:A:95:ILE:HG23	1:B:74:SER:CA	0.44	2.43	13	1
1:B:21:PHE:CD1	1:B:79:LEU:HD22	0.44	2.48	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:ILE:HG22	1:B:74:SER:HB3	0.44	1.89	14	1
1:B:76:TYR:HD1	1:B:79:LEU:HD13	0.44	1.72	17	1
1:A:32:SER:HB2	1:A:71:LEU:CB	0.44	2.43	20	1
1:A:13:ILE:O	1:A:17:VAL:CG1	0.43	2.66	7	11
1:A:91:LYS:CB	1:B:76:TYR:CB	0.43	2.96	2	1
1:A:16:VAL:HG23	1:B:9:LEU:CG	0.43	2.42	6	2
1:A:4:GLU:N	1:A:4:GLU:OE1	0.43	2.51	4	1
1:B:70:GLU:OE1	1:B:79:LEU:CD2	0.43	2.66	4	1
1:A:1:MET:HG2	1:B:39:LYS:CA	0.43	2.43	7	2
1:A:59:LYS:HA	1:B:2:ALA:CB	0.43	2.42	7	2
1:A:70:GLU:OE2	1:A:72:ARG:NE	0.43	2.51	10	3
1:A:38:PHE:O	1:A:41:LEU:CG	0.43	2.66	18	2
1:A:17:VAL:HA	1:A:21:PHE:CD2	0.43	2.48	13	3
1:A:42:ALA:CB	1:B:4:GLU:CG	0.43	2.95	11	1
1:A:23:PHE:CB	1:A:33:LEU:CD2	0.43	2.96	14	1
1:A:52:ASP:O	1:A:53:VAL:CG2	0.43	2.66	14	1
1:A:5:THR:CG2	1:B:89:LYS:CD	0.43	2.95	17	1
1:B:71:LEU:CG	1:B:75:GLU:HB2	0.43	2.44	8	4
1:B:92:ALA:O	1:B:95:ILE:CG1	0.43	2.66	4	6
1:A:15:THR:O	1:A:19:THR:N	0.43	2.51	3	3
1:A:33:LEU:HB3	1:A:70:GLU:OE1	0.43	2.12	15	2
1:A:33:LEU:CB	1:A:70:GLU:OE1	0.43	2.65	5	2
1:B:38:PHE:O	1:B:41:LEU:CG	0.43	2.66	18	2
1:A:82:GLU:OE2	1:A:85:LYS:NZ	0.43	2.50	10	1
1:A:26:ARG:NE	1:A:36:ASN:CB	0.43	2.81	12	1
1:A:33:LEU:CG	1:A:70:GLU:OE2	0.43	2.66	13	1
1:B:66:ASN:OD1	1:B:66:ASN:N	0.43	2.50	14	1
1:A:42:ALA:HB3	1:A:59:LYS:CG	0.43	2.43	16	1
1:A:32:SER:CB	1:A:68:ASP:OD1	0.43	2.67	17	2
1:B:71:LEU:HB3	1:B:75:GLU:HB2	0.43	1.90	18	1
1:A:33:LEU:HG	1:A:70:GLU:CG	0.43	2.43	20	1
1:A:62:THR:CG2	1:A:66:ASN:OD1	0.43	2.67	5	4
1:B:63:LEU:O	1:B:67:GLN:N	0.43	2.51	3	1
1:B:33:LEU:HB3	1:B:70:GLU:OE1	0.43	2.14	5	2
1:B:89:LYS:NZ	1:B:93:LEU:HB3	0.43	2.28	5	1
1:B:95:ILE:O	1:B:95:ILE:CD1	0.43	2.67	6	1
1:A:39:LYS:HD2	1:A:63:LEU:HD11	0.43	1.88	8	1
1:B:45:GLN:N	1:B:45:GLN:NE2	0.43	2.66	14	2
1:A:6:LEU:CD1	1:B:89:LYS:HG3	0.43	2.43	12	2
1:A:86:GLU:OE1	1:B:13:ILE:CB	0.43	2.66	20	2
1:A:59:LYS:HE3	1:B:1:MET:HE2	0.43	1.90	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:42:ALA:HB3	1:B:59:LYS:HD2	0.43	1.90	19	1
1:A:89:LYS:CD	1:B:5:THR:C	0.43	2.87	20	1
1:A:51:LYS:HA	1:B:5:THR:CG2	0.43	2.44	4	3
1:A:23:PHE:CZ	1:A:33:LEU:HD11	0.43	2.48	2	1
1:A:30:LYS:C	1:A:72:ARG:HB2	0.43	2.34	2	1
1:B:13:ILE:O	1:B:17:VAL:CG1	0.43	2.67	5	9
1:A:89:LYS:NZ	1:B:5:THR:O	0.43	2.51	3	1
1:B:65:VAL:O	1:B:78:ARG:NH1	0.43	2.52	3	1
1:A:6:LEU:HD12	1:B:89:LYS:CG	0.43	2.44	4	1
1:A:70:GLU:OE2	1:A:72:ARG:NH1	0.43	2.51	5	7
1:B:2:ALA:O	1:B:4:GLU:N	0.43	2.51	6	1
1:B:70:GLU:OE2	1:B:72:ARG:NE	0.43	2.51	10	3
1:A:20:PHE:CZ	1:A:41:LEU:CG	0.43	3.02	17	2
1:B:33:LEU:O	1:B:68:ASP:HA	0.43	2.14	9	1
1:A:67:GLN:CD	1:A:68:ASP:N	0.43	2.72	17	1
1:B:89:LYS:CE	1:B:90:GLU:OE1	0.43	2.67	18	1
1:B:7:THR:CB	1:B:9:LEU:CD1	0.43	2.97	20	1
1:A:92:ALA:O	1:A:95:ILE:CG1	0.43	2.67	2	6
1:A:5:THR:O	1:B:89:LYS:NZ	0.43	2.51	3	1
1:A:24:ALA:CB	1:A:72:ARG:NH1	0.43	2.81	3	2
1:B:68:ASP:CB	1:B:78:ARG:HG3	0.43	2.44	11	5
1:A:2:ALA:CB	1:B:59:LYS:HA	0.43	2.43	7	2
1:A:95:ILE:CG2	1:B:73:PHE:C	0.43	2.87	9	3
1:B:26:ARG:CD	1:B:37:GLU:HG2	0.43	2.43	7	1
1:A:35:ILE:O	1:A:39:LYS:HG2	0.43	2.14	19	4
1:A:86:GLU:OE2	1:B:7:THR:N	0.43	2.51	16	2
1:A:45:GLN:NE2	1:B:7:THR:CB	0.43	2.82	9	1
1:A:21:PHE:O	1:A:72:ARG:CD	0.43	2.67	13	1
1:A:72:ARG:NE	1:A:72:ARG:HA	0.43	2.29	13	1
1:B:20:PHE:CZ	1:B:38:PHE:CE2	0.43	3.07	13	1
1:A:10:GLU:O	1:A:13:ILE:N	0.43	2.51	14	2
1:A:83:LEU:HD12	1:B:87:VAL:HG23	0.43	1.91	14	1
1:B:26:ARG:HG2	1:B:37:GLU:CG	0.43	2.43	14	1
1:B:71:LEU:CD2	1:B:76:TYR:CE1	0.43	3.02	14	1
1:B:14:GLU:CG	1:B:15:THR:N	0.43	2.82	15	1
1:A:54:GLY:CA	1:B:4:GLU:HG2	0.43	2.43	16	1
1:A:7:THR:HA	1:B:45:GLN:OE1	0.43	2.14	18	2
1:A:97:LYS:HE2	1:B:73:PHE:CB	0.43	2.43	19	1
1:B:7:THR:OG1	1:B:9:LEU:CD1	0.43	2.66	20	1
1:B:35:ILE:HD13	1:B:63:LEU:CD2	0.43	2.44	20	1
1:A:3:ALA:CB	1:B:85:LYS:HE3	0.43	2.43	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:VAL:O	1:B:55:SER:N	0.43	2.51	14	3
1:A:6:LEU:CD1	1:A:10:GLU:HB3	0.43	2.43	2	1
1:A:6:LEU:CG	1:A:10:GLU:HB3	0.43	2.43	2	1
1:A:49:LEU:CD2	1:A:50:LEU:N	0.43	2.81	4	1
1:B:21:PHE:CD2	1:B:79:LEU:CD2	0.43	3.01	19	2
