



Full wwPDB NMR Structure Validation Report ⓘ

Feb 22, 2020 – 01:57 AM EST

PDB ID : 2KMT
Title : NMR solution structure of Vibrio fischeri CcdB
Authors : Zangger, K.
Deposited on : 2009-08-04

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 ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.8
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.8

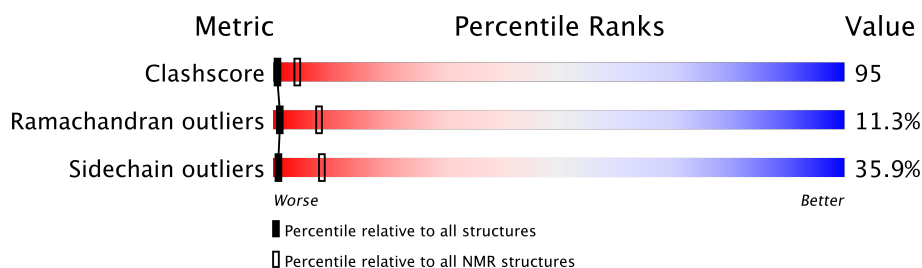
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	105	<div> <div>20%</div> <div>48%</div> <div>30%</div> <div>..</div> </div>
1	B	105	<div> <div>20%</div> <div>50%</div> <div>27%</div> <div>.</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:105, B:1-B:105 (209)	0.58	8

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

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

The models can be grouped into 5 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3386 atoms, of which 1718 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CcdB.

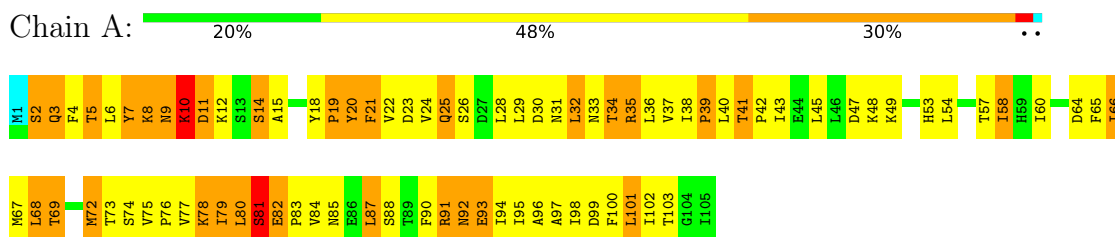
Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1693	538	859	131	161	4	
1	B	105	Total	C	H	N	O	S	0
			1693	538	859	131	161	4	

4 Residue-property plots [i](#)

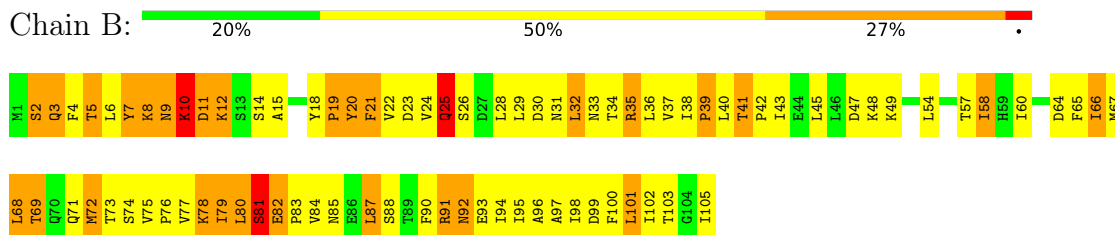
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CcdB



- Molecule 1: CcdB

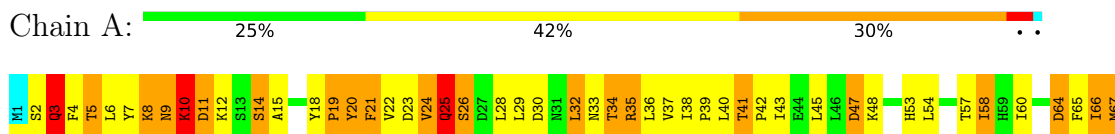


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

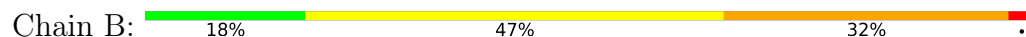
4.2.1 Score per residue for model 1

- Molecule 1: CcdB



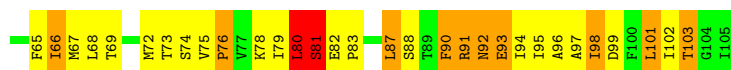
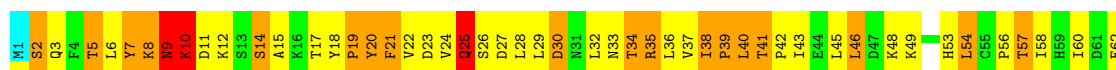
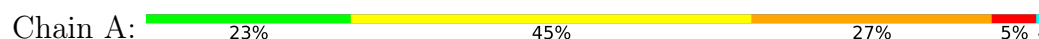


• Molecule 1: CcdB

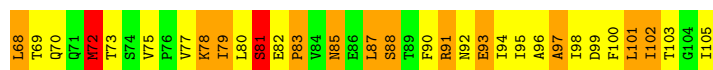


4.2.2 Score per residue for model 2

• Molecule 1: CcdB

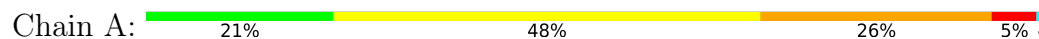


• Molecule 1: CcdB

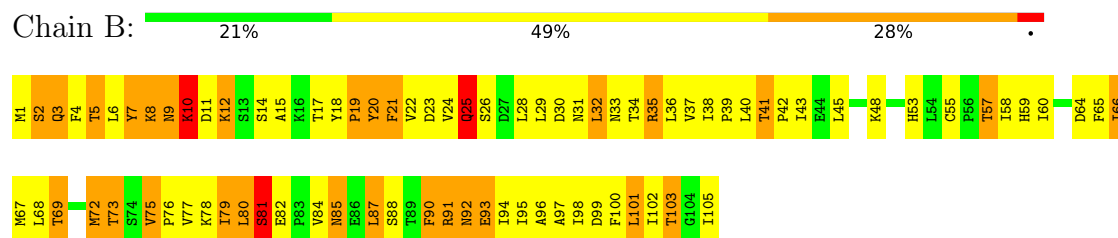


4.2.3 Score per residue for model 3

• Molecule 1: CcdB

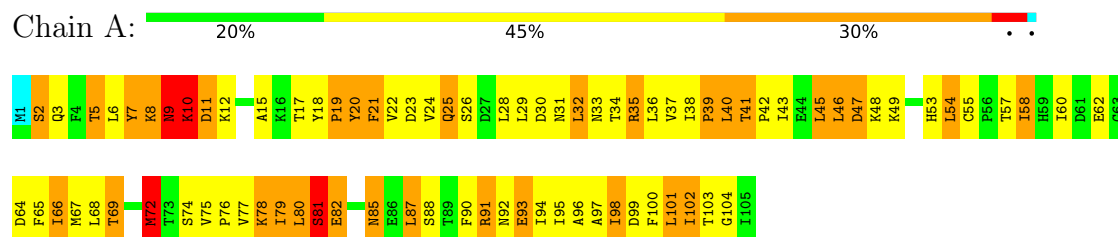


• Molecule 1: CcdB

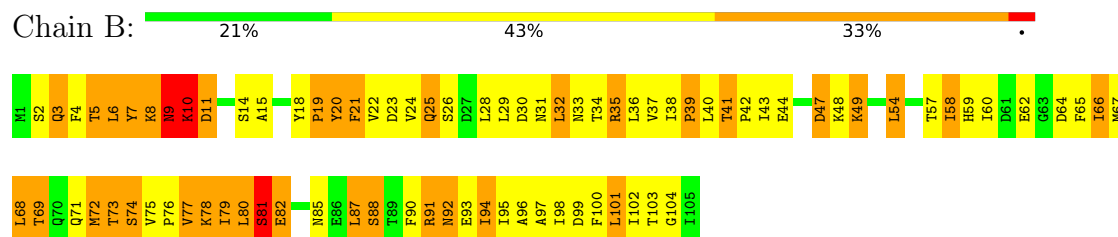


4.2.4 Score per residue for model 4

- Molecule 1: CcdB

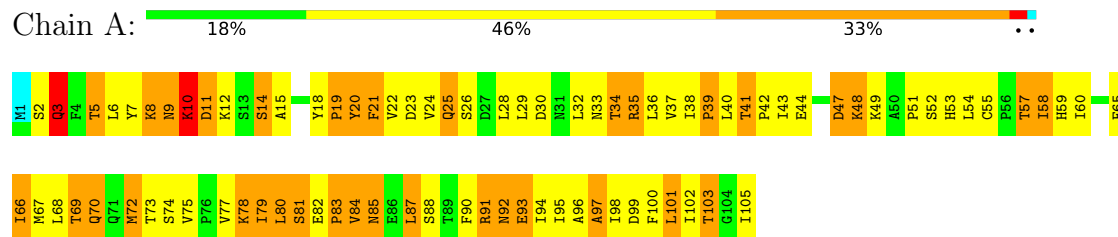


- Molecule 1: CcdB

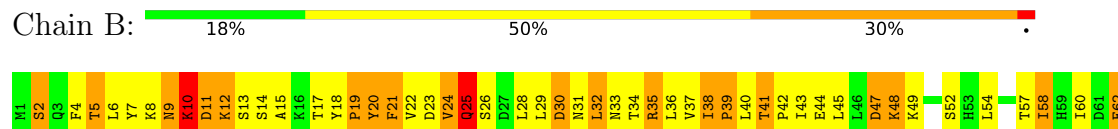


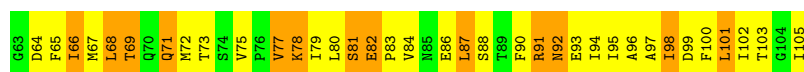
4.2.5 Score per residue for model 5

- Molecule 1: CcdB



- Molecule 1: CcdB

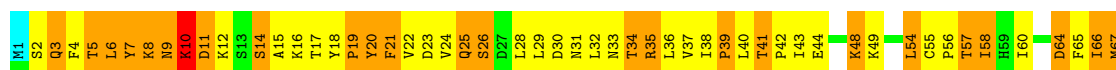




4.2.6 Score per residue for model 6

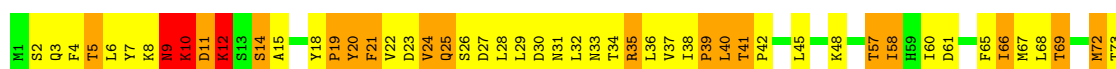
- Molecule 1: CcdB

Chain A: 19% 44% 33% ..



- Molecule 1: CcdB

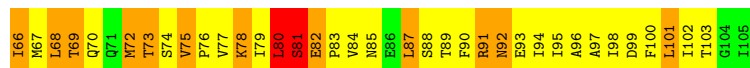
Chain B: 26% 46% 25% .



4.2.7 Score per residue for model 7

- Molecule 1: CcdB

Chain A: 17% 50% 29% ..



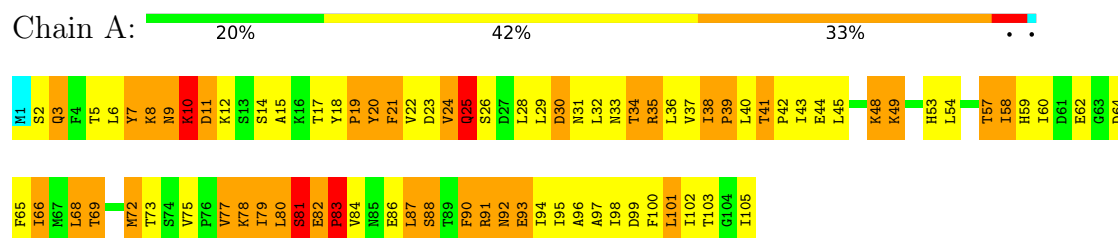
- Molecule 1: CcdB

Chain B: 22% 48% 30% .

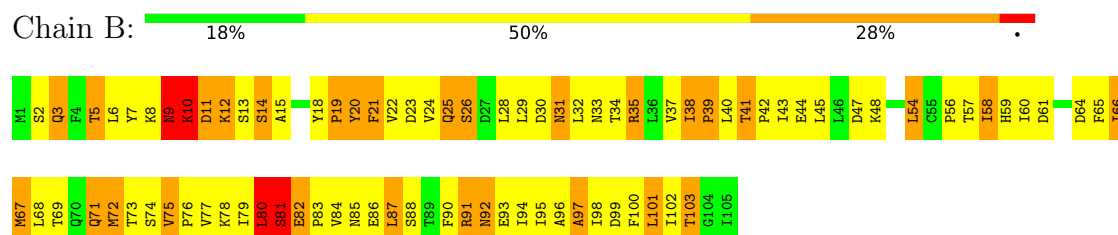


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: CcdB

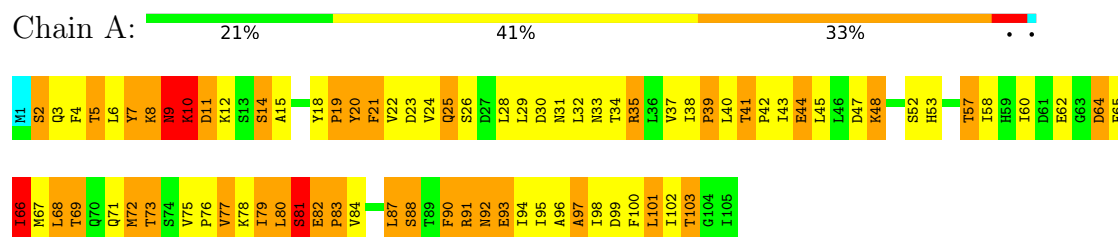


- Molecule 1: CcdB

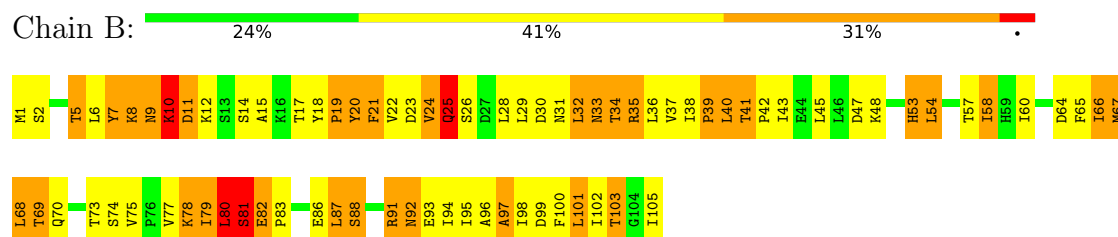


4.2.9 Score per residue for model 9

- Molecule 1: CcdB



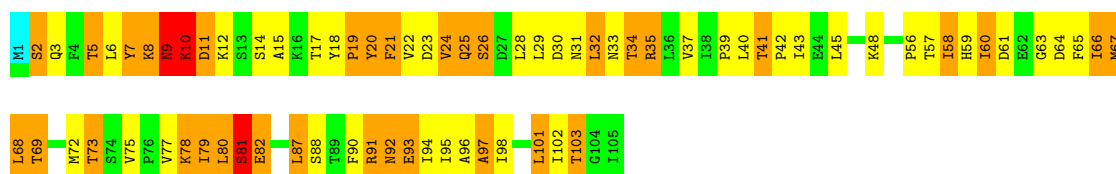
- Molecule 1: CcdB



4.2.10 Score per residue for model 10

- Molecule 1: CcdB





• Molecule 1: CcdB

Chain B: 21% 50% 25% 5%



4.2.11 Score per residue for model 11

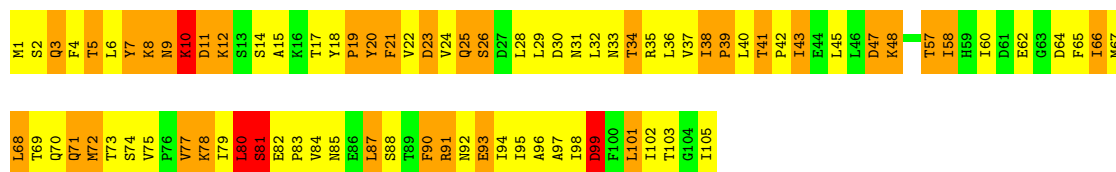
• Molecule 1: CcdB

Chain A: 24% 42% 30%



• Molecule 1: CcdB

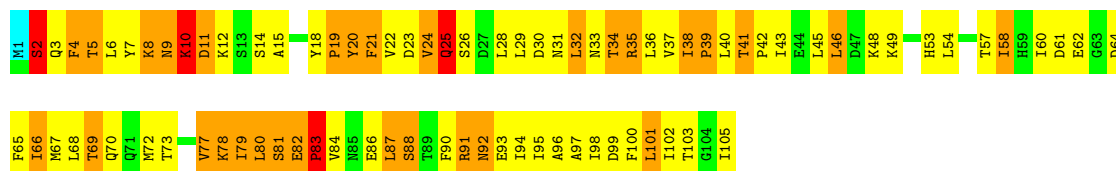
Chain B: 20% 45% 31%



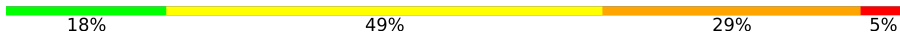
4.2.12 Score per residue for model 12

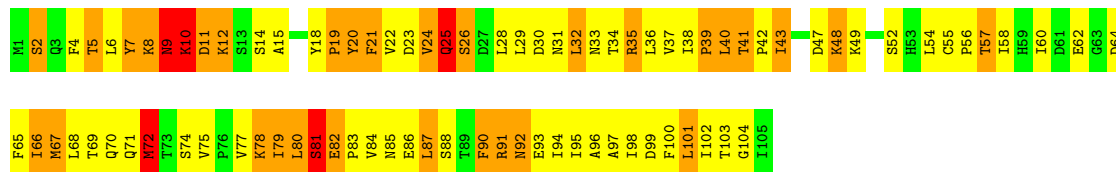
• Molecule 1: CcdB

Chain A: 19% 48% 29%



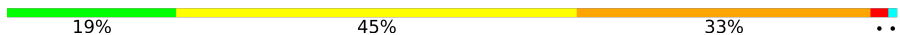
- Molecule 1: CcdB

Chain B: 



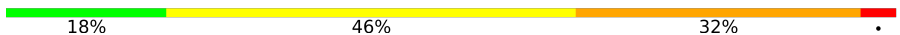
4.2.13 Score per residue for model 13

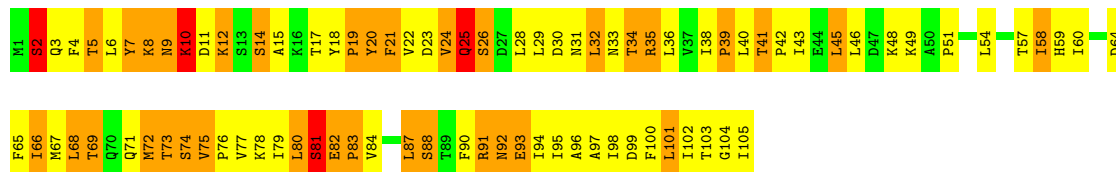
- Molecule 1: CcdB

Chain A: 



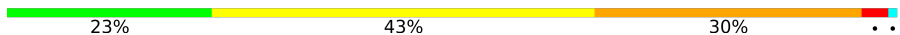
- Molecule 1: CcdB

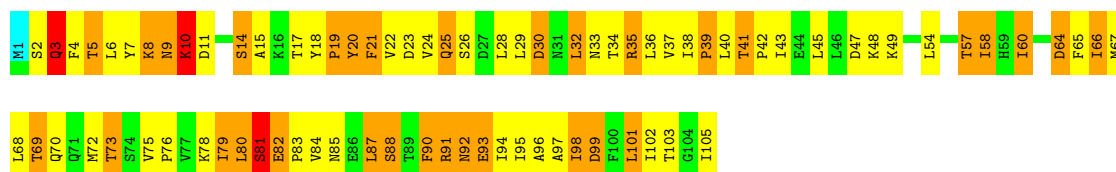
Chain B: 



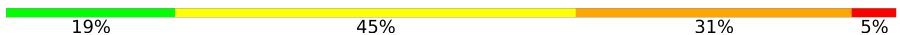
4.2.14 Score per residue for model 14

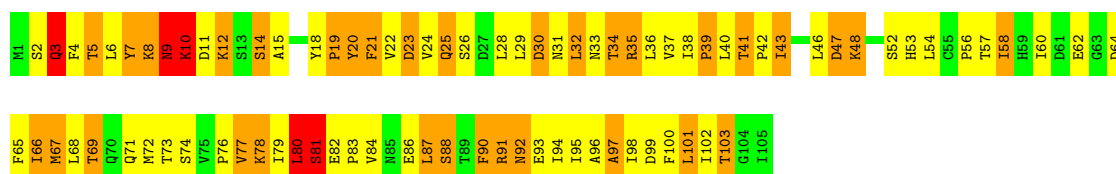
- Molecule 1: CcdB

Chain A: 



- Molecule 1: CcdB

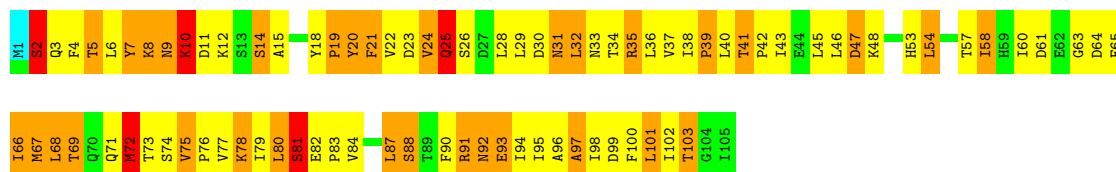
Chain B: 



4.2.15 Score per residue for model 15

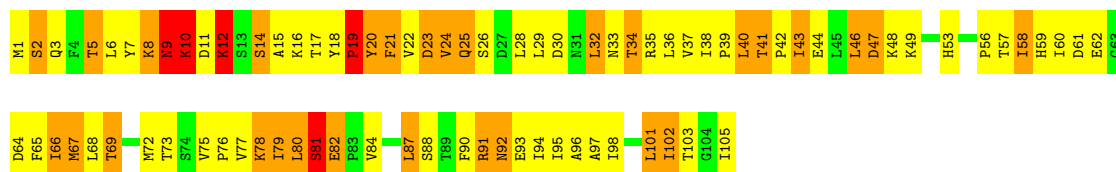
- Molecule 1: CcdB

Chain A: 18% 46% 30% 5%



- Molecule 1: CcdB

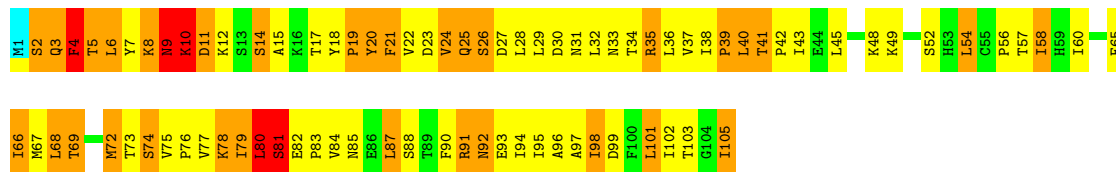
Chain B: 20% 48% 28% 5%



4.2.16 Score per residue for model 16

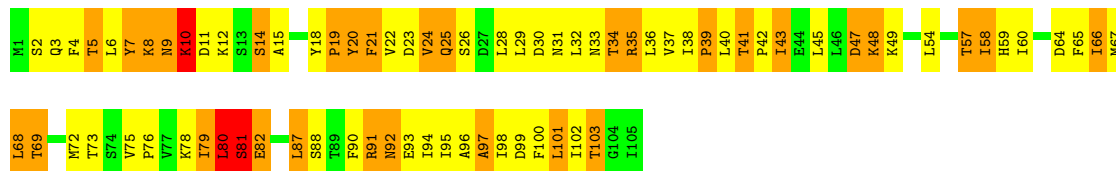
- Molecule 1: CcdB

Chain A: 19% 45% 30% 5%



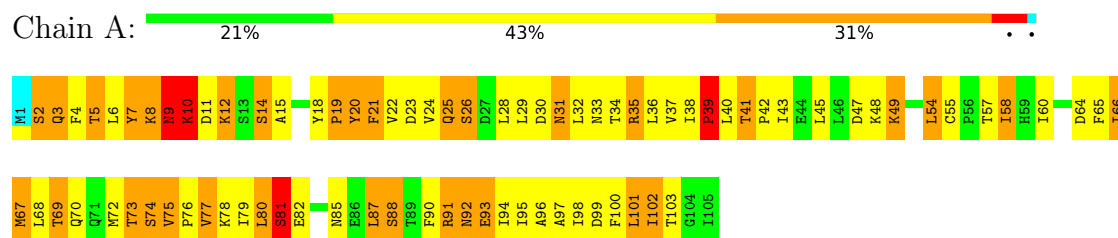
- Molecule 1: CcdB

Chain B: 26% 43% 29%

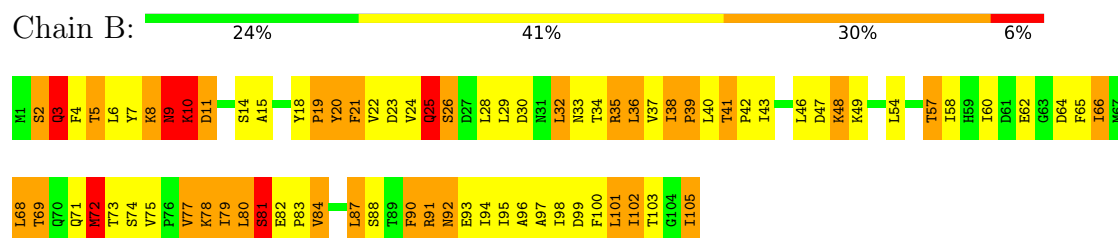


4.2.17 Score per residue for model 17

- Molecule 1: CcdB

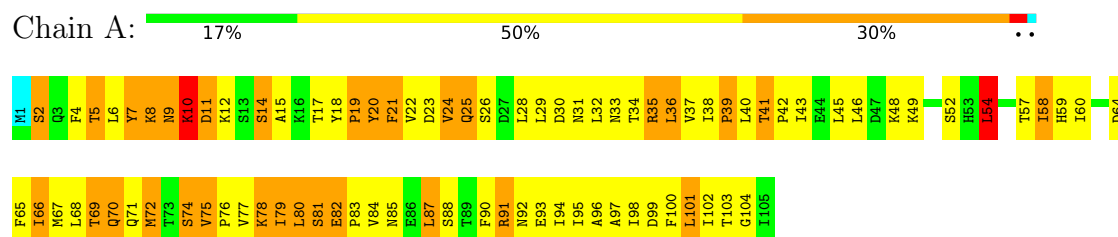


- Molecule 1: CcdB

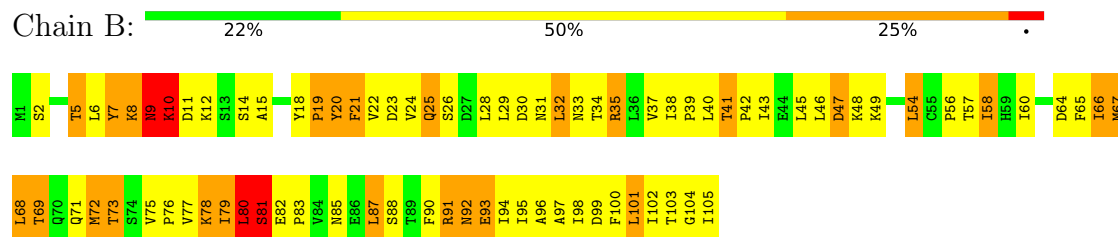


4.2.18 Score per residue for model 18

- Molecule 1: CcdB

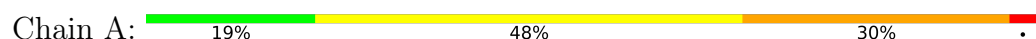


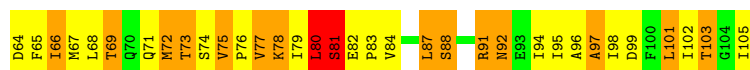
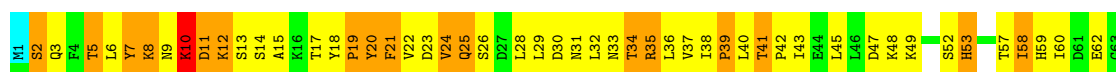
- Molecule 1: CcdB