1:B:36:ASN:O	1:B:39:LYS:HG3	0.43	2.13	10	1
1:B:39:LYS:HE3	1:B:63:LEU:HD11	0.43	1.88	10	1
1:A:4:GLU:OE2	1:B:54:GLY:CA	0.43	2.66	11	1
1:A:20:PHE:CZ	1:A:38:PHE:HA	0.43	2.49	17	2
1:A:24:ALA:HB2	1:A:70:GLU:OE2	0.43	2.13	14	1
1:A:67:GLN:NE2	1:A:68:ASP:OD2	0.43	2.52	17	3
1:B:57:ASP:O	1:B:61:LYS:CG	0.43	2.67	18	2
1:B:66:ASN:N	1:B:66:ASN:OD1	0.43	2.51	15	1
1:A:21:PHE:HB3	1:A:70:GLU:OE2	0.43	2.13	16	1
1:A:54:GLY:O	1:A:59:LYS:CD	0.43	2.67	16	1
1:A:56:LEU:N	1:A:56:LEU:CD2	0.43	2.82	18	1
1:B:71:LEU:HB3	1:B:75:GLU:CB	0.43	2.43	18	1
1:A:70:GLU:OE2	1:A:72:ARG:CD	0.43	2.67	1	1
1:A:33:LEU:HB3	1:A:70:GLU:HG2	0.43	1.90	3	1
1:A:68:ASP:CB	1:A:75:GLU:HG3	0.43	2.44	3	1
1:A:84:ALA:O	1:A:87:VAL:N	0.43	2.52	12	10
1:A:20:PHE:CD2	1:A:21:PHE:CE1	0.43	3.07	4	3
1:A:23:PHE:CE2	1:A:33:LEU:HG	0.43	2.48	15	2
1:A:64:ASP:O	1:A:67:GLN:OE1	0.43	2.36	20	3
1:A:45:GLN:OE1	1:B:7:THR:HA	0.43	2.14	18	3
1:B:35:ILE:CD1	1:B:63:LEU:CD2	0.43	2.95	18	1
1:A:89:LYS:HG2	1:B:5:THR:CG2	0.43	2.44	19	1
1:A:90:GLU:O	1:A:94:GLY:N	0.43	2.50	20	1
1:B:46:LEU:O	1:B:51:LYS:HE2	0.43	2.14	15	3
1:B:71:LEU:CD2	1:B:73:PHE:H	0.43	2.26	15	6
1:A:32:SER:HB3	1:A:73:PHE:CZ	0.43	2.48	4	2
1:B:45:GLN:O	1:B:48:HIS:ND1	0.43	2.52	2	2
1:B:83:LEU:O	1:B:86:GLU:HG2	0.43	2.13	5	4
1:A:34:ASN:HA	1:A:67:GLN:O	0.43	2.14	19	2
1:A:35:ILE:O	1:A:39:LYS:CG	0.43	2.67	9	1
1:A:66:ASN:ND2	1:A:82:GLU:OE1	0.43	2.52	10	1
1:A:67:GLN:NE2	1:A:67:GLN:C	0.43	2.72	11	1
1:B:23:PHE:CB	1:B:33:LEU:CD2	0.43	2.97	14	1
1:B:21:PHE:HA	1:B:23:PHE:CD1	0.43	2.49	18	1
1:B:62:THR:O	1:B:66:ASN:N	0.43	2.50	19	1
1:A:60:MET:O	1:A:63:LEU:CB	0.43	2.66	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:82:GLU:HA	1:B:85:LYS:CD	0.43	2.44	1	2
1:B:68:ASP:CB	1:B:75:GLU:HG3	0.43	2.44	3	1
1:A:70:GLU:OE1	1:A:79:LEU:CD2	0.43	2.66	4	1
1:B:84:ALA:O	1:B:87:VAL:N	0.43	2.52	5	8
1:A:71:LEU:HD21	1:A:73:PHE:C	0.43	2.33	17	3
1:A:83:LEU:HD13	1:B:87:VAL:HG21	0.43	1.90	5	1
1:A:7:THR:CG2	1:B:85:LYS:HE2	0.43	2.44	7	1
1:A:87:VAL:CG1	1:A:87:VAL:O	0.43	2.67	7	3
1:A:45:GLN:NE2	1:B:7:THR:OG1	0.43	2.52	9	3
1:A:54:GLY:CA	1:B:4:GLU:OE2	0.43	2.66	11	1
1:A:81:GLY:C	1:A:85:LYS:HZ3	0.43	2.17	13	1
1:B:24:ALA:HB2	1:B:32:SER:HA	0.43	1.91	13	1
1:B:77:TRP:CD1	1:B:78:ARG:HG2	0.43	2.49	13	4
1:A:68:ASP:HB2	1:A:78:ARG:CG	0.43	2.44	15	1
1:A:4:GLU:HG2	1:B:54:GLY:CA	0.43	2.44	16	1
1:B:39:LYS:O	1:B:43:THR:CG2	0.43	2.67	16	1
1:A:86:GLU:HB2	1:B:13:ILE:HD13	0.43	1.91	19	1
1:A:4:GLU:HG3	1:B:54:GLY:HA2	0.43	1.90	20	1
1:A:7:THR:O	1:A:9:LEU:N	0.43	2.52	5	12
1:A:85:LYS:HD2	1:B:3:ALA:CB	0.43	2.44	2	1
1:A:62:THR:O	1:A:66:ASN:N	0.43	2.51	10	5
1:A:39:LYS:HA	1:B:1:MET:SD	0.43	2.54	9	4
1:A:89:LYS:CE	1:A:90:GLU:OE2	0.43	2.67	5	1
1:A:5:THR:OG1	1:B:52:ASP:N	0.43	2.52	15	3
1:B:21:PHE:HB3	1:B:70:GLU:CD	0.43	2.34	11	1
1:B:41:LEU:O	1:B:45:GLN:CG	0.43	2.67	12	1
1:A:4:GLU:OE1	1:B:54:GLY:N	0.43	2.52	13	1
1:A:20:PHE:CZ	1:A:38:PHE:CE2	0.43	3.07	13	1
1:B:55:SER:OG	1:B:58:GLU:CB	0.43	2.67	15	1
1:A:2:ALA:CB	1:B:58:GLU:O	0.43	2.67	18	1
1:A:38:PHE:O	1:A:41:LEU:CB	0.43	2.67	18	1
1:A:89:LYS:CB	1:B:5:THR:HG23	0.43	2.44	18	1
1:A:38:PHE:CZ	1:B:3:ALA:HB2	0.43	2.49	19	1
1:A:86:GLU:OE1	1:B:7:THR:N	0.42	2.52	10	7
1:B:7:THR:O	1:B:9:LEU:N	0.42	2.52	5	8
1:B:91:LYS:O	1:B:94:GLY:N	0.42	2.51	2	1
1:A:4:GLU:OE2	1:B:45:GLN:HB2	0.42	2.14	3	1
1:B:50:LEU:CD1	1:B:90:GLU:OE1	0.42	2.67	4	1
1:B:59:LYS:O	1:B:63:LEU:HD13	0.42	2.14	4	1
1:A:7:THR:HG21	1:B:85:LYS:CE	0.42	2.44	7	2
1:A:95:ILE:O	1:A:95:ILE:CD1	0.42	2.67	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ASN:OD1	1:A:35:ILE:CD1	0.42	2.67	17	4
1:A:42:ALA:CB	1:A:59:LYS:CD	0.42	2.97	7	1
1:A:87:VAL:HG11	1:B:80:ILE:N	0.42	2.29	10	3
1:A:48:HIS:HB2	1:A:51:LYS:CD	0.42	2.44	8	1
1:A:33:LEU:O	1:A:68:ASP:HA	0.42	2.14	9	1
1:A:6:LEU:HD11	1:B:50:LEU:HD21	0.42	1.89	11	1
1:A:20:PHE:CE1	1:A:70:GLU:HB3	0.42	2.48	13	1
1:B:20:PHE:CE1	1:B:70:GLU:HB3	0.42	2.49	13	1
1:B:54:GLY:O	1:B:59:LYS:CD	0.42	2.67	16	1
1:A:4:GLU:OE2	1:B:42:ALA:CB	0.42	2.67	17	1
1:A:86:GLU:OE1	1:B:10:GLU:N	0.42	2.52	17	1
1:A:23:PHE:CD1	1:A:33:LEU:CD1	0.42	3.02	18	1