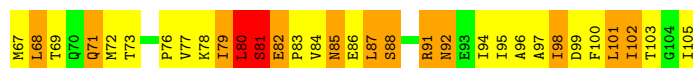
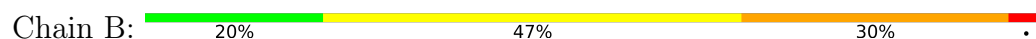
4.2.19 Score per residue for model 19

- Molecule 1: CcdB



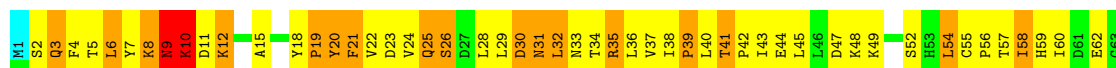
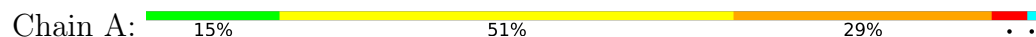


• Molecule 1: CcdB

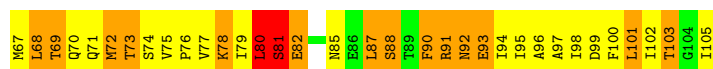
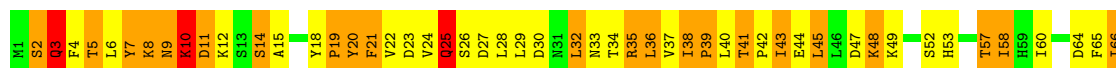
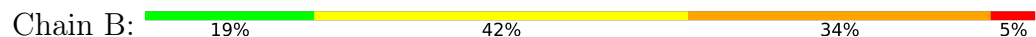


4.2.20 Score per residue for model 20

• Molecule 1: CcdB



• Molecule 1: CcdB



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CNS	structure solution	
CNS	refinement	

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

Chemical shift file(s)	2kmt_cs.cif
Number of chemical shift lists	1
Total number of shifts	2354
Number of shifts mapped to atoms	2354
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	826	848	846	159±11
1	B	834	859	857	164±11
All	All	33200	34140	34060	6359