1:A:7:THR:OG1	1:A:9:LEU:CD1	0.42	2.67	20	1
1:B:66:ASN:CA	1:B:69:SER:OG	0.42	2.67	20	1
1:A:4:GLU:OE2	1:B:45:GLN:CB	0.42	2.68	3	2
1:A:76:TYR:HB2	1:B:91:LYS:CB	0.42	2.44	2	1
1:A:71:LEU:CD2	1:A:73:PHE:H	0.42	2.27	5	3
1:B:70:GLU:OE2	1:B:72:ARG:NH1	0.42	2.52	16	6
1:A:54:GLY:N	1:B:4:GLU:OE1	0.42	2.52	13	2
1:A:73:PHE:CG	1:A:74:SER:N	0.42	2.86	11	2
1:A:41:LEU:O	1:A:45:GLN:HG3	0.42	2.14	8	1
1:A:72:ARG:O	1:B:97:LYS:NZ	0.42	2.52	17	3
1:B:45:GLN:O	1:B:46:LEU:C	0.42	2.57	19	2
1:A:39:LYS:HE3	1:A:63:LEU:CD1	0.42	2.44	10	1
1:B:80:ILE:HG23	1:B:81:GLY:N	0.42	2.29	18	3
1:A:48:HIS:CE1	1:B:6:LEU:HD12	0.42	2.49	14	1
1:A:59:LYS:CG	1:B:4:GLU:OE2	0.42	2.67	17	1
1:B:33:LEU:HG	1:B:70:GLU:CG	0.42	2.44	20	1
1:B:89:LYS:CE	1:B:89:LYS:H	0.42	2.28	20	1
1:A:86:GLU:HG3	1:B:10:GLU:N	0.42	2.29	17	2
1:A:71:LEU:CG	1:A:75:GLU:HB2	0.42	2.45	8	4
1:A:95:ILE:HG21	1:A:98:LYS:HE2	0.42	1.90	3	1
1:B:95:ILE:O	1:B:95:ILE:CG2	0.42	2.66	3	1
1:A:76:TYR:O	1:A:79:LEU:HD12	0.42	2.14	19	5
1:B:87:VAL:CG1	1:B:87:VAL:O	0.42	2.67	7	2
1:A:23:PHE:HB2	1:A:37:GLU:CG	0.42	2.45	9	1
1:A:71:LEU:CD2	1:A:73:PHE:HD1	0.42	2.27	12	1
1:A:70:GLU:CG	1:A:70:GLU:O	0.42	2.68	13	1
1:A:85:LYS:CG	1:B:3:ALA:O	0.42	2.67	14	1
1:B:3:ALA:CB	1:B:7:THR:CG2	0.42	2.97	14	1
1:A:4:GLU:CG	1:B:54:GLY:N	0.42	2.83	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:PHE:CE1	1:B:9:LEU:HD11	0.42	2.49	16	1
1:A:54:GLY:N	1:B:4:GLU:HG2	0.42	2.29	16	1
1:A:17:VAL:HG13	1:A:18:SER:N	0.42	2.29	17	2
1:A:42:ALA:HB3	1:A:59:LYS:HG3	0.42	1.91	18	1
1:A:9:LEU:CD2	1:B:21:PHE:CE1	0.42	3.03	19	1
1:A:21:PHE:CE1	1:B:9:LEU:CD2	0.42	3.02	19	1
1:B:14:GLU:O	1:B:18:SER:CB	0.42	2.67	19	1
1:B:23:PHE:CG	1:B:33:LEU:CD1	0.42	3.03	19	1
1:A:91:LYS:O	1:A:94:GLY:N	0.42	2.53	2	1
1:B:82:GLU:C	1:B:84:ALA:N	0.42	2.73	4	2
1:A:51:LYS:HG2	1:A:53:VAL:N	0.42	2.29	6	5
1:A:91:LYS:O	1:B:74:SER:CA	0.42	2.68	3	2
1:A:50:LEU:CD1	1:A:90:GLU:OE1	0.42	2.67	4	1
1:B:4:GLU:OE1	1:B:4:GLU:N	0.42	2.52	17	2
1:A:7:THR:HG21	1:B:85:LYS:NZ	0.42	2.29	5	1
1:B:89:LYS:NZ	1:B:93:LEU:CB	0.42	2.83	5	1
1:A:86:GLU:OE1	1:B:10:GLU:CB	0.42	2.67	6	1
1:B:34:ASN:OD1	1:B:36:ASN:N	0.42	2.52	10	2
1:B:6:LEU:H	1:B:6:LEU:HD12	0.42	1.74	7	1
1:A:7:THR:N	1:B:86:GLU:OE2	0.42	2.53	16	2
1:A:3:ALA:CB	1:B:85:LYS:NZ	0.42	2.82	10	1
1:A:75:GLU:OE1	1:A:77:TRP:CH2	0.42	2.72	12	2
1:A:70:GLU:O	1:A:70:GLU:HG2	0.42	2.15	13	1
1:A:33:LEU:CG	1:A:70:GLU:HB3	0.42	2.44	15	1
1:A:97:LYS:CD	1:B:30:LYS:HB2	0.42	2.44	15	1
1:A:5:THR:HB	1:B:51:LYS:CD	0.42	2.44	18	2
1:A:50:LEU:HD22	1:A:93:LEU:CD1	0.42	2.45	18	1
1:A:58:GLU:OE2	1:A:59:LYS:NZ	0.42	2.52	18	1
1:B:58:GLU:OE2	1:B:59:LYS:NZ	0.42	2.52	18	1
1:A:7:THR:HA	1:B:45:GLN:NE2	0.42	2.29	19	1
1:A:89:LYS:HB3	1:B:5:THR:CG2	0.42	2.44	19	1
1:A:58:GLU:OE1	1:A:58:GLU:N	0.42	2.53	20	1
1:A:83:LEU:HA	1:B:9:LEU:HD22	0.42	1.90	20	1
1:B:60:MET:O	1:B:63:LEU:CB	0.42	2.67	20	1
1:B:97:LYS:O	1:B:97:LYS:CD	0.42	2.67	20	1
1:B:68:ASP:HB3	1:B:75:GLU:CB	0.42	2.44	9	3
1:A:75:GLU:O	1:A:78:ARG:N	0.42	2.50	2	2
1:A:10:GLU:HA	1:B:86:GLU:HB2	0.42	1.91	5	1
1:A:11:ALA:C	1:B:15:THR:HG21	0.42	2.35	5	1
1:B:23:PHE:HA	1:B:37:GLU:OE2	0.42	2.14	10	5
1:A:90:GLU:HG3	1:B:6:LEU:CD2	0.42	2.42	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:PHE:CD2	1:B:21:PHE:CD1	0.42	3.08	7	1
1:B:68:ASP:O	1:B:70:GLU:N	0.42	2.53	10	3
1:B:45:GLN:O	1:B:51:LYS:HE2	0.42	2.14	8	2
1:B:61:LYS:NZ	1:B:65:VAL:CG2	0.42	2.83	11	1
1:A:24:ALA:CB	1:A:70:GLU:OE2	0.42	2.67	14	1
1:A:45:GLN:HG3	1:B:7:THR:CG2	0.42	2.45	14	1
1:B:16:VAL:HG21	1:B:83:LEU:CD2	0.42	2.45	14	1
1:B:20:PHE:CZ	1:B:38:PHE:HA	0.42	2.49	17	1
1:A:23:PHE:N	1:A:33:LEU:HD13	0.42	2.29	20	1
1:A:71:LEU:HD13	1:A:79:LEU:CD2	0.42	2.42	20	1
1:B:24:ALA:CA	1:B:33:LEU:HB3	0.42	2.44	20	1
1:A:83:LEU:HD13	1:B:83:LEU:HB3	0.42	1.90	1	1
1:A:15:THR:HG21	1:B:12:ALA:HA	0.42	1.91	2	1
1:B:33:LEU:HD23	1:B:34:ASN:O	0.42	2.13	4	2
1:B:47:PRO:HA	1:B:51:LYS:CE	0.42	2.44	4	5
1:B:89:LYS:CE	1:B:90:GLU:OE2	0.42	2.67	5	1
1:A:4:GLU:CD	1:B:42:ALA:HB1	0.42	2.34	9	1
1:A:42:ALA:HB1	1:B:4:GLU:CD	0.42	2.35	9	1
1:A:86:GLU:HG2	1:B:9:LEU:HB2	0.42	1.90	11	1
1:B:75:GLU:HA	1:B:77:TRP:CE2	0.42	2.50	11	2