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 95.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:ILE:HD12	1:B:69:THR:HG23	1.14	1.20	9	3
1:B:8:LYS:HA	1:B:20:TYR:HB3	1.06	1.25	15	18
1:A:58:ILE:HD13	1:A:60:ILE:HG23	1.05	1.19	10	2
1:B:58:ILE:HD13	1:B:60:ILE:HG23	1.05	1.09	1	1
1:B:30:ASP:O	1:B:35:ARG:HB2	1.00	1.57	20	8
1:B:69:THR:HG22	1:B:101:LEU:HD22	1.00	1.33	20	6
1:B:29:LEU:HD23	1:B:32:LEU:HD22	1.00	1.30	6	5
1:B:54:LEU:HD23	1:B:69:THR:HG23	0.99	1.27	8	2
1:A:69:THR:HG22	1:A:101:LEU:HD22	0.97	1.34	4	7
1:A:29:LEU:HD23	1:A:32:LEU:HD22	0.97	1.30	17	7
1:A:22:VAL:HG11	1:A:94:ILE:CG1	0.97	1.89	8	17
1:A:24:VAL:HG21	1:A:98:ILE:HD11	0.95	1.39	18	1
1:B:43:ILE:HD11	1:B:57:THR:OG1	0.94	1.62	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:22:VAL:HG11	1:B:94:ILE:CG1	0.94	1.92	19	15
1:A:60:ILE:HD11	1:A:87:LEU:HD23	0.94	1.36	15	1
1:B:41:THR:HG23	1:B:66:ILE:CD1	0.93	1.94	15	15
1:A:43:ILE:HD11	1:A:57:THR:OG1	0.92	1.63	10	12
1:A:58:ILE:HD12	1:A:59:HIS:N	0.92	1.80	19	2
1:A:58:ILE:HG23	1:A:90:PHE:CE2	0.91	1.99	4	8
1:A:29:LEU:HD23	1:A:32:LEU:HD12	0.91	1.42	18	5
1:A:41:THR:HG23	1:A:66:ILE:CD1	0.91	1.96	5	18
1:A:58:ILE:HG21	1:A:87:LEU:HD12	0.90	1.42	14	7
1:B:58:ILE:HG21	1:B:87:LEU:HD12	0.90	1.41	7	4
1:A:6:LEU:HD11	1:A:60:ILE:HD13	0.89	1.44	12	8
1:A:6:LEU:HD21	1:A:60:ILE:HD13	0.88	1.43	17	2
1:B:10:LYS:N	1:B:81:SER:HA	0.86	1.86	3	20
1:A:10:LYS:N	1:A:81:SER:HA	0.86	1.84	14	19
1:B:29:LEU:HD23	1:B:32:LEU:HD12	0.86	1.47	18	5
1:B:101:LEU:C	1:B:101:LEU:HD22	0.86	1.91	13	1
1:B:101:LEU:HD22	1:B:101:LEU:C	0.86	1.91	14	2
1:A:79:ILE:O	1:A:79:ILE:HG12	0.86	1.68	18	3
1:A:58:ILE:CD1	1:A:60:ILE:HG23	0.86	2.00	19	2
1:B:54:LEU:CD2	1:B:69:THR:HG23	0.85	1.99	2	2
1:B:22:VAL:CG1	1:B:94:ILE:HD13	0.85	2.00	1	3
1:A:40:LEU:HD21	1:A:67:MET:CE	0.85	2.02	13	2
1:A:45:LEU:HD12	1:A:45:LEU:O	0.85	1.72	4	1
1:B:58:ILE:HG23	1:B:90:PHE:CE2	0.85	2.07	18	9
1:A:8:LYS:HA	1:A:20:TYR:HB3	0.85	1.47	16	17
1:B:29:LEU:HD23	1:B:32:LEU:CD1	0.85	2.02	18	7
1:B:45:LEU:HD12	1:B:45:LEU:O	0.85	1.72	13	1
1:B:101:LEU:HD13	1:B:102:ILE:HG13	0.84	1.49	13	3
1:B:36:LEU:HD13	1:B:37:VAL:N	0.84	1.88	7	2
1:A:101:LEU:HD22	1:A:101:LEU:C	0.84	1.91	15	1
1:B:58:ILE:HG21	1:B:87:LEU:HD23	0.84	1.48	18	7
1:B:22:VAL:HG11	1:B:94:ILE:HG13	0.84	1.50	12	15
1:A:54:LEU:HD23	1:A:69:THR:HG23	0.83	1.48	3	1
1:A:22:VAL:HG11	1:A:94:ILE:HG12	0.83	1.50	5	16
1:A:29:LEU:HD23	1:A:32:LEU:CD1	0.83	2.03	15	5
1:A:38:ILE:HD12	1:A:69:THR:HG23	0.83	1.50	18	2
1:B:58:ILE:HD11	1:B:65:PHE:HB2	0.82	1.50	8	7
1:A:8:LYS:O	1:A:20:TYR:HA	0.82	1.74	15	6
1:A:57:THR:OG1	1:A:66:ILE:HG23	0.82	1.74	13	13
1:B:75:VAL:HG23	1:B:79:ILE:HD13	0.82	1.49	3	7
1:A:22:VAL:HG11	1:A:94:ILE:HD13	0.82	1.50	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:THR:HB	1:A:7:TYR:CE1	0.82	2.09	20	20
1:B:45:LEU:O	1:B:45:LEU:HD12	0.82	1.72	2	1
1:B:58:ILE:HD12	1:B:87:LEU:HD22	0.82	1.51	18	4
1:B:8:LYS:O	1:B:20:TYR:HA	0.82	1.73	13	2
1:A:43:ILE:HD11	1:A:57:THR:CG2	0.81	2.05	19	1
1:A:25:GLN:OE1	1:B:101:LEU:HD12	0.81	1.75	8	3
1:A:30:ASP:O	1:A:35:ARG:HB2	0.81	1.75	2	5
1:A:75:VAL:HG23	1:A:79:ILE:HD13	0.81	1.53	6	5
1:B:36:LEU:HD11	1:B:72:MET:HE3	0.81	1.49	14	1
1:A:58:ILE:HG21	1:A:87:LEU:HD23	0.81	1.52	17	4
1:A:10:LYS:HG2	1:A:79:ILE:HG22	0.81	1.52	13	1
1:B:102:ILE:HD12	1:B:103:THR:HG23	0.81	1.52	19	1
1:B:8:LYS:O	1:B:82:GLU:N	0.81	2.14	17	18
1:A:6:LEU:HD12	1:A:84:VAL:HG23	0.81	1.51	20	1
1:A:58:ILE:HA	1:A:90:PHE:CZ	0.80	2.11	8	14
1:B:58:ILE:CG2	1:B:60:ILE:HG23	0.80	2.06	16	5
1:B:10:LYS:HG2	1:B:79:ILE:HG22	0.80	1.53	20	3
1:A:101:LEU:HD12	1:B:25:GLN:OE1	0.80	1.77	1	1
1:A:22:VAL:HG11	1:A:94:ILE:HG13	0.80	1.53	8	12
1:A:58:ILE:CG2	1:A:60:ILE:HG23	0.80	2.06	18	5
1:A:60:ILE:HD11	1:A:87:LEU:CD2	0.80	2.07	15	1
1:B:6:LEU:HD21	1:B:60:ILE:HD13	0.80	1.53	19	4
1:A:101:LEU:HD13	1:A:102:ILE:HG13	0.80	1.51	15	1
1:A:35:ARG:HA	1:A:35:ARG:NE	0.79	1.92	3	2
1:A:22:VAL:HG11	1:A:94:ILE:CD1	0.79	2.06	10	6
1:A:8:LYS:O	1:A:82:GLU:N	0.79	2.14	9	12
1:B:22:VAL:HG11	1:B:94:ILE:HG12	0.79	1.54	9	15
1:B:25:GLN:NE2	1:B:36:LEU:HD22	0.79	1.91	14	1
1:B:31:ASN:OD1	1:B:80:LEU:HD12	0.79	1.78	14	2
1:A:30:ASP:O	1:A:35:ARG:HB3	0.79	1.76	8	7
1:A:43:ILE:HD12	1:A:57:THR:OG1	0.79	1.78	6	4
1:B:22:VAL:HG11	1:B:94:ILE:HD13	0.79	1.52	10	3
1:B:57:THR:OG1	1:B:66:ILE:HG23	0.79	1.75	13	14
1:B:72:MET:HE1	1:B:101:LEU:HD21	0.79	1.52	2	2
1:A:58:ILE:C	1:A:58:ILE:HD12	0.79	1.98	19	1
1:A:22:VAL:CG1	1:A:94:ILE:HD13	0.79	2.08	3	5
1:B:29:LEU:CD2	1:B:32:LEU:HD22	0.79	2.08	7	3
1:A:102:ILE:HG21	1:B:102:ILE:HD13	0.79	1.52	9	3
1:A:35:ARG:CZ	1:A:80:LEU:HD22	0.78	2.08	6	4
1:B:5:THR:HB	1:B:7:TYR:CE1	0.78	2.14	5	20
1:B:23:ASP:OD1	1:B:80:LEU:HD11	0.78	1.79	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:58:ILE:HA	1:B:90:PHE:CZ	0.78	2.14	11	15
1:B:58:ILE:HG23	1:B:90:PHE:CD2	0.78	2.14	14	8
1:B:36:LEU:HD21	1:B:72:MET:CE	0.78	2.08	4	3
1:B:38:ILE:HG21	1:B:69:THR:HG23	0.78	1.54	1	10
1:A:58:ILE:HD11	1:A:65:PHE:HB2	0.78	1.55	13	8
1:A:43:ILE:HD11	1:A:57:THR:HB	0.78	1.56	18	2
1:B:57:THR:HA	1:B:65:PHE:O	0.77	1.79	3	14
1:A:10:LYS:CD	1:A:10:LYS:N	0.77	2.47	20	7
1:B:24:VAL:HG22	1:B:98:ILE:HD12	0.77	1.56	5	4
1:B:43:ILE:HD11	1:B:57:THR:HG23	0.77	1.54	1	1
1:B:38:ILE:CD1	1:B:69:THR:HG23	0.77	2.06	9	2
1:B:58:ILE:HD13	1:B:60:ILE:CG2	0.77	2.03	1	1
1:B:41:THR:HG23	1:B:66:ILE:HD13	0.77	1.55	4	13
1:B:23:ASP:OD2	1:B:80:LEU:HD21	0.77	1.80	2	1
1:B:58:ILE:C	1:B:58:ILE:HD12	0.76	2.00	1	1
1:A:29:LEU:HD23	1:A:32:LEU:HD13	0.76	1.55	7	4
1:A:58:ILE:HG22	1:A:60:ILE:HG23	0.76	1.57	8	7
1:A:10:LYS:N	1:A:10:LYS:CD	0.76	2.47	14	10
1:A:6:LEU:HD11	1:A:20:TYR:CD2	0.76	2.14	4	1
1:A:102:ILE:CD1	1:A:103:THR:HG23	0.76	2.11	6	4
1:B:20:TYR:CE1	1:B:40:LEU:HB2	0.76	2.15	15	1
1:A:41:THR:HG23	1:A:66:ILE:HD13	0.76	1.56	9	16
1:B:35:ARG:HA	1:B:35:ARG:NE	0.76	1.95	18	2
1:B:4:PHE:CD1	1:B:94:ILE:HD12	0.76	2.15	10	2
1:A:58:ILE:HG23	1:A:90:PHE:CD2	0.76	2.16	4	7
1:A:38:ILE:HG21	1:A:69:THR:HG23	0.76	1.58	11	9
1:A:10:LYS:N	1:A:10:LYS:HD2	0.76	1.95	18	5
1:A:7:TYR:C	1:A:81:SER:HB3	0.76	2.01	17	5
1:B:9:ASN:OD1	1:B:19:PRO:HA	0.76	1.81	14	4
1:B:6:LEU:CD1	1:B:60:ILE:HG21	0.75	2.11	5	6
1:B:6:LEU:HD12	1:B:60:ILE:HG21	0.75	1.58	7	4
1:B:22:VAL:O	1:B:24:VAL:HG13	0.75	1.80	17	2
1:A:9:ASN:OD1	1:A:11:ASP:O	0.75	2.04	19	1
1:B:10:LYS:CD	1:B:10:LYS:N	0.75	2.48	13	9
1:A:91:ARG:HA	1:A:94:ILE:HD12	0.75	1.56	2	4
1:A:24:VAL:CG1	1:A:94:ILE:HG23	0.75	2.11	18	1
1:B:24:VAL:HG11	1:B:38:ILE:HD11	0.75	1.59	20	3
1:B:6:LEU:HD11	1:B:60:ILE:HD13	0.74	1.57	5	4
1:A:89:THR:HG23	1:A:90:PHE:CD1	0.74	2.16	7	1
1:B:10:LYS:HG2	1:B:79:ILE:CD1	0.74	2.11	7	1
1:A:73:THR:OG1	1:B:73:THR:HG22	0.74	1.82	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:TYR:OH	1:B:65:PHE:CE1	0.74	2.39	4	15
1:B:38:ILE:CG2	1:B:69:THR:HG23	0.74	2.13	13	12
1:A:73:THR:CB	1:B:73:THR:HG22	0.74	2.12	11	2
1:B:58:ILE:HD13	1:B:90:PHE:CE2	0.74	2.18	17	2
1:A:10:LYS:HB3	1:A:79:ILE:HG12	0.74	1.58	18	1
1:B:30:ASP:O	1:B:35:ARG:HB3	0.74	1.83	17	4
1:B:102:ILE:CD1	1:B:103:THR:HG23	0.74	2.12	10	3
1:A:6:LEU:CD1	1:A:60:ILE:HD13	0.74	2.13	3	6
1:B:29:LEU:HD23	1:B:32:LEU:HD13	0.74	1.56	17	6
1:A:69:THR:OG1	1:A:101:LEU:HD22	0.74	1.82	3	3
1:B:42:PRO:HA	1:B:65:PHE:CD1	0.74	2.17	15	1
1:B:43:ILE:HG23	1:B:48:LYS:HG2	0.74	1.60	17	1
1:B:10:LYS:N	1:B:10:LYS:HD3	0.74	1.98	11	7
1:A:73:THR:HB	1:B:73:THR:HG22	0.74	1.60	11	2
1:B:58:ILE:HD13	1:B:90:PHE:CD2	0.74	2.17	20	3
1:B:99:ASP:CG	1:B:105:ILE:HD11	0.74	2.03	9	3
1:A:35:ARG:NH1	1:A:80:LEU:HD22	0.74	1.96	6	3
1:B:36:LEU:HD11	1:B:72:MET:HG2	0.73	1.59	11	4
1:B:79:ILE:O	1:B:79:ILE:HG12	0.73	1.82	17	6
1:B:10:LYS:N	1:B:10:LYS:HD2	0.73	1.99	8	3
1:A:8:LYS:CE	1:A:15:ALA:HB2	0.73	2.13	18	1
1:B:33:ASN:O	1:B:34:THR:HG23	0.73	1.82	19	8
1:A:35:ARG:NH1	1:A:80:LEU:HD11	0.73	1.98	16	1
1:B:22:VAL:C	1:B:37:VAL:HG12	0.73	2.03	5	12
1:B:101:LEU:CD2	1:B:101:LEU:C	0.73	2.56	6	2
1:B:29:LEU:HD23	1:B:32:LEU:CD2	0.73	2.10	6	2
1:A:22:VAL:HG21	1:A:67:MET:CE	0.73	2.12	17	2
1:A:40:LEU:HD21	1:A:67:MET:HE3	0.73	1.59	13	1
1:B:7:TYR:C	1:B:81:SER:HB3	0.73	2.04	16	7
1:A:38:ILE:CG2	1:A:69:THR:HG23	0.73	2.13	5	11
1:B:69:THR:HG22	1:B:101:LEU:HD12	0.73	1.60	6	2
1:A:35:ARG:CZ	1:A:75:VAL:HB	0.73	2.13	18	1
1:A:99:ASP:O	1:A:103:THR:HG23	0.73	1.83	20	1
1:B:7:TYR:CD2	1:B:80:LEU:HD12	0.73	2.18	18	5
1:B:58:ILE:HD12	1:B:87:LEU:CD2	0.73	2.14	20	4
1:A:69:THR:HG21	1:A:97:ALA:HB1	0.73	1.58	13	4
1:A:20:TYR:OH	1:A:65:PHE:CE1	0.73	2.41	15	18
1:B:76:PRO:O	1:B:79:ILE:HD12	0.73	1.83	15	10
1:B:40:LEU:HD21	1:B:67:MET:CE	0.73	2.13	8	1
1:A:58:ILE:HD12	1:A:58:ILE:C	0.72	2.03	10	1
1:B:69:THR:OG1	1:B:101:LEU:HD22	0.72	1.84	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ASP:CG	1:A:105:ILE:HD11	0.72	2.04	5	2
1:B:6:LEU:HD12	1:B:87:LEU:HD13	0.72	1.60	13	1
1:B:24:VAL:CG1	1:B:94:ILE:HG23	0.72	2.14	15	1
1:A:22:VAL:C	1:A:37:VAL:HG12	0.72	2.04	4	13
1:B:24:VAL:HG21	1:B:38:ILE:CD1	0.72	2.14	15	1
1:B:24:VAL:HG21	1:B:98:ILE:HD11	0.72	1.61	17	2
1:A:75:VAL:HG12	1:A:79:ILE:HD13	0.72	1.58	15	4
1:B:72:MET:SD	1:B:101:LEU:HD11	0.72	2.24	14	2
1:B:75:VAL:HG12	1:B:79:ILE:HD13	0.72	1.59	15	3
1:B:8:LYS:HE3	1:B:15:ALA:HB2	0.72	1.61	2	1
1:B:4:PHE:CZ	1:B:95:ILE:HD11	0.72	2.20	5	6
1:B:24:VAL:HG11	1:B:38:ILE:CD1	0.72	2.15	17	5
1:A:101:LEU:CD2	1:A:101:LEU:C	0.72	2.57	15	1
1:A:6:LEU:HD13	1:A:60:ILE:HD13	0.72	1.62	18	3
1:B:40:LEU:HD23	1:B:67:MET:HG2	0.72	1.61	15	4
1:A:58:ILE:HD13	1:A:90:PHE:CD2	0.71	2.20	3	3
1:A:24:VAL:HG11	1:A:38:ILE:HD11	0.71	1.61	8	6
1:A:25:GLN:NE2	1:B:101:LEU:HD11	0.71	1.99	18	5
1:A:6:LEU:CD1	1:A:60:ILE:HG21	0.71	2.15	18	2
1:B:101:LEU:C	1:B:101:LEU:CD2	0.71	2.57	14	1
1:A:22:VAL:O	1:A:37:VAL:HG12	0.71	1.85	1	6
1:B:10:LYS:HB3	1:B:79:ILE:HB	0.71	1.61	15	4
1:B:21:PHE:CD2	1:B:75:VAL:HG21	0.71	2.19	18	1
1:B:56:PRO:HD2	1:B:67:MET:HB2	0.71	1.62	12	4
1:A:33:ASN:O	1:A:34:THR:HG23	0.71	1.85	18	8
1:A:29:LEU:HD23	1:A:32:LEU:CD2	0.71	2.13	17	3
1:B:43:ILE:HG23	1:B:66:ILE:HG13	0.71	1.63	15	1
1:A:7:TYR:C	1:A:81:SER:HB2	0.71	2.05	2	11
1:A:57:THR:HA	1:A:65:PHE:O	0.71	1.86	5	16
1:A:101:LEU:HD12	1:B:25:GLN:NE2	0.71	2.01	5	3
1:B:22:VAL:O	1:B:37:VAL:HG12	0.71	1.86	6	5
1:B:38:ILE:HD12	1:B:67:MET:HE1	0.71	1.62	10	2
1:B:10:LYS:HD2	1:B:10:LYS:N	0.71	2.00	18	4
1:B:8:LYS:C	1:B:19:PRO:O	0.71	2.30	1	2
1:A:22:VAL:O	1:A:24:VAL:HG13	0.71	1.86	18	1
1:B:58:ILE:HG22	1:B:60:ILE:HG23	0.70	1.62	20	6
1:B:8:LYS:HG3	1:B:9:ASN:ND2	0.70	2.00	12	4
1:B:41:THR:HG21	1:B:68:LEU:HD13	0.70	1.60	11	7
1:A:54:LEU:HD12	1:A:100:PHE:CE2	0.70	2.21	15	4
1:A:8:LYS:C	1:A:19:PRO:O	0.70	2.29	8	6
1:B:37:VAL:HG11	1:B:75:VAL:HG22	0.70	1.63	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:O	1:A:32:LEU:HD12	0.70	1.86	20	2
1:B:58:ILE:HD12	1:B:59:HIS:N	0.70	2.01	1	1
1:B:37:VAL:HG22	1:B:73:THR:O	0.70	1.87	7	8
1:B:58:ILE:HG23	1:B:67:MET:HE1	0.70	1.60	9	1
1:A:38:ILE:HD12	1:A:69:THR:CG2	0.70	2.15	18	2
1:A:24:VAL:HG22	1:A:98:ILE:HD12	0.70	1.63	10	11
1:B:97:ALA:O	1:B:101:LEU:HB3	0.70	1.87	19	19
1:A:103:THR:OG1	1:A:105:ILE:HG23	0.70	1.87	19	1
1:A:97:ALA:O	1:A:101:LEU:HB3	0.70	1.87	7	18
1:B:9:ASN:OD1	1:B:9:ASN:O	0.70	2.09	5	4
1:B:22:VAL:HG23	1:B:40:LEU:HD11	0.70	1.62	9	3
1:B:35:ARG:NH2	1:B:75:VAL:HG13	0.70	2.00	3	1
1:A:58:ILE:HD12	1:A:87:LEU:CD2	0.70	2.17	3	3
1:A:37:VAL:HG22	1:A:73:THR:O	0.70	1.87	7	5
1:A:102:ILE:HD13	1:A:103:THR:HG23	0.70	1.63	6	1
1:A:76:PRO:O	1:A:79:ILE:HD12	0.69	1.86	16	9
1:A:6:LEU:HD12	1:A:60:ILE:HG21	0.69	1.62	18	1
1:A:72:MET:SD	1:A:101:LEU:HD21	0.69	2.26	5	4
1:A:6:LEU:CD2	1:A:60:ILE:HD13	0.69	2.17	4	2
1:A:26:SER:O	1:A:30:ASP:N	0.69	2.25	16	9
1:B:38:ILE:HG23	1:B:69:THR:HG23	0.69	1.63	7	5
1:A:54:LEU:HD21	1:A:101:LEU:HD22	0.69	1.63	14	1
1:A:30:ASP:O	1:A:35:ARG:HG2	0.69	1.86	11	4
1:A:39:PRO:O	1:A:68:LEU:HB2	0.69	1.86	5	20
1:A:24:VAL:HG12	1:A:94:ILE:HG23	0.69	1.63	18	1
1:B:39:PRO:O	1:B:68:LEU:HB2	0.69	1.87	15	20
1:B:102:ILE:HG13	1:B:103:THR:HG23	0.69	1.65	2	3
1:B:6:LEU:HD23	1:B:85:ASN:HB3	0.69	1.65	20	4
1:A:4:PHE:CZ	1:A:95:ILE:HD11	0.69	2.22	14	6
1:B:6:LEU:CD1	1:B:60:ILE:HD13	0.69	2.17	14	8
1:A:19:PRO:CG	1:A:42:PRO:HD3	0.69	2.18	15	20
1:B:10:LYS:HA	1:B:82:GLU:N	0.69	2.03	2	13
1:A:8:LYS:O	1:A:81:SER:HB3	0.69	1.88	19	4
1:A:10:LYS:HA	1:A:82:GLU:N	0.69	2.03	9	6
1:A:35:ARG:CG	1:A:80:LEU:HD11	0.69	2.17	12	1
1:A:38:ILE:HD12	1:A:67:MET:HG2	0.68	1.62	1	1
1:A:58:ILE:O	1:A:64:ASP:HA	0.68	1.87	10	4
1:A:10:LYS:HD3	1:A:10:LYS:N	0.68	2.01	8	2
1:B:7:TYR:O	1:B:20:TYR:HB2	0.68	1.88	15	1
1:A:69:THR:O	1:A:101:LEU:HD13	0.68	1.88	3	3
1:B:20:TYR:CG	1:B:40:LEU:HD12	0.68	2.23	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:VAL:CG2	1:A:98:ILE:HD11	0.68	2.16	18	1
1:B:72:MET:CE	1:B:101:LEU:HD21	0.68	2.19	2	4
1:A:10:LYS:HG2	1:A:79:ILE:CG2	0.68	2.19	13	1
1:B:102:ILE:HD13	1:B:103:THR:HG23	0.68	1.65	10	2
1:B:8:LYS:CA	1:B:20:TYR:HB3	0.68	2.19	2	4
1:B:43:ILE:HD11	1:B:57:THR:HG1	0.68	1.47	18	3
1:A:58:ILE:HG22	1:A:90:PHE:CG	0.68	2.24	11	3
1:B:8:LYS:HA	1:B:20:TYR:CB	0.68	2.14	15	16
1:B:68:LEU:HD23	1:B:71:GLN:HB2	0.68	1.64	19	3
1:A:40:LEU:HD21	1:A:67:MET:SD	0.68	2.28	1	2
1:B:10:LYS:HD3	1:B:11:ASP:H	0.68	1.48	2	14
1:B:98:ILE:HG13	1:B:102:ILE:HD12	0.68	1.65	4	4
1:B:69:THR:HG21	1:B:97:ALA:HB1	0.68	1.64	4	2
1:B:87:LEU:HD12	1:B:87:LEU:H	0.68	1.48	3	5
1:A:58:ILE:HD12	1:A:87:LEU:HD22	0.68	1.65	17	3
1:A:10:LYS:HD3	1:A:11:ASP:N	0.68	2.03	11	9
1:B:30:ASP:HA	1:B:35:ARG:CD	0.68	2.19	14	3
1:B:72:MET:O	1:B:73:THR:HG23	0.68	1.89	13	1
1:A:72:MET:CE	1:A:101:LEU:HD21	0.67	2.19	2	3
1:B:7:TYR:C	1:B:81:SER:HB2	0.67	2.09	7	12
1:B:94:ILE:O	1:B:97:ALA:HB3	0.67	1.89	3	4
1:A:6:LEU:HD11	1:A:85:ASN:CB	0.67	2.19	20	1
1:B:26:SER:CB	1:B:29:LEU:HB2	0.67	2.19	5	20
1:B:35:ARG:HD2	1:B:37:VAL:HG13	0.67	1.64	17	1
1:A:22:VAL:O	1:A:24:VAL:HG12	0.67	1.90	3	19
1:B:6:LEU:CD2	1:B:60:ILE:HD13	0.67	2.20	18	1
1:A:102:ILE:HD12	1:A:103:THR:N	0.67	2.05	6	2
1:B:75:VAL:O	1:B:80:LEU:HD22	0.67	1.89	9	1
1:A:8:LYS:HE3	1:A:15:ALA:HB2	0.67	1.67	18	1
1:B:8:LYS:C	1:B:81:SER:HB3	0.67	2.10	1	3
1:B:69:THR:CG2	1:B:101:LEU:HD22	0.67	2.20	17	11
1:A:75:VAL:HG23	1:A:79:ILE:CD1	0.67	2.18	6	3
1:A:101:LEU:HD11	1:B:25:GLN:NE2	0.67	2.04	18	3
1:A:10:LYS:HD3	1:A:11:ASP:H	0.67	1.49	20	11
1:B:36:LEU:HD11	1:B:72:MET:CG	0.67	2.20	4	2
1:B:40:LEU:HD21	1:B:58:ILE:HG13	0.67	1.64	7	3
1:A:36:LEU:HD11	1:B:72:MET:HE2	0.67	1.66	4	1
1:A:102:ILE:HG23	1:B:25:GLN:OE1	0.67	1.90	12	1
1:B:10:LYS:N	1:B:10:LYS:CD	0.67	2.57	20	11
1:A:10:LYS:HD2	1:A:10:LYS:N	0.67	2.04	16	2
1:B:22:VAL:O	1:B:24:VAL:HG12	0.66	1.89	14	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:LYS:HG3	1:B:79:ILE:O	0.66	1.90	5	4
1:B:102:ILE:HD12	1:B:103:THR:N	0.66	2.05	11	2
1:A:24:VAL:HG21	1:A:98:ILE:CD1	0.66	2.18	18	1
1:B:100:PHE:HB2	1:B:105:ILE:HG22	0.66	1.67	19	1
1:A:101:LEU:HD11	1:B:25:GLN:CD	0.66	2.11	13	2
1:B:43:ILE:HD12	1:B:57:THR:CG2	0.66	2.20	17	1
1:A:6:LEU:HD12	1:A:87:LEU:HB3	0.66	1.67	2	1
1:B:43:ILE:HD12	1:B:64:ASP:OD2	0.66	1.90	18	1
1:B:72:MET:SD	1:B:101:LEU:HD21	0.66	2.31	3	2
1:B:4:PHE:CD2	1:B:94:ILE:HD12	0.66	2.26	4	1
1:A:9:ASN:N	1:A:81:SER:OG	0.66	2.28	6	5
1:A:10:LYS:HG2	1:A:79:ILE:CG1	0.66	2.21	18	1
1:A:25:GLN:OE1	1:A:36:LEU:HD22	0.66	1.90	20	1
1:B:24:VAL:HB	1:B:94:ILE:HG23	0.66	1.68	7	4
1:B:37:VAL:CG1	1:B:75:VAL:HG22	0.66	2.21	4	1
1:B:103:THR:HG22	1:B:105:ILE:HG23	0.66	1.67	13	3
1:A:102:ILE:HG13	1:A:103:THR:HG23	0.66	1.66	3	3
1:B:19:PRO:CG	1:B:42:PRO:HD3	0.66	2.21	15	19
1:A:98:ILE:HG13	1:A:102:ILE:HD12	0.66	1.66	18	3
1:A:40:LEU:HD23	1:A:66:ILE:C	0.65	2.11	14	6
1:A:103:THR:HG22	1:A:105:ILE:HG23	0.65	1.68	12	1
1:B:35:ARG:NH2	1:B:80:LEU:HD22	0.65	2.06	13	2
1:B:20:TYR:CD1	1:B:20:TYR:N	0.65	2.64	20	13
1:A:10:LYS:CG	1:A:79:ILE:HB	0.65	2.21	2	10
1:B:20:TYR:N	1:B:20:TYR:CD1	0.65	2.64	12	7
1:A:36:LEU:HD22	1:A:74:SER:HB3	0.65	1.67	18	1
1:B:69:THR:O	1:B:101:LEU:HD13	0.65	1.91	8	4
1:B:9:ASN:C	1:B:82:GLU:H	0.65	1.95	1	6
1:B:92:ASN:HA	1:B:95:ILE:HD12	0.65	1.68	2	11
1:B:41:THR:O	1:B:66:ILE:HD12	0.65	1.91	7	19
1:B:98:ILE:HA	1:B:101:LEU:HD23	0.65	1.68	8	9
1:A:54:LEU:CD2	1:A:69:THR:HG23	0.65	2.21	3	1
1:B:76:PRO:HD2	1:B:79:ILE:HD11	0.65	1.67	20	6
1:B:58:ILE:HD11	1:B:67:MET:SD	0.65	2.32	18	2
1:A:79:ILE:HG12	1:A:79:ILE:O	0.65	1.91	12	5
1:A:7:TYR:CD2	1:A:80:LEU:HD12	0.65	2.27	7	5
1:A:73:THR:HG22	1:B:73:THR:OG1	0.65	1.91	5	1
1:A:103:THR:HG1	1:A:105:ILE:HG23	0.65	1.51	19	1
1:A:79:ILE:O	1:A:81:SER:N	0.65	2.30	2	11
1:B:79:ILE:O	1:B:81:SER:N	0.65	2.29	10	12
1:A:25:GLN:OE1	1:B:102:ILE:HG23	0.65	1.92	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:LYS:N	1:B:82:GLU:H	0.65	1.90	5	8
1:B:31:ASN:CG	1:B:77:VAL:HG23	0.65	2.12	18	2
1:A:6:LEU:HD23	1:A:87:LEU:N	0.65	2.07	20	1
1:A:20:TYR:CD1	1:A:20:TYR:N	0.65	2.65	4	9
1:B:99:ASP:CG	1:B:105:ILE:HD12	0.65	2.12	19	1
1:B:23:ASP:OD1	1:B:80:LEU:HD21	0.64	1.93	1	1
1:A:92:ASN:O	1:A:96:ALA:N	0.64	2.29	20	20
1:B:33:ASN:O	1:B:34:THR:HG22	0.64	1.92	9	9
1:A:92:ASN:HA	1:A:95:ILE:HD12	0.64	1.69	7	9
1:B:6:LEU:HD13	1:B:60:ILE:HD13	0.64	1.68	16	5
1:A:98:ILE:HA	1:A:101:LEU:HD23	0.64	1.68	3	8
1:B:87:LEU:H	1:B:87:LEU:HD12	0.64	1.52	12	8
1:B:10:LYS:HD3	1:B:11:ASP:N	0.64	2.06	2	12
1:B:92:ASN:O	1:B:96:ALA:N	0.64	2.30	13	20
1:B:8:LYS:O	1:B:81:SER:HB3	0.64	1.93	13	2
1:A:8:LYS:O	1:A:10:LYS:N	0.64	2.31	5	1
1:B:58:ILE:HD13	1:B:90:PHE:CD1	0.64	2.27	18	3
1:B:10:LYS:H	1:B:81:SER:HA	0.64	1.52	7	5
1:B:2:SER:O	1:B:3:GLN:CB	0.64	2.46	8	7
1:B:40:LEU:HD23	1:B:67:MET:CG	0.64	2.22	15	4
1:A:5:THR:HB	1:A:7:TYR:CZ	0.64	2.26	13	20
1:A:9:ASN:O	1:A:11:ASP:N	0.64	2.31	7	19
1:B:9:ASN:ND2	1:B:15:ALA:HB2	0.64	2.07	7	1
1:B:75:VAL:HG23	1:B:79:ILE:CD1	0.64	2.21	3	2
1:B:101:LEU:HD13	1:B:102:ILE:CG1	0.64	2.23	14	3
1:A:20:TYR:OH	1:A:65:PHE:CE2	0.64	2.51	6	5
1:B:24:VAL:CG2	1:B:98:ILE:HD12	0.64	2.23	5	3
1:A:10:LYS:N	1:A:10:LYS:HD3	0.64	2.08	9	8
1:A:9:ASN:OD1	1:A:12:LYS:HA	0.64	1.92	3	1
1:B:58:ILE:HG21	1:B:87:LEU:CD2	0.64	2.23	18	5
1:A:94:ILE:O	1:A:97:ALA:HB3	0.64	1.94	3	4
1:A:10:LYS:CG	1:A:79:ILE:CG1	0.64	2.76	18	7
1:B:60:ILE:HD12	1:B:62:GLU:HB2	0.64	1.69	12	2
1:A:75:VAL:HG13	1:A:80:LEU:HD22	0.64	1.69	9	1
1:B:41:THR:OG1	1:B:42:PRO:HD2	0.63	1.92	20	20
1:B:20:TYR:OH	1:B:65:PHE:CG	0.63	2.47	6	3
1:A:54:LEU:HD13	1:A:54:LEU:O	0.63	1.92	4	1
1:A:20:TYR:N	1:A:20:TYR:CD1	0.63	2.66	17	11
1:A:102:ILE:HD12	1:A:103:THR:HG23	0.63	1.69	4	2
1:A:23:ASP:OD2	1:A:80:LEU:HD21	0.63	1.93	11	3
1:B:9:ASN:O	1:B:11:ASP:N	0.63	2.31	13	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:LYS:CG	1:B:79:ILE:HB	0.63	2.24	18	8
1:B:58:ILE:HG23	1:B:60:ILE:HG23	0.63	1.71	4	3
1:A:9:ASN:N	1:A:19:PRO:O	0.63	2.32	1	14
1:A:41:THR:OG1	1:A:42:PRO:HD2	0.63	1.94	2	20
1:A:26:SER:CB	1:A:29:LEU:HB2	0.63	2.23	13	19
1:B:43:ILE:CD1	1:B:57:THR:HG22	0.63	2.23	3	1
1:A:102:ILE:HD12	1:B:102:ILE:HD13	0.63	1.70	10	1
1:A:40:LEU:HD22	1:A:58:ILE:HD12	0.63	1.71	13	3
1:B:30:ASP:O	1:B:35:ARG:HD3	0.63	1.93	19	1
1:A:69:THR:CG2	1:A:101:LEU:HD22	0.63	2.23	1	12
1:A:4:PHE:HD1	1:A:94:ILE:HD12	0.63	1.54	3	1
1:B:8:LYS:O	1:B:9:ASN:O	0.63	2.17	3	9
1:B:10:LYS:HD2	1:B:11:ASP:N	0.63	2.08	5	1
1:A:87:LEU:H	1:A:87:LEU:HD12	0.63	1.53	9	6
1:B:19:PRO:HB2	1:B:20:TYR:CE1	0.63	2.29	1	17
1:B:20:TYR:OH	1:B:65:PHE:CD1	0.63	2.52	17	12
1:B:58:ILE:N	1:B:58:ILE:HD12	0.63	2.08	12	1
1:B:10:LYS:HG2	1:B:79:ILE:CB	0.63	2.24	6	3
1:B:6:LEU:HG	1:B:87:LEU:HD13	0.63	1.70	7	2
1:B:4:PHE:HD1	1:B:94:ILE:HD12	0.62	1.54	10	2
1:A:40:LEU:HD21	1:A:58:ILE:HG13	0.62	1.70	14	3
1:A:6:LEU:HG	1:A:60:ILE:HD13	0.62	1.68	15	1
1:A:57:THR:HG1	1:A:66:ILE:HG23	0.62	1.53	20	6
1:B:7:TYR:O	1:B:20:TYR:HB3	0.62	1.94	5	17
1:A:35:ARG:NH2	1:A:80:LEU:HD22	0.62	2.09	14	2
1:A:31:ASN:OD1	1:A:77:VAL:HG23	0.62	1.94	8	2
1:B:3:GLN:HA	1:B:35:ARG:NH1	0.62	2.09	10	1
1:B:35:ARG:HA	1:B:35:ARG:CZ	0.62	2.23	18	2
1:B:6:LEU:HD11	1:B:60:ILE:HG21	0.62	1.71	9	2
1:B:35:ARG:O	1:B:74:SER:HA	0.62	1.94	11	3
1:A:101:LEU:HD13	1:A:102:ILE:CG1	0.62	2.24	15	1
1:A:7:TYR:HB3	1:A:81:SER:HB2	0.62	1.71	12	5
1:B:80:LEU:O	1:B:81:SER:O	0.62	2.16	18	10
1:B:98:ILE:HG23	1:B:102:ILE:CG1	0.62	2.24	10	2
1:B:35:ARG:NE	1:B:35:ARG:HA	0.62	2.09	20	2
1:B:10:LYS:CG	1:B:79:ILE:HA	0.62	2.24	2	6
1:B:42:PRO:HG3	1:B:45:LEU:HD23	0.62	1.71	2	2
1:B:35:ARG:HD2	1:B:80:LEU:HD21	0.62	1.72	9	1
1:A:40:LEU:HG	1:A:67:MET:HG2	0.62	1.72	3	1
1:A:29:LEU:CD2	1:A:32:LEU:HD22	0.62	2.24	12	2
1:B:43:ILE:HD11	1:B:57:THR:CG2	0.62	2.25	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HD12	1:A:58:ILE:N	0.62	2.10	2	1
1:B:6:LEU:HD13	1:B:87:LEU:HD13	0.62	1.72	19	2
1:A:7:TYR:CD2	1:A:80:LEU:HD11	0.62	2.29	19	2
1:A:58:ILE:CD1	1:A:60:ILE:N	0.62	2.63	10	2
1:A:41:THR:HG21	1:A:68:LEU:HD13	0.61	1.71	13	8
1:B:54:LEU:HD12	1:B:100:PHE:CE2	0.61	2.30	13	3
1:B:79:ILE:HG12	1:B:79:ILE:O	0.61	1.94	9	2
1:B:31:ASN:OD1	1:B:77:VAL:HG23	0.61	1.95	14	4
1:A:34:THR:HG22	1:A:76:PRO:HA	0.61	1.71	9	3
1:A:80:LEU:O	1:A:81:SER:O	0.61	2.18	13	9
1:B:38:ILE:HG23	1:B:38:ILE:O	0.61	1.95	2	2
1:A:102:ILE:HG21	1:B:102:ILE:CD1	0.61	2.24	9	1
1:A:75:VAL:HG12	1:A:79:ILE:CD1	0.61	2.26	20	4
1:B:10:LYS:CG	1:B:79:ILE:HG12	0.61	2.26	1	6
1:B:40:LEU:HD23	1:B:66:ILE:C	0.61	2.14	7	7
1:A:30:ASP:O	1:A:35:ARG:CB	0.61	2.47	14	6
1:B:7:TYR:O	1:B:20:TYR:CB	0.61	2.48	2	12
1:B:9:ASN:N	1:B:19:PRO:O	0.61	2.34	16	18
1:A:10:LYS:CB	1:A:79:ILE:HG12	0.61	2.26	18	2
1:A:99:ASP:O	1:A:105:ILE:HD13	0.61	1.94	14	1
1:A:87:LEU:HD12	1:A:87:LEU:H	0.61	1.55	5	5
1:B:30:ASP:O	1:B:34:THR:O	0.61	2.18	8	4
1:A:98:ILE:HA	1:A:102:ILE:HG23	0.61	1.70	17	4
1:B:41:THR:HG21	1:B:68:LEU:HD23	0.61	1.72	17	2
1:A:38:ILE:CD1	1:A:69:THR:HG23	0.61	2.23	18	1
1:A:41:THR:O	1:A:66:ILE:HD12	0.61	1.94	13	20
1:A:19:PRO:HB2	1:A:20:TYR:CE1	0.61	2.31	14	20
1:A:21:PHE:CD2	1:A:75:VAL:HG21	0.61	2.30	15	2
1:A:54:LEU:HD11	1:A:101:LEU:HD13	0.61	1.71	18	1
1:A:42:PRO:CG	1:A:45:LEU:HD12	0.61	2.25	8	9
1:A:43:ILE:HD12	1:A:64:ASP:HB3	0.61	1.72	3	2
1:A:99:ASP:HA	1:A:103:THR:HG23	0.61	1.71	1	6
1:A:10:LYS:HA	1:A:81:SER:HA	0.61	1.73	1	2
1:A:58:ILE:HD12	1:A:59:HIS:CA	0.61	2.25	19	2
1:A:10:LYS:CA	1:A:81:SER:HA	0.60	2.26	1	2
1:B:8:LYS:CE	1:B:15:ALA:HB2	0.60	2.26	2	1
1:A:7:TYR:O	1:A:20:TYR:HB3	0.60	1.96	17	15
1:A:5:THR:CB	1:A:7:TYR:CE1	0.60	2.84	12	13
1:A:97:ALA:O	1:A:101:LEU:CB	0.60	2.48	10	1
1:B:29:LEU:HD23	1:B:32:LEU:HG	0.60	1.72	5	2
1:A:8:LYS:HE2	1:A:84:VAL:HG13	0.60	1.70	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:LEU:O	1:B:32:LEU:HD13	0.60	1.97	6	3
1:B:6:LEU:CD1	1:B:87:LEU:HD13	0.60	2.26	13	2
1:B:98:ILE:HA	1:B:102:ILE:HG23	0.60	1.72	2	4
1:B:25:GLN:NE2	1:B:36:LEU:HD23	0.60	2.11	20	1
1:B:58:ILE:CD1	1:B:60:ILE:HG23	0.60	2.05	1	1
1:A:33:ASN:O	1:A:34:THR:HG22	0.60	1.97	13	10
1:A:76:PRO:HD2	1:A:79:ILE:HD11	0.60	1.72	15	6
1:A:10:LYS:HG2	1:A:79:ILE:HA	0.60	1.73	12	6
1:B:10:LYS:HG2	1:B:79:ILE:CG2	0.60	2.25	20	3
1:B:43:ILE:HG23	1:B:66:ILE:CG1	0.60	2.26	15	1
1:A:20:TYR:CD1	1:A:40:LEU:HD13	0.60	2.31	16	1
1:B:58:ILE:O	1:B:64:ASP:HA	0.60	1.96	1	6
1:B:10:LYS:HG2	1:B:79:ILE:HA	0.60	1.72	5	7
1:A:24:VAL:O	1:A:25:GLN:CB	0.60	2.48	2	6
1:B:58:ILE:HG22	1:B:90:PHE:CD1	0.60	2.31	6	2
1:B:9:ASN:OD1	1:B:15:ALA:N	0.60	2.35	12	5
1:A:2:SER:O	1:A:3:GLN:CB	0.60	2.50	20	10
1:B:30:ASP:O	1:B:35:ARG:CB	0.60	2.49	17	2
1:A:22:VAL:HG23	1:A:40:LEU:HD11	0.60	1.73	4	1
1:B:99:ASP:HA	1:B:103:THR:OG1	0.60	1.95	11	2
1:B:28:LEU:N	1:B:28:LEU:HD12	0.59	2.12	19	4
1:B:6:LEU:HD13	1:B:87:LEU:HD21	0.59	1.72	18	3
1:A:23:ASP:OD1	1:A:80:LEU:HD21	0.59	1.96	15	3
1:A:10:LYS:HG2	1:A:79:ILE:CB	0.59	2.27	13	1
1:B:58:ILE:HG12	1:B:90:PHE:CD2	0.59	2.32	16	3
1:A:38:ILE:HG23	1:A:69:THR:HG23	0.59	1.74	15	7
1:B:5:THR:HB	1:B:7:TYR:CZ	0.59	2.32	1	20
1:B:33:ASN:O	1:B:34:THR:CG2	0.59	2.51	6	12
1:B:19:PRO:HG3	1:B:42:PRO:HD3	0.59	1.74	6	13
1:B:9:ASN:ND2	1:B:19:PRO:HA	0.59	2.12	10	5
1:A:10:LYS:H	1:A:81:SER:HA	0.59	1.56	8	8
1:B:43:ILE:HG23	1:B:48:LYS:CG	0.59	2.27	17	1
1:A:9:ASN:O	1:A:10:LYS:C	0.59	2.39	7	15
1:A:20:TYR:O	1:A:40:LEU:N	0.59	2.36	14	15
1:B:7:TYR:CD2	1:B:80:LEU:HD22	0.59	2.32	14	1
1:B:57:THR:CG2	1:B:58:ILE:N	0.59	2.66	5	15
1:B:22:VAL:HG21	1:B:67:MET:HE3	0.59	1.72	6	6
1:B:9:ASN:N	1:B:81:SER:OG	0.59	2.35	16	4
1:A:79:ILE:O	1:A:79:ILE:CG1	0.59	2.47	18	3
1:A:58:ILE:HG13	1:A:90:PHE:CE1	0.59	2.33	18	3
1:B:77:VAL:HA	1:B:80:LEU:HD23	0.59	1.75	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:THR:HG23	1:A:86:GLU:HG2	0.59	1.74	8	1
1:A:75:VAL:CG1	1:A:79:ILE:HD13	0.59	2.28	11	1
1:A:57:THR:CG2	1:A:58:ILE:N	0.59	2.65	19	14
1:A:58:ILE:H	1:A:58:ILE:HD13	0.59	1.58	13	4
1:B:24:VAL:HG21	1:B:98:ILE:HD13	0.59	1.75	3	9
1:A:30:ASP:O	1:A:34:THR:O	0.59	2.21	20	6
1:B:75:VAL:HG12	1:B:79:ILE:CD1	0.59	2.27	18	3
1:B:38:ILE:CD1	1:B:67:MET:HB3	0.59	2.28	2	3
1:B:38:ILE:HD13	1:B:67:MET:HB3	0.59	1.75	2	1
1:A:54:LEU:HD21	1:A:100:PHE:CD2	0.59	2.31	6	1
1:A:99:ASP:HA	1:A:103:THR:OG1	0.59	1.97	6	1
1:A:25:GLN:HE22	1:B:101:LEU:HD11	0.59	1.58	12	1
1:B:9:ASN:O	1:B:10:LYS:C	0.59	2.40	13	14
1:B:36:LEU:HD21	1:B:72:MET:SD	0.59	2.38	4	2
1:A:35:ARG:NE	1:A:80:LEU:HD22	0.59	2.13	17	1
1:B:28:LEU:O	1:B:32:LEU:HD23	0.59	1.98	5	1
1:A:6:LEU:HD23	1:A:85:ASN:HB3	0.58	1.74	1	3
1:B:10:LYS:HD2	1:B:11:ASP:H	0.58	1.56	5	1
1:A:69:THR:HB	1:A:101:LEU:HD13	0.58	1.74	1	2
1:B:58:ILE:HG23	1:B:90:PHE:CD1	0.58	2.33	15	1
1:A:38:ILE:HD13	1:A:97:ALA:CB	0.58	2.27	3	2
1:B:38:ILE:HD13	1:B:97:ALA:CB	0.58	2.27	16	3
1:A:2:SER:O	1:A:30:ASP:HB2	0.58	1.98	11	4
1:B:22:VAL:CG2	1:B:40:LEU:HD11	0.58	2.28	12	2
1:A:6:LEU:O	1:A:6:LEU:HD13	0.58	1.99	15	1
1:B:24:VAL:CG2	1:B:98:ILE:HD13	0.58	2.27	7	10
1:A:31:ASN:HD21	1:A:77:VAL:HG23	0.58	1.59	13	1
1:B:24:VAL:HG23	1:B:24:VAL:O	0.58	1.98	15	1
1:A:6:LEU:HD11	1:A:85:ASN:HB3	0.58	1.75	20	1
1:B:9:ASN:HD21	1:B:15:ALA:HB2	0.58	1.58	7	1
1:A:29:LEU:HD13	1:B:54:LEU:HD12	0.58	1.75	7	1
1:B:40:LEU:HA	1:B:66:ILE:O	0.58	1.98	15	1
1:B:75:VAL:CG2	1:B:79:ILE:HG23	0.58	2.28	17	1
1:A:46:LEU:HD21	1:A:68:LEU:CD1	0.58	2.29	18	1
1:B:5:THR:CB	1:B:7:TYR:CE1	0.58	2.86	17	17
1:B:40:LEU:CD2	1:B:58:ILE:HD11	0.58	2.29	3	1
1:A:24:VAL:HG11	1:A:38:ILE:CD1	0.58	2.29	17	9
1:A:55:CYS:SG	1:A:68:LEU:HD23	0.58	2.38	5	1
1:A:25:GLN:CD	1:B:101:LEU:HD12	0.58	2.19	9	1
1:A:24:VAL:HG11	1:A:94:ILE:HG22	0.58	1.75	2	6
1:A:87:LEU:N	1:A:87:LEU:CD2	0.58	2.66	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ASP:O	1:A:103:THR:OG1	0.58	2.21	11	3
1:A:29:LEU:HD13	1:B:70:GLN:CG	0.58	2.28	10	1
1:A:28:LEU:HD12	1:A:28:LEU:N	0.58	2.13	7	3
1:A:29:LEU:HA	1:A:32:LEU:HD23	0.58	1.76	6	1
1:A:28:LEU:N	1:A:28:LEU:HD12	0.58	2.13	11	4
1:A:20:TYR:OH	1:A:60:ILE:HD11	0.58	1.99	16	1
1:A:33:ASN:O	1:A:34:THR:CG2	0.58	2.52	17	10
1:B:6:LEU:HD13	1:B:87:LEU:HG	0.58	1.76	6	1
1:A:72:MET:SD	1:A:102:ILE:HD11	0.58	2.39	18	2
1:A:6:LEU:HG	1:A:87:LEU:HD13	0.58	1.74	18	1
1:A:105:ILE:OXT	1:A:105:ILE:HD12	0.58	1.99	1	1
1:A:25:GLN:OE1	1:B:101:LEU:HD11	0.58	1.99	15	2
1:A:10:LYS:CG	1:A:79:ILE:HG12	0.58	2.29	11	7
1:B:10:LYS:HB3	1:B:79:ILE:O	0.58	1.98	7	2
1:A:98:ILE:CG2	1:A:102:ILE:HD11	0.58	2.28	16	2
1:B:40:LEU:HD21	1:B:67:MET:HE2	0.58	1.75	8	1
1:A:58:ILE:N	1:A:58:ILE:HD13	0.58	2.13	12	5
1:B:30:ASP:O	1:B:35:ARG:HD2	0.57	1.99	8	1
1:B:64:ASP:O	1:B:65:PHE:CD1	0.57	2.58	3	14
1:B:2:SER:CB	1:B:30:ASP:HB2	0.57	2.29	19	1
1:B:10:LYS:HD3	1:B:10:LYS:N	0.57	2.14	1	7
1:B:20:TYR:CG	1:B:40:LEU:HD13	0.57	2.34	6	2
1:B:28:LEU:HD12	1:B:28:LEU:N	0.57	2.14	3	2
1:B:72:MET:HE1	1:B:98:ILE:HD11	0.57	1.76	12	1
1:A:75:VAL:O	1:A:75:VAL:HG23	0.57	1.99	1	3
1:B:20:TYR:O	1:B:40:LEU:N	0.57	2.38	4	15
1:A:25:GLN:HB2	1:A:36:LEU:CB	0.57	2.29	17	7
1:A:79:ILE:CG1	1:A:79:ILE:O	0.57	2.52	12	5
1:A:97:ALA:O	1:A:101:LEU:N	0.57	2.32	10	5
1:A:24:VAL:HG21	1:A:98:ILE:HD13	0.57	1.75	12	4
1:A:10:LYS:HD2	1:A:79:ILE:CG1	0.57	2.29	10	6
1:A:9:ASN:C	1:A:82:GLU:H	0.57	2.02	8	3
1:A:43:ILE:HD11	1:A:57:THR:HG1	0.57	1.60	1	3
1:A:98:ILE:O	1:A:102:ILE:HB	0.57	2.00	20	10
1:A:40:LEU:HD22	1:A:58:ILE:CD1	0.57	2.30	1	3
1:B:42:PRO:CG	1:B:45:LEU:HD12	0.57	2.29	8	4
1:A:21:PHE:CD2	1:A:75:VAL:HG11	0.57	2.35	1	6
1:A:35:ARG:CZ	1:A:35:ARG:HA	0.57	2.29	3	3
1:A:7:TYR:CD2	1:A:80:LEU:CD1	0.57	2.87	20	5
1:B:58:ILE:HD13	1:B:58:ILE:N	0.57	2.15	9	3
1:A:25:GLN:NE2	1:B:101:LEU:HD12	0.57	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HA	1:A:90:PHE:CE2	0.57	2.34	2	2
1:B:10:LYS:CD	1:B:79:ILE:HG13	0.57	2.30	17	6
1:B:6:LEU:HD12	1:B:85:ASN:HB2	0.57	1.76	4	1
1:A:36:LEU:HD11	1:A:72:MET:HE3	0.57	1.76	5	2
1:B:23:ASP:N	1:B:37:VAL:HG12	0.57	2.15	19	2
1:A:87:LEU:HD22	1:A:87:LEU:N	0.57	2.14	4	1
1:A:79:ILE:O	1:A:80:LEU:C	0.57	2.43	16	3
1:B:30:ASP:O	1:B:35:ARG:HG2	0.57	2.00	12	1
1:A:24:VAL:CG2	1:A:98:ILE:HD12	0.56	2.31	1	6
1:A:58:ILE:HG21	1:A:87:LEU:CD2	0.56	2.27	17	3
1:B:79:ILE:O	1:B:79:ILE:CG1	0.56	2.52	1	3
1:B:99:ASP:HA	1:B:103:THR:HG23	0.56	1.77	1	4
1:A:19:PRO:HG3	1:A:42:PRO:HD3	0.56	1.76	5	11
1:A:7:TYR:O	1:A:20:TYR:CB	0.56	2.53	16	10
1:B:36:LEU:HD21	1:B:72:MET:HE1	0.56	1.75	16	3
1:A:102:ILE:CG2	1:B:102:ILE:HD13	0.56	2.30	8	1
1:B:62:GLU:OE1	1:B:84:VAL:HG21	0.56	2.00	10	1
1:A:43:ILE:HD11	1:A:57:THR:HG21	0.56	1.76	19	1
1:B:53:HIS:C	1:B:54:LEU:HD12	0.56	2.20	1	1
1:A:58:ILE:HD13	1:A:58:ILE:N	0.56	2.15	6	2
1:A:20:TYR:OH	1:A:65:PHE:CZ	0.56	2.59	10	12
1:A:80:LEU:HD12	1:A:80:LEU:O	0.56	2.00	10	2
1:B:69:THR:HG1	1:B:101:LEU:HD22	0.56	1.58	2	1
1:A:19:PRO:HG2	1:A:42:PRO:HD3	0.56	1.76	2	5
1:A:69:THR:OG1	1:A:101:LEU:CD2	0.56	2.53	16	3
1:A:58:ILE:HD13	1:A:90:PHE:CG	0.56	2.35	4	1
1:B:54:LEU:HD21	1:B:69:THR:CG2	0.56	2.28	12	1
1:B:40:LEU:HD11	1:B:67:MET:CE	0.56	2.31	14	1
1:B:43:ILE:HG23	1:B:64:ASP:OD1	0.56	2.00	16	1
1:A:35:ARG:NH1	1:A:75:VAL:O	0.56	2.39	19	3
1:B:72:MET:CE	1:B:102:ILE:HD11	0.56	2.31	18	1
1:B:45:LEU:C	1:B:45:LEU:HD12	0.56	2.21	2	1
1:A:28:LEU:N	1:A:28:LEU:HD22	0.56	2.16	4	6
1:A:10:LYS:CG	1:A:79:ILE:HA	0.56	2.30	10	5
1:B:75:VAL:HG13	1:B:79:ILE:CD1	0.56	2.31	8	1
1:B:10:LYS:HB3	1:B:79:ILE:CB	0.56	2.31	15	7
1:B:54:LEU:HD23	1:B:69:THR:CG2	0.56	2.18	8	1
1:B:30:ASP:O	1:B:35:ARG:HG3	0.56	2.00	9	2
1:A:8:LYS:HG3	1:A:19:PRO:O	0.56	1.99	19	13
1:B:79:ILE:O	1:B:80:LEU:C	0.56	2.44	3	6
1:A:98:ILE:O	1:A:102:ILE:CG1	0.56	2.54	17	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:LYS:HB3	1:B:84:VAL:HG13	0.56	1.78	6	4
1:B:10:LYS:CB	1:B:79:ILE:HG12	0.56	2.31	7	1
1:A:36:LEU:HD22	1:A:74:SER:CB	0.56	2.30	18	1
1:B:28:LEU:HD22	1:B:28:LEU:N	0.56	2.16	20	5
1:B:22:VAL:HG21	1:B:67:MET:SD	0.56	2.40	4	1
1:A:23:ASP:OD1	1:A:80:LEU:HD11	0.56	2.00	11	3
1:A:38:ILE:HD13	1:A:72:MET:HG3	0.56	1.76	20	1
1:B:40:LEU:HD22	1:B:65:PHE:HB2	0.56	1.78	1	1
1:A:28:LEU:HD22	1:A:28:LEU:N	0.56	2.16	10	4
1:B:8:LYS:O	1:B:9:ASN:C	0.56	2.43	17	18
1:B:40:LEU:HD21	1:B:58:ILE:HD11	0.56	1.77	3	1
1:A:96:ALA:O	1:A:100:PHE:N	0.56	2.38	20	10
1:B:38:ILE:HG23	1:B:69:THR:CG2	0.56	2.31	7	1
1:A:58:ILE:HG12	1:A:87:LEU:HD12	0.56	1.77	20	1
1:A:8:LYS:HA	1:A:20:TYR:CB	0.56	2.27	16	18
1:A:21:PHE:HA	1:A:39:PRO:HA	0.56	1.78	18	20
1:B:9:ASN:ND2	1:B:15:ALA:N	0.56	2.54	10	4
1:B:28:LEU:N	1:B:28:LEU:HD22	0.56	2.16	11	3
1:B:27:ASP:OD1	1:B:28:LEU:HD22	0.56	2.01	6	1
1:A:26:SER:O	1:A:30:ASP:CB	0.56	2.54	20	7
1:B:67:MET:HE1	1:B:93:GLU:HB3	0.56	1.78	18	1
1:A:101:LEU:HD23	1:A:102:ILE:HG13	0.56	1.77	20	1
1:B:21:PHE:HA	1:B:39:PRO:HA	0.55	1.78	7	18
1:A:5:THR:CB	1:A:7:TYR:CZ	0.55	2.89	13	19
1:A:8:LYS:O	1:A:81:SER:CB	0.55	2.54	3	6
1:B:6:LEU:HB2	1:B:87:LEU:HD22	0.55	1.76	2	4
1:B:75:VAL:O	1:B:75:VAL:HG23	0.55	2.00	5	5
1:A:75:VAL:HG13	1:A:79:ILE:CD1	0.55	2.32	13	1