1:A:24:ALA:HB3	1:A:72:ARG:CG	0.42	2.42	13	1
1:B:41:LEU:CB	1:B:45:GLN:OE1	0.42	2.68	13	1
1:A:75:GLU:OE1	1:A:78:ARG:HG2	0.42	2.14	14	1
1:B:10:GLU:O	1:B:13:ILE:N	0.42	2.52	14	1
1:B:52:ASP:O	1:B:53:VAL:CG2	0.42	2.67	14	1
1:A:87:VAL:CG1	1:B:79:LEU:HB2	0.42	2.44	17	1
1:A:6:LEU:HD11	1:B:89:LYS:HZ2	0.42	1.73	18	1
1:A:58:GLU:O	1:B:2:ALA:CB	0.42	2.67	18	1
1:A:1:MET:HE2	1:B:43:THR:CG2	0.42	2.43	19	1
1:A:5:THR:C	1:B:89:LYS:CD	0.42	2.88	20	1
1:A:35:ILE:HD13	1:A:63:LEU:CD2	0.42	2.44	20	1
1:B:20:PHE:CD2	1:B:21:PHE:CE1	0.42	3.08	7	5
1:B:67:GLN:NE2	1:B:68:ASP:OD1	0.42	2.52	4	1
1:A:95:ILE:CD1	1:A:98:LYS:HE3	0.42	2.45	6	1
1:B:95:ILE:CD1	1:B:98:LYS:HE3	0.42	2.45	6	1
1:B:33:LEU:CB	1:B:70:GLU:HG3	0.42	2.45	19	3
1:A:91:LYS:HG3	1:A:92:ALA:N	0.42	2.29	18	5
1:A:13:ILE:CG1	1:B:86:GLU:OE1	0.42	2.68	9	1
1:A:35:ILE:CG2	1:A:63:LEU:O	0.42	2.64	11	1
1:A:61:LYS:NZ	1:A:65:VAL:CG2	0.42	2.82	11	1
1:A:95:ILE:O	1:A:98:LYS:HG3	0.42	2.15	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:76:TYR:O	1:B:79:LEU:HG	0.42	2.14	13	1
1:A:13:ILE:CB	1:B:86:GLU:OE1	0.42	2.67	14	1
1:A:90:GLU:CG	1:B:6:LEU:CD2	0.42	2.98	15	2
1:B:67:GLN:CD	1:B:68:ASP:N	0.42	2.73	14	1
1:A:30:LYS:HB2	1:B:97:LYS:CD	0.42	2.45	15	1
1:A:89:LYS:HZ2	1:B:6:LEU:HD11	0.42	1.75	18	1
1:B:56:LEU:N	1:B:56:LEU:CD2	0.42	2.82	18	1
1:A:13:ILE:CB	1:B:86:GLU:OE2	0.42	2.67	20	1
1:B:46:LEU:CD1	1:B:47:PRO:HD3	0.42	2.45	20	1
1:B:58:GLU:N	1:B:58:GLU:OE1	0.42	2.52	20	1
1:A:74:SER:CB	1:B:95:ILE:CG2	0.42	2.98	13	2
1:A:91:LYS:HB2	1:B:76:TYR:HB2	0.42	1.92	2	1
1:B:6:LEU:CD1	1:B:10:GLU:HB3	0.42	2.44	2	1
1:A:20:PHE:CD2	1:A:21:PHE:CD1	0.42	3.08	6	1
1:A:67:GLN:CG	1:A:68:ASP:N	0.42	2.83	9	2
1:A:56:LEU:O	1:A:60:MET:N	0.42	2.53	20	2
1:A:10:GLU:HA	1:B:86:GLU:CB	0.42	2.45	9	1
1:A:89:LYS:HD3	1:B:5:THR:HG22	0.42	1.91	10	2
1:A:36:ASN:O	1:A:39:LYS:HG3	0.42	2.15	10	1
1:A:54:GLY:HA3	1:B:4:GLU:HG3	0.42	1.92	10	1
1:A:52:ASP:N	1:B:5:THR:OG1	0.42	2.52	11	2
1:A:23:PHE:CA	1:A:37:GLU:OE1	0.42	2.68	12	1
1:B:68:ASP:C	1:B:70:GLU:N	0.42	2.72	18	3
1:A:29:ARG:HD3	1:A:29:ARG:N	0.42	2.30	15	1
1:B:70:GLU:C	1:B:79:LEU:HD11	0.42	2.35	17	2
1:A:15:THR:O	1:A:18:SER:N	0.42	2.53	16	1
1:B:17:VAL:CG1	1:B:18:SER:N	0.42	2.83	17	1
1:A:71:LEU:CD2	1:A:73:PHE:O	0.42	2.68	18	1
1:B:38:PHE:O	1:B:41:LEU:CB	0.42	2.68	18	1
1:A:6:LEU:HD22	1:A:10:GLU:HB3	0.42	1.92	19	1
1:A:97:LYS:CE	1:B:30:LYS:O	0.42	2.68	3	1
1:B:91:LYS:HG3	1:B:92:ALA:N	0.42	2.30	14	5
1:B:26:ARG:HG3	1:B:37:GLU:CG	0.42	2.45	19	2
1:B:68:ASP:HB3	1:B:75:GLU:HB3	0.42	1.91	13	2
1:A:41:LEU:HD13	1:B:8:GLU:OE1	0.42	2.14	8	1
1:A:89:LYS:HG2	1:A:90:GLU:N	0.42	2.29	8	1
1:B:85:LYS:O	1:B:88:ARG:N	0.42	2.50	9	1
1:A:42:ALA:HA	1:A:45:GLN:CG	0.42	2.45	10	1
1:A:39:LYS:CA	1:B:1:MET:HG2	0.42	2.45	12	1
1:A:33:LEU:CG	1:A:34:ASN:N	0.42	2.83	13	2
1:A:41:LEU:HB3	1:A:45:GLN:OE1	0.42	2.14	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:ALA:CB	1:B:70:GLU:OE2	0.42	2.67	14	1
1:A:23:PHE:CD1	1:A:23:PHE:O	0.42	2.73	16	1
1:A:42:ALA:CB	1:B:4:GLU:OE2	0.42	2.68	17	1
1:A:6:LEU:HG	1:B:89:LYS:HG2	0.42	1.91	18	1
1:A:7:THR:HB	1:A:9:LEU:HD12	0.42	1.91	20	1
1:A:68:ASP:HB3	1:A:75:GLU:CB	0.42	2.45	9	3
1:B:50:LEU:HD11	1:B:89:LYS:C	0.42	2.35	2	1
1:A:21:PHE:CE2	1:A:79:LEU:HB3	0.42	2.50	3	2
1:A:82:GLU:HB3	1:B:9:LEU:CD1	0.42	2.44	3	4
1:B:23:PHE:CE2	1:B:38:PHE:HB2	0.42	2.49	11	2
1:A:15:THR:HG21	1:B:11:ALA:C	0.42	2.35	5	1
1:A:80:ILE:CG1	1:B:84:ALA:CB	0.42	2.95	5	1
1:A:97:LYS:HE2	1:B:72:ARG:O	0.42	2.15	6	1
1:B:42:ALA:CA	1:B:45:GLN:HB2	0.42	2.44	9	1
1:B:42:ALA:HA	1:B:45:GLN:CG	0.42	2.45	10	1
1:B:57:ASP:O	1:B:61:LYS:N	0.42	2.51	10	1
1:A:1:MET:SD	1:B:59:LYS:CE	0.42	3.08	17	1
1:B:32:SER:CB	1:B:68:ASP:OD1	0.42	2.68	17	2
1:A:69:SER:HA	1:A:78:ARG:CB	0.42	2.44	20	1
1:A:7:THR:OG1	1:B:85:LYS:NZ	0.41	2.53	1	1
1:A:95:ILE:HG13	1:A:95:ILE:O	0.41	2.15	1	1
1:A:39:LYS:HA	1:B:1:MET:CB	0.41	2.45	2	3
1:A:67:GLN:HE21	1:A:68:ASP:H	0.41	1.56	2	1
1:A:65:VAL:O	1:A:78:ARG:NH1	0.41	2.53	3	1
1:A:71:LEU:HD22	1:A:73:PHE:H	0.41	1.75	5	2
1:A:87:VAL:HG21	1:B:83:LEU:HD13	0.41	1.92	5	1
1:A:2:ALA:O	1:A:4:GLU:N	0.41	2.53	6	2