1:A:3:GLN:O	1:A:4:PHE:HB2	0.55	2.00	12	5
1:A:20:TYR:HB2	1:A:40:LEU:CD1	0.55	2.31	2	2
1:B:30:ASP:HA	1:B:35:ARG:NH1	0.55	2.16	8	1
1:A:88:SER:O	1:A:91:ARG:CG	0.55	2.54	10	20
1:A:36:LEU:HD13	1:B:72:MET:HE2	0.55	1.77	3	1
1:A:58:ILE:CG2	1:A:59:HIS:N	0.55	2.69	5	3
1:A:54:LEU:HD11	1:A:101:LEU:HB2	0.55	1.78	8	4
1:A:10:LYS:HG3	1:A:79:ILE:HG12	0.55	1.77	11	3
1:A:2:SER:OG	1:A:80:LEU:HD21	0.55	2.01	11	1
1:A:9:ASN:C	1:A:10:LYS:HD2	0.55	2.21	18	2
1:B:58:ILE:CD1	1:B:58:ILE:C	0.55	2.71	1	1
1:A:92:ASN:O	1:A:95:ILE:N	0.55	2.40	20	18
1:A:9:ASN:ND2	1:A:21:PHE:CE1	0.55	2.75	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:35:ARG:HG3	1:B:80:LEU:HD23	0.55	1.79	4	1
1:A:21:PHE:CD2	1:A:81:SER:OG	0.55	2.59	14	2
1:A:10:LYS:CB	1:A:79:ILE:HG22	0.55	2.31	17	4
1:B:38:ILE:HD11	1:B:67:MET:HB3	0.55	1.78	18	1
1:B:98:ILE:O	1:B:102:ILE:CG1	0.55	2.54	17	4
1:B:76:PRO:CD	1:B:79:ILE:HD11	0.55	2.31	20	5
1:B:69:THR:OG1	1:B:101:LEU:CD2	0.55	2.55	12	1
1:B:60:ILE:HD11	1:B:65:PHE:CD2	0.55	2.36	20	2
1:A:40:LEU:HD21	1:A:67:MET:HE2	0.55	1.76	13	1
1:A:98:ILE:HG23	1:A:102:ILE:HD12	0.55	1.79	7	4
1:B:58:ILE:N	1:B:58:ILE:HD13	0.55	2.16	2	4
1:B:3:GLN:O	1:B:4:PHE:HB2	0.55	2.01	13	7
1:A:58:ILE:HG12	1:A:90:PHE:CD2	0.55	2.37	20	3
1:B:88:SER:O	1:B:91:ARG:CG	0.55	2.55	19	20
1:B:10:LYS:CG	1:B:79:ILE:CG1	0.55	2.84	12	7
1:A:25:GLN:CG	1:A:36:LEU:HB2	0.55	2.32	17	6
1:A:102:ILE:CG1	1:A:103:THR:HG23	0.55	2.31	11	2
1:A:29:LEU:CD1	1:B:54:LEU:HD22	0.55	2.31	5	1
1:B:9:ASN:O	1:B:9:ASN:OD1	0.55	2.24	7	1
1:A:38:ILE:CD1	1:A:94:ILE:HG23	0.55	2.32	14	4
1:B:40:LEU:HD11	1:B:67:MET:HE3	0.55	1.79	14	1
1:A:26:SER:HB3	1:A:29:LEU:HB2	0.55	1.79	14	13
1:A:17:THR:HG22	1:A:18:TYR:CE1	0.55	2.37	4	8
1:A:5:THR:HG23	1:A:86:GLU:HA	0.55	1.77	20	1
1:A:80:LEU:O	1:A:81:SER:C	0.54	2.45	16	8
1:B:9:ASN:H	1:B:20:TYR:HA	0.54	1.62	7	4
1:A:41:THR:OG1	1:A:46:LEU:HD12	0.54	2.02	4	1
1:B:37:VAL:HG11	1:B:75:VAL:CG2	0.54	2.32	4	1
1:A:6:LEU:HD23	1:A:84:VAL:HG23	0.54	1.78	5	1
1:B:22:VAL:CG2	1:B:40:LEU:HD21	0.54	2.32	6	1
1:B:103:THR:HG22	1:B:105:ILE:H	0.54	1.61	7	1
1:A:10:LYS:CD	1:A:11:ASP:H	0.54	2.15	18	2
1:B:25:GLN:HB2	1:B:36:LEU:HB3	0.54	1.79	1	6
1:B:22:VAL:O	1:B:37:VAL:HA	0.54	2.03	19	9
1:A:64:ASP:O	1:A:65:PHE:CD1	0.54	2.60	9	10
1:B:38:ILE:HD12	1:B:69:THR:CG2	0.54	2.32	18	2
1:A:54:LEU:HD23	1:A:70:GLN:NE2	0.54	2.17	12	1
1:A:8:LYS:O	1:A:9:ASN:C	0.54	2.45	4	13
1:B:96:ALA:O	1:B:100:PHE:N	0.54	2.40	14	16
1:B:40:LEU:HD23	1:B:67:MET:N	0.54	2.17	16	8
1:A:10:LYS:HG3	1:A:79:ILE:O	0.54	2.02	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:SER:O	1:A:30:ASP:CA	0.54	2.56	13	13
1:B:2:SER:O	1:B:30:ASP:HB2	0.54	2.02	4	5
1:A:24:VAL:HG11	1:A:38:ILE:HG12	0.54	1.79	18	1
1:B:43:ILE:HD12	1:B:57:THR:HG22	0.54	1.78	17	2
1:B:26:SER:O	1:B:30:ASP:CA	0.54	2.56	6	9
1:B:10:LYS:CG	1:B:79:ILE:O	0.54	2.55	6	2
1:A:36:LEU:HD21	1:A:72:MET:HE2	0.54	1.79	16	1
1:A:35:ARG:HH21	1:A:77:VAL:HG23	0.54	1.61	17	1
1:A:7:TYR:CE1	1:A:23:ASP:HB2	0.54	2.37	4	7
1:B:20:TYR:OH	1:B:65:PHE:CZ	0.54	2.61	8	10
1:A:72:MET:HE1	1:A:101:LEU:HD21	0.54	1.80	6	1
1:B:20:TYR:HB2	1:B:40:LEU:HD12	0.54	1.79	12	3
1:A:87:LEU:HD12	1:A:87:LEU:N	0.54	2.18	8	5
1:B:69:THR:HG22	1:B:101:LEU:CD1	0.54	2.31	6	2
1:B:36:LEU:HD21	1:B:72:MET:HG2	0.54	1.79	7	1
1:B:72:MET:CE	1:B:98:ILE:HD11	0.54	2.33	12	2
1:B:60:ILE:HD11	1:B:62:GLU:HB2	0.54	1.80	11	2
1:B:6:LEU:HD12	1:B:60:ILE:HD13	0.54	1.80	11	1
1:A:40:LEU:HD21	1:A:58:ILE:CG2	0.54	2.32	19	1
1:B:29:LEU:HA	1:B:32:LEU:HD23	0.54	1.79	1	1
1:A:102:ILE:HG21	1:B:102:ILE:HG21	0.54	1.79	8	5
1:B:40:LEU:HD22	1:B:58:ILE:HD12	0.54	1.80	5	2
1:A:98:ILE:HG23	1:A:102:ILE:CG1	0.54	2.33	6	2
1:B:10:LYS:HG2	1:B:79:ILE:HD11	0.54	1.79	7	1
1:A:58:ILE:CD1	1:A:59:HIS:N	0.54	2.67	10	2
1:B:101:LEU:O	1:B:101:LEU:HD22	0.54	2.03	13	1
1:B:58:ILE:CD1	1:B:60:ILE:N	0.54	2.71	1	1
1:B:58:ILE:HG22	1:B:90:PHE:CG	0.54	2.37	6	3
1:B:22:VAL:HG11	1:B:94:ILE:HD12	0.54	1.79	18	2
1:A:36:LEU:HD21	1:A:72:MET:CE	0.54	2.33	17	2
1:B:8:LYS:CA	1:B:19:PRO:O	0.53	2.56	1	1
1:B:15:ALA:HA	1:B:19:PRO:CA	0.53	2.33	17	17
1:A:15:ALA:HA	1:A:19:PRO:CA	0.53	2.33	8	18
1:B:7:TYR:CE1	1:B:23:ASP:HB2	0.53	2.38	8	10
1:B:37:VAL:CG2	1:B:73:THR:HG23	0.53	2.33	4	1
1:B:58:ILE:CG2	1:B:59:HIS:N	0.53	2.71	13	3
1:B:7:TYR:HB2	1:B:81:SER:OG	0.53	2.03	7	8
1:B:101:LEU:HD22	1:B:101:LEU:O	0.53	2.03	14	2
1:B:9:ASN:CB	1:B:14:SER:HB3	0.53	2.33	8	3
1:A:28:LEU:O	1:A:32:LEU:HD13	0.53	2.03	17	3
1:B:6:LEU:CG	1:B:87:LEU:HG	0.53	2.33	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:SER:HB2	1:B:35:ARG:CD	0.53	2.33	14	1
1:A:21:PHE:HD2	1:A:81:SER:HG	0.53	1.46	15	1
1:A:68:LEU:HD22	1:A:70:GLN:CG	0.53	2.33	5	1
1:A:24:VAL:HB	1:A:94:ILE:CG2	0.53	2.32	7	6
1:B:58:ILE:H	1:B:58:ILE:HD13	0.53	1.63	8	1
1:B:7:TYR:HB3	1:B:81:SER:CB	0.53	2.33	2	9
1:B:22:VAL:HG21	1:B:67:MET:CE	0.53	2.34	2	3
1:B:40:LEU:HD21	1:B:67:MET:HG3	0.53	1.79	3	1
1:A:7:TYR:CB	1:A:81:SER:OG	0.53	2.56	15	8
1:A:42:PRO:HG3	1:A:45:LEU:HD23	0.53	1.78	4	1
1:B:42:PRO:N	1:B:65:PHE:CD2	0.53	2.76	6	3
1:A:89:THR:HG23	1:A:90:PHE:HD1	0.53	1.61	7	1
1:B:17:THR:HG23	1:B:18:TYR:N	0.53	2.18	13	1
1:A:101:LEU:HD22	1:A:101:LEU:O	0.53	2.03	15	1
1:A:25:GLN:HB2	1:A:36:LEU:HB3	0.53	1.80	6	9
1:B:15:ALA:HA	1:B:19:PRO:N	0.53	2.19	17	12
1:A:72:MET:HE3	1:A:101:LEU:HD21	0.53	1.79	2	1
1:B:38:ILE:HD12	1:B:97:ALA:HB1	0.53	1.80	2	1
1:B:54:LEU:O	1:B:69:THR:HG21	0.53	2.03	8	1
1:B:35:ARG:CZ	1:B:80:LEU:HD13	0.53	2.32	17	1
1:A:8:LYS:HA	1:A:19:PRO:O	0.53	2.04	5	6
1:A:41:THR:O	1:A:65:PHE:HB3	0.53	2.04	13	8
1:B:24:VAL:O	1:B:25:GLN:HB2	0.53	2.03	15	8
1:B:68:LEU:HD23	1:B:71:GLN:CB	0.53	2.33	5	3
1:A:7:TYR:CB	1:A:81:SER:HB3	0.53	2.33	6	3
1:B:24:VAL:HA	1:B:35:ARG:NH1	0.53	2.19	10	1
1:A:38:ILE:HD12	1:A:94:ILE:HG23	0.53	1.80	11	3
1:B:58:ILE:HG12	1:B:87:LEU:HD12	0.53	1.81	13	1
1:A:8:LYS:CA	1:A:20:TYR:HB3	0.53	2.29	16	1
1:B:10:LYS:CA	1:B:82:GLU:H	0.53	2.17	5	7
1:A:58:ILE:CG2	1:A:90:PHE:CE2	0.53	2.91	17	2
1:B:4:PHE:HZ	1:B:95:ILE:HD11	0.53	1.64	11	1
1:A:56:PRO:HD2	1:A:67:MET:HB2	0.53	1.81	16	4
1:B:80:LEU:O	1:B:81:SER:C	0.53	2.46	16	8
1:B:2:SER:OG	1:B:31:ASN:HB2	0.53	2.04	4	2
1:A:10:LYS:HB2	1:A:79:ILE:HG12	0.53	1.79	5	1
1:A:29:LEU:HD13	1:B:70:GLN:HG2	0.53	1.81	10	1
1:A:35:ARG:CD	1:A:80:LEU:HD11	0.53	2.34	12	1
1:A:60:ILE:CD1	1:A:87:LEU:HD23	0.53	2.24	15	1
1:B:87:LEU:N	1:B:87:LEU:HD12	0.53	2.17	3	8
1:B:101:LEU:HG	1:B:102:ILE:N	0.53	2.19	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:VAL:O	1:A:25:GLN:HB2	0.53	2.03	4	10
1:A:45:LEU:HD12	1:A:45:LEU:C	0.53	2.23	4	1
1:A:2:SER:O	1:A:3:GLN:HB3	0.53	2.03	5	2
1:A:7:TYR:HB3	1:A:81:SER:HB3	0.53	1.80	8	1
1:B:9:ASN:HD21	1:B:12:LYS:HA	0.53	1.64	14	3
1:A:72:MET:HB3	1:B:36:LEU:HD21	0.53	1.81	17	1
1:A:2:SER:HB3	1:A:30:ASP:HB3	0.53	1.81	20	1
1:B:58:ILE:HB	1:B:90:PHE:CE2	0.53	2.38	1	2
1:A:23:ASP:HA	1:A:37:VAL:HG12	0.53	1.80	18	6
1:A:35:ARG:CG	1:A:37:VAL:HG13	0.53	2.33	1	1
1:A:7:TYR:CE1	1:A:23:ASP:CB	0.53	2.91	19	5
1:A:24:VAL:CG2	1:A:98:ILE:HD13	0.53	2.34	12	6
1:A:56:PRO:HD2	1:A:67:MET:CB	0.53	2.34	13	2
1:A:68:LEU:HD23	1:A:71:GLN:HB2	0.53	1.81	20	1
1:B:38:ILE:CG2	1:B:67:MET:HB3	0.52	2.34	11	5
1:A:98:ILE:HG22	1:A:99:ASP:N	0.52	2.19	20	7
1:B:9:ASN:OD1	1:B:12:LYS:HA	0.52	2.04	5	5
1:A:98:ILE:HG23	1:A:102:ILE:HG12	0.52	1.81	11	4
1:B:58:ILE:HD13	1:B:58:ILE:H	0.52	1.65	10	4
1:B:40:LEU:HD22	1:B:58:ILE:CD1	0.52	2.34	15	2
1:B:2:SER:OG	1:B:31:ASN:HB3	0.52	2.04	19	2
1:B:26:SER:O	1:B:30:ASP:N	0.52	2.42	13	8
1:B:39:PRO:O	1:B:68:LEU:CB	0.52	2.57	15	4
1:B:2:SER:HB3	1:B:30:ASP:OD2	0.52	2.04	6	1
1:B:24:VAL:HG21	1:B:38:ILE:HD12	0.52	1.82	15	1
1:B:20:TYR:HB2	1:B:40:LEU:CD1	0.52	2.34	2	2
1:A:87:LEU:N	1:A:87:LEU:HD12	0.52	2.20	7	6
1:A:35:ARG:CD	1:A:37:VAL:HG13	0.52	2.33	8	1
1:A:101:LEU:HD23	1:A:102:ILE:CG2	0.52	2.34	10	1
1:A:23:ASP:OD2	1:A:80:LEU:HD11	0.52	2.04	15	1
1:A:84:VAL:HG22	1:A:85:ASN:OD1	0.52	2.05	16	1
1:B:92:ASN:O	1:B:95:ILE:N	0.52	2.43	18	17
1:B:36:LEU:HD13	1:B:36:LEU:C	0.52	2.24	7	2
1:A:81:SER:O	1:A:83:PRO:HD3	0.52	2.04	12	3
1:A:7:TYR:HB2	1:A:81:SER:OG	0.52	2.05	15	9
1:B:17:THR:HG22	1:B:18:TYR:CE1	0.52	2.40	11	5
1:A:8:LYS:HB3	1:A:82:GLU:O	0.52	2.05	7	3
1:A:30:ASP:O	1:A:35:ARG:CG	0.52	2.58	20	4
1:A:7:TYR:C	1:A:81:SER:CB	0.52	2.78	4	5
1:A:21:PHE:CE2	1:A:81:SER:OG	0.52	2.60	6	1
1:B:101:LEU:CD1	1:B:102:ILE:CG1	0.52	2.88	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TYR:C	1:A:40:LEU:HD12	0.52	2.24	16	1
1:A:58:ILE:HD12	1:A:87:LEU:CD1	0.52	2.34	14	2
1:A:43:ILE:HG12	1:A:57:THR:HG22	0.52	1.82	7	2
1:A:10:LYS:HD2	1:A:79:ILE:HG13	0.52	1.80	10	1
1:B:64:ASP:O	1:B:65:PHE:HD1	0.52	1.88	15	1
1:A:54:LEU:HD21	1:A:100:PHE:CE2	0.52	2.40	6	1
1:B:9:ASN:ND2	1:B:12:LYS:HA	0.52	2.20	6	4
1:A:22:VAL:CG1	1:A:94:ILE:CG1	0.52	2.88	18	1
1:B:31:ASN:ND2	1:B:77:VAL:HG23	0.52	2.20	18	1
1:B:100:PHE:CB	1:B:105:ILE:HG22	0.52	2.34	19	1
1:B:10:LYS:HD2	1:B:79:ILE:CG1	0.52	2.35	2	6
1:B:8:LYS:N	1:B:81:SER:HB3	0.52	2.19	2	1
1:B:58:ILE:HD12	1:B:58:ILE:N	0.52	2.20	3	1
1:B:37:VAL:HG21	1:B:75:VAL:HG13	0.52	1.81	11	2
1:A:38:ILE:N	1:A:38:ILE:HD12	0.52	2.19	6	1
1:B:54:LEU:HD23	1:B:55:CYS:SG	0.52	2.43	12	1
1:B:38:ILE:HG23	1:B:69:THR:HB	0.52	1.81	12	1
1:B:43:ILE:HG23	1:B:48:LYS:CD	0.52	2.35	17	1
1:A:35:ARG:NE	1:A:80:LEU:HD23	0.52	2.19	20	1
1:A:15:ALA:HA	1:A:19:PRO:N	0.52	2.20	4	16
1:A:101:LEU:HG	1:A:102:ILE:N	0.52	2.20	9	8
1:A:38:ILE:CG2	1:A:67:MET:HB3	0.52	2.35	14	6
1:A:26:SER:HB2	1:A:29:LEU:HB2	0.52	1.82	6	1
1:A:67:MET:HE1	1:A:94:ILE:HD12	0.52	1.82	12	1
1:B:43:ILE:HB	1:B:66:ILE:HG13	0.52	1.80	17	1
1:A:35:ARG:NH2	1:A:80:LEU:HD13	0.52	2.20	1	1
1:B:6:LEU:HD21	1:B:40:LEU:HD13	0.52	1.82	1	2
1:B:38:ILE:HD11	1:B:94:ILE:HG23	0.52	1.81	3	1
1:B:28:LEU:CD1	1:B:28:LEU:N	0.52	2.73	19	4
1:A:8:LYS:HB2	1:A:84:VAL:CG1	0.52	2.35	8	4
1:A:58:ILE:HG23	1:A:60:ILE:HG23	0.52	1.82	5	2
1:B:6:LEU:HD13	1:B:87:LEU:CD2	0.52	2.34	6	2
1:B:58:ILE:CG2	1:B:90:PHE:CE2	0.52	2.90	7	3
1:A:2:SER:OG	1:A:31:ASN:HB2	0.52	2.05	9	1
1:A:58:ILE:N	1:A:58:ILE:HD12	0.52	2.19	9	1
1:A:75:VAL:HG11	1:A:79:ILE:HD13	0.52	1.81	11	1
1:B:8:LYS:HB3	1:B:82:GLU:O	0.52	2.04	13	1
1:A:36:LEU:HD22	1:B:72:MET:CE	0.52	2.35	14	1
1:A:41:THR:O	1:A:66:ILE:CD1	0.51	2.58	16	8
1:A:98:ILE:O	1:A:102:ILE:N	0.51	2.41	8	13
1:B:20:TYR:OH	1:B:65:PHE:CE2	0.51	2.60	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:7:TYR:CD2	1:B:80:LEU:CD1	0.51	2.93	7	5
1:B:99:ASP:O	1:B:103:THR:HB	0.51	2.04	13	9
1:A:36:LEU:HD21	1:B:72:MET:CE	0.51	2.35	6	1
1:A:105:ILE:HD12	1:A:105:ILE:OXT	0.51	2.05	8	1
1:B:33:ASN:O	1:B:77:VAL:HG12	0.51	2.05	20	1
1:A:54:LEU:HD21	1:A:69:THR:CG2	0.51	2.35	2	1
1:B:17:THR:HG22	1:B:18:TYR:CZ	0.51	2.40	2	3
1:B:79:ILE:CG1	1:B:79:ILE:O	0.51	2.58	9	4
1:B:24:VAL:HB	1:B:94:ILE:CG2	0.51	2.35	14	8
1:A:7:TYR:CB	1:A:81:SER:CB	0.51	2.88	13	6
1:A:58:ILE:HD13	1:A:90:PHE:CD1	0.51	2.40	17	1
1:B:26:SER:O	1:B:30:ASP:HB2	0.51	2.05	17	3
1:B:24:VAL:O	1:B:25:GLN:CB	0.51	2.59	10	7
1:B:10:LYS:NZ	1:B:79:ILE:HD11	0.51	2.20	5	1
1:B:25:GLN:HB2	1:B:36:LEU:CB	0.51	2.35	6	4
1:A:22:VAL:O	1:A:37:VAL:HA	0.51	2.05	17	3
1:B:8:LYS:O	1:B:81:SER:CB	0.51	2.59	13	1
1:B:9:ASN:CG	1:B:19:PRO:O	0.51	2.49	15	1
1:B:58:ILE:CD1	1:B:60:ILE:H	0.51	2.17	1	1
1:A:10:LYS:N	1:A:82:GLU:N	0.51	2.59	8	2
1:B:25:GLN:CG	1:B:36:LEU:HB2	0.51	2.35	6	3
1:B:2:SER:CB	1:B:31:ASN:HB3	0.51	2.36	13	4
1:A:7:TYR:CE2	1:A:23:ASP:OD2	0.51	2.64	9	5
1:A:25:GLN:CD	1:A:36:LEU:HB2	0.51	2.25	17	1
1:A:7:TYR:HB3	1:A:81:SER:CB	0.51	2.36	8	8
1:A:76:PRO:CD	1:A:79:ILE:HD11	0.51	2.35	15	3
1:A:7:TYR:CE2	1:A:80:LEU:CD2	0.51	2.94	17	1
1:B:24:VAL:HG22	1:B:98:ILE:CD1	0.51	2.36	1	5
1:A:72:MET:CE	1:A:102:ILE:HD11	0.51	2.35	12	4
1:B:58:ILE:HA	1:B:90:PHE:CE2	0.51	2.41	12	3
1:B:75:VAL:HG23	1:B:79:ILE:HG23	0.51	1.82	17	3
1:B:24:VAL:HG12	1:B:94:ILE:HG23	0.51	1.82	17	2
1:B:72:MET:HE3	1:B:101:LEU:HD21	0.51	1.83	19	1
1:B:99:ASP:HB3	1:B:105:ILE:HD11	0.51	1.82	1	1
1:A:9:ASN:H	1:A:20:TYR:HA	0.51	1.66	18	4
1:A:8:LYS:CA	1:A:19:PRO:O	0.51	2.59	5	6
1:A:20:TYR:OH	1:A:65:PHE:CD2	0.51	2.63	13	4
1:B:38:ILE:HD12	1:B:67:MET:SD	0.51	2.46	5	3
1:A:7:TYR:CZ	1:A:23:ASP:OD2	0.51	2.64	12	6
1:A:69:THR:HG22	1:A:101:LEU:CD2	0.51	2.24	4	1
1:A:28:LEU:CD1	1:A:28:LEU:N	0.51	2.74	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:LEU:HD13	1:B:87:LEU:CG	0.51	2.35	6	1
1:A:28:LEU:N	1:A:28:LEU:CD1	0.51	2.74	11	4
1:A:70:GLN:OE1	1:B:29:LEU:HD13	0.51	2.05	14	1
1:B:43:ILE:CG2	1:B:66:ILE:HG23	0.51	2.35	15	1
1:B:35:ARG:CD	1:B:37:VAL:HG13	0.51	2.34	17	1
1:B:5:THR:CB	1:B:7:TYR:CZ	0.51	2.94	20	16
1:A:67:MET:HE1	1:A:94:ILE:HG13	0.51	1.83	2	1
1:A:10:LYS:CD	1:A:79:ILE:CG1	0.51	2.89	12	6
1:A:58:ILE:CD1	1:A:58:ILE:C	0.51	2.74	10	1
1:B:29:LEU:O	1:B:34:THR:O	0.51	2.29	10	1
1:B:7:TYR:CZ	1:B:23:ASP:HB2	0.51	2.41	14	2
1:A:101:LEU:CD1	1:A:102:ILE:CG1	0.51	2.89	15	1
1:A:35:ARG:NH2	1:A:80:LEU:HA	0.51	2.19	18	1
1:A:35:ARG:CZ	1:A:37:VAL:HG11	0.51	2.36	1	1
1:B:8:LYS:HG3	1:B:19:PRO:O	0.51	2.05	12	12
1:B:54:LEU:HD23	1:B:101:LEU:HD13	0.51	1.83	4	1
1:B:101:LEU:HD22	1:B:102:ILE:N	0.51	2.21	6	3
1:B:54:LEU:HD23	1:B:55:CYS:N	0.51	2.21	12	1
1:A:7:TYR:OH	1:A:35:ARG:NH1	0.51	2.44	13	1
1:B:45:LEU:HD12	1:B:45:LEU:C	0.51	2.26	13	1
1:A:98:ILE:HA	1:A:102:ILE:HG13	0.50	1.83	14	11
1:B:7:TYR:CD1	1:B:7:TYR:N	0.50	2.79	2	6
1:B:38:ILE:HD12	1:B:97:ALA:CB	0.50	2.36	2	1
1:B:10:LYS:CD	1:B:79:ILE:CG1	0.50	2.89	12	6
1:B:25:GLN:HG3	1:B:36:LEU:CB	0.50	2.36	9	5
1:B:34:THR:HG22	1:B:76:PRO:HA	0.50	1.82	4	3
1:A:34:THR:HA	1:A:77:VAL:HG13	0.50	1.83	9	1
1:A:62:GLU:OE2	1:A:84:VAL:HG22	0.50	2.06	9	1
1:A:43:ILE:HD11	1:A:57:THR:HG23	0.50	1.80	19	1
1:A:24:VAL:HG22	1:A:98:ILE:CD1	0.50	2.36	4	4
1:A:8:LYS:N	1:A:81:SER:HB3	0.50	2.22	12	6
1:A:40:LEU:HD23	1:A:67:MET:HG2	0.50	1.84	2	1
1:B:10:LYS:HG3	1:B:79:ILE:HG12	0.50	1.83	2	5
1:B:38:ILE:CD1	1:B:69:THR:HB	0.50	2.36	2	1
1:B:38:ILE:HD11	1:B:94:ILE:O	0.50	2.06	5	1
1:A:97:ALA:O	1:A:101:LEU:HB2	0.50	2.06	19	2
1:A:101:LEU:CD2	1:A:101:LEU:O	0.50	2.59	15	1
1:A:58:ILE:C	1:A:58:ILE:CD1	0.50	2.69	19	1
1:B:7:TYR:CB	1:B:81:SER:OG	0.50	2.60	17	11
1:B:35:ARG:CZ	1:B:35:ARG:HA	0.50	2.37	2	1
1:A:8:LYS:O	1:A:9:ASN:O	0.50	2.30	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:TYR:CZ	1:A:23:ASP:CG	0.50	2.85	8	4
1:B:35:ARG:HG2	1:B:36:LEU:N	0.50	2.22	3	1
1:B:41:THR:O	1:B:65:PHE:HB3	0.50	2.07	5	6
1:B:6:LEU:H	1:B:86:GLU:HA	0.50	1.66	19	3
1:A:54:LEU:HD21	1:A:101:LEU:HB2	0.50	1.84	13	1
1:A:8:LYS:C	1:A:8:LYS:HD2	0.50	2.27	5	1
1:A:38:ILE:CD1	1:A:67:MET:CB	0.50	2.90	7	1
1:B:98:ILE:HA	1:B:101:LEU:HD13	0.50	1.84	13	2
1:A:35:ARG:HG3	1:A:37:VAL:HG13	0.50	1.83	1	1
1:B:3:GLN:O	1:B:23:ASP:O	0.50	2.29	3	2
1:B:38:ILE:HD13	1:B:67:MET:CB	0.50	2.37	2	1
1:B:28:LEU:N	1:B:28:LEU:CD1	0.50	2.74	9	2
1:B:10:LYS:HG2	1:B:79:ILE:CA	0.50	2.37	5	1
1:B:41:THR:O	1:B:66:ILE:N	0.50	2.44	9	5
1:A:75:VAL:HG23	1:A:79:ILE:HG23	0.50	1.83	8	2
1:A:6:LEU:HD13	1:A:6:LEU:O	0.50	2.07	10	1
1:A:60:ILE:HD11	1:A:65:PHE:CE2	0.50	2.42	12	1
1:A:6:LEU:HD13	1:A:87:LEU:HD21	0.50	1.84	17	1
1:A:2:SER:HB2	1:A:31:ASN:HB3	0.50	1.84	18	1
1:A:5:THR:O	1:A:7:TYR:CD1	0.50	2.65	5	17
1:B:15:ALA:HA	1:B:18:TYR:C	0.50	2.27	9	19
1:B:26:SER:HB3	1:B:29:LEU:HB2	0.50	1.83	5	12
1:A:75:VAL:HG23	1:A:75:VAL:O	0.50	2.07	4	2
1:A:6:LEU:CD2	1:A:20:TYR:CD2	0.50	2.95	16	4
1:A:35:ARG:NH2	1:A:75:VAL:HG21	0.49	2.21	1	1
1:A:6:LEU:HD13	1:A:87:LEU:HD13	0.49	1.82	1	1
1:B:40:LEU:CD2	1:B:67:MET:HG2	0.49	2.36	2	3
1:A:24:VAL:HG11	1:A:94:ILE:CG2	0.49	2.37	11	4
1:A:20:TYR:OH	1:A:65:PHE:CD1	0.49	2.65	7	7
1:A:35:ARG:HD2	1:A:37:VAL:HG13	0.49	1.84	8	1
1:B:42:PRO:HG2	1:B:45:LEU:HD12	0.49	1.83	19	3
1:A:105:ILE:OXT	1:A:105:ILE:HG22	0.49	2.07	13	1
1:B:29:LEU:O	1:B:35:ARG:NH2	0.49	2.46	18	2
1:B:7:TYR:CZ	1:B:23:ASP:OD2	0.49	2.65	19	10
1:B:7:TYR:CB	1:B:81:SER:CB	0.49	2.89	11	9
1:B:2:SER:HB3	1:B:30:ASP:HB2	0.49	1.83	4	2
1:A:30:ASP:OD2	1:A:35:ARG:CZ	0.49	2.60	5	1
1:B:37:VAL:CG2	1:B:75:VAL:HG13	0.49	2.37	5	2
1:B:38:ILE:HG23	1:B:69:THR:CB	0.49	2.36	7	1
1:B:8:LYS:O	1:B:8:LYS:HD2	0.49	2.08	11	1
1:A:35:ARG:HD2	1:A:75:VAL:O	0.49	2.07	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LEU:HD21	1:A:69:THR:HB	0.49	1.83	5	1
1:A:2:SER:O	1:A:3:GLN:CG	0.49	2.60	20	2
1:A:43:ILE:HG23	1:A:48:LYS:HG2	0.49	1.83	6	1
1:A:71:GLN:O	1:A:72:MET:O	0.49	2.30	11	5
1:A:38:ILE:HD13	1:A:67:MET:CB	0.49	2.36	7	1
1:B:3:GLN:HB2	1:B:35:ARG:NH1	0.49	2.23	11	1
1:B:60:ILE:HD11	1:B:65:PHE:HD2	0.49	1.67	12	1
1:B:9:ASN:ND2	1:B:9:ASN:O	0.49	2.42	12	1
1:A:99:ASP:O	1:A:105:ILE:CD1	0.49	2.60	14	1
1:A:30:ASP:HA	1:A:35:ARG:CD	0.49	2.37	15	2
1:A:22:VAL:CG2	1:A:40:LEU:HD11	0.49	2.37	4	1
1:A:22:VAL:HG11	1:A:94:ILE:HD12	0.49	1.83	13	2
1:A:72:MET:CE	1:B:36:LEU:HD21	0.49	2.37	5	1
1:A:43:ILE:CG2	1:A:48:LYS:CD	0.49	2.90	6	1
1:A:8:LYS:CD	1:A:20:TYR:CD2	0.49	2.95	15	2
1:B:54:LEU:HD11	1:B:101:LEU:HD13	0.49	1.84	12	1
1:B:101:LEU:O	1:B:101:LEU:CD2	0.49	2.60	14	1
1:A:10:LYS:HG2	1:A:79:ILE:HB	0.49	1.85	15	2
1:B:24:VAL:HG21	1:B:38:ILE:HD11	0.49	1.82	15	1
1:B:35:ARG:CZ	1:B:35:ARG:HB3	0.49	2.38	17	1
1:B:8:LYS:N	1:B:81:SER:HB2	0.49	2.22	20	6
1:A:58:ILE:HD13	1:A:58:ILE:H	0.49	1.67	6	2
1:A:38:ILE:HG23	1:A:38:ILE:O	0.49	2.08	7	1
1:A:24:VAL:N	1:A:35:ARG:NH1	0.49	2.61	10	1
1:A:60:ILE:HG22	1:A:61:ASP:N	0.49	2.23	15	1
1:A:3:GLN:O	1:A:4:PHE:CG	0.49	2.66	16	1
1:B:98:ILE:O	1:B:102:ILE:N	0.49	2.41	5	7
1:B:33:ASN:C	1:B:34:THR:HG22	0.49	2.28	13	5
1:B:41:THR:O	1:B:66:ILE:CD1	0.49	2.61	9	11
1:B:10:LYS:HE2	1:B:79:ILE:HG12	0.49	1.82	5	1
1:B:58:ILE:HD12	1:B:87:LEU:CD1	0.49	2.36	7	1
1:A:94:ILE:HD13	1:A:94:ILE:N	0.49	2.23	13	1
1:A:35:ARG:HD3	1:A:36:LEU:H	0.49	1.68	3	1
1:B:23:ASP:CA	1:B:35:ARG:HD2	0.49	2.36	3	1
1:B:9:ASN:N	1:B:81:SER:CB	0.49	2.76	5	3
1:A:38:ILE:HD11	1:A:69:THR:OG1	0.49	2.07	7	1
1:B:20:TYR:CD1	1:B:40:LEU:HD12	0.49	2.42	15	1
1:A:38:ILE:HG23	1:A:69:THR:CA	0.49	2.38	18	2
1:A:10:LYS:HG2	1:A:79:ILE:HG13	0.49	1.84	18	1
1:A:6:LEU:HB2	1:A:87:LEU:HD13	0.49	1.84	4	1
1:B:54:LEU:HD11	1:B:101:LEU:CA	0.49	2.38	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:7:TYR:CB	1:B:81:SER:HB3	0.49	2.37	16	5
1:A:58:ILE:HD11	1:A:67:MET:SD	0.49	2.48	17	1
1:A:35:ARG:CD	1:A:35:ARG:O	0.49	2.61	18	1
1:B:5:THR:O	1:B:7:TYR:CD1	0.49	2.66	10	16
1:B:30:ASP:O	1:B:35:ARG:CG	0.49	2.60	9	4
1:B:10:LYS:HA	1:B:82:GLU:CB	0.49	2.38	2	1
1:B:87:LEU:HD12	1:B:87:LEU:N	0.49	2.23	6	4
1:A:58:ILE:HG23	1:A:67:MET:HE1	0.49	1.83	6	1
1:A:98:ILE:HA	1:A:101:LEU:HD13	0.49	1.83	15	1
1:B:99:ASP:HB3	1:B:105:ILE:HG21	0.49	1.84	19	1
1:A:58:ILE:HG23	1:A:90:PHE:CZ	0.49	2.42	3	4
1:A:8:LYS:HB2	1:A:84:VAL:HB	0.49	1.82	3	3
1:B:58:ILE:HG23	1:B:90:PHE:CG	0.49	2.43	15	2
1:B:101:LEU:CD2	1:B:101:LEU:O	0.49	2.61	13	2
1:B:71:GLN:O	1:B:72:MET:O	0.49	2.30	7	4
1:A:5:THR:HG23	1:A:86:GLU:CG	0.49	2.37	8	1
1:B:17:THR:CG2	1:B:18:TYR:N	0.49	2.76	13	1
1:A:40:LEU:HD23	1:A:67:MET:N	0.49	2.23	18	5
1:B:38:ILE:CG1	1:B:69:THR:HG23	0.49	2.38	18	1
1:B:10:LYS:N	1:B:82:GLU:N	0.48	2.60	1	1
1:B:9:ASN:C	1:B:11:ASP:N	0.48	2.66	4	9
1:A:15:ALA:HA	1:A:18:TYR:C	0.48	2.28	16	19
1:A:98:ILE:CA	1:A:101:LEU:HD23	0.48	2.38	3	4
1:B:99:ASP:O	1:B:103:THR:OG1	0.48	2.30	17	3
1:A:26:SER:HB2	1:A:35:ARG:CZ	0.48	2.38	3	2
1:A:9:ASN:C	1:A:11:ASP:N	0.48	2.65	12	6
1:B:54:LEU:HD21	1:B:101:LEU:HB2	0.48	1.85	5	3
1:A:25:GLN:HG3	1:A:36:LEU:CB	0.48	2.37	14	5
1:B:8:LYS:HG3	1:B:9:ASN:OD1	0.48	2.08	7	1
1:B:41:THR:OG1	1:B:46:LEU:HD22	0.48	2.08	18	2
1:B:58:ILE:HD13	1:B:90:PHE:CG	0.48	2.43	18	2
1:A:72:MET:O	1:A:73:THR:HG23	0.48	2.08	16	1
1:A:66:ILE:HD12	1:A:66:ILE:N	0.48	2.23	17	1
1:B:6:LEU:HD21	1:B:60:ILE:CD1	0.48	2.33	19	1
1:B:98:ILE:CA	1:B:101:LEU:HD23	0.48	2.38	2	2
1:B:20:TYR:O	1:B:21:PHE:CD1	0.48	2.66	7	7
1:A:7:TYR:N	1:A:7:TYR:CD1	0.48	2.81	15	6
1:B:21:PHE:HA	1:B:38:ILE:O	0.48	2.08	4	1
1:B:8:LYS:CB	1:B:84:VAL:HB	0.48	2.38	7	1
1:B:98:ILE:CG2	1:B:102:ILE:HD11	0.48	2.39	10	2
1:A:75:VAL:HG22	1:A:79:ILE:CD1	0.48	2.38	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LYS:CG	1:A:19:PRO:O	0.48	2.61	1	8
1:B:42:PRO:HG3	1:B:45:LEU:HD12	0.48	1.83	6	8
1:A:58:ILE:HG23	1:A:90:PHE:CG	0.48	2.43	9	3
1:B:21:PHE:HD2	1:B:81:SER:HG	0.48	1.51	13	2
1:A:58:ILE:HG23	1:A:59:HIS:N	0.48	2.23	5	3
1:A:23:ASP:HB3	1:A:35:ARG:HD3	0.48	1.85	7	1
1:A:43:ILE:HD11	1:A:66:ILE:HG23	0.48	1.82	8	1
1:B:30:ASP:HA	1:B:35:ARG:HD2	0.48	1.86	14	1
1:A:38:ILE:CG2	1:A:69:THR:HB	0.48	2.38	3	2
1:B:36:LEU:HD12	1:B:73:THR:O	0.48	2.08	3	1
1:B:58:ILE:CG1	1:B:90:PHE:CD2	0.48	2.96	4	3
1:B:2:SER:HB2	1:B:31:ASN:HB2	0.48	1.84	5	1
1:B:26:SER:O	1:B:35:ARG:NH1	0.48	2.47	15	1
1:A:42:PRO:N	1:A:65:PHE:CD2	0.48	2.82	16	1
1:B:26:SER:O	1:B:30:ASP:HB3	0.48	2.07	4	3
1:B:2:SER:CB	1:B:31:ASN:CB	0.48	2.91	6	4
1:B:66:ILE:N	1:B:66:ILE:HD12	0.48	2.23	7	5
1:A:35:ARG:CZ	1:A:35:ARG:HB3	0.48	2.39	8	1
1:A:38:ILE:O	1:A:38:ILE:HG12	0.48	2.09	12	1
1:B:57:THR:HG23	1:B:58:ILE:N	0.48	2.23	12	2
1:B:75:VAL:HG13	1:B:80:LEU:HD22	0.48	1.85	12	1
1:A:23:ASP:HA	1:A:35:ARG:HG3	0.48	1.85	16	1
1:B:26:SER:O	1:B:30:ASP:CB	0.48	2.62	16	1
1:B:22:VAL:HG12	1:B:94:ILE:HG21	0.48	1.84	18	1
1:B:23:ASP:OD2	1:B:35:ARG:NE	0.48	2.47	19	1
1:A:10:LYS:CD	1:A:10:LYS:C	0.48	2.82	5	2
1:A:99:ASP:OD1	1:A:105:ILE:HD11	0.48	2.07	5	1
1:B:60:ILE:HD11	1:B:87:LEU:HD23	0.48	1.84	15	1
1:A:6:LEU:HG	1:A:87:LEU:HG	0.48	1.86	16	1
1:A:66:ILE:N	1:A:66:ILE:HD12	0.48	2.23	3	5
1:B:79:ILE:O	1:B:80:LEU:O	0.48	2.32	6	1
1:A:102:ILE:C	1:A:102:ILE:HD12	0.48	2.29	16	2
1:B:21:PHE:CD2	1:B:75:VAL:HG11	0.48	2.44	11	2
1:A:23:ASP:CA	1:A:35:ARG:HD2	0.48	2.39	11	1
1:A:10:LYS:HB2	1:A:79:ILE:CG1	0.48	2.39	1	1
1:B:7:TYR:HB3	1:B:81:SER:HB2	0.48	1.86	2	4
1:A:10:LYS:HB3	1:A:79:ILE:CB	0.48	2.39	2	6
1:A:58:ILE:HD13	1:A:90:PHE:CE2	0.48	2.44	3	1
1:A:67:MET:HE3	1:A:94:ILE:CD1	0.48	2.39	7	1
1:B:8:LYS:HB3	1:B:84:VAL:HB	0.48	1.86	12	4
1:A:58:ILE:CD1	1:A:60:ILE:H	0.48	2.21	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:57:THR:HA	1:B:66:ILE:CG2	0.48	2.39	11	1
1:B:8:LYS:CD	1:B:20:TYR:CD2	0.48	2.96	13	1
1:A:31:ASN:ND2	1:A:80:LEU:HD21	0.48	2.24	3	1
1:B:23:ASP:CB	1:B:35:ARG:HD3	0.48	2.39	3	1
1:A:101:LEU:CD1	1:A:102:ILE:HG23	0.48	2.39	6	2
1:B:40:LEU:HG	1:B:67:MET:HG2	0.48	1.85	7	3
1:B:2:SER:O	1:B:3:GLN:HB2	0.48	2.08	17	2
1:B:102:ILE:C	1:B:102:ILE:HD12	0.48	2.29	10	1
1:B:24:VAL:HG11	1:B:38:ILE:HD12	0.48	1.85	12	1
1:B:24:VAL:HG22	1:B:36:LEU:O	0.48	2.09	20	2
1:B:7:TYR:C	1:B:81:SER:CB	0.47	2.82	2	6
1:B:102:ILE:CG1	1:B:103:THR:HG23	0.47	2.38	15	3
1:B:19:PRO:HG2	1:B:41:THR:HA	0.47	1.85	6	5
1:A:38:ILE:HD12	1:A:67:MET:SD	0.47	2.49	3	1
1:B:60:ILE:HD12	1:B:85:ASN:ND2	0.47	2.24	11	1
1:A:69:THR:HB	1:A:101:LEU:HD22	0.47	1.86	12	3
1:A:58:ILE:HG21	1:A:87:LEU:CD1	0.47	2.28	14	1
1:A:39:PRO:O	1:A:68:LEU:CB	0.47	2.61	17	9
1:B:43:ILE:HD11	1:B:57:THR:HG22	0.47	1.84	3	1
1:A:15:ALA:CB	1:A:19:PRO:HB3	0.47	2.39	8	7
1:A:94:ILE:N	1:A:94:ILE:HD13	0.47	2.24	4	1
1:B:7:TYR:CE1	1:B:23:ASP:CB	0.47	2.98	4	1
1:B:35:ARG:NH1	1:B:80:LEU:HD23	0.47	2.24	6	1
1:A:38:ILE:HG21	1:A:67:MET:HB3	0.47	1.85	19	2
1:B:60:ILE:HG22	1:B:61:ASP:N	0.47	2.25	15	1
1:A:6:LEU:HD22	1:A:87:LEU:HG	0.47	1.86	17	1
1:A:2:SER:O	1:A:30:ASP:CB	0.47	2.62	3	2
1:A:9:ASN:CG	1:A:21:PHE:CZ	0.47	2.87	5	1
1:B:58:ILE:CA	1:B:90:PHE:CZ	0.47	2.97	6	1
1:A:98:ILE:O	1:A:102:ILE:HG13	0.47	2.10	16	3
1:A:25:GLN:CB	1:A:36:LEU:HB3	0.47	2.40	11	2
1:B:25:GLN:OE1	1:B:36:LEU:HD22	0.47	2.09	11	1
1:A:46:LEU:HD22	1:A:66:ILE:HD13	0.47	1.86	18	1
1:B:67:MET:HE1	1:B:93:GLU:C	0.47	2.29	18	1
1:A:38:ILE:HG23	1:A:69:THR:HA	0.47	1.85	16	6
1:B:2:SER:CB	1:B:31:ASN:HB2	0.47	2.40	5	4
1:B:29:LEU:HA	1:B:32:LEU:HD13	0.47	1.84	9	2
1:A:44:GLU:HA	1:A:48:LYS:HG2	0.47	1.86	8	2
1:A:35:ARG:HD3	1:A:37:VAL:HG13	0.47	1.86	18	1
1:B:99:ASP:O	1:B:104:GLY:N	0.47	2.47	10	7
1:B:35:ARG:HG3	1:B:36:LEU:N	0.47	2.24	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HD12	1:A:87:LEU:HD12	0.47	1.86	4	1
1:B:82:GLU:O	1:B:84:VAL:N	0.47	2.47	7	3
1:A:2:SER:CB	1:A:31:ASN:HB2	0.47	2.39	9	3
1:A:67:MET:HE1	1:A:93:GLU:HB3	0.47	1.84	9	1
1:A:103:THR:HG22	1:B:103:THR:CG2	0.47	2.40	10	1
1:B:101:LEU:CD1	1:B:102:ILE:HG23	0.47	2.39	10	2
1:B:99:ASP:CB	1:B:105:ILE:HD12	0.47	2.39	10	1
1:B:24:VAL:HG13	1:B:98:ILE:HD11	0.47	1.85	11	1
1:B:41:THR:HG21	1:B:68:LEU:HD22	0.47	1.85	12	1
1:B:58:ILE:CG2	1:B:90:PHE:CG	0.47	2.98	15	1
1:A:72:MET:CB	1:B:36:LEU:HD21	0.47	2.39	17	1
1:B:41:THR:CG2	1:B:68:LEU:HD13	0.47	2.38	19	1
1:B:10:LYS:HG2	1:B:79:ILE:CG1	0.47	2.39	7	2
1:A:41:THR:HG21	1:A:68:LEU:HD22	0.47	1.87	18	2
1:B:35:ARG:CD	1:B:80:LEU:CD1	0.47	2.92	1	1
1:A:33:ASN:C	1:A:34:THR:HG22	0.47	2.30	5	9
1:B:33:ASN:C	1:B:34:THR:CG2	0.47	2.83	11	9
1:A:88:SER:O	1:A:91:ARG:HG2	0.47	2.10	14	13
1:B:94:ILE:N	1:B:94:ILE:HD12	0.47	2.25	14	3
1:B:26:SER:HB2	1:B:35:ARG:CZ	0.47	2.39	18	3
1:A:22:VAL:CG1	1:A:94:ILE:CG2	0.47	2.93	3	3
1:B:94:ILE:HD13	1:B:94:ILE:N	0.47	2.25	3	1
1:B:20:TYR:C	1:B:21:PHE:CD1	0.47	2.88	7	6
1:A:67:MET:HE3	1:A:94:ILE:HD12	0.47	1.85	4	1
1:B:58:ILE:HG13	1:B:90:PHE:CE1	0.47	2.44	13	3
1:B:22:VAL:CG1	1:B:94:ILE:CG1	0.47	2.87	6	3
1:A:2:SER:HB2	1:A:31:ASN:HB2	0.47	1.85	7	2
1:A:29:LEU:HD22	1:B:70:GLN:HE21	0.47	1.69	9	1
1:A:59:HIS:CE1	1:A:90:PHE:CZ	0.47	3.03	10	1
1:B:7:TYR:N	1:B:7:TYR:CD1	0.47	2.82	12	3
1:B:10:LYS:O	1:B:82:GLU:HB2	0.47	2.10	16	3
1:A:70:GLN:HG2	1:B:29:LEU:HD13	0.47	1.87	12	1
1:A:54:LEU:O	1:A:56:PRO:HD3	0.47	2.10	13	1
1:A:98:ILE:HG12	1:A:102:ILE:HD12	0.47	1.86	13	1
1:B:97:ALA:O	1:B:101:LEU:N	0.47	2.43	13	2
1:A:19:PRO:HG2	1:A:20:TYR:CE1	0.47	2.45	14	2
1:A:35:ARG:NE	1:A:36:LEU:H	0.47	2.06	15	1
1:B:54:LEU:HD21	1:B:101:LEU:HD13	0.47	1.86	18	1
1:B:98:ILE:O	1:B:102:ILE:HB	0.47	2.10	1	7
1:B:98:ILE:HG23	1:B:102:ILE:HD12	0.47	1.87	3	3
1:A:8:LYS:N	1:A:81:SER:OG	0.47	2.48	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD21	1:A:72:MET:SD	0.47	2.50	7	1
1:A:58:ILE:HG22	1:A:90:PHE:CD2	0.47	2.45	11	1
1:B:43:ILE:HG12	1:B:48:LYS:CD	0.47	2.40	14	5
1:B:21:PHE:N	1:B:21:PHE:CD1	0.47	2.83	12	1
1:B:80:LEU:HD12	1:B:80:LEU:O	0.47	2.10	12	1
1:A:24:VAL:HG11	1:A:38:ILE:HD12	0.47	1.85	14	1
1:B:24:VAL:HG11	1:B:94:ILE:HG23	0.47	1.84	15	1
1:B:8:LYS:HB2	1:B:84:VAL:CG1	0.47	2.40	1	7
1:B:88:SER:O	1:B:91:ARG:HG2	0.47	2.10	11	15
1:A:24:VAL:N	1:A:35:ARG:HD2	0.47	2.25	5	1
1:A:79:ILE:O	1:A:80:LEU:O	0.47	2.32	6	1
1:A:36:LEU:HD11	1:A:72:MET:SD	0.47	2.50	8	1
1:B:40:LEU:HD23	1:B:67:MET:SD	0.47	2.50	9	1
1:B:101:LEU:HG	1:B:102:ILE:HG23	0.47	1.85	10	2
1:A:72:MET:HE3	1:A:102:ILE:HD11	0.47	1.85	12	2
1:B:94:ILE:N	1:B:94:ILE:CD1	0.47	2.77	20	4
1:A:60:ILE:HD11	1:A:65:PHE:CD2	0.47	2.45	14	1
1:A:40:LEU:HD21	1:A:58:ILE:HG23	0.47	1.85	19	1
1:A:21:PHE:CG	1:A:75:VAL:HG11	0.47	2.44	5	1
1:A:58:ILE:HG22	1:A:90:PHE:CD1	0.47	2.44	15	3
1:B:43:ILE:HD12	1:B:64:ASP:HB2	0.46	1.87	1	1
1:B:35:ARG:CD	1:B:80:LEU:HD11	0.46	2.40	1	1
1:A:33:ASN:C	1:A:34:THR:CG2	0.46	2.84	12	10
1:B:2:SER:HB2	1:B:31:ASN:HB3	0.46	1.86	13	3
1:A:19:PRO:CG	1:A:42:PRO:CD	0.46	2.92	2	2
1:A:7:TYR:CB	1:A:81:SER:HB2	0.46	2.40	2	5
1:B:23:ASP:HA	1:B:35:ARG:HD2	0.46	1.86	3	1
1:A:10:LYS:CD	1:A:79:ILE:HG13	0.46	2.41	4	3
1:A:17:THR:HG22	1:A:18:TYR:CZ	0.46	2.45	16	3
1:B:36:LEU:HD11	1:B:72:MET:CE	0.46	2.32	14	1
1:B:59:HIS:N	1:B:90:PHE:CZ	0.46	2.84	15	1
1:A:20:TYR:CG	1:A:40:LEU:HD13	0.46	2.44	16	1
1:B:2:SER:O	1:B:3:GLN:HB3	0.46	2.10	20	1
1:A:41:THR:O	1:A:66:ILE:N	0.46	2.48	18	6
1:B:43:ILE:HD11	1:B:66:ILE:HG23	0.46	1.86	3	1
1:A:26:SER:O	1:A:30:ASP:HB2	0.46	2.10	20	3
1:B:37:VAL:HG23	1:B:73:THR:HG23	0.46	1.87	4	1
1:A:28:LEU:O	1:A:32:LEU:HD21	0.46	2.11	5	1
1:B:4:PHE:CE2	1:B:91:ARG:HB2	0.46	2.46	11	6
1:A:67:MET:SD	1:A:94:ILE:HD12	0.46	2.50	20	2
1:A:9:ASN:ND2	1:A:21:PHE:CZ	0.46	2.84	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:LEU:HD22	1:B:84:VAL:CG1	0.46	2.39	8	3
1:B:40:LEU:HD21	1:B:67:MET:HE3	0.46	1.85	8	2
1:B:3:GLN:CB	1:B:35:ARG:NH2	0.46	2.78	15	1
1:B:58:ILE:HD12	1:B:59:HIS:CA	0.46	2.39	1	1
1:A:40:LEU:HA	1:A:67:MET:HA	0.46	1.87	16	2
1:B:87:LEU:CG	1:B:87:LEU:O	0.46	2.63	5	3
1:A:10:LYS:HD2	1:A:79:ILE:HG12	0.46	1.85	12	5
1:A:42:PRO:HG2	1:A:45:LEU:HD12	0.46	1.86	8	3
1:A:35:ARG:HG3	1:A:80:LEU:HD11	0.46	1.87	12	1
1:A:57:THR:HG22	1:A:58:ILE:N	0.46	2.24	19	2
1:A:6:LEU:HD13	1:A:87:LEU:CD2	0.46	2.41	17	1
1:B:10:LYS:CA	1:B:82:GLU:N	0.46	2.78	9	4
1:B:7:TYR:CB	1:B:81:SER:HB2	0.46	2.40	11	4
1:B:23:ASP:HB3	1:B:35:ARG:CD	0.46	2.40	8	2
1:B:57:THR:HG22	1:B:58:ILE:N	0.46	2.25	8	3
1:B:10:LYS:CD	1:B:79:ILE:HG12	0.46	2.41	1	1
1:B:69:THR:HB	1:B:101:LEU:HD22	0.46	1.88	4	1
1:A:8:LYS:C	1:A:81:SER:HB3	0.46	2.30	12	3
1:A:40:LEU:HD21	1:A:67:MET:HE1	0.46	1.87	6	1
1:A:44:GLU:CG	1:A:48:LYS:HG3	0.46	2.40	6	1
1:B:10:LYS:HG2	1:B:79:ILE:HB	0.46	1.87	6	1
1:B:4:PHE:CE1	1:B:95:ILE:HD11	0.46	2.45	14	1
1:B:90:PHE:O	1:B:94:ILE:HD13	0.46	2.11	16	1
1:B:35:ARG:NH1	1:B:80:LEU:HD13	0.46	2.26	17	1
1:A:10:LYS:HB3	1:A:79:ILE:HG22	0.46	1.88	7	5
1:A:43:ILE:HD12	1:A:57:THR:HG1	0.46	1.69	6	1
1:B:27:ASP:CG	1:B:28:LEU:HD22	0.46	2.31	6	1
1:A:95:ILE:O	1:A:99:ASP:N	0.46	2.46	16	3
1:B:101:LEU:CD2	1:B:102:ILE:HG12	0.46	2.41	13	3
1:B:6:LEU:CD2	1:B:20:TYR:CD2	0.46	2.99	17	4
1:B:102:ILE:HD12	1:B:102:ILE:C	0.46	2.31	11	1
1:A:30:ASP:O	1:A:35:ARG:CD	0.46	2.64	13	2
1:A:6:LEU:N	1:A:87:LEU:HD22	0.46	2.26	20	2
1:A:7:TYR:CD2	1:A:80:LEU:HD22	0.46	2.46	16	1
1:A:2:SER:CB	1:A:31:ASN:HB3	0.46	2.40	20	2
1:B:98:ILE:HA	1:B:102:ILE:HG13	0.46	1.88	4	13
1:B:15:ALA:CB	1:B:19:PRO:HB3	0.46	2.41	4	3
1:B:25:GLN:HG2	1:B:36:LEU:HD23	0.46	1.87	2	1
1:B:21:PHE:CB	1:B:37:VAL:HB	0.46	2.40	4	14
1:A:6:LEU:CD1	1:A:40:LEU:HD13	0.46	2.40	4	1
1:A:40:LEU:CD2	1:A:58:ILE:CD1	0.46	2.94	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:ILE:O	1:A:96:ALA:C	0.46	2.54	14	11
1:B:41:THR:OG1	1:B:42:PRO:CD	0.46	2.62	20	9
1:A:101:LEU:HD12	1:B:25:GLN:HE22	0.46	1.70	5	1
1:A:25:GLN:NE2	1:B:101:LEU:CD2	0.46	2.79	6	2
1:A:99:ASP:O	1:A:103:THR:HB	0.46	2.11	12	4
1:A:7:TYR:CE1	1:A:23:ASP:CG	0.46	2.89	14	2
1:B:43:ILE:HD11	1:B:48:LYS:HG3	0.46	1.86	20	3
1:A:75:VAL:HG22	1:A:79:ILE:HD11	0.46	1.86	13	1
1:A:40:LEU:HD22	1:A:65:PHE:CB	0.46	2.41	19	1
1:A:10:LYS:HA	1:A:81:SER:CA	0.46	2.39	1	1
1:B:75:VAL:HG21	1:B:79:ILE:O	0.46	2.11	12	3
1:A:98:ILE:CA	1:A:102:ILE:HG23	0.46	2.41	3	2
1:B:58:ILE:HG23	1:B:59:HIS:N	0.46	2.26	16	3
1:A:23:ASP:N	1:A:37:VAL:HG12	0.46	2.26	5	7
1:B:6:LEU:HD23	1:B:6:LEU:O	0.46	2.11	5	1
1:A:94:ILE:N	1:A:94:ILE:HD12	0.46	2.26	7	3
1:A:58:ILE:HD13	1:A:65:PHE:O	0.46	2.10	7	1
1:B:30:ASP:HA	1:B:35:ARG:CG	0.46	2.41	7	1
1:A:7:TYR:O	1:A:21:PHE:N	0.46	2.46	8	1
1:A:23:ASP:HB3	1:A:35:ARG:CD	0.46	2.41	13	1
1:A:101:LEU:CD2	1:A:102:ILE:HG12	0.46	2.40	15	1
1:A:7:TYR:CZ	1:A:23:ASP:CB	0.46	2.99	17	2
1:B:38:ILE:CD1	1:B:67:MET:CB	0.46	2.94	2	1
1:B:35:ARG:NE	1:B:35:ARG:CA	0.46	2.77	20	2
1:B:8:LYS:C	1:B:81:SER:OG	0.46	2.54	11	2
1:A:9:ASN:ND2	1:A:15:ALA:N	0.46	2.64	3	1
1:A:10:LYS:CD	1:A:79:ILE:HG12	0.46	2.41	12	4
1:A:10:LYS:HG2	1:A:79:ILE:CA	0.46	2.41	13	1
1:A:23:ASP:CG	1:A:80:LEU:HD21	0.46	2.31	15	1
1:A:8:LYS:CB	1:A:84:VAL:HG13	0.46	2.41	15	1
1:A:35:ARG:HG3	1:A:80:LEU:CD2	0.46	2.40	20	1
1:B:98:ILE:O	1:B:102:ILE:HG23	0.45	2.11	17	3
1:B:71:GLN:OE1	1:B:73:THR:HG23	0.45	2.11	11	1
1:A:35:ARG:NE	1:A:80:LEU:HD13	0.45	2.25	14	1
1:A:22:VAL:HG11	1:A:94:ILE:HD11	0.45	1.87	18	1
1:B:57:THR:OG1	1:B:66:ILE:CG2	0.45	2.64	1	2
1:A:40:LEU:CA	1:A:67:MET:HA	0.45	2.41	16	2
1:A:98:ILE:O	1:A:102:ILE:HG23	0.45	2.11	3	2
1:B:75:VAL:CG2	1:B:80:LEU:HD22	0.45	2.42	4	1