1:A:10:GLU:CB	1:B:86:GLU:OE1	0.41	2.68	6	1
1:A:95:ILE:CA	1:B:73:PHE:O	0.41	2.68	10	1
1:B:30:LYS:N	1:B:30:LYS:HD2	0.41	2.29	10	1
1:B:87:VAL:O	1:B:87:VAL:HG12	0.41	2.15	12	1
1:B:26:ARG:NH2	1:B:37:GLU:OE1	0.41	2.52	13	1
1:B:62:THR:O	1:B:65:VAL:N	0.41	2.53	13	1
1:B:70:GLU:CG	1:B:70:GLU:O	0.41	2.67	13	1
1:B:86:GLU:OE1	1:B:86:GLU:CA	0.41	2.68	13	1
1:A:86:GLU:OE1	1:B:13:ILE:CA	0.41	2.68	14	1
1:B:75:GLU:OE1	1:B:78:ARG:HG2	0.41	2.15	14	1
1:A:90:GLU:CG	1:B:6:LEU:HD11	0.41	2.45	17	1
1:A:20:PHE:CE2	1:A:23:PHE:CD2	0.41	3.07	19	1
1:B:80:ILE:HD13	1:B:80:ILE:O	0.41	2.14	20	1
1:A:35:ILE:CG2	1:A:66:ASN:O	0.41	2.68	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:SER:C	1:A:22:THR:HG23	0.41	2.36	6	3
1:B:47:PRO:HA	1:B:51:LYS:HE3	0.41	1.90	6	2
1:A:26:ARG:CD	1:A:37:GLU:HG2	0.41	2.45	7	1
1:A:3:ALA:O	1:B:85:LYS:NZ	0.41	2.50	8	1
1:A:61:LYS:HD3	1:A:61:LYS:N	0.41	2.31	8	1
1:B:42:ALA:O	1:B:46:LEU:CA	0.41	2.69	8	1
1:B:61:LYS:O	1:B:64:ASP:N	0.41	2.52	9	1
1:A:86:GLU:HG3	1:B:9:LEU:C	0.41	2.36	10	1
1:B:55:SER:O	1:B:58:GLU:N	0.41	2.53	10	1
1:B:66:ASN:ND2	1:B:82:GLU:OE1	0.41	2.54	10	1
1:A:7:THR:N	1:B:86:GLU:OE1	0.41	2.53	16	2
1:B:7:THR:O	1:B:10:GLU:HG2	0.41	2.15	12	1
1:A:10:GLU:OE1	1:A:11:ALA:N	0.41	2.54	17	1
1:A:33:LEU:CD2	1:A:34:ASN:O	0.41	2.68	18	1
1:A:14:GLU:O	1:A:18:SER:CB	0.41	2.67	19	1
1:A:97:LYS:CD	1:A:97:LYS:O	0.41	2.68	20	1
1:B:14:GLU:CA	1:B:17:VAL:HG12	0.41	2.45	20	1
1:B:23:PHE:CE2	1:B:70:GLU:HG3	0.41	2.51	20	1
1:A:46:LEU:HB3	1:A:47:PRO:HD3	0.41	1.92	1	3
1:B:70:GLU:OE2	1:B:72:ARG:CD	0.41	2.68	1	1
1:A:39:LYS:CE	1:A:63:LEU:HD21	0.41	2.46	3	2
1:B:73:PHE:CE1	1:B:75:GLU:HB2	0.41	2.50	14	3
1:B:65:VAL:O	1:B:78:ARG:NH2	0.41	2.52	5	1
1:A:5:THR:O	1:B:89:LYS:CE	0.41	2.68	6	1
1:A:13:ILE:HA	1:A:16:VAL:CG1	0.41	2.45	10	2
1:A:42:ALA:CB	1:B:1:MET:HB3	0.41	2.46	7	2
1:A:73:PHE:C	1:B:95:ILE:CG2	0.41	2.89	7	1
1:A:68:ASP:C	1:A:70:GLU:N	0.41	2.72	19	4
1:B:7:THR:HG22	1:B:8:GLU:OE1	0.41	2.15	8	1
1:B:71:LEU:HD11	1:B:76:TYR:N	0.41	2.30	8	1
1:A:95:ILE:CG2	1:B:74:SER:OG	0.41	2.67	9	1
1:A:34:ASN:OD1	1:A:36:ASN:N	0.41	2.53	10	1
1:B:26:ARG:NE	1:B:37:GLU:CG	0.41	2.83	10	1
1:A:26:ARG:NH2	1:A:37:GLU:OE1	0.41	2.53	13	1
1:A:54:GLY:CA	1:B:4:GLU:OE1	0.41	2.67	13	1
1:A:53:VAL:O	1:A:55:SER:N	0.41	2.53	14	1
1:A:17:VAL:CG1	1:A:18:SER:N	0.41	2.82	17	1
1:A:87:VAL:HA	1:A:90:GLU:HB2	0.41	1.91	19	1
1:B:72:ARG:NE	1:B:72:ARG:CA	0.41	2.83	19	1
1:A:21:PHE:O	1:A:33:LEU:CD2	0.41	2.68	20	1
1:B:46:LEU:N	1:B:47:PRO:CD	0.41	2.83	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:CD1	1:A:10:GLU:CB	0.41	2.97	2	1
1:A:50:LEU:O	1:A:50:LEU:HG	0.41	2.16	2	1
1:B:39:LYS:CE	1:B:63:LEU:HD21	0.41	2.44	2	2
1:B:68:ASP:O	1:B:69:SER:C	0.41	2.58	2	1
1:A:1:MET:HB3	1:B:42:ALA:CB	0.41	2.46	14	2
1:A:32:SER:OG	1:A:73:PHE:CZ	0.41	2.67	6	1
1:A:18:SER:C	1:A:22:THR:CG2	0.41	2.89	17	2
1:B:56:LEU:O	1:B:60:MET:N	0.41	2.53	8	2
1:A:6:LEU:HB3	1:A:10:GLU:HB3	0.41	1.92	13	1
1:B:5:THR:CG2	1:B:6:LEU:CD1	0.41	2.95	13	1
1:A:21:PHE:O	1:A:70:GLU:CD	0.41	2.59	17	3
1:B:21:PHE:O	1:B:70:GLU:CD	0.41	2.59	14	2
1:B:67:GLN:NE2	1:B:68:ASP:OD2	0.41	2.53	16	2
1:A:21:PHE:CZ	1:B:9:LEU:HD11	0.41	2.50	17	1
1:A:85:LYS:O	1:A:89:LYS:HE2	0.41	2.15	17	1
1:A:66:ASN:CA	1:A:69:SER:OG	0.41	2.68	20	1
1:B:65:VAL:O	1:B:67:GLN:OE1	0.41	2.38	20	1
1:A:67:GLN:NE2	1:A:68:ASP:H	0.41	2.13	2	1
1:A:68:ASP:O	1:A:69:SER:C	0.41	2.59	2	1
1:B:92:ALA:O	1:B:95:ILE:HG12	0.41	2.15	13	5
1:A:90:GLU:HG2	1:B:6:LEU:CD2	0.41	2.46	13	2
1:A:59:LYS:O	1:A:63:LEU:HD13	0.41	2.16	4	1
1:B:68:ASP:HB2	1:B:78:ARG:HG3	0.41	1.93	5	2
1:B:82:GLU:HA	1:B:85:LYS:HD3	0.41	1.92	15	2
1:B:39:LYS:HE3	1:B:63:LEU:CD1	0.41	2.44	10	1
1:A:41:LEU:O	1:A:45:GLN:CG	0.41	2.68	12	1
1:A:42:ALA:CA	1:A:45:GLN:HG3	0.41	2.45	12	1
1:B:85:LYS:CG	1:B:86:GLU:OE2	0.41	2.69	12	1
1:A:97:LYS:NZ	1:B:72:ARG:O	0.41	2.53	13	2
1:A:1:MET:HG3	1:B:59:LYS:HD2	0.41	1.92	14	1
1:A:16:VAL:HG21	1:A:83:LEU:CD2	0.41	2.46	14	1
1:B:35:ILE:HA	1:B:38:PHE:HB2	0.41	1.92	14	1
1:A:4:GLU:HG2	1:B:54:GLY:N	0.41	2.31	16	1
1:B:53:VAL:O	1:B:53:VAL:HG12	0.41	2.16	17	1
1:A:20:PHE:CD2	1:A:41:LEU:HD21	0.41	2.49	19	1
1:A:21:PHE:O	1:A:70:GLU:HG2	0.41	2.16	19	1
1:A:1:MET:CG	1:B:39:LYS:HA	0.41	2.45	6	2
1:B:71:LEU:HD21	1:B:73:PHE:C	0.41	2.36	5	2
1:A:52:ASP:OD2	1:A:88:ARG:NH2	0.41	2.53	6	1
1:A:89:LYS:CE	1:B:5:THR:O	0.41	2.69	6	1
1:A:42:ALA:O	1:A:46:LEU:CA	0.41	2.69	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:LEU:O	1:B:45:GLN:HG3	0.41	2.15	8	1
1:B:45:GLN:OE1	1:B:51:LYS:HE3	0.41	2.16	8	1
1:A:7:THR:CB	1:B:45:GLN:NE2	0.41	2.84	9	1
1:A:39:LYS:NZ	1:A:63:LEU:HD11	0.41	2.31	9	1
1:A:74:SER:CA	1:B:95:ILE:HG23	0.41	2.45	13	1
1:A:5:THR:CG2	1:A:6:LEU:N	0.41	2.77	14	1
1:A:87:VAL:CG2	1:B:83:LEU:HD12	0.41	2.45	14	1
1:A:79:LEU:N	1:A:79:LEU:CD1	0.41	2.84	15	1
1:B:71:LEU:HD21	1:B:73:PHE:CG	0.41	2.50	15	1
1:A:10:GLU:N	1:B:86:GLU:OE1	0.41	2.53	17	1
1:A:6:LEU:CA	1:B:86:GLU:OE1	0.41	2.68	18	1
1:A:24:ALA:CA	1:A:33:LEU:HB3	0.41	2.44	20	1
1:A:55:SER:O	1:A:58:GLU:N	0.41	2.54	3	1
1:A:89:LYS:NZ	1:A:93:LEU:HB3	0.41	2.30	5	1
1:B:23:PHE:CE2	1:B:33:LEU:HG	0.41	2.51	5	2
1:B:71:LEU:HD22	1:B:73:PHE:H	0.41	1.75	5	2
1:A:68:ASP:HB3	1:A:75:GLU:HB3	0.41	1.91	13	2
1:B:41:LEU:O	1:B:44:GLN:N	0.41	2.53	14	2
1:B:42:ALA:HA	1:B:45:GLN:HG3	0.41	1.92	8	2
1:B:26:ARG:NE	1:B:36:ASN:HB3	0.41	2.31	12	1
1:B:32:SER:OG	1:B:73:PHE:CE1	0.41	2.67	12	1
1:A:6:LEU:CD2	1:B:90:GLU:HG2	0.41	2.45	13	1
1:A:19:THR:O	1:A:22:THR:OG1	0.41	2.39	13	1
1:A:33:LEU:CD2	1:A:37:GLU:HG3	0.41	2.45	13	1
1:A:38:PHE:CD1	1:A:41:LEU:HG	0.41	2.50	13	1
1:A:57:ASP:O	1:A:61:LYS:CG	0.41	2.69	14	2
1:A:71:LEU:CG	1:A:75:GLU:N	0.41	2.82	15	1
1:B:23:PHE:CD1	1:B:33:LEU:CD1	0.41	3.03	18	1
1:B:50:LEU:CD1	1:B:89:LYS:O	0.41	2.69	2	1
1:B:70:GLU:CB	1:B:79:LEU:HD21	0.41	2.45	2	1
1:A:23:PHE:CE2	1:A:38:PHE:HB2	0.41	2.50	5	4
1:B:38:PHE:CD1	1:B:41:LEU:HG	0.41	2.51	13	2
1:A:3:ALA:HB3	1:B:85:LYS:CE	0.41	2.45	8	1
1:A:42:ALA:HA	1:A:45:GLN:HG3	0.41	1.92	12	1
1:A:4:GLU:OE2	1:B:53:VAL:N	0.41	2.50	13	1
1:A:52:ASP:OD1	1:B:5:THR:CB	0.41	2.69	14	1
1:B:67:GLN:NE2	1:B:68:ASP:H	0.41	2.13	19	2
1:B:75:GLU:OE1	1:B:75:GLU:CA	0.41	2.68	14	1
1:A:23:PHE:HA	1:A:37:GLU:OE2	0.41	2.15	15	1
1:B:15:THR:O	1:B:18:SER:N	0.41	2.53	16	1
1:A:4:GLU:OE2	1:B:42:ALA:HB2	0.41	2.16	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ALA:HB2	1:B:4:GLU:OE2	0.41	2.16	17	1
1:B:17:VAL:HG13	1:B:18:SER:N	0.41	2.30	17	2
1:B:71:LEU:HD21	1:B:76:TYR:CE2	0.41	2.49	18	1
1:A:87:VAL:HG23	1:B:13:ILE:HD11	0.41	1.91	19	1
1:A:14:GLU:CA	1:A:17:VAL:HG12	0.41	2.45	20	1
1:A:89:LYS:CE	1:A:89:LYS:H	0.41	2.28	20	1
1:B:7:THR:CB	1:B:9:LEU:HD12	0.41	2.46	20	1
1:A:54:GLY:O	1:A:59:LYS:HD2	0.41	2.16	1	1
1:A:60:MET:O	1:A:63:LEU:CD1	0.41	2.68	1	1
1:A:70:GLU:CD	1:A:71:LEU:N	0.41	2.74	1	1
1:A:61:LYS:HD2	1:A:61:LYS:N	0.41	2.31	2	1
1:A:95:ILE:CG2	1:B:74:SER:HB3	0.41	2.46	13	2
1:B:50:LEU:O	1:B:50:LEU:HG	0.41	2.16	2	1
1:A:80:ILE:CD1	1:B:88:ARG:N	0.41	2.84	3	1
1:A:89:LYS:NZ	1:B:4:GLU:O	0.41	2.52	3	1
1:A:9:LEU:CD2	1:A:9:LEU:N	0.41	2.84	4	1
1:A:45:GLN:OE1	1:B:6:LEU:O	0.41	2.39	4	1
1:A:50:LEU:HD11	1:A:89:LYS:HD2	0.41	1.90	5	1
1:A:82:GLU:O	1:B:9:LEU:HD12	0.41	2.16	5	1
1:A:54:GLY:CA	1:B:4:GLU:HB3	0.41	2.46	6	1
1:B:6:LEU:CD2	1:B:10:GLU:HB3	0.41	2.46	6	1
1:A:41:LEU:O	1:A:42:ALA:C	0.41	2.60	7	2
1:A:48:HIS:CD2	1:B:5:THR:HB	0.41	2.51	7	1
1:A:45:GLN:OE1	1:A:51:LYS:HE3	0.41	2.16	8	1
1:A:4:GLU:OE1	1:B:42:ALA:O	0.41	2.38	9	1
1:A:61:LYS:O	1:A:64:ASP:N	0.41	2.54	9	1
1:B:26:ARG:NE	1:B:37:GLU:HG2	0.41	2.31	10	1
1:A:50:LEU:HD13	1:A:93:LEU:HB2	0.41	1.92	11	1
1:A:71:LEU:O	1:A:72:ARG:NE	0.41	2.52	11	1
1:B:41:LEU:C	1:B:45:GLN:HG2	0.41	2.37	12	1
1:A:4:GLU:OE1	1:B:54:GLY:CA	0.41	2.69	13	1
1:A:7:THR:O	1:B:86:GLU:OE2	0.41	2.38	13	1
1:A:62:THR:O	1:A:65:VAL:N	0.41	2.53	13	1
1:B:19:THR:OG1	1:B:20:PHE:N	0.41	2.53	13	1
1:B:21:PHE:CZ	1:B:79:LEU:HD13	0.41	2.42	13	1
1:B:31:GLY:HA2	1:B:73:PHE:HB3	0.41	1.93	13	1
1:A:74:SER:HB3	1:B:95:ILE:HG22	0.41	1.93	14	1
1:B:23:PHE:HB2	1:B:70:GLU:OE1	0.41	2.16	14	1
1:A:97:LYS:CD	1:B:30:LYS:HB3	0.41	2.46	15	1
1:B:33:LEU:CG	1:B:70:GLU:HB3	0.41	2.46	15	1
1:B:68:ASP:HB2	1:B:78:ARG:CG	0.41	2.46	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:HD11	1:B:21:PHE:CE1	0.41	2.51	16	1