1:B:57:THR:HG1	1:B:66:ILE:HG23	0.45	1.70	9	3
1:B:6:LEU:HB2	1:B:87:LEU:HG	0.45	1.88	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:HD21	1:A:67:MET:CG	0.45	2.41	7	1
1:B:25:GLN:HG2	1:B:26:SER:N	0.45	2.25	11	2
1:A:38:ILE:HD11	1:A:98:ILE:CD1	0.45	2.41	20	1
1:A:105:ILE:HD12	1:A:105:ILE:C	0.45	2.31	1	1
1:B:6:LEU:HD13	1:B:84:VAL:CG1	0.45	2.41	1	1
1:A:77:VAL:HG13	1:A:78:LYS:N	0.45	2.27	5	12
1:B:64:ASP:C	1:B:65:PHE:CD1	0.45	2.89	5	2
1:B:58:ILE:HG23	1:B:90:PHE:CZ	0.45	2.47	7	4
1:A:60:ILE:HD11	1:A:62:GLU:HB2	0.45	1.87	4	1
1:A:37:VAL:CG2	1:A:75:VAL:HG13	0.45	2.41	4	1
1:A:98:ILE:CG2	1:A:102:ILE:HG12	0.45	2.41	11	2
1:A:8:LYS:O	1:A:81:SER:HB2	0.45	2.10	8	2
1:B:20:TYR:CE1	1:B:65:PHE:CD2	0.45	3.05	9	1
1:B:41:THR:HG23	1:B:66:ILE:HD11	0.45	1.85	15	1
1:A:34:THR:C	1:A:35:ARG:HG2	0.45	2.31	20	1
1:A:9:ASN:HA	1:A:21:PHE:CZ	0.45	2.47	1	1
1:A:6:LEU:HB2	1:A:87:LEU:HD22	0.45	1.87	1	1
1:B:77:VAL:HG13	1:B:78:LYS:N	0.45	2.27	9	13
1:A:22:VAL:HG12	1:A:94:ILE:HG21	0.45	1.87	3	2
1:B:35:ARG:HB3	1:B:35:ARG:CZ	0.45	2.41	3	1
1:A:9:ASN:ND2	1:A:21:PHE:CE2	0.45	2.84	5	1
1:A:2:SER:CB	1:A:30:ASP:HB2	0.45	2.41	7	3
1:B:24:VAL:O	1:B:36:LEU:HD12	0.45	2.12	7	1
1:A:23:ASP:CB	1:A:35:ARG:NH1	0.45	2.80	13	1
1:A:10:LYS:HD2	1:A:11:ASP:H	0.45	1.71	18	1
1:A:21:PHE:CB	1:A:37:VAL:HB	0.45	2.42	9	16
1:B:2:SER:HB2	1:B:31:ASN:CA	0.45	2.41	9	2
1:A:35:ARG:HD3	1:A:36:LEU:N	0.45	2.26	11	1
1:B:9:ASN:ND2	1:B:21:PHE:CZ	0.45	2.85	18	2
1:A:35:ARG:NE	1:A:80:LEU:CD1	0.45	2.79	14	1
1:B:43:ILE:HD11	1:B:48:LYS:HD2	0.45	1.87	14	1
1:A:65:PHE:CD1	1:A:65:PHE:N	0.45	2.85	16	1
1:B:38:ILE:HG23	1:B:69:THR:HA	0.45	1.88	15	4
1:A:72:MET:HE1	1:A:98:ILE:CD1	0.45	2.42	3	1
1:B:24:VAL:HB	1:B:94:ILE:HG22	0.45	1.88	18	2
1:A:30:ASP:O	1:A:35:ARG:HG3	0.45	2.12	5	1
1:B:6:LEU:HD21	1:B:20:TYR:CD2	0.45	2.46	9	3
1:A:10:LYS:O	1:A:82:GLU:HB2	0.45	2.12	18	3
1:B:22:VAL:CG1	1:B:94:ILE:HG13	0.45	2.40	7	3
1:B:37:VAL:CG2	1:B:73:THR:O	0.45	2.63	7	1
1:A:38:ILE:CG2	1:A:69:THR:CG2	0.45	2.95	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASP:CG	1:A:35:ARG:HD2	0.45	2.32	9	1
1:B:87:LEU:H	1:B:87:LEU:CD2	0.45	2.25	16	1
1:B:35:ARG:HB2	1:B:35:ARG:NH1	0.45	2.27	19	1
1:A:38:ILE:HD11	1:A:94:ILE:HA	0.45	1.87	1	1
1:B:10:LYS:HD2	1:B:79:ILE:HG12	0.45	1.89	1	1
1:B:9:ASN:CA	1:B:81:SER:HA	0.45	2.41	1	1
1:A:35:ARG:HG3	1:A:36:LEU:N	0.45	2.26	2	1
1:B:55:CYS:O	1:B:66:ILE:HG22	0.45	2.12	3	1
1:A:10:LYS:CA	1:A:82:GLU:N	0.45	2.79	10	5
1:A:25:GLN:HE21	1:A:36:LEU:HD22	0.45	1.72	5	2
1:A:55:CYS:CB	1:A:67:MET:O	0.45	2.65	6	2
1:A:35:ARG:HD2	1:A:80:LEU:CD2	0.45	2.42	9	1
1:B:58:ILE:CD1	1:B:58:ILE:N	0.45	2.80	12	1
1:A:94:ILE:HD12	1:A:94:ILE:N	0.45	2.26	1	3
1:A:58:ILE:HB	1:A:90:PHE:CE2	0.45	2.47	11	5
1:B:17:THR:HG22	1:B:18:TYR:CE2	0.45	2.46	2	1
1:A:21:PHE:N	1:A:21:PHE:CD1	0.45	2.84	4	1
1:A:2:SER:O	1:A:35:ARG:NH1	0.45	2.50	4	1
1:B:35:ARG:NH2	1:B:77:VAL:HB	0.45	2.27	5	1
1:A:90:PHE:O	1:A:94:ILE:HD13	0.45	2.12	6	3
1:A:9:ASN:CB	1:A:14:SER:HB3	0.45	2.41	16	3
1:A:67:MET:HE1	1:A:94:ILE:CD1	0.45	2.41	12	1
1:A:99:ASP:O	1:A:104:GLY:N	0.45	2.49	13	2
1:A:101:LEU:HD22	1:A:102:ILE:N	0.45	2.25	15	1
1:B:21:PHE:CD1	1:B:21:PHE:N	0.45	2.84	15	1
1:B:58:ILE:CD1	1:B:90:PHE:CD2	0.45	2.99	17	1
1:B:54:LEU:CG	1:B:69:THR:HG23	0.45	2.42	2	1
1:B:23:ASP:CB	1:B:35:ARG:CD	0.45	2.95	3	1
1:A:8:LYS:HG2	1:A:19:PRO:O	0.45	2.10	5	1
1:B:31:ASN:O	1:B:31:ASN:CG	0.45	2.55	6	1
1:A:7:TYR:CE1	1:A:23:ASP:HB3	0.45	2.47	19	2
1:B:25:GLN:NE2	1:B:26:SER:CB	0.45	2.80	8	1
1:B:30:ASP:CB	1:B:35:ARG:NE	0.45	2.80	11	1
1:B:57:THR:HA	1:B:66:ILE:HG23	0.45	1.87	11	1
1:B:8:LYS:O	1:B:81:SER:CA	0.45	2.65	11	1
1:B:7:TYR:CE2	1:B:80:LEU:CD2	0.45	3.00	15	1
1:A:11:ASP:O	1:A:13:SER:N	0.45	2.50	19	1
1:B:7:TYR:HB3	1:B:81:SER:OG	0.45	2.12	1	1
1:B:99:ASP:CB	1:B:105:ILE:HD11	0.45	2.42	1	1
1:A:88:SER:O	1:A:91:ARG:CD	0.45	2.65	16	8
1:A:57:THR:OG1	1:A:65:PHE:O	0.45	2.31	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:98:ILE:CA	1:B:102:ILE:HG23	0.45	2.42	2	3
1:A:20:TYR:O	1:A:21:PHE:CD1	0.45	2.70	3	4
1:B:66:ILE:HD12	1:B:66:ILE:N	0.45	2.27	4	1
1:B:87:LEU:HB2	1:B:90:PHE:HB2	0.45	1.89	14	3
1:A:25:GLN:NE2	1:B:101:LEU:CD1	0.45	2.80	19	2
1:B:23:ASP:C	1:B:35:ARG:NH1	0.45	2.71	12	1
1:A:38:ILE:HG12	1:A:69:THR:HG23	0.45	1.88	13	1
1:A:24:VAL:HG13	1:A:24:VAL:O	0.45	2.11	16	2
1:A:6:LEU:CG	1:A:87:LEU:HD13	0.45	2.42	18	1
1:B:2:SER:O	1:B:35:ARG:HD2	0.45	2.12	19	1
1:A:19:PRO:HG2	1:A:41:THR:HA	0.44	1.89	5	3
1:B:7:TYR:CZ	1:B:23:ASP:CG	0.44	2.91	5	6
1:B:17:THR:CG2	1:B:18:TYR:CE2	0.44	3.00	15	2
1:B:24:VAL:CG2	1:B:98:ILE:CD1	0.44	2.95	3	9
1:A:10:LYS:N	1:A:82:GLU:H	0.44	2.09	12	5
1:B:19:PRO:HG2	1:B:42:PRO:HD3	0.44	1.88	9	5
1:B:7:TYR:HB3	1:B:81:SER:O	0.44	2.12	5	1
1:A:25:GLN:NE2	1:B:101:LEU:HD23	0.44	2.27	6	1
1:B:24:VAL:O	1:B:36:LEU:HB3	0.44	2.12	7	1
1:B:10:LYS:CA	1:B:81:SER:HA	0.44	2.42	7	1
1:A:2:SER:O	1:A:3:GLN:HB2	0.44	2.11	8	3
1:B:8:LYS:CG	1:B:19:PRO:O	0.44	2.65	16	4
1:B:95:ILE:O	1:B:99:ASP:N	0.44	2.47	11	2
1:A:6:LEU:H	1:A:86:GLU:HA	0.44	1.72	13	1
1:B:43:ILE:CG2	1:B:66:ILE:CG2	0.44	2.95	15	1
1:B:5:THR:O	1:B:7:TYR:CE1	0.44	2.70	2	7
1:A:9:ASN:CB	1:A:14:SER:HB2	0.44	2.42	18	4
1:A:35:ARG:CA	1:A:35:ARG:NE	0.44	2.74	3	2
1:A:43:ILE:CD1	1:A:57:THR:OG1	0.44	2.65	14	4
1:B:20:TYR:OH	1:B:65:PHE:CD2	0.44	2.69	15	3
1:B:98:ILE:HG23	1:B:102:ILE:HG12	0.44	1.88	10	2
1:A:98:ILE:O	1:A:102:ILE:CB	0.44	2.64	20	2
1:A:92:ASN:O	1:A:93:GLU:C	0.44	2.56	20	8
1:A:29:LEU:O	1:A:35:ARG:NH2	0.44	2.50	3	1
1:A:102:ILE:HG12	1:B:102:ILE:HG21	0.44	1.89	6	1
1:B:99:ASP:HA	1:B:103:THR:HB	0.44	1.88	6	1
1:A:9:ASN:OD1	1:A:21:PHE:CE1	0.44	2.70	14	2
1:A:4:PHE:CD2	1:A:91:ARG:HB3	0.44	2.48	14	1
1:B:105:ILE:HD12	1:B:105:ILE:O	0.44	2.13	17	1
1:A:95:ILE:O	1:A:98:ILE:N	0.44	2.51	2	1
1:B:23:ASP:HB3	1:B:35:ARG:HD3	0.44	1.90	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:7:TYR:CE1	1:B:23:ASP:HB3	0.44	2.47	4	1
1:B:21:PHE:HD1	1:B:81:SER:HG	0.44	1.53	4	1
1:A:58:ILE:CG1	1:A:90:PHE:CD2	0.44	3.00	20	2
1:B:69:THR:CG2	1:B:101:LEU:CD2	0.44	2.95	7	2
1:B:98:ILE:O	1:B:102:ILE:HG13	0.44	2.12	10	3
1:A:29:LEU:O	1:A:35:ARG:NH1	0.44	2.50	15	1
1:A:10:LYS:HB3	1:A:79:ILE:CG1	0.44	2.39	18	1
1:A:24:VAL:CB	1:A:94:ILE:HG23	0.44	2.42	18	1
1:A:41:THR:OG1	1:A:42:PRO:CD	0.44	2.66	3	4
1:A:8:LYS:C	1:A:20:TYR:HA	0.44	2.32	3	1
1:B:58:ILE:CG1	1:B:90:PHE:CE2	0.44	3.00	4	1
1:B:8:LYS:HB2	1:B:20:TYR:CD2	0.44	2.48	9	6
1:A:9:ASN:HB2	1:A:14:SER:HB3	0.44	1.88	5	1
1:A:21:PHE:HB2	1:A:37:VAL:HB	0.44	1.90	5	1
1:B:95:ILE:O	1:B:96:ALA:C	0.44	2.56	19	4
1:B:9:ASN:OD1	1:B:15:ALA:HB2	0.44	2.12	6	1
1:A:2:SER:CB	1:A:30:ASP:C	0.44	2.85	9	3
1:B:38:ILE:HG21	1:B:67:MET:SD	0.44	2.52	12	1
1:B:8:LYS:HB2	1:B:84:VAL:HB	0.44	1.89	13	1
1:A:8:LYS:CD	1:A:20:TYR:CE2	0.44	3.00	15	1
1:A:31:ASN:HB2	1:A:35:ARG:CZ	0.44	2.43	17	1
1:B:24:VAL:HG11	1:B:38:ILE:HD13	0.44	1.87	17	1
1:B:24:VAL:CB	1:B:94:ILE:HG22	0.44	2.42	18	1
1:B:22:VAL:CG1	1:B:94:ILE:CG2	0.44	2.95	1	5
1:B:15:ALA:HB1	1:B:19:PRO:HB3	0.44	1.89	4	3
1:B:19:PRO:HD2	1:B:40:LEU:O	0.44	2.13	5	3
1:A:6:LEU:HD21	1:A:20:TYR:CD2	0.44	2.47	16	4
1:B:6:LEU:C	1:B:6:LEU:HD23	0.44	2.33	9	2
1:A:75:VAL:O	1:A:80:LEU:HD22	0.44	2.12	10	1
1:B:2:SER:O	1:B:30:ASP:CB	0.44	2.66	10	2
1:B:10:LYS:O	1:B:82:GLU:CB	0.44	2.65	11	1
1:A:4:PHE:CD2	1:A:91:ARG:CB	0.44	3.00	14	2
1:B:87:LEU:N	1:B:87:LEU:CD2	0.44	2.80	16	1
1:A:4:PHE:CD1	1:A:4:PHE:N	0.44	2.84	18	1
1:B:3:GLN:N	1:B:7:TYR:OH	0.44	2.46	2	1
1:B:81:SER:O	1:B:83:PRO:HD3	0.44	2.13	2	2
1:B:26:SER:HB2	1:B:35:ARG:NE	0.44	2.27	20	2
1:A:31:ASN:ND2	1:A:80:LEU:CD2	0.44	2.81	3	2
1:A:33:ASN:O	1:A:77:VAL:HG12	0.44	2.12	3	1
1:B:92:ASN:O	1:B:93:GLU:C	0.44	2.56	3	6
1:B:58:ILE:HG13	1:B:90:PHE:CZ	0.44	2.47	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:58:ILE:HA	1:B:90:PHE:CE1	0.44	2.46	6	1
1:B:38:ILE:CG1	1:B:72:MET:HE2	0.44	2.42	8	1
1:B:6:LEU:HD12	1:B:87:LEU:HG	0.44	1.90	8	1
1:A:103:THR:CG2	1:B:103:THR:HG22	0.44	2.43	10	1
1:B:10:LYS:HA	1:B:82:GLU:H	0.44	1.72	18	3
1:B:6:LEU:HD23	1:B:85:ASN:CB	0.44	2.41	19	2
1:B:101:LEU:HG	1:B:102:ILE:CG1	0.44	2.43	8	5
1:B:21:PHE:CD2	1:B:81:SER:OG	0.44	2.71	5	1
1:B:20:TYR:CE1	1:B:65:PHE:HD2	0.44	2.30	15	1
1:A:6:LEU:HD22	1:A:84:VAL:CG1	0.44	2.42	19	1
1:A:101:LEU:HD23	1:A:102:ILE:CG1	0.44	2.42	20	1
1:A:42:PRO:HG3	1:A:45:LEU:HD12	0.44	1.89	1	8
1:A:60:ILE:HD12	1:A:62:GLU:HB2	0.44	1.90	2	2
1:A:30:ASP:HA	1:A:35:ARG:NE	0.44	2.27	3	1
1:B:35:ARG:NH1	1:B:35:ARG:HB3	0.44	2.28	3	2
1:B:24:VAL:CG1	1:B:38:ILE:CG1	0.44	2.96	4	1
1:B:24:VAL:HG11	1:B:94:ILE:HG22	0.44	1.90	4	1
1:A:6:LEU:HD22	1:A:85:ASN:HB3	0.44	1.90	5	1
1:A:24:VAL:HG13	1:A:98:ILE:HD11	0.44	1.90	8	3
1:B:98:ILE:HA	1:B:102:ILE:CD1	0.44	2.42	14	2
1:B:41:THR:HG21	1:B:68:LEU:HD12	0.44	1.90	18	1
1:A:54:LEU:HD22	1:B:29:LEU:CD1	0.44	2.43	1	1
1:A:64:ASP:C	1:A:65:PHE:CD1	0.44	2.91	1	3
1:A:15:ALA:HB1	1:A:19:PRO:HB3	0.44	1.89	3	5
1:A:77:VAL:HA	1:A:80:LEU:HD23	0.44	1.90	3	1
1:B:40:LEU:CD2	1:B:58:ILE:CD1	0.44	2.96	3	1
1:A:87:LEU:HD22	1:A:87:LEU:H	0.44	1.73	4	1
1:B:44:GLU:HA	1:B:48:LYS:HG2	0.44	1.90	10	2
1:A:40:LEU:CD2	1:A:58:ILE:HD11	0.44	2.43	9	1
1:A:3:GLN:O	1:A:23:ASP:O	0.44	2.36	10	2
1:B:38:ILE:CG2	1:B:69:THR:CG2	0.44	2.95	19	2
1:A:3:GLN:N	1:A:35:ARG:NH1	0.44	2.65	13	1
1:B:8:LYS:HD2	1:B:20:TYR:CD2	0.44	2.48	13	1
1:A:42:PRO:CA	1:A:65:PHE:CD2	0.44	3.00	16	1
1:B:54:LEU:HD21	1:B:69:THR:HB	0.44	1.89	16	1
1:A:30:ASP:HA	1:A:35:ARG:HG2	0.43	1.90	4	1
1:A:67:MET:CE	1:A:94:ILE:HD12	0.43	2.42	12	1
1:A:67:MET:HE2	1:A:94:ILE:CD1	0.43	2.43	15	1
1:B:3:GLN:HA	1:B:23:ASP:HB2	0.43	1.90	16	1
1:A:10:LYS:CB	1:A:79:ILE:CG1	0.43	2.95	18	1
1:A:46:LEU:HD21	1:A:68:LEU:HD11	0.43	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HD11	1:A:67:MET:HG3	0.43	1.90	2	1
1:B:96:ALA:O	1:B:100:PHE:HB3	0.43	2.12	4	3
1:A:101:LEU:HG	1:A:102:ILE:CG1	0.43	2.44	7	3
1:B:20:TYR:OH	1:B:60:ILE:HD11	0.43	2.13	6	1
1:A:87:LEU:H	1:A:87:LEU:CD2	0.43	2.27	18	3
1:A:102:ILE:HD13	1:B:102:ILE:HG21	0.43	1.90	7	1
1:A:34:THR:HG21	1:B:71:GLN:OE1	0.43	2.13	8	1
1:A:69:THR:CG2	1:A:101:LEU:HD13	0.43	2.44	10	1
1:A:7:TYR:CD1	1:A:7:TYR:N	0.43	2.86	13	2
1:B:38:ILE:CG2	1:B:69:THR:HB	0.43	2.43	12	1
1:A:6:LEU:HB2	1:A:87:LEU:HG	0.43	1.89	15	2
1:B:46:LEU:O	1:B:46:LEU:HD23	0.43	2.13	15	1
1:A:69:THR:HG21	1:A:101:LEU:CD2	0.43	2.42	19	1
1:A:40:LEU:CD2	1:A:67:MET:HG2	0.43	2.43	4	1
1:B:31:ASN:CG	1:B:31:ASN:O	0.43	2.56	4	1
1:B:14:SER:O	1:B:18:TYR:N	0.43	2.49	13	3
1:A:8:LYS:HA	1:A:20:TYR:CA	0.43	2.43	5	1
1:A:98:ILE:HG22	1:A:102:ILE:HD11	0.43	1.89	16	2
1:B:19:PRO:CG	1:B:42:PRO:CD	0.43	2.94	15	2
1:A:40:LEU:HD21	1:A:67:MET:HG3	0.43	1.90	9	1
1:B:8:LYS:HG2	1:B:19:PRO:O	0.43	2.12	11	1
1:B:60:ILE:HG21	1:B:87:LEU:HB3	0.43	1.89	11	1
1:B:54:LEU:HD21	1:B:69:THR:HG23	0.43	1.89	12	1
1:B:10:LYS:HB3	1:B:79:ILE:HG22	0.43	1.90	13	1
1:B:35:ARG:CZ	1:B:80:LEU:HD22	0.43	2.43	13	1
1:B:36:LEU:HD12	1:B:72:MET:CG	0.43	2.43	17	1
1:B:75:VAL:HG23	1:B:75:VAL:O	0.43	2.14	20	1
1:A:99:ASP:HA	1:A:103:THR:CG2	0.43	2.43	20	3
1:B:9:ASN:N	1:B:81:SER:HB3	0.43	2.28	4	2
1:B:57:THR:CA	1:B:65:PHE:O	0.43	2.66	17	3
1:A:60:ILE:HD11	1:A:65:PHE:CE1	0.43	2.48	6	1
1:A:38:ILE:CD1	1:A:67:MET:HB3	0.43	2.43	7	1
1:A:4:PHE:CE2	1:A:91:ARG:HB2	0.43	2.48	7	3
1:B:38:ILE:HG12	1:B:72:MET:HE2	0.43	1.90	8	1
1:A:56:PRO:HB2	1:A:93:GLU:HG3	0.43	1.91	10	1
1:A:30:ASP:O	1:A:35:ARG:HD2	0.43	2.14	17	1
1:A:87:LEU:CG	1:A:87:LEU:O	0.43	2.65	1	3
1:B:8:LYS:HG3	1:B:9:ASN:N	0.43	2.28	1	1
1:B:98:ILE:HG22	1:B:99:ASP:N	0.43	2.29	2	4
1:A:84:VAL:HG13	1:A:85:ASN:N	0.43	2.29	3	1
1:A:2:SER:HB2	1:A:31:ASN:CB	0.43	2.44	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:LYS:CG	1:B:9:ASN:ND2	0.43	2.81	15	2
1:A:25:GLN:CG	1:A:36:LEU:CB	0.43	2.97	16	5
1:B:5:THR:HG23	1:B:86:GLU:HG2	0.43	1.90	9	1
1:A:76:PRO:HB3	1:A:78:LYS:CE	0.43	2.44	16	1
1:B:23:ASP:HA	1:B:37:VAL:HG12	0.43	1.89	16	1
1:B:38:ILE:CG2	1:B:38:ILE:O	0.43	2.66	2	1
1:A:14:SER:O	1:A:18:TYR:N	0.43	2.45	3	3
1:B:25:GLN:CB	1:B:36:LEU:CB	0.43	2.97	4	1
1:B:67:MET:CE	1:B:94:ILE:HG13	0.43	2.44	7	1
1:A:8:LYS:C	1:A:81:SER:OG	0.43	2.57	9	1
1:A:9:ASN:CA	1:A:81:SER:HA	0.43	2.44	12	1
1:A:101:LEU:HD11	1:B:25:GLN:OE1	0.43	2.12	13	3
1:A:6:LEU:CD2	1:A:87:LEU:HB3	0.43	2.43	20	1
1:A:24:VAL:CG2	1:A:98:ILE:CD1	0.43	2.97	12	3
1:B:37:VAL:HG22	1:B:73:THR:C	0.43	2.34	4	1
1:B:6:LEU:CD2	1:B:6:LEU:O	0.43	2.67	15	2
1:B:20:TYR:CG	1:B:40:LEU:CD1	0.43	3.01	6	1
1:B:10:LYS:CB	1:B:79:ILE:O	0.43	2.66	7	2
1:A:5:THR:O	1:A:7:TYR:CE1	0.43	2.72	10	4
1:B:69:THR:HG22	1:B:101:LEU:HG	0.43	1.90	13	1
1:B:58:ILE:HG13	1:B:90:PHE:CE2	0.43	2.48	3	1
1:A:54:LEU:C	1:A:54:LEU:HD22	0.43	2.34	4	1
1:B:10:LYS:HG2	1:B:79:ILE:HG12	0.43	1.89	7	1
1:A:7:TYR:CZ	1:A:23:ASP:HB2	0.43	2.49	13	5
1:A:102:ILE:CG2	1:B:102:ILE:HG21	0.43	2.43	8	1
1:B:98:ILE:HG13	1:B:102:ILE:CD1	0.43	2.44	9	1
1:A:3:GLN:O	1:A:4:PHE:CD1	0.43	2.72	11	1
1:A:98:ILE:HG23	1:A:102:ILE:HD11	0.43	1.91	16	1
1:B:67:MET:HE1	1:B:94:ILE:HD13	0.43	1.91	18	1
1:A:54:LEU:CD2	1:A:69:THR:HG22	0.43	2.44	16	2
1:B:59:HIS:CD2	1:B:59:HIS:N	0.43	2.86	3	1
1:B:10:LYS:CB	1:B:79:ILE:HG22	0.43	2.44	14	5
1:A:2:SER:CB	1:A:31:ASN:CB	0.43	2.97	6	2
1:B:94:ILE:CD1	1:B:94:ILE:N	0.43	2.81	9	4
1:A:58:ILE:O	1:A:64:ASP:CA	0.43	2.63	10	2
1:B:25:GLN:CB	1:B:36:LEU:HB3	0.43	2.43	11	2
1:A:31:ASN:OD1	1:A:31:ASN:O	0.43	2.36	12	1
1:B:9:ASN:CB	1:B:14:SER:HB2	0.43	2.44	15	3
1:A:87:LEU:HG	1:A:87:LEU:O	0.43	2.14	13	2
1:B:21:PHE:CD2	1:B:81:SER:HB3	0.43	2.49	5	1
1:B:2:SER:HB2	1:B:31:ASN:N	0.43	2.28	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ARG:HG2	1:A:37:VAL:HG13	0.43	1.89	6	1
1:A:2:SER:OG	1:A:31:ASN:ND2	0.43	2.52	7	1
1:B:57:THR:HG23	1:B:65:PHE:O	0.43	2.14	15	3
1:A:71:GLN:HA	1:B:74:SER:OG	0.43	2.14	9	1
1:B:24:VAL:O	1:B:25:GLN:CG	0.43	2.67	12	1
1:B:41:THR:HG23	1:B:66:ILE:HD12	0.43	1.86	15	1
1:B:94:ILE:HD12	1:B:94:ILE:N	0.43	2.28	17	1
1:A:22:VAL:CG1	1:A:94:ILE:HG13	0.43	2.43	18	1
1:B:2:SER:HB3	1:B:31:ASN:N	0.43	2.28	18	1
1:A:54:LEU:O	1:A:56:PRO:CD	0.43	2.67	20	1
1:B:10:LYS:CG	1:B:79:ILE:CA	0.43	2.97	20	1
1:B:19:PRO:HB2	1:B:20:TYR:CZ	0.42	2.49	1	1
1:B:9:ASN:HA	1:B:81:SER:HA	0.42	1.90	1	1
1:B:9:ASN:C	1:B:81:SER:HA	0.42	2.33	3	1
1:B:21:PHE:CD2	1:B:81:SER:CB	0.42	3.02	5	1
1:A:56:PRO:HD2	1:A:67:MET:HB3	0.42	1.91	6	1
1:A:35:ARG:O	1:A:74:SER:HA	0.42	2.14	7	2
1:A:40:LEU:CD2	1:A:67:MET:CG	0.42	2.97	7	1
1:B:19:PRO:HG2	1:B:20:TYR:CE1	0.42	2.49	11	3
1:A:46:LEU:O	1:A:46:LEU:HD23	0.42	2.14	12	1
1:A:62:GLU:HB2	1:A:65:PHE:CZ	0.42	2.49	20	2
1:A:101:LEU:HD12	1:A:101:LEU:O	0.42	2.13	18	1
1:A:8:LYS:CB	1:A:84:VAL:HB	0.42	2.44	18	1
1:A:26:SER:HB2	1:A:35:ARG:NE	0.42	2.29	2	1
1:A:20:TYR:HB2	1:A:40:LEU:HD12	0.42	1.91	4	1
1:A:38:ILE:HD12	1:A:72:MET:HG3	0.42	1.90	4	1
1:B:21:PHE:HB3	1:B:37:VAL:HB	0.42	1.91	6	1
1:B:5:THR:O	1:B:22:VAL:HG13	0.42	2.13	6	1
1:B:84:VAL:HG13	1:B:85:ASN:N	0.42	2.29	12	2
1:A:67:MET:CE	1:A:94:ILE:CD1	0.42	2.97	12	2
1:A:10:LYS:HA	1:A:82:GLU:CB	0.42	2.44	11	1
1:A:2:SER:OG	1:A:35:ARG:CD	0.42	2.67	12	1
1:A:35:ARG:NH2	1:A:77:VAL:HG23	0.42	2.28	17	1
1:A:6:LEU:HD13	1:A:87:LEU:CG	0.42	2.44	17	1
1:A:99:ASP:CA	1:A:103:THR:HG23	0.42	2.44	19	1
1:A:57:THR:HG23	1:A:65:PHE:O	0.42	2.14	19	1
1:B:87:LEU:O	1:B:87:LEU:HG	0.42	2.13	19	1
1:B:2:SER:HB3	1:B:35:ARG:CD	0.42	2.45	1	1
1:A:67:MET:CE	1:A:94:ILE:HG13	0.42	2.45	2	1
1:A:38:ILE:CG2	1:A:69:THR:CB	0.42	2.96	2	1
1:B:3:GLN:H	1:B:7:TYR:HH	0.42	1.57	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:VAL:CG1	1:A:94:ILE:HG21	0.42	2.43	3	1
1:B:2:SER:CB	1:B:30:ASP:C	0.42	2.88	3	3
1:A:87:LEU:CD2	1:A:87:LEU:H	0.42	2.25	4	1
1:B:10:LYS:CG	1:B:79:ILE:HG13	0.42	2.45	5	2
1:A:76:PRO:HB2	1:A:78:LYS:HG2	0.42	1.89	6	1
1:A:4:PHE:HZ	1:A:95:ILE:HD11	0.42	1.73	12	2
1:A:30:ASP:HA	1:A:35:ARG:NH2	0.42	2.29	11	1
1:A:87:LEU:CD2	1:A:87:LEU:N	0.42	2.82	14	1
1:B:43:ILE:HG23	1:B:66:ILE:HG23	0.42	1.91	15	1
1:B:36:LEU:CD2	1:B:72:MET:HE1	0.42	2.44	16	1
1:A:102:ILE:HG13	1:A:103:THR:N	0.42	2.28	17	1
1:B:10:LYS:CB	1:B:79:ILE:CG2	0.42	2.98	18	1
1:B:8:LYS:O	1:B:19:PRO:O	0.42	2.37	1	1
1:B:38:ILE:CG1	1:B:67:MET:HB3	0.42	2.45	2	1
1:A:100:PHE:HA	1:A:104:GLY:HA2	0.42	1.89	4	1
1:A:30:ASP:HA	1:A:35:ARG:CG	0.42	2.43	5	2
1:A:51:PRO:O	1:A:53:HIS:N	0.42	2.52	5	1
1:B:32:LEU:HD23	1:B:33:ASN:ND2	0.42	2.29	9	1
1:A:101:LEU:HD23	1:A:102:ILE:HG23	0.42	1.90	10	1
1:B:102:ILE:CD1	1:B:102:ILE:C	0.42	2.88	11	1
1:B:24:VAL:HG13	1:B:98:ILE:CD1	0.42	2.45	11	1
1:B:25:GLN:HG3	1:B:36:LEU:HB3	0.42	1.90	12	1
1:B:69:THR:HG22	1:B:101:LEU:CG	0.42	2.44	13	1
1:B:10:LYS:HD2	1:B:79:ILE:HG13	0.42	1.91	17	1
1:A:35:ARG:CZ	1:A:80:LEU:CD1	0.42	2.97	1	1
1:B:35:ARG:CG	1:B:36:LEU:N	0.42	2.82	2	1
1:B:7:TYR:CE1	1:B:23:ASP:OD1	0.42	2.72	17	2
1:A:36:LEU:HD21	1:B:72:MET:HE1	0.42	1.90	6	1
1:A:8:LYS:HB3	1:A:84:VAL:HG13	0.42	1.91	6	1
1:A:19:PRO:HD2	1:A:40:LEU:O	0.42	2.15	8	3
1:A:10:LYS:CA	1:A:82:GLU:HB2	0.42	2.45	8	1
1:B:75:VAL:HG22	1:B:79:ILE:CD1	0.42	2.44	8	1
1:B:31:ASN:CB	1:B:35:ARG:NH2	0.42	2.83	13	1
1:A:17:THR:HG22	1:A:18:TYR:CD1	0.42	2.49	14	1
1:A:25:GLN:O	1:A:27:ASP:N	0.42	2.53	16	1
1:A:80:LEU:HD12	1:A:80:LEU:C	0.42	2.35	19	1
1:B:31:ASN:HB3	1:B:35:ARG:NH1	0.42	2.30	19	1
1:A:8:LYS:O	1:A:81:SER:HA	0.42	2.15	1	1
1:B:36:LEU:HD13	1:B:74:SER:OG	0.42	2.14	1	1
1:A:46:LEU:HD23	1:A:46:LEU:O	0.42	2.14	2	1
1:A:58:ILE:HG23	1:A:90:PHE:CE1	0.42	2.50	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:78:LYS:H	1:B:78:LYS:CD	0.42	2.27	4	2
1:B:2:SER:HB2	1:B:31:ASN:CB	0.42	2.45	6	1
1:B:7:TYR:CD2	1:B:80:LEU:HD11	0.42	2.50	6	1
1:A:10:LYS:CE	1:A:79:ILE:HG13	0.42	2.45	8	1
1:A:2:SER:OG	1:A:35:ARG:HD3	0.42	2.15	9	1
1:B:100:PHE:CE1	1:B:105:ILE:HD12	0.42	2.49	9	1
1:A:75:VAL:HG23	1:A:80:LEU:HD22	0.42	1.91	10	1
1:A:26:SER:N	1:A:35:ARG:HH21	0.42	2.12	11	1
1:A:8:LYS:HB2	1:A:84:VAL:HG13	0.42	1.90	15	1
1:A:101:LEU:HD23	1:B:25:GLN:NE2	0.42	2.28	15	1
1:B:58:ILE:HG22	1:B:90:PHE:CE2	0.42	2.49	15	1
1:B:28:LEU:O	1:B:32:LEU:HD12	0.42	2.13	19	1
1:A:2:SER:HB2	1:A:30:ASP:CG	0.42	2.35	1	1
1:A:69:THR:OG1	1:A:72:MET:CE	0.42	2.68	2	1
1:B:40:LEU:HA	1:B:67:MET:HA	0.42	1.90	2	1
1:B:68:LEU:HD23	1:B:70:GLN:HG3	0.42	1.91	2	1
1:B:7:TYR:CZ	1:B:23:ASP:OD1	0.42	2.73	15	2
1:A:6:LEU:CG	1:A:87:LEU:HG	0.42	2.44	3	1
1:A:9:ASN:OD1	1:A:9:ASN:O	0.42	2.37	3	1
1:A:2:SER:O	1:A:30:ASP:OD2	0.42	2.38	5	1
1:A:8:LYS:HD2	1:A:20:TYR:CD2	0.42	2.49	15	2
1:A:9:ASN:OD1	1:A:21:PHE:CZ	0.42	2.72	15	3
1:B:65:PHE:N	1:B:65:PHE:CD1	0.42	2.88	9	1
1:B:43:ILE:CD1	1:B:57:THR:OG1	0.42	2.61	10	1
1:A:101:LEU:CD1	1:B:25:GLN:NE2	0.42	2.82	16	2
1:B:38:ILE:HD13	1:B:67:MET:SD	0.42	2.55	15	1
1:B:24:VAL:O	1:B:25:GLN:HB3	0.42	2.15	17	1
1:A:24:VAL:HG23	1:A:25:GLN:N	0.42	2.29	18	1
1:A:38:ILE:HG23	1:A:69:THR:CG2	0.42	2.44	18	1
1:B:96:ALA:HA	1:B:105:ILE:HG21	0.42	1.90	19	1
1:A:77:VAL:O	1:A:80:LEU:HB2	0.42	2.14	1	1
1:B:6:LEU:HG	1:B:87:LEU:HG	0.42	1.91	1	1
1:B:88:SER:O	1:B:91:ARG:CD	0.42	2.68	15	5
1:A:38:ILE:O	1:A:40:LEU:N	0.42	2.53	2	1
1:B:23:ASP:HA	1:B:35:ARG:CD	0.42	2.45	3	1
1:A:3:GLN:N	1:A:7:TYR:OH	0.42	2.53	4	1
1:A:73:THR:HG22	1:B:73:THR:CB	0.42	2.44	5	1
1:B:78:LYS:CD	1:B:78:LYS:H	0.42	2.27	5	1
1:A:37:VAL:CG2	1:A:73:THR:O	0.42	2.68	15	2
1:A:38:ILE:HG21	1:A:67:MET:HG2	0.42	1.90	17	1
1:A:35:ARG:CZ	1:A:80:LEU:CD2	0.42	2.97	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HG12	1:A:90:PHE:CG	0.42	2.49	18	1
1:B:9:ASN:HB2	1:B:14:SER:CB	0.42	2.45	8	1
1:A:80:LEU:O	1:A:80:LEU:HD12	0.42	2.14	9	1
1:A:2:SER:OG	1:A:31:ASN:HB3	0.42	2.15	10	2
1:A:6:LEU:HD23	1:A:87:LEU:HD21	0.42	1.92	10	1
1:A:58:ILE:HD12	1:A:87:LEU:HD11	0.42	1.92	14	1
1:A:36:LEU:CD2	1:B:72:MET:CE	0.42	2.97	14	1
1:A:94:ILE:N	1:A:94:ILE:CD1	0.42	2.83	17	1
1:A:10:LYS:HG2	1:A:79:ILE:CD1	0.42	2.45	18	1
1:A:46:LEU:CD2	1:A:68:LEU:HD13	0.42	2.45	18	1
1:B:19:PRO:HB2	1:B:20:TYR:CD1	0.42	2.49	4	3
1:A:69:THR:OG1	1:A:101:LEU:CB	0.42	2.68	3	1
1:B:6:LEU:CB	1:B:87:LEU:HD22	0.42	2.45	9	2
1:A:57:THR:CG2	1:A:59:HIS:CE1	0.42	3.03	8	1
1:B:56:PRO:HD2	1:B:67:MET:CB	0.42	2.44	8	3
1:B:76:PRO:O	1:B:79:ILE:CD1	0.42	2.68	8	1
1:A:29:LEU:HD22	1:B:70:GLN:NE2	0.42	2.29	9	1
1:A:25:GLN:HG3	1:B:102:ILE:HG22	0.42	1.91	10	1
1:A:63:GLY:O	1:A:65:PHE:CZ	0.42	2.73	15	1
1:A:34:THR:HA	1:A:35:ARG:NH2	0.42	2.30	16	1
1:A:26:SER:O	1:A:30:ASP:HB3	0.42	2.13	17	2
1:B:42:PRO:CA	1:B:65:PHE:CD2	0.42	3.03	19	1
1:A:31:ASN:CB	1:A:35:ARG:NE	0.42	2.83	20	1
1:B:4:PHE:CZ	1:B:91:ARG:HB2	0.41	2.50	1	2
1:B:69:THR:OG1	1:B:101:LEU:CB	0.41	2.68	2	1
1:A:20:TYR:C	1:A:21:PHE:CD1	0.41	2.94	14	5
1:B:75:VAL:CG2	1:B:75:VAL:O	0.41	2.68	5	1
1:A:44:GLU:HG3	1:A:48:LYS:CG	0.41	2.45	6	1
1:A:3:GLN:HB2	1:A:35:ARG:NH1	0.41	2.29	7	1
1:B:38:ILE:CD1	1:B:97:ALA:CB	0.41	2.98	7	3
1:A:35:ARG:NH1	1:A:80:LEU:CD2	0.41	2.83	8	1
1:A:72:MET:CE	1:B:36:LEU:CD2	0.41	2.98	9	1
1:B:23:ASP:O	1:B:35:ARG:NH1	0.41	2.53	11	1
1:B:37:VAL:O	1:B:72:MET:CG	0.41	2.67	14	1
1:A:58:ILE:HD11	1:A:65:PHE:CB	0.41	2.41	15	1
1:A:8:LYS:HD3	1:A:20:TYR:CD2	0.41	2.50	15	1
1:B:20:TYR:CZ	1:B:65:PHE:HD2	0.41	2.32	15	1
1:B:24:VAL:CG2	1:B:24:VAL:O	0.41	2.68	15	1
1:B:7:TYR:O	1:B:21:PHE:N	0.41	2.46	1	1
1:A:7:TYR:CG	1:A:23:ASP:OD1	0.41	2.73	5	1
1:B:35:ARG:NH1	1:B:80:LEU:HD22	0.41	2.29	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:ILE:HD12	1:B:67:MET:CE	0.41	2.45	5	1
1:B:6:LEU:CA	1:B:87:LEU:HD22	0.41	2.45	19	2
1:A:8:LYS:HE2	1:A:84:VAL:HG21	0.41	1.92	9	1
1:B:25:GLN:CG	1:B:36:LEU:CB	0.41	2.98	13	2
1:B:67:MET:SD	1:B:94:ILE:HD12	0.41	2.54	11	1
1:A:58:ILE:N	1:A:58:ILE:CD1	0.41	2.83	12	1
1:B:54:LEU:HD21	1:B:69:THR:HG22	0.41	1.91	12	1
1:B:7:TYR:CE2	1:B:23:ASP:OD2	0.41	2.73	20	4
1:A:4:PHE:CZ	1:A:95:ILE:CD1	0.41	2.99	14	1
1:A:6:LEU:CD1	1:A:6:LEU:O	0.41	2.68	15	1
1:A:22:VAL:HG21	1:A:67:MET:HE2	0.41	1.88	17	1
1:B:2:SER:O	1:B:3:GLN:CG	0.41	2.68	20	1
1:A:78:LYS:CD	1:A:78:LYS:H	0.41	2.28	10	2
1:A:94:ILE:CD1	1:A:94:ILE:N	0.41	2.84	9	2
1:B:41:THR:CG2	1:B:68:LEU:HD12	0.41	2.45	2	1
1:B:54:LEU:CD2	1:B:101:LEU:HD13	0.41	2.45	4	1
1:B:73:THR:OG1	1:B:74:SER:N	0.41	2.53	4	1
1:B:69:THR:CG2	1:B:101:LEU:HD12	0.41	2.40	6	1
1:B:59:HIS:N	1:B:59:HIS:CD2	0.41	2.88	7	1
1:A:8:LYS:C	1:A:81:SER:HB2	0.41	2.36	20	2
1:B:7:TYR:CD2	1:B:80:LEU:HG	0.41	2.51	15	1
1:A:74:SER:N	1:B:71:GLN:O	0.41	2.53	17	1
1:A:20:TYR:O	1:A:39:PRO:HA	0.41	2.14	19	1
1:B:7:TYR:CD1	1:B:23:ASP:OD1	0.41	2.74	2	2
1:B:10:LYS:HG3	1:B:79:ILE:HA	0.41	1.92	2	1
1:A:4:PHE:CE2	1:A:91:ARG:NH1	0.41	2.88	3	1
1:A:8:LYS:HB2	1:A:84:VAL:CB	0.41	2.46	3	1
1:B:10:LYS:HG2	1:B:79:ILE:HG13	0.41	1.91	5	1
1:B:6:LEU:CG	1:B:87:LEU:HD13	0.41	2.43	7	2
1:B:38:ILE:HG23	1:B:69:THR:CA	0.41	2.45	8	2
1:A:35:ARG:NH1	1:A:80:LEU:CD1	0.41	2.83	12	1
1:B:43:ILE:CG1	1:B:48:LYS:CD	0.41	2.98	14	1
1:A:26:SER:CB	1:A:35:ARG:CZ	0.41	2.99	2	1
1:A:34:THR:HB	1:A:76:PRO:HA	0.41	1.93	2	1
1:A:58:ILE:HG13	1:A:90:PHE:CE2	0.41	2.51	2	2
1:A:44:GLU:HA	1:A:48:LYS:HD3	0.41	1.93	5	1
1:A:9:ASN:C	1:A:81:SER:HA	0.41	2.36	10	1
1:B:25:GLN:HG3	1:B:36:LEU:HD23	0.41	1.91	12	1
1:B:54:LEU:CD2	1:B:69:THR:HG22	0.41	2.46	12	1
1:B:43:ILE:HG22	1:B:65:PHE:CA	0.41	2.45	20	4
1:B:42:PRO:CG	1:B:45:LEU:HG	0.41	2.45	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ASN:HA	1:A:35:ARG:CD	0.41	2.45	17	1
1:A:36:LEU:HD21	1:A:72:MET:HE3	0.41	1.92	17	1
1:A:5:THR:CG2	1:A:85:ASN:O	0.41	2.69	20	1
1:B:10:LYS:CG	1:B:79:ILE:CB	0.41	2.98	20	1
1:B:20:TYR:CD1	1:B:40:LEU:HB2	0.41	2.50	20	1
1:A:26:SER:HB3	1:A:29:LEU:N	0.41	2.31	16	3
1:A:90:PHE:CE2	1:A:93:GLU:CG	0.41	3.03	2	1
1:B:42:PRO:HG3	1:B:45:LEU:CD2	0.41	2.44	2	1
1:A:25:GLN:N	1:A:35:ARG:NE	0.41	2.69	5	1
1:A:63:GLY:O	1:A:65:PHE:CE2	0.41	2.74	10	1
1:A:24:VAL:CG1	1:A:38:ILE:HD13	0.41	2.46	12	1
1:A:35:ARG:HA	1:A:35:ARG:NH1	0.41	2.31	15	1
1:A:98:ILE:HA	1:A:102:ILE:CD1	0.41	2.45	15	1
1:B:20:TYR:N	1:B:20:TYR:HD1	0.41	2.10	15	1
1:B:25:GLN:CG	1:B:26:SER:N	0.41	2.82	15	1
1:B:25:GLN:HE21	1:B:36:LEU:HD22	0.41	1.75	15	1
1:A:31:ASN:HB2	1:A:77:VAL:HG21	0.41	1.92	18	1
1:A:35:ARG:NE	1:A:80:LEU:CD2	0.41	2.84	20	1
1:A:5:THR:HG23	1:A:86:GLU:CA	0.41	2.45	20	1
1:A:7:TYR:HB3	1:A:81:SER:O	0.41	2.16	20	1
1:A:7:TYR:CG	1:A:35:ARG:NH1	0.41	2.89	1	1
1:A:54:LEU:HD22	1:B:29:LEU:HD11	0.41	1.92	1	1
1:A:25:GLN:HB3	1:A:35:ARG:HH11	0.41	1.76	2	1
1:A:35:ARG:CG	1:A:36:LEU:N	0.41	2.84	2	1
1:B:8:LYS:C	1:B:81:SER:HB2	0.41	2.35	6	1
1:A:38:ILE:HD13	1:A:67:MET:HB3	0.41	1.92	7	1
1:B:24:VAL:CB	1:B:94:ILE:HG23	0.41	2.44	7	1
1:A:10:LYS:HE2	1:A:11:ASP:HB2	0.41	1.91	8	1
1:B:64:ASP:C	1:B:65:PHE:CD2	0.41	2.94	8	1
1:B:88:SER:O	1:B:91:ARG:N	0.41	2.46	8	1
1:A:8:LYS:N	1:A:81:SER:HB2	0.41	2.30	10	1
1:B:102:ILE:C	1:B:102:ILE:CD1	0.41	2.89	10	1
1:B:9:ASN:OD1	1:B:21:PHE:CE1	0.41	2.74	16	1
1:A:9:ASN:OD1	1:A:14:SER:CB	0.41	2.69	18	1
1:B:38:ILE:CD1	1:B:69:THR:OG1	0.41	2.69	18	1
1:A:31:ASN:HB2	1:A:35:ARG:NE	0.41	2.31	20	1
1:B:10:LYS:O	1:B:82:GLU:CG	0.41	2.69	20	1
1:B:63:GLY:O	1:B:65:PHE:CE2	0.41	2.74	1	1
1:B:38:ILE:CG2	1:B:67:MET:CE	0.41	2.99	2	1
1:A:42:PRO:HG3	1:A:45:LEU:CD2	0.41	2.46	4	1
1:A:21:PHE:HB2	1:A:37:VAL:CB	0.41	2.45	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:THR:HG22	1:A:72:MET:HE1	0.41	1.93	6	1
1:B:8:LYS:CA	1:B:81:SER:HB2	0.41	2.45	6	1
1:A:25:GLN:HG3	1:B:102:ILE:HG23	0.41	1.93	7	1
1:B:54:LEU:HD21	1:B:101:LEU:HD22	0.41	1.92	7	1
1:A:103:THR:CG2	1:B:103:THR:CG2	0.41	2.99	10	1
1:A:102:ILE:CD1	1:A:103:THR:CG2	0.41	2.97	11	1
1:A:8:LYS:HG3	1:A:9:ASN:N	0.41	2.30	12	1
1:B:35:ARG:NH2	1:B:80:LEU:CD2	0.41	2.80	13	2
1:A:34:THR:CA	1:A:35:ARG:NH2	0.41	2.83	19	1
1:B:45:LEU:N	1:B:45:LEU:HD23	0.41	2.30	20	1
1:B:2:SER:OG	1:B:31:ASN:CB	0.41	2.68	1	1
1:B:59:HIS:H	1:B:90:PHE:HE2	0.41	1.59	1	1
1:A:24:VAL:HB	1:A:94:ILE:HG22	0.41	1.92	3	1
1:A:38:ILE:CD1	1:A:97:ALA:CB	0.41	2.99	3	3
1:A:92:ASN:ND2	1:A:93:GLU:N	0.41	2.69	4	4
1:B:20:TYR:CD1	1:B:40:LEU:HB3	0.41	2.51	4	1
1:A:46:LEU:HD22	1:A:46:LEU:O	0.41	2.16	4	1
1:A:78:LYS:H	1:A:78:LYS:CD	0.41	2.28	4	1
1:A:8:LYS:HA	1:A:20:TYR:HA	0.41	1.93	5	1
1:B:65:PHE:CD1	1:B:65:PHE:N	0.41	2.89	5	1
1:B:25:GLN:HG3	1:B:36:LEU:HB2	0.41	1.93	6	1
1:A:57:THR:HG23	1:A:58:ILE:N	0.41	2.30	6	1
1:B:35:ARG:CZ	1:B:80:LEU:CD2	0.41	2.99	6	1
1:A:9:ASN:OD1	1:A:10:LYS:HD2	0.41	2.15	7	1
1:B:69:THR:HG21	1:B:101:LEU:CD2	0.41	2.45	7	1
1:A:54:LEU:HD23	1:A:69:THR:OG1	0.41	2.15	8	1
1:A:75:VAL:CG2	1:A:79:ILE:HG23	0.41	2.46	8	1
1:B:10:LYS:C	1:B:82:GLU:HB2	0.41	2.36	9	1
1:A:25:GLN:CG	1:A:26:SER:N	0.41	2.84	11	2
1:A:67:MET:HB2	1:A:67:MET:HE2	0.41	1.71	11	1
1:B:22:VAL:CG2	1:B:67:MET:CE	0.41	2.99	12	1
1:A:8:LYS:HD3	1:A:20:TYR:CE2	0.41	2.51	15	2
1:A:101:LEU:CD2	1:B:25:GLN:NE2	0.41	2.84	15	1
1:A:99:ASP:OD2	1:A:105:ILE:HG21	0.41	2.16	16	1
1:B:9:ASN:ND2	1:B:14:SER:CB	0.41	2.84	17	1
1:B:35:ARG:NH1	1:B:80:LEU:CD1	0.41	2.84	17	1
1:A:31:ASN:CB	1:A:35:ARG:NH1	0.41	2.84	17	1
1:B:3:GLN:HA	1:B:23:ASP:CB	0.41	2.46	17	1
1:A:25:GLN:HE21	1:B:101:LEU:HD11	0.41	1.68	18	1
1:A:7:TYR:HB3	1:A:81:SER:OG	0.41	2.16	19	1
1:A:2:SER:HB3	1:A:31:ASN:CB	0.41	2.46	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD12	1:A:84:VAL:CG2	0.41	2.36	20	1
1:B:92:ASN:ND2	1:B:93:GLU:N	0.41	2.69	2	3
1:A:69:THR:HG1	1:A:101:LEU:HD22	0.41	1.72	3	1
1:B:29:LEU:CD2	1:B:32:LEU:HD13	0.41	2.42	3	1
1:B:75:VAL:HG22	1:B:80:LEU:HA	0.41	1.93	3	1
1:B:21:PHE:CA	1:B:39:PRO:HA	0.41	2.46	7	1
1:A:31:ASN:ND2	1:A:35:ARG:NH1	0.41	2.69	12	1
1:A:35:ARG:CD	1:A:80:LEU:CD1	0.41	2.99	12	1
1:A:11:ASP:O	1:A:14:SER:HB2	0.40	2.16	1	2
1:B:21:PHE:HB3	1:B:37:VAL:CG2	0.40	2.46	1	1
1:B:15:ALA:HA	1:B:19:PRO:HA	0.40	1.94	9	4
1:A:9:ASN:N	1:A:81:SER:HB3	0.40	2.30	4	1
1:B:42:PRO:CG	1:B:45:LEU:CD1	0.40	3.00	8	1
1:A:20:TYR:CD1	1:A:40:LEU:HB2	0.40	2.51	10	1
1:A:69:THR:CB	1:A:101:LEU:HD22	0.40	2.45	12	1
1:A:38:ILE:CD1	1:A:94:ILE:CG2	0.40	2.99	13	2
1:A:35:ARG:CD	1:A:80:LEU:HD21	0.40	2.45	16	1
1:A:22:VAL:HG22	1:A:40:LEU:HD21	0.40	1.91	16	1
1:A:22:VAL:O	1:A:24:VAL:CG1	0.40	2.65	18	1
1:A:58:ILE:HD11	1:A:60:ILE:HG12	0.40	1.91	19	1
1:A:64:ASP:O	1:A:65:PHE:CG	0.40	2.73	10	2
1:A:17:THR:HG22	1:A:18:TYR:CE2	0.40	2.51	2	1
1:A:67:MET:CE	1:A:94:ILE:CG1	0.40	3.00	2	1
1:B:54:LEU:O	1:B:69:THR:HG22	0.40	2.16	2	1
1:A:90:PHE:CE2	1:A:93:GLU:OE1	0.40	2.74	3	1
1:A:2:SER:N	1:A:30:ASP:OD2	0.40	2.54	9	1
1:A:72:MET:CE	1:A:101:LEU:HD22	0.40	2.45	10	1
1:A:28:LEU:CD2	1:A:28:LEU:N	0.40	2.85	10	1
1:A:102:ILE:CD1	1:B:102:ILE:HD13	0.40	2.46	11	1
1:A:101:LEU:HD11	1:B:25:GLN:HE22	0.40	1.74	12	1
1:B:56:PRO:HD2	1:B:67:MET:HB3	0.40	1.93	14	1
1:B:43:ILE:CG2	1:B:66:ILE:CG1	0.40	2.98	15	1
1:B:3:GLN:HG2	1:B:4:PHE:CD1	0.40	2.51	17	1
1:A:52:SER:O	1:A:53:HIS:CG	0.40	2.75	19	1
1:B:28:LEU:CD2	1:B:28:LEU:N	0.40	2.84	20	1
1:B:54:LEU:HD12	1:B:54:LEU:N	0.40	2.32	1	1
1:B:10:LYS:CA	1:B:82:GLU:HB2	0.40	2.47	1	1
1:A:24:VAL:CB	1:A:94:ILE:HG22	0.40	2.46	3	1
1:B:20:TYR:C	1:B:40:LEU:HD12	0.40	2.36	6	1
1:A:23:ASP:OD2	1:A:35:ARG:HD2	0.40	2.16	9	2
1:A:3:GLN:CB	1:A:23:ASP:O	0.40	2.69	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:SER:O	1:A:91:ARG:N	0.40	2.47	9	1
1:A:24:VAL:CA	1:A:35:ARG:NH1	0.40	2.84	10	1
1:A:8:LYS:HB2	1:A:20:TYR:CD2	0.40	2.52	10	1
1:A:28:LEU:N	1:A:28:LEU:CD2	0.40	2.84	12	1
1:A:35:ARG:CZ	1:A:80:LEU:HD12	0.40	2.46	12	1
1:B:9:ASN:OD1	1:B:10:LYS:CE	0.40	2.69	13	1
1:A:74:SER:CB	1:B:71:GLN:O	0.40	2.69	13	1
1:B:9:ASN:OD1	1:B:10:LYS:HD2	0.40	2.16	13	1
1:B:20:TYR:O	1:B:39:PRO:HA	0.40	2.17	15	1
1:A:35:ARG:NH2	1:A:77:VAL:N	0.40	2.70	16	1
1:B:43:ILE:HG22	1:B:65:PHE:HA	0.40	1.93	16	1
1:A:54:LEU:CD2	1:A:70:GLN:N	0.40	2.84	18	1
1:A:96:ALA:O	1:A:100:PHE:HB3	0.40	2.16	20	1
1:B:20:TYR:CD1	1:B:40:LEU:CB	0.40	3.04	20	1
1:B:45:LEU:CD2	1:B:45:LEU:N	0.40	2.84	20	1
1:B:28:LEU:N	1:B:28:LEU:CD2	0.40	2.85	1	1
1:B:20:TYR:CD2	1:B:84:VAL:HG11	0.40	2.51	3	1
1:B:7:TYR:CZ	1:B:23:ASP:HB3	0.40	2.51	4	1
1:B:8:LYS:HA	1:B:19:PRO:O	0.40	2.16	4	1
1:A:2:SER:O	1:A:35:ARG:HD3	0.40	2.16	7	1
1:A:19:PRO:HB2	1:A:20:TYR:CD1	0.40	2.52	8	1
1:B:66:ILE:HD12	1:B:66:ILE:H	0.40	1.76	8	1
1:A:65:PHE:O	1:A:66:ILE:HG23	0.40	2.16	9	1
1:A:36:LEU:HD13	1:A:74:SER:OG	0.40	2.16	11	1
1:A:22:VAL:HG22	1:A:40:LEU:HD11	0.40	1.93	11	1
1:A:35:ARG:NH1	1:A:80:LEU:HD12	0.40	2.32	12	1
1:A:23:ASP:HB3	1:A:35:ARG:CZ	0.40	2.46	13	1
1:A:9:ASN:ND2	1:A:14:SER:CB	0.40	2.85	15	1
1:A:35:ARG:CZ	1:A:80:LEU:HG	0.40	2.46	16	1
1:B:41:THR:HG21	1:B:68:LEU:CD1	0.40	2.46	18	1
1:B:99:ASP:OD2	1:B:105:ILE:HD12	0.40	2.14	19	1
1:B:35:ARG:HD2	1:B:80:LEU:HD11	0.40	1.94	1	1
1:B:75:VAL:HG13	1:B:80:LEU:HD13	0.40	1.94	2	1
1:A:33:ASN:C	1:A:34:THR:HG23	0.40	2.37	4	1
1:B:23:ASP:OD2	1:B:35:ARG:CD	0.40	2.69	4	1
1:B:98:ILE:HG12	1:B:102:ILE:HD12	0.40	1.93	5	1
1:B:35:ARG:CD	1:B:80:LEU:CD2	0.40	3.00	6	1
1:B:84:VAL:HG23	1:B:85:ASN:N	0.40	2.31	6	1
1:B:66:ILE:N	1:B:66:ILE:CD1	0.40	2.85	7	1
1:B:58:ILE:HG22	1:B:90:PHE:CD2	0.40	2.51	8	1
1:B:9:ASN:CB	1:B:14:SER:CB	0.40	2.99	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:VAL:N	1:A:35:ARG:HH11	0.40	2.15	10	1
1:B:36:LEU:CD2	1:B:72:MET:CE	0.40	3.00	10	1
1:B:33:ASN:C	1:B:34:THR:HG23	0.40	2.37	12	1
1:A:19:PRO:HB2	1:A:20:TYR:CZ	0.40	2.52	14	1
1:A:20:TYR:CD2	1:A:84:VAL:HG11	0.40	2.51	14	1
1:B:54:LEU:HD11	1:B:101:LEU:HA	0.40	1.93	14	1
1:A:2:SER:HB3	1:A:31:ASN:HB3	0.40	1.94	16	1
1:A:10:LYS:CB	1:A:79:ILE:CG2	0.40	3.00	17	1
1:B:3:GLN:NE2	1:B:4:PHE:CE2	0.40	2.90	19	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/105 (98%)	68±3 (66±3%)	23±3 (22±3%)	12±2 (12±2%)	1	7
1	B	103/105 (98%)	68±4 (66±4%)	24±3 (23±3%)	11±2 (11±2%)	1	9
All	All	4120/4200 (98%)	2724 (66%)	932 (23%)	464 (11%)	1	8

All 51 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	19	PRO	20
1	B	10	LYS	20
1	B	25	GLN	20
1	A	19	PRO	20
1	A	25	GLN	20
1	A	10	LYS	20
1	A	81	SER	19
1	A	39	PRO	18
1	B	81	SER	18
1	B	9	ASN	17
1	A	83	PRO	16
1	B	39	PRO	16

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Mol	Chain	Res	Type	Models (Total)
1	B	80	LEU	14
1	A	72	MET	14
1	A	9	ASN	14
1	B	83	PRO	14
1	A	80	LEU	13
1	A	3	GLN	12
1	B	47	ASP	12
1	B	72	MET	11
1	A	47	ASP	11
1	B	77	VAL	10
1	B	3	GLN	9
1	B	24	VAL	9
1	B	12	LYS	8
1	A	24	VAL	8
1	A	53	HIS	7
1	A	77	VAL	7
1	A	49	LYS	7
1	B	97	ALA	6
1	A	12	LYS	6
1	A	8	LYS	6
1	A	97	ALA	6
1	B	26	SER	4
1	A	2	SER	4
1	A	26	SER	4
1	A	54	LEU	3
1	B	53	HIS	3
1	B	8	LYS	2
1	A	76	PRO	2
1	B	33	ASN	2
1	B	49	LYS	2
1	A	4	PHE	2
1	A	66	ILE	1
1	A	52	SER	1
1	A	55	CYS	1
1	B	32	LEU	1
1	B	2	SER	1
1	B	99	ASP	1
1	B	51	PRO	1
1	B	54	LEU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	98/99 (99%)	63±2 (64±2%)	35±2 (36±2%)	1	9
1	B	99/99 (100%)	63±4 (64±4%)	36±4 (36±4%)	1	8
All	All	3940/3960 (99%)	2526 (64%)	1414 (36%)	1	8