1:A:67:GLN:NE2	1:A:68:ASP:CG	0.41	2.75	16	1
1:B:7:THR:O	1:B:10:GLU:HG3	0.41	2.16	17	1
1:A:57:ASP:O	1:A:61:LYS:HG3	0.41	2.16	18	1
1:B:24:ALA:CA	1:B:33:LEU:CD1	0.41	2.92	18	1
1:A:66:ASN:O	1:A:70:GLU:OE2	0.41	2.38	20	1
1:B:21:PHE:O	1:B:33:LEU:CD2	0.41	2.68	20	1
1:B:60:MET:O	1:B:63:LEU:CD1	0.41	2.69	1	1
1:A:76:TYR:CB	1:B:91:LYS:CB	0.41	2.98	2	1
1:A:33:LEU:CB	1:A:70:GLU:HG2	0.41	2.46	3	1
1:A:92:ALA:O	1:A:95:ILE:HG13	0.41	2.16	6	1
1:A:15:THR:O	1:A:19:THR:CG2	0.41	2.67	8	1
1:B:63:LEU:C	1:B:63:LEU:HD23	0.41	2.36	9	1
1:A:9:LEU:HD21	1:B:20:PHE:HB3	0.41	1.92	13	1
1:B:32:SER:HB2	1:B:70:GLU:O	0.41	2.16	13	1
1:B:55:SER:O	1:B:59:LYS:CE	0.41	2.69	13	1
1:A:4:GLU:HB3	1:B:52:ASP:HB2	0.41	1.93	14	1
1:A:89:LYS:HE2	1:B:6:LEU:CG	0.41	2.46	14	1
1:B:23:PHE:HB3	1:B:37:GLU:HB2	0.41	1.92	14	1
1:B:46:LEU:HD23	1:B:54:GLY:H	0.41	1.76	14	1
1:B:29:ARG:N	1:B:29:ARG:HD3	0.41	2.31	15	1
1:A:32:SER:HA	1:A:72:ARG:HG2	0.41	1.92	16	1
1:A:10:GLU:N	1:B:86:GLU:HG3	0.41	2.31	17	1
1:A:21:PHE:CG	1:A:70:GLU:HB2	0.41	2.51	17	1
1:A:5:THR:O	1:B:89:LYS:CD	0.41	2.69	20	1
1:A:74:SER:HB3	1:B:95:ILE:CG2	0.40	2.47	1	1
1:A:10:GLU:O	1:A:13:ILE:CB	0.40	2.69	2	1
1:B:35:ILE:CD1	1:B:35:ILE:C	0.40	2.90	2	1
1:A:6:LEU:HD13	1:B:48:HIS:NE2	0.40	2.31	4	1
1:A:68:ASP:HB2	1:A:78:ARG:HG3	0.40	1.91	5	2
1:A:97:LYS:CE	1:B:73:PHE:HB3	0.40	2.46	5	1
1:A:2:ALA:N	1:B:59:LYS:HA	0.40	2.30	6	1
1:B:41:LEU:O	1:B:42:ALA:C	0.40	2.59	7	1
1:B:48:HIS:HB2	1:B:51:LYS:CG	0.40	2.46	8	1
1:A:53:VAL:HG12	1:A:53:VAL:O	0.40	2.16	10	1
1:A:86:GLU:OE1	1:B:7:THR:O	0.40	2.39	10	1
1:B:83:LEU:O	1:B:86:GLU:HG3	0.40	2.15	11	1
1:A:19:THR:OG1	1:A:20:PHE:N	0.40	2.54	13	1
1:A:35:ILE:HA	1:A:38:PHE:CB	0.40	2.46	13	1
1:B:90:GLU:OE2	1:B:93:LEU:HD22	0.40	2.16	13	1
1:A:1:MET:CB	1:B:39:LYS:HA	0.40	2.46	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LYS:O	1:B:1:MET:HG3	0.40	2.16	17	1
1:B:42:ALA:CB	1:B:59:LYS:CD	0.40	2.99	19	1
1:A:1:MET:N	1:B:39:LYS:HA	0.40	2.31	11	3
1:A:76:TYR:HB2	1:B:91:LYS:CA	0.40	2.47	2	1
1:A:23:PHE:CD2	1:A:33:LEU:CD2	0.40	3.02	3	1
1:A:23:PHE:HB2	1:A:37:GLU:CB	0.40	2.47	3	2
1:B:90:GLU:OE1	1:B:93:LEU:HD22	0.40	2.16	4	1
1:A:38:PHE:HA	1:A:41:LEU:HG	0.40	1.94	6	1
1:A:10:GLU:N	1:B:86:GLU:OE2	0.40	2.54	8	1
1:A:57:ASP:O	1:A:61:LYS:N	0.40	2.50	10	1
1:A:45:GLN:OE1	1:B:2:ALA:O	0.40	2.39	12	1
1:A:4:GLU:CD	1:B:54:GLY:N	0.40	2.74	13	1
1:A:86:GLU:O	1:A:90:GLU:HB2	0.40	2.16	14	1
1:B:69:SER:OG	1:B:82:GLU:HG3	0.40	2.17	14	1
1:A:45:GLN:NE2	1:B:7:THR:HA	0.40	2.30	19	1
1:A:89:LYS:HE2	1:B:6:LEU:CD1	0.40	2.43	19	1
1:B:9:LEU:N	1:B:9:LEU:HD23	0.40	2.30	1	2
1:B:35:ILE:HB	1:B:63:LEU:HD23	0.40	1.93	1	1
1:A:35:ILE:CD1	1:A:35:ILE:C	0.40	2.90	2	1
1:A:18:SER:HA	1:A:22:THR:CG2	0.40	2.46	4	1
1:A:82:GLU:C	1:A:84:ALA:N	0.40	2.74	4	1
1:A:85:LYS:NZ	1:B:7:THR:HG21	0.40	2.31	5	1
1:B:58:GLU:O	1:B:62:THR:N	0.40	2.51	5	1
1:A:5:THR:O	1:B:89:LYS:HE3	0.40	2.15	6	1
1:A:41:LEU:CD1	1:B:7:THR:CG2	0.40	2.91	6	1
1:B:60:MET:HA	1:B:63:LEU:CD1	0.40	2.46	6	1
1:A:89:LYS:HG3	1:B:5:THR:CG2	0.40	2.45	8	1
1:B:13:ILE:N	1:B:13:ILE:CD1	0.40	2.84	8	1
1:B:15:THR:O	1:B:19:THR:CG2	0.40	2.66	9	1
1:B:39:LYS:NZ	1:B:63:LEU:HD11	0.40	2.32	9	1
1:B:13:ILE:HA	1:B:16:VAL:CG1	0.40	2.47	10	2
1:B:67:GLN:NE2	1:B:67:GLN:C	0.40	2.74	11	1
1:B:56:LEU:HD23	1:B:56:LEU:O	0.40	2.16	12	1
1:B:57:ASP:O	1:B:61:LYS:HG2	0.40	2.16	12	1
1:B:23:PHE:CZ	1:B:41:LEU:CD2	0.40	3.04	13	1
1:A:74:SER:CA	1:B:91:LYS:O	0.40	2.69	14	1
1:B:34:ASN:C	1:B:35:ILE:HD13	0.40	2.36	16	1
1:A:50:LEU:CD2	1:A:93:LEU:HD13	0.40	2.46	18	1
1:A:72:ARG:N	1:A:72:ARG:HD2	0.40	2.31	20	1
1:A:91:LYS:O	1:B:74:SER:O	0.40	2.39	20	1
1:B:67:GLN:O	1:B:70:GLU:OE2	0.40	2.39	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:MET:O	1:B:63:LEU:HD13	0.40	2.17	1	1
1:B:6:LEU:CG	1:B:10:GLU:HB3	0.40	2.46	2	1
1:B:66:ASN:HB3	1:B:69:SER:HB3	0.40	1.92	2	1
1:A:51:LYS:CG	1:A:52:ASP:N	0.40	2.84	3	1
1:A:97:LYS:HE3	1:B:73:PHE:CB	0.40	2.46	3	1
1:B:24:ALA:HA	1:B:33:LEU:CD2	0.40	2.45	3	1
1:A:65:VAL:O	1:A:78:ARG:NH2	0.40	2.55	5	1
1:B:24:ALA:O	1:B:26:ARG:N	0.40	2.54	7	1