All 154 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	B	101	LEU	20
1	B	87	LEU	20
1	B	91	ARG	20
1	B	66	ILE	20
1	A	20	TYR	20
1	A	66	ILE	20
1	B	10	LYS	20
1	B	21	PHE	20
1	A	41	THR	20
1	A	48	LYS	20
1	A	91	ARG	20
1	B	5	THR	20
1	B	78	LYS	20
1	B	48	LYS	20
1	A	10	LYS	20
1	B	41	THR	20
1	A	21	PHE	20
1	B	20	TYR	20
1	A	101	LEU	20
1	A	87	LEU	20
1	A	78	LYS	20
1	A	35	ARG	20
1	B	93	GLU	19
1	A	93	GLU	19
1	B	81	SER	19
1	A	14	SER	18
1	B	14	SER	18
1	A	58	ILE	18

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Mol	Chain	Res	Type	Models (Total)
1	B	92	ASN	18
1	A	5	THR	18
1	A	81	SER	17
1	A	12	LYS	17
1	B	58	ILE	17
1	A	92	ASN	17
1	B	35	ARG	17
1	B	32	LEU	17
1	A	69	THR	16
1	B	12	LYS	15
1	A	80	LEU	14
1	A	8	LYS	14
1	B	80	LEU	14
1	B	69	THR	14
1	B	8	LYS	14
1	A	11	ASP	14
1	A	7	TYR	14
1	B	7	TYR	14
1	A	82	GLU	14
1	A	32	LEU	13
1	B	68	LEU	13
1	B	79	ILE	13
1	B	73	THR	13
1	A	68	LEU	12
1	A	9	ASN	12
1	B	82	GLU	12
1	A	79	ILE	12
1	B	11	ASP	11
1	B	9	ASN	11
1	B	49	LYS	11
1	B	25	GLN	10
1	A	103	THR	10
1	A	49	LYS	10
1	A	73	THR	10
1	A	74	SER	10
1	A	34	THR	10
1	A	2	SER	10
1	B	2	SER	9
1	A	88	SER	9
1	B	88	SER	9
1	A	54	LEU	9
1	B	72	MET	9

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Mol	Chain	Res	Type	Models (Total)
1	B	34	THR	8
1	B	3	GLN	8
1	B	103	THR	8
1	B	47	ASP	8
1	A	75	VAL	8
1	B	57	THR	7
1	A	85	ASN	7
1	B	71	GLN	7
1	B	40	LEU	7
1	A	64	ASP	7
1	A	47	ASP	7
1	B	74	SER	6
1	B	43	ILE	6
1	B	90	PHE	6
1	B	54	LEU	6
1	A	57	THR	6
1	A	98	ILE	6
1	A	6	LEU	6
1	B	67	MET	6
1	A	67	MET	6
1	A	52	SER	5
1	B	38	ILE	5
1	B	1	MET	5
1	A	90	PHE	5
1	B	52	SER	5
1	B	28	LEU	5
1	B	62	GLU	5
1	A	30	ASP	5
1	B	105	ILE	5
1	B	44	GLU	5
1	A	3	GLN	5
1	A	25	GLN	5
1	B	102	ILE	4
1	B	46	LEU	4
1	B	45	LEU	4
1	B	85	ASN	4
1	A	38	ILE	4
1	A	70	GLN	4
1	A	83	PRO	4
1	B	70	GLN	4
1	A	72	MET	4
1	A	46	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	B	75	VAL	4
1	A	102	ILE	4
1	B	86	GLU	3
1	B	23	ASP	3
1	A	31	ASN	3
1	A	61	ASP	3
1	A	26	SER	3
1	B	13	SER	3
1	A	28	LEU	3
1	B	98	ILE	3
1	A	40	LEU	3
1	B	53	HIS	3
1	A	27	ASP	2
1	A	105	ILE	2
1	B	31	ASN	2
1	A	84	VAL	2
1	B	61	ASP	2
1	A	99	ASP	2
1	A	53	HIS	2
1	A	60	ILE	2
1	A	45	LEU	2
1	B	36	LEU	2
1	B	6	LEU	2
1	B	94	ILE	2
1	B	30	ASP	2
1	A	62	GLU	2
1	A	44	GLU	2
1	B	99	ASP	2
1	A	86	GLU	1
1	A	55	CYS	1
1	A	36	LEU	1
1	B	19	PRO	1
1	A	71	GLN	1
1	A	24	VAL	1
1	B	26	SER	1
1	B	59	HIS	1
1	B	84	VAL	1
1	A	16	LYS	1
1	A	39	PRO	1
1	B	27	ASP	1
1	B	16	LYS	1
1	A	4	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: 2kmt_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2354
Number of shifts mapped to atoms	2354
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	208	0.14 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	200	0.30 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	206	0.25 ± 0.15	None needed (< 0.5 ppm)
^{15}N	188	0.49 ± 0.42	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 2180 atoms were assigned a chemical shift out of a possible 2597. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	986/1017 (97%)	384/404 (95%)	414/418 (99%)	188/195 (96%)
Sidechain	1072/1410 (76%)	630/821 (77%)	434/545 (80%)	8/44 (18%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	122/170 (72%)	62/90 (69%)	60/72 (83%)	0/8 (0%)
Overall	2180/2597 (84%)	1076/1315 (82%)	908/1035 (88%)	196/247 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 2180 atoms were assigned a chemical shift out of a possible 2610. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	986/1022 (96%)	384/406 (95%)	414/420 (99%)	188/196 (96%)
Sidechain	1072/1418 (76%)	630/826 (76%)	434/548 (79%)	8/44 (18%)
Aromatic	122/170 (72%)	62/90 (69%)	60/72 (83%)	0/8 (0%)
Overall	2180/2610 (84%)	1076/1322 (81%)	908/1040 (87%)	196/248 (79%)

7.1.4 Statistically unusual chemical shifts ⓘ

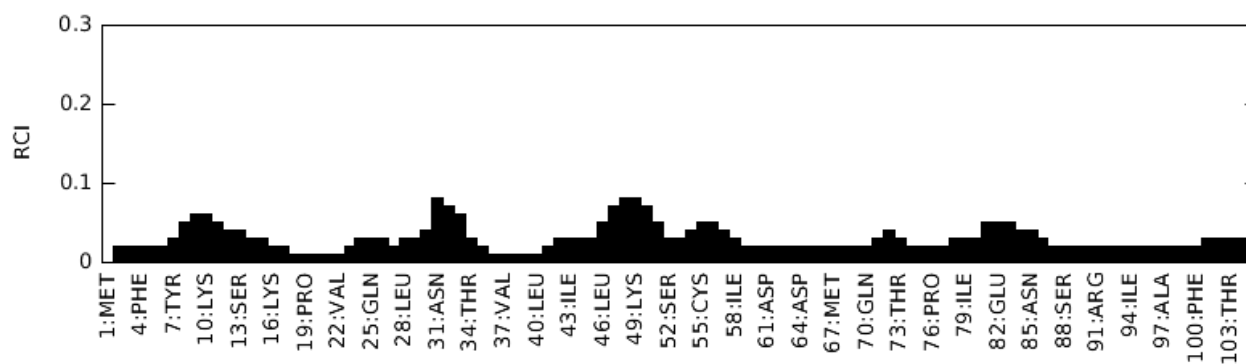
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	41	THR	CG2	15.70	27.15 – 15.95	-5.2
1	B	41	THR	CG2	15.70	27.15 – 15.95	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