1:A:42:ALA:CB	1:B:1:MET:HG3	0.40	2.38	9	1
1:A:30:LYS:N	1:A:30:LYS:HD2	0.40	2.30	10	1
1:B:82:GLU:OE2	1:B:85:LYS:NZ	0.40	2.52	10	1
1:A:26:ARG:CD	1:A:36:ASN:CB	0.40	2.99	12	1
1:B:31:GLY:O	1:B:72:ARG:HB2	0.40	2.15	12	1
1:A:86:GLU:OE1	1:A:86:GLU:CA	0.40	2.70	13	1
1:A:86:GLU:OE2	1:B:7:THR:O	0.40	2.39	13	1
1:B:33:LEU:O	1:B:70:GLU:HG2	0.40	2.16	13	1
1:A:3:ALA:O	1:B:85:LYS:CG	0.40	2.70	14	1
1:B:63:LEU:CD2	1:B:64:ASP:N	0.40	2.84	14	1
1:B:71:LEU:CD2	1:B:73:PHE:O	0.40	2.69	18	1
1:A:3:ALA:HB2	1:B:38:PHE:CZ	0.40	2.51	19	1
1:A:7:THR:C	1:A:9:LEU:N	0.40	2.75	19	1
1:B:7:THR:HB	1:B:9:LEU:CD1	0.40	2.46	20	1
1:B:69:SER:HA	1:B:78:ARG:CB	0.40	2.46	20	1
1:A:24:ALA:HA	1:A:33:LEU:CD1	0.40	2.46	3	1
1:A:4:GLU:HB3	1:B:54:GLY:N	0.40	2.32	7	1
1:B:46:LEU:O	1:B:51:LYS:HE3	0.40	2.17	7	1
1:A:4:GLU:OE1	1:B:46:LEU:HA	0.40	2.16	9	1
1:A:56:LEU:HD23	1:A:56:LEU:O	0.40	2.16	12	1
1:B:23:PHE:CD1	1:B:23:PHE:O	0.40	2.74	16	1
1:A:26:ARG:HD2	1:A:37:GLU:CG	0.40	2.46	17	1
1:B:56:LEU:HG	1:B:57:ASP:N	0.40	2.32	17	1
1:A:66:ASN:CB	1:A:69:SER:OG	0.40	2.70	20	1
1:A:93:LEU:HD23	1:A:93:LEU:O	0.40	2.16	20	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	96/98 (98%)	62±2 (64±3%)	25±3 (26±4%)	9±2 (9±2%)	1 11
1	B	96/98 (98%)	62±3 (65±3%)	26±3 (27±3%)	9±2 (9±3%)	1 12
All	All	3840/3920 (98%)	2472 (64%)	1016 (26%)	352 (9%)	1 11

All 43 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	95	ILE	20
1	B	95	ILE	20
1	A	41	LEU	19
1	A	53	VAL	19
1	B	53	VAL	19
1	B	51	LYS	17
1	A	4	GLU	16
1	A	51	LYS	16
1	B	4	GLU	16
1	A	29	ARG	13
1	B	29	ARG	13
1	A	28	GLY	11
1	B	28	GLY	11
1	B	54	GLY	10
1	B	5	THR	10
1	B	25	GLY	9
1	B	46	LEU	9
1	A	5	THR	9
1	B	75	GLU	8
1	A	65	VAL	7
1	A	75	GLU	7
1	A	76	TYR	7
1	B	76	TYR	7
1	A	63	LEU	6
1	B	63	LEU	6
1	A	46	LEU	6
1	A	42	ALA	6
1	A	54	GLY	5
1	B	65	VAL	5
1	B	8	GLU	4
1	A	8	GLU	3
1	A	88	ARG	2
1	A	25	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	49	LEU	2
1	B	41	LEU	2
1	A	56	LEU	2
1	B	56	LEU	2
1	A	62	THR	1
1	B	88	ARG	1
1	A	7	THR	1
1	B	7	THR	1
1	A	55	SER	1
1	B	55	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	84/84 (100%)	64±3 (76±4%)	20±3 (24±4%)	2 26
1	B	84/84 (100%)	64±3 (76±4%)	20±3 (24±4%)	2 26
All	All	3360/3360 (100%)	2549 (76%)	811 (24%)	2 26

All 114 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	10	GLU	20
1	A	89	LYS	20
1	B	10	GLU	20
1	B	89	LYS	20
1	A	7	THR	19
1	B	7	THR	19
1	A	23	PHE	18
1	A	76	TYR	18
1	B	1	MET	18
1	B	23	PHE	18
1	B	76	TYR	18
1	A	1	MET	17
1	B	48	HIS	16
1	B	71	LEU	16

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Mol	Chain	Res	Type	Models (Total)
1	B	97	LYS	16
1	A	48	HIS	15
1	A	71	LEU	15
1	A	97	LYS	15
1	A	13	ILE	14
1	B	13	ILE	14
1	A	35	ILE	14
1	A	79	LEU	14
1	A	57	ASP	13
1	B	67	GLN	13
1	B	79	LEU	13
1	A	4	GLU	12
1	A	67	GLN	12
1	B	4	GLU	12
1	B	57	ASP	12
1	B	35	ILE	12
1	A	73	PHE	11
1	B	73	PHE	10
1	A	33	LEU	9
1	B	33	LEU	9
1	A	63	LEU	8
1	B	61	LYS	8
1	B	63	LEU	8
1	A	5	THR	7
1	A	66	ASN	7
1	B	5	THR	7
1	A	43	THR	7
1	A	53	VAL	6
1	B	53	VAL	6
1	A	6	LEU	6
1	A	20	PHE	6
1	B	20	PHE	6
1	B	51	LYS	6
1	A	32	SER	6
1	A	85	LYS	6
1	B	85	LYS	6
1	A	72	ARG	6
1	B	72	ARG	6
1	A	40	GLU	5
1	B	40	GLU	5
1	A	96	ARG	5
1	B	96	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	B	32	SER	5
1	B	66	ASN	5
1	B	74	SER	5
1	A	45	GLN	5
1	B	45	GLN	5
1	A	50	LEU	4
1	B	50	LEU	4
1	A	86	GLU	4
1	B	59	LYS	4
1	B	26	ARG	4
1	A	61	LYS	4
1	A	51	LYS	4
1	B	6	LEU	4
1	A	38	PHE	4
1	B	38	PHE	4
1	A	9	LEU	4
1	B	9	LEU	4
1	B	43	THR	3
1	A	59	LYS	3
1	A	75	GLU	3
1	B	75	GLU	3
1	A	26	ARG	3
1	A	69	SER	3
1	B	69	SER	3
1	A	93	LEU	3
1	B	93	LEU	3
1	A	88	ARG	3
1	B	88	ARG	3
1	A	41	LEU	3
1	B	41	LEU	3
1	B	46	LEU	3
1	A	74	SER	3
1	B	86	GLU	3
1	A	29	ARG	3
1	B	29	ARG	3
1	A	68	ASP	2
1	B	68	ASP	2
1	A	46	LEU	2
1	A	78	ARG	2
1	B	78	ARG	2
1	A	70	GLU	2
1	B	70	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	58	GLU	2
1	B	58	GLU	2
1	A	87	VAL	2
1	B	87	VAL	2
1	A	55	SER	1
1	B	55	SER	1
1	A	95	ILE	1
1	B	95	ILE	1
1	A	52	ASP	1
1	B	52	ASP	1
1	A	8	GLU	1
1	A	56	LEU	1
1	B	39	LYS	1
1	B	56	LEU	1
1	A	80	ILE	1
1	B	80	ILE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided