



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:29 PM BST

PDB ID : 1I4V
Title : SOLUTION STRUCTURE OF THE UMUD' HOMODIMER
Authors : Ferentz, A.E.; Walker, G.C.; Wagner, G.
Deposited on : 2001-02-23

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

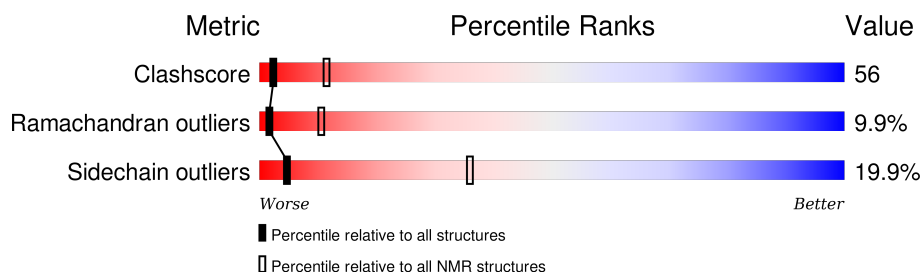
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 66%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	115	
1	B	115	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 6 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:38-A:139, B:38-B:139 (204)	0.79	6

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3474 atoms, of which 1744 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UMUD' PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	115	Total	C	H	N	O	S	0
			1737	550	872	141	171	3	
1	B	115	Total	C	H	N	O	S	0
			1737	550	872	141	171	3	

There are 2 discrepancies between the modelled and reference sequences:

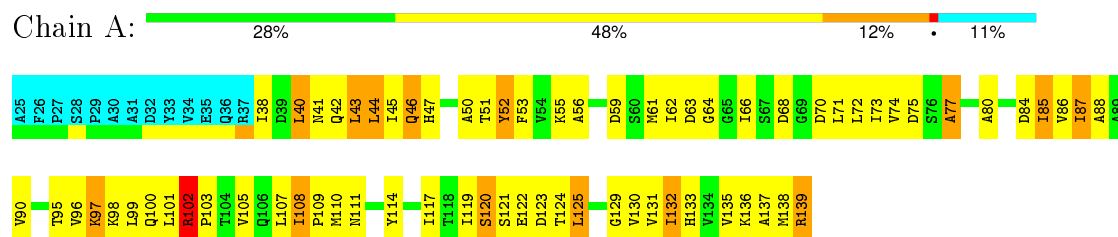
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	GLY	ENGINEERED	UNP P04153
B	25	ALA	GLY	ENGINEERED	UNP P04153

4 Residue-property plots [i](#)

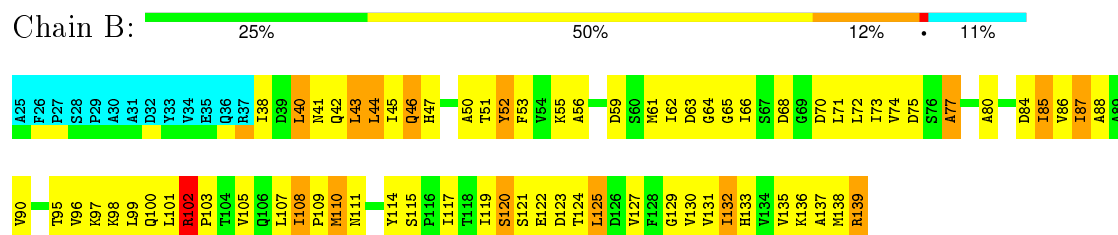
4.1 Average score per residue in the NMR ensemble

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: UMUD' PROTEIN



• Molecule 1: UMUD' PROTEIN

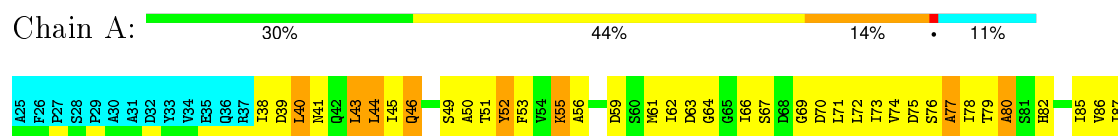


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

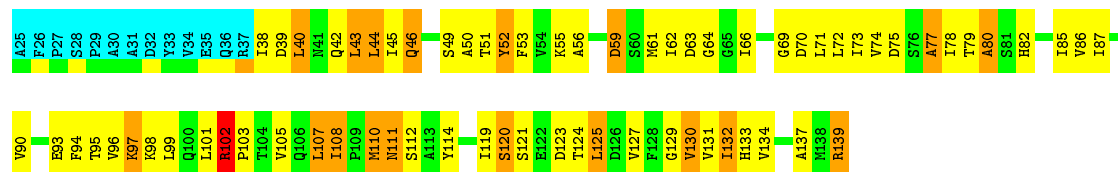
4.2.1 Score per residue for model 1

• Molecule 1: UMUD' PROTEIN



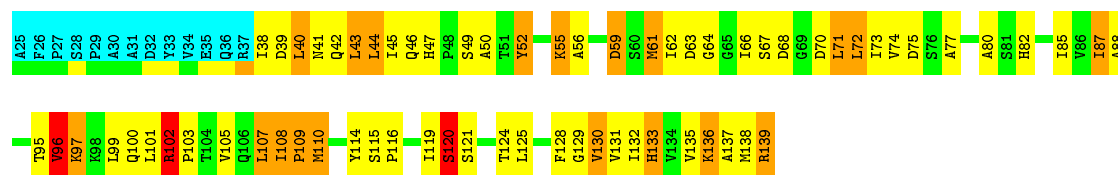


• Molecule 1: UMUD' PROTEIN

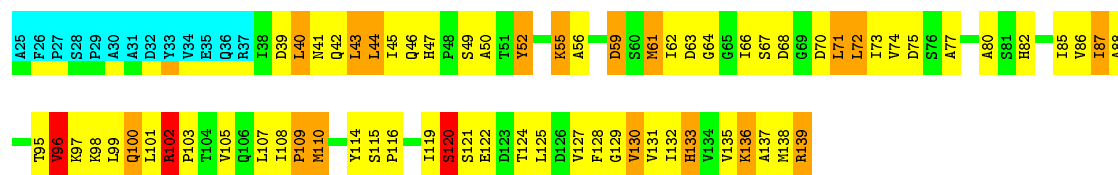


4.2.2 Score per residue for model 2

• Molecule 1: UMUD' PROTEIN

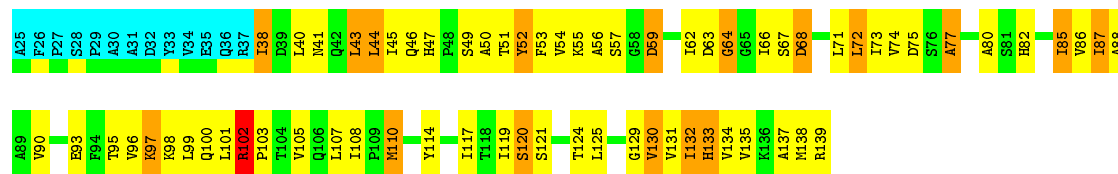
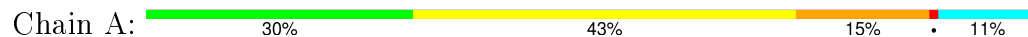


• Molecule 1: UMUD' PROTEIN

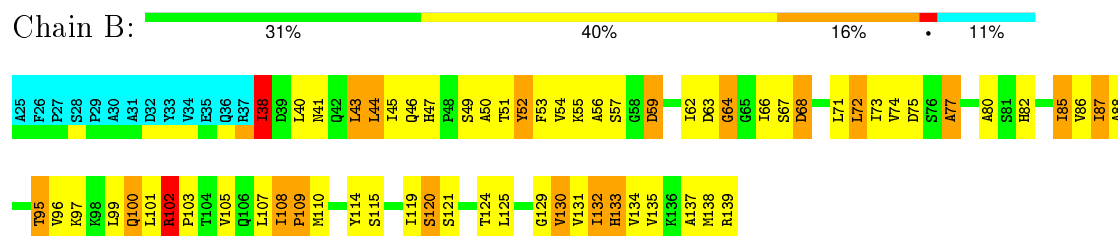


4.2.3 Score per residue for model 3

• Molecule 1: UMUD' PROTEIN

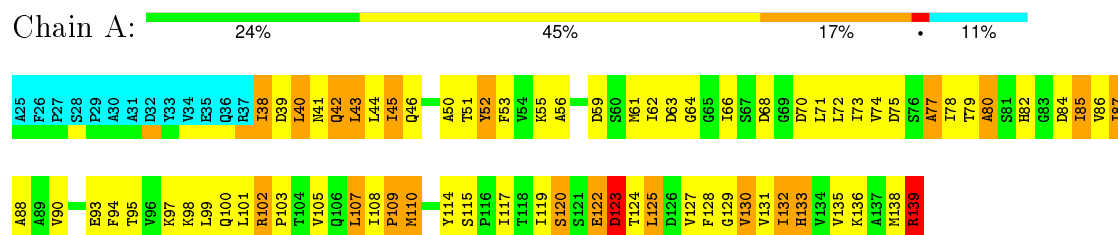


• Molecule 1: UMUD' PROTEIN

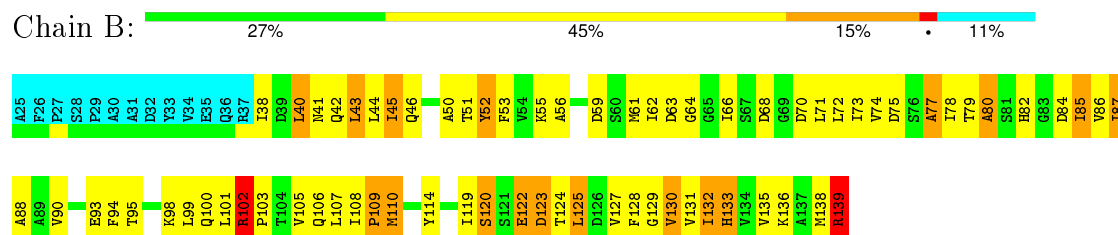


4.2.4 Score per residue for model 4

- Molecule 1: UMUD' PROTEIN

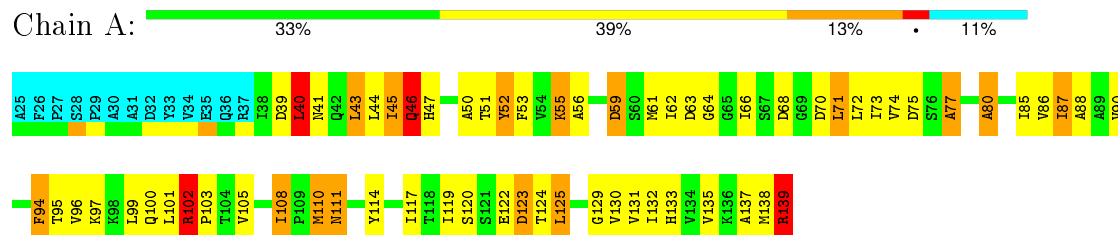


- Molecule 1: UMUD' PROTEIN

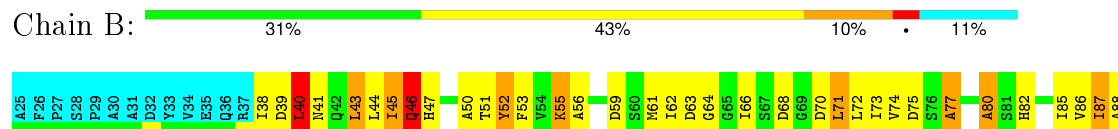


4.2.5 Score per residue for model 5

- Molecule 1: UMUD' PROTEIN



- Molecule 1: UMUD' PROTEIN





4.2.6 Score per residue for model 6 (medoid)

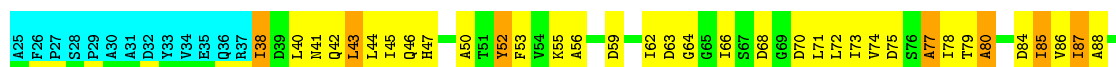
- Molecule 1: UMUD' PROTEIN

Chain A: 30% 47% 10% 11%



- Molecule 1: UMUD' PROTEIN

Chain B: 30% 45% 11% 11%



4.2.7 Score per residue for model 7

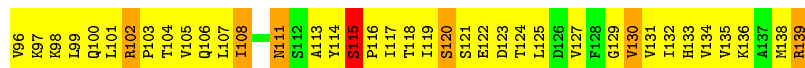
- Molecule 1: UMUD' PROTEIN

Chain A: 21% 54% 10% 11%



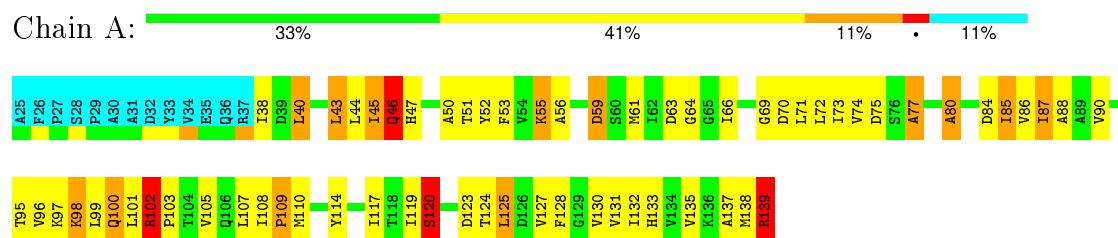
- Molecule 1: UMUD' PROTEIN

Chain B: 22% 53% 11% 11%

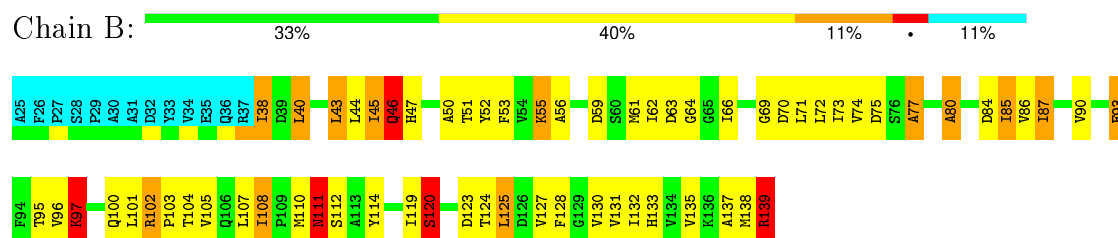


4.2.8 Score per residue for model 8

• Molecule 1: UMUD' PROTEIN

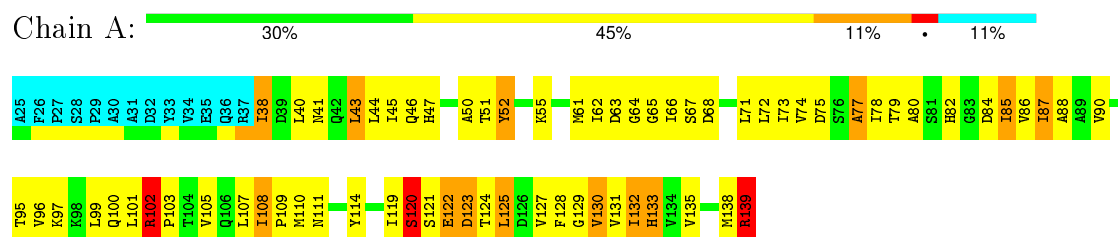


• Molecule 1: UMUD' PROTEIN

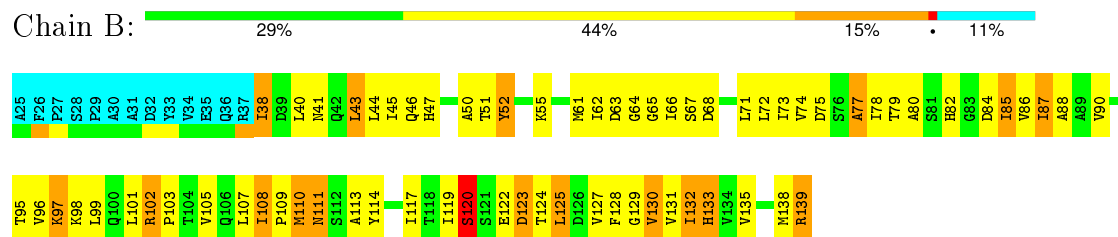


4.2.9 Score per residue for model 9

• Molecule 1: UMUD' PROTEIN



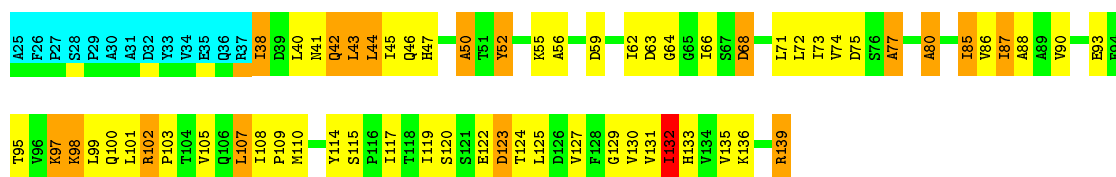
• Molecule 1: UMUD' PROTEIN



4.2.10 Score per residue for model 10

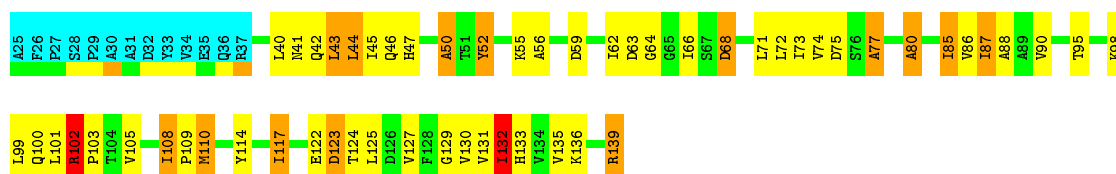
• Molecule 1: UMUD' PROTEIN





• Molecule 1: UMUD' PROTEIN

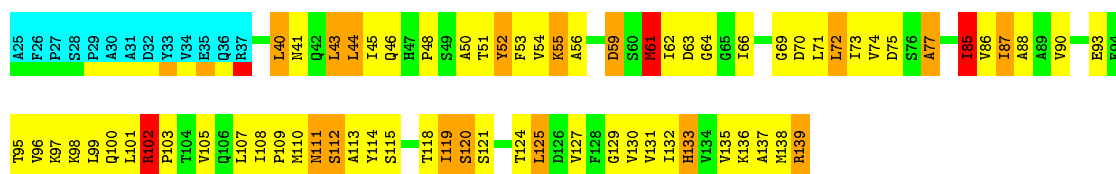
Chain B: 40% 35% 12% 11%



4.2.11 Score per residue for model 11

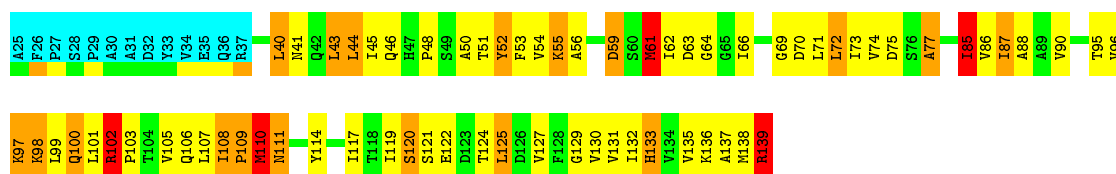
• Molecule 1: UMUD' PROTEIN

Chain A: 28% 44% 14% 11%



• Molecule 1: UMUD' PROTEIN

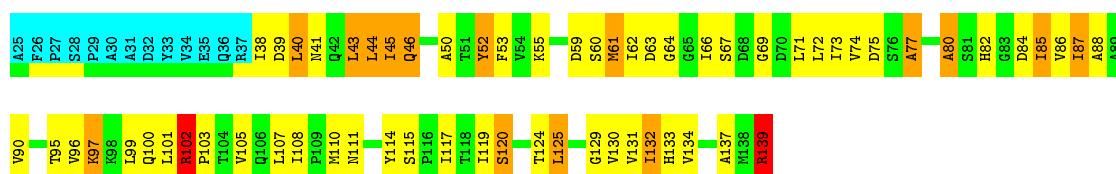
Chain B: 30% 39% 16% 11%



4.2.12 Score per residue for model 12

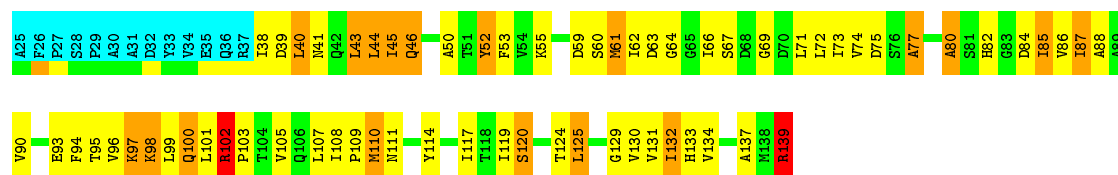
• Molecule 1: UMUD' PROTEIN

Chain A: 34% 40% 13% 11%



- Molecule 1: UMUD' PROTEIN

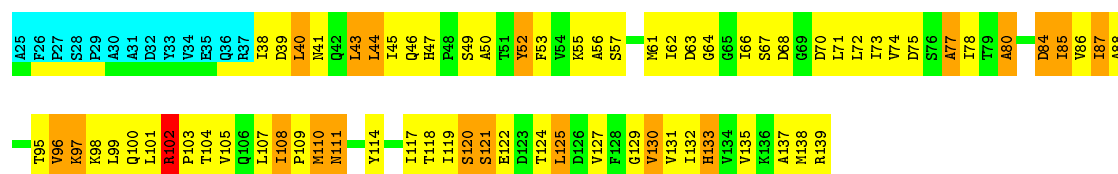
Chain B:



4.2.13 Score per residue for model 13

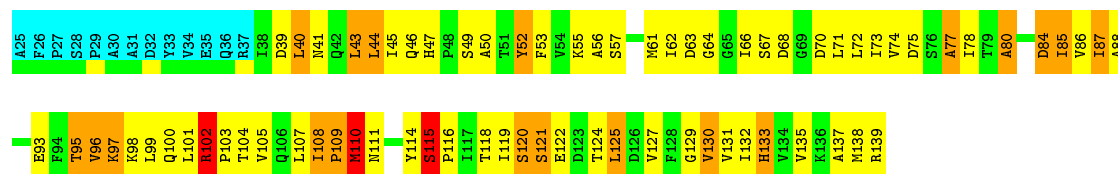
- Molecule 1: UMUD' PROTEIN

Chain A:



- Molecule 1: UMUD' PROTEIN

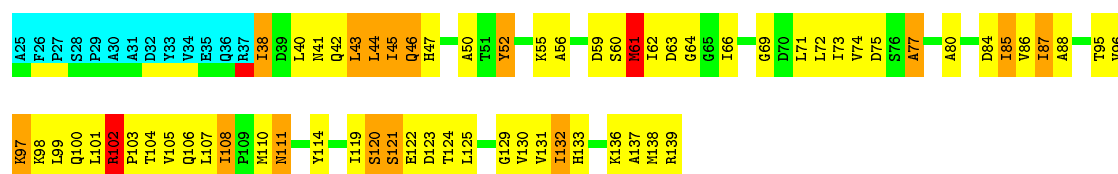
Chain B:



4.2.14 Score per residue for model 14

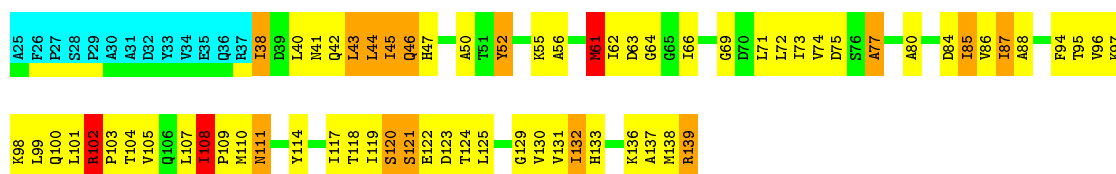
- Molecule 1: UMUD' PROTEIN

Chain A:



- Molecule 1: UMUD' PROTEIN

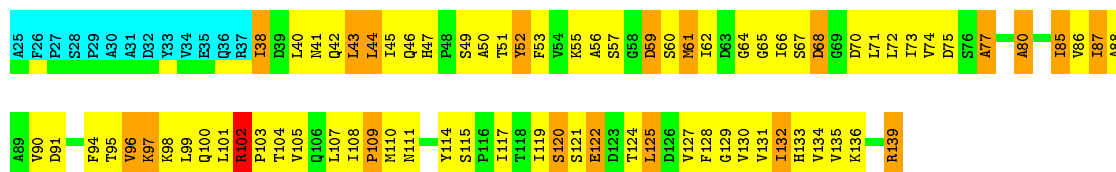
Chain B:



4.2.15 Score per residue for model 15

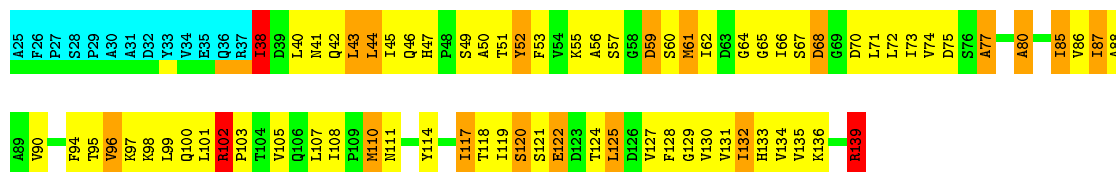
- Molecule 1: UMUD' PROTEIN

Chain A: 22% 50% 17% 11%



- Molecule 1: UMUD' PROTEIN

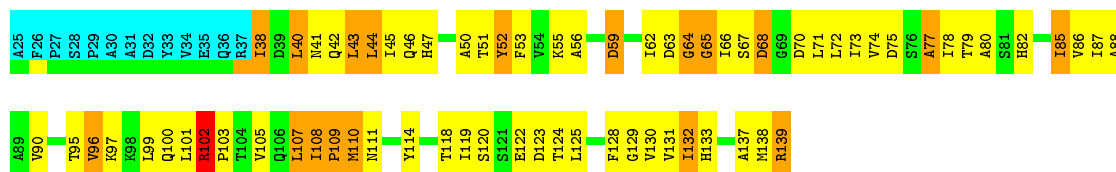
Chain B: 24% 47% 15% 11%



4.2.16 Score per residue for model 16

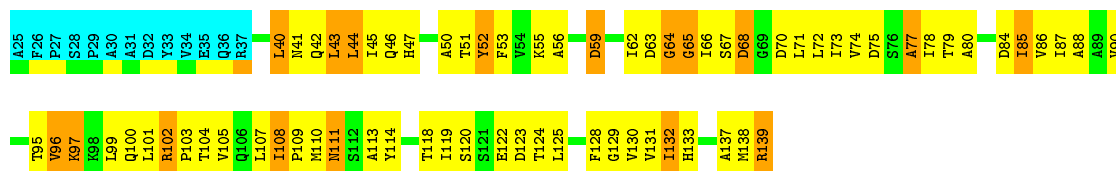
- Molecule 1: UMUD' PROTEIN

Chain A: 28% 44% 16% 11%



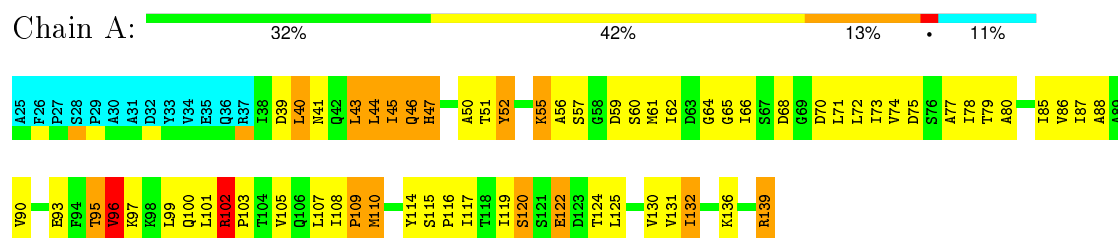
- Molecule 1: UMUD' PROTEIN

Chain B: 27% 47% 15% 11%

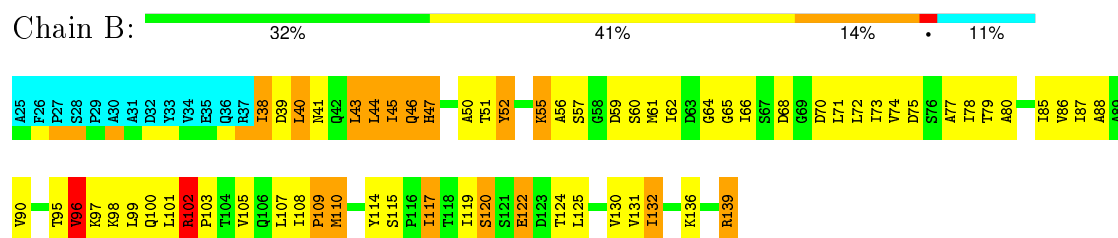


4.2.17 Score per residue for model 17

• Molecule 1: UMUD' PROTEIN

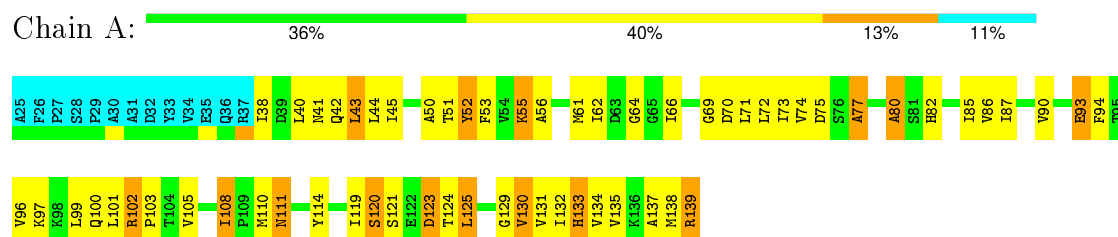


• Molecule 1: UMUD' PROTEIN

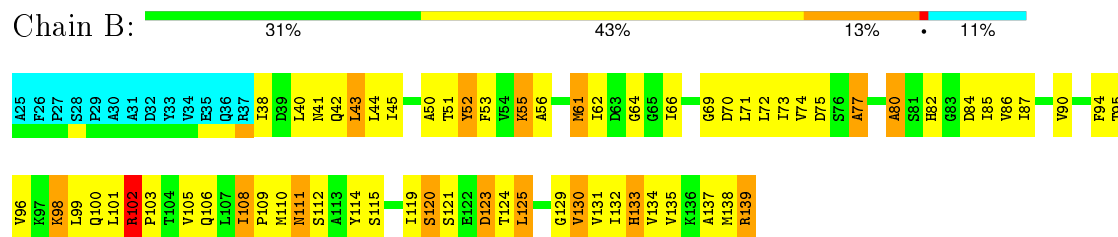


4.2.18 Score per residue for model 18

• Molecule 1: UMUD' PROTEIN



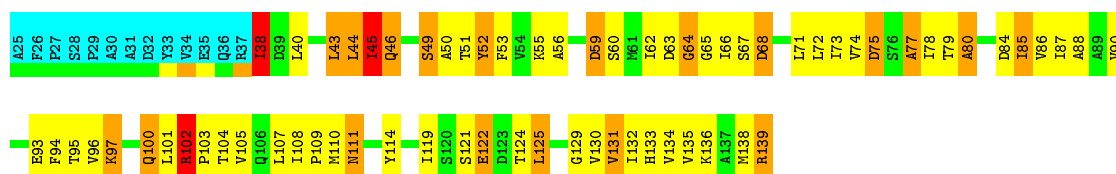
• Molecule 1: UMUD' PROTEIN



4.2.19 Score per residue for model 19

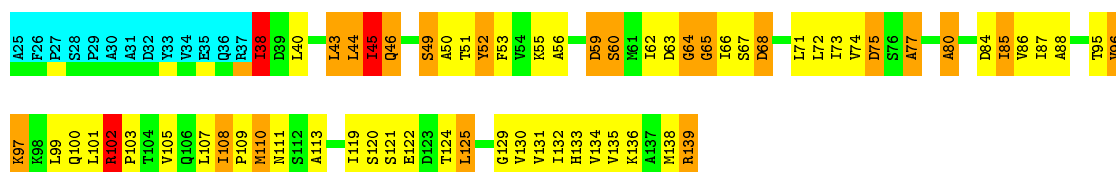
• Molecule 1: UMUD' PROTEIN





• Molecule 1: UMUD' PROTEIN

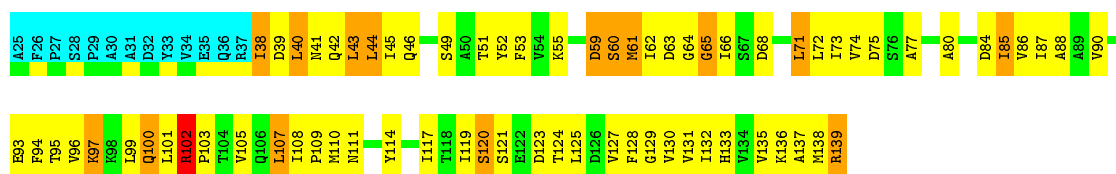
Chain B: 32% 37% 17% 11%



4.2.20 Score per residue for model 20

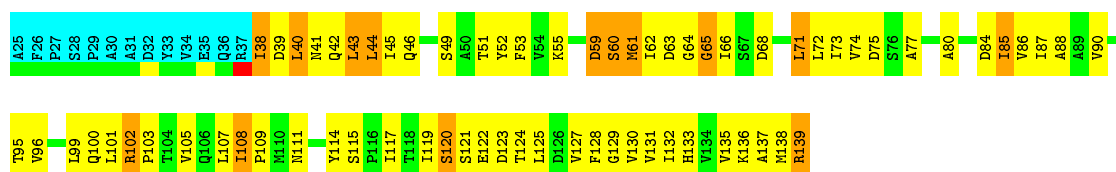
• Molecule 1: UMUD' PROTEIN

Chain A: 26% 49% 13% 11%



• Molecule 1: UMUD' PROTEIN

Chain B: 28% 49% 12% 11%



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 least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851

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

Chemical shift file(s)	BMRB entry 5022
Number of chemical shift lists	1
Total number of shifts	1958
Number of shifts mapped to atoms	1958
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.0±0.0
1	B	0.0±0.0	2.0±0.0
All	All	0	80

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	139	ARG	Sidechain	20
1	B	102	ARG	Sidechain	20
1	A	102	ARG	Sidechain	20
1	A	139	ARG	Sidechain	20

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	763	778	778	100±9
1	B	763	778	778	101±11
All	All	30520	31120	31120	3481

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:HD11	1:B:40:LEU:HD13	1.05	1.27	11	3
1:A:44:LEU:HD23	1:B:44:LEU:HD23	1.04	1.20	8	12
1:B:107:LEU:HD13	1:B:119:ILE:HD11	1.01	1.26	11	2
1:A:40:LEU:HD13	1:B:45:ILE:HD11	1.00	1.29	11	3
1:B:95:THR:HG21	1:B:107:LEU:HD23	1.00	1.29	9	2
1:A:72:LEU:HD11	1:A:132:ILE:HG23	0.96	1.37	10	3
1:A:45:ILE:HD12	1:B:40:LEU:HD13	0.95	1.38	13	1
1:A:40:LEU:HD13	1:B:45:ILE:HD12	0.95	1.38	13	1
1:B:72:LEU:HD11	1:B:132:ILE:HG23	0.94	1.37	10	3
1:A:135:VAL:HG12	1:B:133:HIS:CD2	0.94	1.98	2	1
1:A:133:HIS:CD2	1:B:135:VAL:HG12	0.93	1.98	2	1
1:A:135:VAL:HG22	1:B:135:VAL:HG22	0.93	1.39	10	8
1:A:88:ALA:HB3	1:A:95:THR:CG2	0.91	1.95	2	1
1:B:43:LEU:HD13	1:B:44:LEU:N	0.91	1.80	13	3
1:A:40:LEU:HD23	1:B:40:LEU:HD23	0.90	1.42	18	2
1:A:43:LEU:HD13	1:A:44:LEU:N	0.90	1.80	13	3
1:B:45:ILE:HD13	1:B:51:THR:HG21	0.89	1.44	17	4
1:A:40:LEU:HD11	1:B:45:ILE:HD11	0.89	1.43	7	4
1:A:135:VAL:HG22	1:B:135:VAL:HG13	0.89	1.45	5	9
1:B:95:THR:HG21	1:B:107:LEU:HD11	0.89	1.43	5	1
1:A:40:LEU:HD12	1:B:45:ILE:HD13	0.89	1.43	2	1
1:A:43:LEU:CD1	1:A:44:LEU:HD22	0.88	1.98	11	2
1:A:45:ILE:HD13	1:B:40:LEU:HD12	0.88	1.44	2	1
1:B:43:LEU:CD1	1:B:44:LEU:HD22	0.88	1.98	11	2
1:A:66:ILE:HG23	1:A:72:LEU:HD12	0.88	1.45	5	6
1:B:66:ILE:HG23	1:B:72:LEU:HD12	0.88	1.43	4	6
1:A:62:ILE:HD12	1:A:111:ASN:ND2	0.88	1.82	18	3
1:A:40:LEU:CD1	1:A:44:LEU:HD22	0.88	1.98	8	3
1:A:40:LEU:CD1	1:B:45:ILE:HD11	0.87	1.99	4	5
1:A:107:LEU:HD23	1:A:119:ILE:HD11	0.87	1.43	14	1
1:A:135:VAL:HG13	1:B:135:VAL:HG22	0.87	1.45	5	8
1:A:72:LEU:HD13	1:A:73:ILE:N	0.87	1.84	17	4
1:A:45:ILE:HD11	1:B:40:LEU:CD1	0.87	2.00	4	5
1:B:62:ILE:HD12	1:B:111:ASN:ND2	0.87	1.85	18	5
1:A:107:LEU:HD13	1:A:119:ILE:HD11	0.87	1.46	11	1
1:B:72:LEU:HD23	1:B:73:ILE:N	0.87	1.85	6	14
1:A:45:ILE:HD13	1:A:51:THR:HG21	0.87	1.44	17	4
1:B:88:ALA:HB3	1:B:95:THR:OG1	0.87	1.70	11	15
1:B:40:LEU:CD1	1:B:44:LEU:HD22	0.86	1.99	8	3
1:A:88:ALA:HB3	1:A:95:THR:OG1	0.86	1.71	20	14
1:B:43:LEU:HD11	1:B:44:LEU:HD22	0.86	1.46	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:72:LEU:HD13	1:B:73:ILE:N	0.86	1.85	17	4
1:A:45:ILE:HD11	1:B:40:LEU:HD11	0.85	1.43	7	4
1:A:44:LEU:HD23	1:B:44:LEU:CD2	0.85	2.02	18	5
1:A:44:LEU:CD2	1:B:44:LEU:HD23	0.85	2.02	18	5
1:A:43:LEU:HD11	1:A:44:LEU:HD22	0.85	1.46	11	2
1:B:38:ILE:HD12	1:B:40:LEU:HD23	0.85	1.49	12	1
1:A:72:LEU:HD23	1:A:73:ILE:N	0.84	1.85	6	14
1:B:99:LEU:HD12	1:B:101:LEU:HD21	0.83	1.51	1	8
1:A:64:GLY:O	1:A:96:VAL:HG11	0.83	1.73	3	2
1:B:72:LEU:HD12	1:B:73:ILE:N	0.83	1.88	3	1
1:A:72:LEU:HD12	1:A:73:ILE:N	0.82	1.88	3	1
1:B:107:LEU:HD13	1:B:119:ILE:HD12	0.82	1.50	7	1
1:A:43:LEU:HD13	1:A:44:LEU:HD13	0.82	1.52	10	2
1:B:95:THR:HG21	1:B:107:LEU:CD2	0.82	2.04	9	4
1:A:62:ILE:HG23	1:A:67:SER:OG	0.82	1.74	16	2
1:A:80:ALA:HB1	1:A:86:VAL:HG11	0.81	1.53	4	14
1:A:41:ASN:CB	1:B:40:LEU:HD13	0.81	2.05	5	1
1:A:100:GLN:O	1:A:101:LEU:HD23	0.81	1.73	20	17
1:A:40:LEU:HD13	1:B:41:ASN:CB	0.81	2.04	5	1
1:B:62:ILE:HD12	1:B:111:ASN:CG	0.81	1.96	9	11
1:B:43:LEU:HD22	1:B:43:LEU:O	0.81	1.76	11	2
1:A:40:LEU:HD12	1:A:41:ASN:N	0.81	1.90	15	4
1:B:62:ILE:HG23	1:B:67:SER:OG	0.81	1.76	16	2
1:B:80:ALA:HB1	1:B:86:VAL:HG11	0.81	1.53	4	14
1:A:101:LEU:HD12	1:A:102:ARG:N	0.80	1.91	7	1
1:A:106:GLN:O	1:A:107:LEU:HD12	0.80	1.76	7	1
1:B:40:LEU:HD12	1:B:41:ASN:N	0.80	1.91	3	4
1:B:43:LEU:HD13	1:B:44:LEU:HD13	0.80	1.52	10	2
1:A:43:LEU:HD22	1:A:43:LEU:O	0.80	1.76	11	2
1:A:132:ILE:HG23	1:B:138:MET:O	0.80	1.75	20	1
1:A:45:ILE:HD13	1:A:51:THR:CG2	0.79	2.08	17	3
1:A:138:MET:O	1:B:132:ILE:HG23	0.79	1.75	20	1
1:A:45:ILE:CD1	1:B:40:LEU:HD13	0.79	2.07	13	4
1:B:80:ALA:CB	1:B:86:VAL:HG11	0.78	2.08	10	16
1:A:43:LEU:HD21	1:B:71:LEU:HD11	0.78	1.53	3	1
1:B:100:GLN:O	1:B:101:LEU:HD23	0.78	1.78	6	18
1:A:80:ALA:CB	1:A:86:VAL:HG11	0.78	2.08	10	15
1:A:71:LEU:HD11	1:B:43:LEU:HD21	0.78	1.53	3	1
1:B:45:ILE:HD13	1:B:51:THR:CG2	0.78	2.07	17	3
1:A:40:LEU:HD13	1:B:45:ILE:CD1	0.78	2.07	13	4
1:B:63:ASP:OD2	1:B:108:ILE:HD11	0.78	1.77	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:85:ILE:O	1:B:132:ILE:HD13	0.77	1.79	12	12
1:A:44:LEU:HD11	1:B:73:ILE:HD11	0.77	1.56	18	7
1:A:40:LEU:HD11	1:B:45:ILE:HD12	0.77	1.53	16	3
1:B:64:GLY:O	1:B:96:VAL:HG11	0.77	1.78	3	2
1:A:85:ILE:O	1:A:132:ILE:HD13	0.77	1.79	12	12
1:A:41:ASN:HB3	1:B:40:LEU:HD21	0.77	1.57	2	1
1:A:45:ILE:CD1	1:B:40:LEU:HD21	0.77	2.09	8	5
1:A:40:LEU:HD21	1:B:41:ASN:HB3	0.77	1.57	2	1
1:A:40:LEU:HD21	1:B:45:ILE:CD1	0.76	2.09	8	5
1:A:97:LYS:HD2	1:A:107:LEU:HD12	0.76	1.56	14	1
1:B:88:ALA:HB3	1:B:95:THR:HB	0.76	1.56	5	2
1:A:131:VAL:C	1:A:132:ILE:HD12	0.76	2.01	11	17
1:A:45:ILE:HD12	1:B:40:LEU:HD11	0.76	1.53	16	3
1:A:105:VAL:HG23	1:A:118:THR:HG1	0.76	1.40	16	1
1:B:131:VAL:C	1:B:132:ILE:HD12	0.76	2.01	11	17
1:B:53:PHE:HB3	1:B:73:ILE:HD13	0.76	1.56	11	11
1:A:41:ASN:HA	1:B:40:LEU:HD22	0.76	1.58	18	6
1:A:73:ILE:HD11	1:B:44:LEU:HD11	0.76	1.56	8	7
1:B:64:GLY:O	1:B:85:ILE:HD11	0.76	1.81	6	5
1:A:53:PHE:HB3	1:A:73:ILE:HD13	0.76	1.56	11	11
1:A:64:GLY:O	1:A:85:ILE:HD11	0.75	1.81	6	5
1:A:44:LEU:HB3	1:B:44:LEU:HD23	0.75	1.57	9	8
1:A:82:HIS:NE2	1:A:101:LEU:HD11	0.75	1.97	7	1
1:B:95:THR:HG23	1:B:109:PRO:HB3	0.75	1.58	12	1
1:B:101:LEU:HD13	1:B:125:LEU:O	0.75	1.82	19	10
1:B:64:GLY:HA3	1:B:96:VAL:HG11	0.74	1.58	15	7
1:B:105:VAL:HG11	1:B:120:SER:O	0.74	1.82	11	5
1:A:105:VAL:HG11	1:A:122:GLU:N	0.74	1.97	16	5
1:A:44:LEU:HD23	1:B:44:LEU:HB3	0.74	1.57	9	6
1:B:87:ILE:O	1:B:127:VAL:HG13	0.74	1.83	20	4
1:A:105:VAL:HG23	1:A:118:THR:OG1	0.74	1.81	16	3
1:A:97:LYS:CD	1:A:107:LEU:HD12	0.74	2.12	14	1
1:A:87:ILE:O	1:A:127:VAL:HG13	0.74	1.83	20	4
1:B:45:ILE:CD1	1:B:51:THR:HG21	0.74	2.13	17	1
1:A:45:ILE:HD12	1:B:40:LEU:CD1	0.74	2.13	13	3
1:A:62:ILE:HD12	1:A:111:ASN:CG	0.73	2.03	13	9
1:A:40:LEU:HD22	1:B:41:ASN:HA	0.73	1.58	18	6
1:A:40:LEU:CD1	1:B:45:ILE:HD12	0.73	2.13	13	3
1:A:105:VAL:HG11	1:A:120:SER:O	0.73	1.84	11	3
1:B:62:ILE:HD12	1:B:111:ASN:OD1	0.73	1.82	11	5
1:A:139:ARG:OXT	1:B:85:ILE:HG22	0.72	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:CD1	1:A:51:THR:HG21	0.72	2.13	17	1
1:B:45:ILE:HG23	1:B:51:THR:HG21	0.72	1.60	15	5
1:B:106:GLN:O	1:B:107:LEU:HD12	0.72	1.84	7	1
1:B:75:ASP:HB3	1:B:131:VAL:HG12	0.72	1.62	3	2
1:A:45:ILE:HG21	1:A:51:THR:OG1	0.72	1.85	4	2
1:A:61:MET:HG2	1:A:96:VAL:HG21	0.71	1.60	7	2
1:B:86:VAL:HG12	1:B:130:VAL:HG13	0.71	1.62	20	1
1:B:45:ILE:HG21	1:B:51:THR:OG1	0.71	1.85	4	2
1:A:40:LEU:HD13	1:B:41:ASN:HB3	0.71	1.61	5	1
1:A:133:HIS:NE2	1:B:137:ALA:HB1	0.71	2.01	20	1
1:A:62:ILE:HG23	1:A:67:SER:HB2	0.71	1.62	15	1
1:B:75:ASP:HB2	1:B:131:VAL:HG12	0.71	1.63	12	16
1:B:62:ILE:HG23	1:B:67:SER:HB2	0.71	1.63	15	1
1:A:41:ASN:HB3	1:B:40:LEU:HD13	0.71	1.61	5	1
1:A:137:ALA:HB1	1:B:133:HIS:NE2	0.71	2.00	20	1
1:A:45:ILE:HG23	1:A:51:THR:HG21	0.71	1.60	15	5
1:A:40:LEU:CD2	1:B:40:LEU:HD23	0.70	2.16	18	1
1:A:40:LEU:HD23	1:B:40:LEU:CD2	0.70	2.16	18	1
1:A:64:GLY:CA	1:A:96:VAL:HG11	0.70	2.15	18	4
1:A:71:LEU:HD13	1:A:72:LEU:N	0.70	2.02	19	2
1:A:88:ALA:HB3	1:A:95:THR:HG23	0.70	1.62	2	1
1:A:90:VAL:HB	1:A:125:LEU:HD22	0.70	1.62	12	5
1:B:99:LEU:CB	1:B:107:LEU:HD12	0.70	2.16	3	7
1:A:62:ILE:HD12	1:A:111:ASN:OD1	0.70	1.86	16	8
1:A:108:ILE:HD13	1:A:108:ILE:O	0.70	1.86	18	3
1:B:61:MET:N	1:B:66:ILE:HD11	0.70	2.01	14	6
1:A:64:GLY:HA3	1:A:96:VAL:HG11	0.70	1.63	15	9
1:B:90:VAL:HB	1:B:125:LEU:HD22	0.70	1.62	12	4
1:A:75:ASP:HB3	1:A:131:VAL:HG12	0.70	1.62	3	2
1:A:85:ILE:HG22	1:B:139:ARG:OXT	0.70	1.86	8	1
1:A:75:ASP:N	1:A:131:VAL:HG12	0.70	2.02	19	1
1:B:50:ALA:HB1	1:B:77:ALA:HB2	0.69	1.65	12	17
1:A:86:VAL:HG12	1:A:130:VAL:HG13	0.69	1.63	20	1
1:A:47:HIS:CB	1:A:50:ALA:HB3	0.69	2.18	9	2
1:B:47:HIS:CB	1:B:50:ALA:HB3	0.69	2.18	9	3
1:B:71:LEU:HD13	1:B:72:LEU:N	0.69	2.02	19	2
1:B:108:ILE:HD13	1:B:108:ILE:O	0.69	1.88	1	2
1:B:75:ASP:N	1:B:131:VAL:HG12	0.69	2.02	19	1
1:A:75:ASP:HB2	1:A:131:VAL:HG12	0.69	1.63	12	16
1:A:61:MET:N	1:A:66:ILE:HD11	0.69	2.03	14	6
1:A:45:ILE:HG13	1:B:40:LEU:HD21	0.69	1.63	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:ILE:HG23	1:B:138:MET:C	0.69	2.08	20	1
1:A:99:LEU:CB	1:A:107:LEU:HD12	0.69	2.18	16	5
1:A:45:ILE:CG1	1:B:40:LEU:HD21	0.69	2.17	17	3
1:B:72:LEU:CD1	1:B:132:ILE:HG23	0.69	2.17	10	1
1:A:72:LEU:CD1	1:A:132:ILE:HG23	0.68	2.16	10	1
1:B:64:GLY:CA	1:B:96:VAL:HG11	0.68	2.18	18	3
1:A:40:LEU:HD21	1:B:45:ILE:CG1	0.68	2.17	17	3
1:B:59:ASP:CA	1:B:62:ILE:HD11	0.68	2.18	3	10
1:A:59:ASP:CA	1:A:62:ILE:HD11	0.68	2.19	3	9
1:B:62:ILE:HD12	1:B:111:ASN:HD21	0.68	1.48	18	3
1:A:138:MET:C	1:B:132:ILE:HG23	0.68	2.07	20	1
1:A:50:ALA:HB1	1:A:77:ALA:HB2	0.68	1.65	9	17
1:A:66:ILE:CG2	1:A:72:LEU:HD12	0.68	2.19	18	7
1:A:44:LEU:CD1	1:B:71:LEU:HD12	0.68	2.18	16	11
1:B:99:LEU:HB3	1:B:107:LEU:HD12	0.67	1.66	3	4
1:A:137:ALA:HB2	1:B:133:HIS:CE1	0.67	2.24	2	1
1:B:119:ILE:HD13	1:B:125:LEU:HG	0.67	1.64	14	6
1:B:38:ILE:CD1	1:B:40:LEU:HD23	0.67	2.19	12	1
1:A:133:HIS:CE1	1:B:137:ALA:HB2	0.67	2.24	2	1
1:A:62:ILE:HD12	1:A:111:ASN:HD21	0.67	1.50	18	2
1:B:66:ILE:CG2	1:B:72:LEU:HD12	0.67	2.19	5	6
1:B:66:ILE:O	1:B:66:ILE:HD12	0.67	1.90	3	10
1:A:40:LEU:HD21	1:B:45:ILE:HG13	0.67	1.64	17	3
1:A:71:LEU:HD12	1:B:44:LEU:CD1	0.67	2.18	16	11
1:B:39:ASP:O	1:B:43:LEU:HD12	0.67	1.89	13	1
1:A:66:ILE:O	1:A:66:ILE:HD12	0.67	1.89	3	11
1:A:47:HIS:HB3	1:A:50:ALA:HB3	0.67	1.66	6	7
1:A:71:LEU:HD12	1:B:44:LEU:HD11	0.67	1.66	9	7
1:B:47:HIS:HB3	1:B:50:ALA:HB3	0.66	1.66	6	7
1:B:72:LEU:HD21	1:B:132:ILE:CG2	0.66	2.20	10	3
1:A:71:LEU:HD11	1:A:73:ILE:HD11	0.66	1.67	3	4
1:B:74:VAL:HG23	1:B:131:VAL:HB	0.66	1.67	20	1
1:A:99:LEU:HD21	1:A:127:VAL:HG22	0.66	1.67	13	1
1:B:71:LEU:HD11	1:B:73:ILE:HD11	0.66	1.68	3	4
1:A:74:VAL:HG23	1:A:131:VAL:HB	0.66	1.67	20	1
1:A:85:ILE:HG23	1:A:85:ILE:O	0.66	1.91	8	13
1:B:80:ALA:HB2	1:B:130:VAL:HA	0.66	1.67	6	7
1:A:64:GLY:HA2	1:A:85:ILE:HD11	0.66	1.65	5	5
1:B:85:ILE:HG23	1:B:85:ILE:O	0.66	1.90	11	6
1:A:119:ILE:HD13	1:A:125:LEU:HG	0.66	1.68	2	5
1:A:99:LEU:HD12	1:A:101:LEU:HD21	0.66	1.67	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:HD12	1:B:40:LEU:CG	0.66	2.21	16	4
1:A:40:LEU:CG	1:B:45:ILE:HD12	0.66	2.21	16	4
1:A:85:ILE:O	1:A:85:ILE:HG23	0.66	1.90	11	7
1:B:131:VAL:O	1:B:132:ILE:HD13	0.66	1.91	13	2
1:A:40:LEU:HD13	1:B:41:ASN:HA	0.65	1.67	15	4
1:A:99:LEU:HB2	1:A:107:LEU:HD12	0.65	1.66	16	5
1:A:44:LEU:HD11	1:B:71:LEU:HD12	0.65	1.66	9	7
1:A:131:VAL:O	1:A:132:ILE:HD13	0.65	1.91	13	2
1:B:64:GLY:HA2	1:B:85:ILE:HD11	0.65	1.66	5	5
1:A:73:ILE:HD11	1:B:43:LEU:CD1	0.65	2.21	4	6
1:A:72:LEU:HD21	1:A:132:ILE:CG2	0.65	2.20	10	3
1:A:105:VAL:HG12	1:A:119:ILE:HB	0.65	1.68	2	2
1:A:43:LEU:CD1	1:B:73:ILE:HD11	0.65	2.22	4	6
1:A:44:LEU:HD23	1:B:44:LEU:HB2	0.65	1.66	2	4
1:A:105:VAL:HG13	1:A:105:VAL:O	0.65	1.92	7	2
1:B:61:MET:HG2	1:B:96:VAL:HG21	0.65	1.69	9	2
1:A:44:LEU:HB2	1:B:44:LEU:HD23	0.65	1.67	2	4
1:A:131:VAL:HG21	1:A:133:HIS:NE2	0.65	2.07	1	4
1:B:88:ALA:HB2	1:B:99:LEU:HD22	0.65	1.67	7	1
1:A:80:ALA:HB2	1:A:130:VAL:HA	0.65	1.67	6	7
1:B:99:LEU:HB2	1:B:107:LEU:HD12	0.65	1.69	14	5
1:A:39:ASP:O	1:A:43:LEU:HD12	0.65	1.92	13	1
1:B:105:VAL:HG13	1:B:105:VAL:O	0.64	1.92	14	2
1:A:105:VAL:HG11	1:A:122:GLU:H	0.64	1.52	19	5
1:A:84:ASP:O	1:A:86:VAL:HG22	0.64	1.93	7	2
1:A:41:ASN:HA	1:B:40:LEU:HD13	0.64	1.68	15	4
1:B:52:TYR:O	1:B:74:VAL:HG12	0.64	1.92	2	19
1:B:85:ILE:O	1:B:85:ILE:HG23	0.64	1.91	8	14
1:A:99:LEU:HD22	1:A:127:VAL:CG2	0.64	2.23	7	1
1:A:138:MET:HB3	1:B:85:ILE:HD13	0.64	1.68	13	1
1:B:66:ILE:HD12	1:B:66:ILE:O	0.64	1.93	19	10
1:A:52:TYR:O	1:A:74:VAL:HG12	0.64	1.92	2	19
1:A:108:ILE:HD13	1:A:116:PRO:N	0.64	2.08	2	3
1:A:107:LEU:O	1:A:117:ILE:HG22	0.64	1.91	13	1
1:B:131:VAL:HG21	1:B:133:HIS:NE2	0.64	2.07	1	4
1:A:85:ILE:HD13	1:B:138:MET:HB3	0.64	1.69	13	1
1:A:61:MET:CG	1:A:96:VAL:HG21	0.64	2.22	7	1
1:A:105:VAL:HG11	1:A:119:ILE:O	0.64	1.92	7	1
1:B:61:MET:H	1:B:66:ILE:HD11	0.64	1.53	1	9
1:A:132:ILE:HD12	1:A:132:ILE:N	0.64	2.08	19	1
1:B:84:ASP:O	1:B:86:VAL:HG22	0.63	1.93	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:105:VAL:HG22	1:B:119:ILE:HB	0.63	1.70	18	2
1:A:64:GLY:HA2	1:A:96:VAL:HG11	0.63	1.71	18	1
1:B:61:MET:SD	1:B:95:THR:HG22	0.63	2.33	18	1
1:A:45:ILE:HD11	1:B:40:LEU:HD21	0.63	1.70	1	4
1:B:105:VAL:HG21	1:B:120:SER:O	0.63	1.94	20	5
1:A:131:VAL:HG23	1:B:139:ARG:HB3	0.63	1.69	5	7
1:B:95:THR:HG23	1:B:109:PRO:HG3	0.63	1.70	5	1
1:A:139:ARG:HB3	1:B:131:VAL:HG23	0.63	1.70	5	7
1:A:66:ILE:HD12	1:A:66:ILE:O	0.63	1.93	19	9
1:A:72:LEU:N	1:A:72:LEU:HD23	0.63	2.09	11	1
1:A:40:LEU:HD21	1:B:45:ILE:HD11	0.63	1.69	1	4
1:A:101:LEU:HD13	1:A:125:LEU:O	0.63	1.94	18	11
1:B:132:ILE:HD12	1:B:132:ILE:N	0.63	2.09	19	2
1:A:99:LEU:HB3	1:A:107:LEU:HD12	0.62	1.70	4	1
1:B:108:ILE:O	1:B:108:ILE:HG23	0.62	1.94	7	5
1:A:82:HIS:CE1	1:A:101:LEU:HD11	0.62	2.28	7	1
1:A:59:ASP:CB	1:A:62:ILE:HD11	0.62	2.25	19	8
1:A:133:HIS:CE1	1:B:137:ALA:HB1	0.62	2.29	18	4
1:A:105:VAL:O	1:A:105:VAL:HG13	0.62	1.94	10	1
1:B:95:THR:HG23	1:B:109:PRO:CB	0.62	2.23	12	1
1:A:61:MET:H	1:A:66:ILE:HD11	0.62	1.52	1	9
1:A:87:ILE:HD11	1:A:94:PHE:CD2	0.62	2.29	5	1
1:A:63:ASP:OD2	1:A:108:ILE:HD11	0.62	1.95	11	1
1:A:43:LEU:C	1:A:43:LEU:HD13	0.62	2.15	11	1
1:B:72:LEU:HD23	1:B:72:LEU:N	0.62	2.10	11	1
1:A:40:LEU:CG	1:A:44:LEU:HD22	0.62	2.25	18	1
1:A:59:ASP:HB2	1:A:62:ILE:HD11	0.62	1.71	16	8
1:A:87:ILE:HD11	1:A:94:PHE:CE2	0.62	2.30	5	1
1:B:97:LYS:CG	1:B:108:ILE:HG23	0.62	2.25	15	1
1:B:59:ASP:HB2	1:B:62:ILE:HD11	0.61	1.71	16	8
1:B:43:LEU:HD13	1:B:43:LEU:C	0.61	2.15	11	3
1:B:105:VAL:O	1:B:105:VAL:HG13	0.61	1.95	18	1
1:B:97:LYS:HG2	1:B:108:ILE:HG23	0.61	1.72	15	1
1:B:59:ASP:CB	1:B:62:ILE:HD11	0.61	2.25	4	7
1:A:105:VAL:O	1:A:105:VAL:HG23	0.61	1.95	15	6
1:A:43:LEU:C	1:A:43:LEU:HD22	0.61	2.14	11	1
1:B:43:LEU:HD22	1:B:43:LEU:C	0.61	2.15	11	2
1:B:108:ILE:O	1:B:108:ILE:HD13	0.61	1.96	18	1
1:A:133:HIS:CD2	1:B:137:ALA:HB1	0.61	2.31	5	1
1:A:71:LEU:HD11	1:B:43:LEU:HD22	0.61	1.73	20	4
1:A:41:ASN:CB	1:B:40:LEU:HD21	0.61	2.25	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:LEU:HD12	1:B:40:LEU:C	0.61	2.15	9	1
1:B:105:VAL:HG23	1:B:105:VAL:O	0.61	1.96	20	8
1:A:43:LEU:HD22	1:A:43:LEU:C	0.61	2.14	3	1
1:B:99:LEU:HD21	1:B:127:VAL:HG22	0.61	1.72	13	1
1:B:82:HIS:CE1	1:B:101:LEU:HD11	0.61	2.31	9	1
1:A:137:ALA:HB1	1:B:133:HIS:CE1	0.61	2.31	18	4
1:A:105:VAL:HG21	1:A:122:GLU:HA	0.61	1.73	10	1
1:A:124:THR:O	1:A:125:LEU:HD22	0.61	1.96	17	14
1:A:64:GLY:O	1:A:132:ILE:HG21	0.61	1.96	3	3
1:A:71:LEU:HD22	1:A:72:LEU:N	0.60	2.11	5	6
1:A:105:VAL:HG23	1:A:105:VAL:O	0.60	1.96	6	8
1:A:108:ILE:C	1:A:108:ILE:HD13	0.60	2.16	1	2
1:A:85:ILE:HD11	1:A:96:VAL:CG1	0.60	2.26	3	1
1:B:71:LEU:HD22	1:B:72:LEU:N	0.60	2.11	5	6
1:B:88:ALA:CB	1:B:107:LEU:HD11	0.60	2.26	14	1
1:B:105:VAL:O	1:B:105:VAL:HG23	0.60	1.96	15	7
1:B:101:LEU:HD23	1:B:125:LEU:HB3	0.60	1.72	9	1
1:B:108:ILE:C	1:B:108:ILE:HD13	0.60	2.16	18	3
1:A:40:LEU:HD21	1:B:41:ASN:CB	0.60	2.25	13	2
1:A:40:LEU:HG	1:A:43:LEU:HD12	0.60	1.72	11	1
1:A:43:LEU:HD11	1:A:44:LEU:CD1	0.60	2.27	5	5
1:B:72:LEU:HD21	1:B:132:ILE:HG23	0.60	1.72	16	4
1:B:108:ILE:HD13	1:B:110:MET:N	0.60	2.11	14	1
1:A:43:LEU:HD13	1:A:43:LEU:C	0.60	2.15	13	2
1:A:72:LEU:HD21	1:A:132:ILE:HG23	0.60	1.73	16	4
1:A:43:LEU:HD22	1:B:71:LEU:HD11	0.60	1.73	20	4
1:B:108:ILE:HG23	1:B:108:ILE:O	0.60	1.96	9	7
1:B:99:LEU:HD22	1:B:127:VAL:CG2	0.60	2.27	9	1
1:B:43:LEU:HD11	1:B:44:LEU:CD1	0.60	2.26	5	5
1:B:132:ILE:O	1:B:132:ILE:HG22	0.60	1.97	8	6
1:A:124:THR:C	1:A:125:LEU:HD22	0.60	2.17	10	3
1:B:40:LEU:HG	1:B:43:LEU:HD12	0.60	1.73	11	1
1:B:43:LEU:CD2	1:B:44:LEU:HD13	0.60	2.26	13	1
1:B:64:GLY:O	1:B:132:ILE:HG21	0.60	1.96	3	2
1:B:124:THR:O	1:B:125:LEU:HD22	0.60	1.96	17	14
1:B:130:VAL:O	1:B:130:VAL:HG22	0.60	1.97	13	9
1:B:132:ILE:HG22	1:B:132:ILE:O	0.59	1.97	3	10
1:A:38:ILE:HG23	1:A:38:ILE:O	0.59	1.96	13	5
1:B:101:LEU:HD13	1:B:125:LEU:HB3	0.59	1.72	13	2
1:A:43:LEU:CD2	1:A:44:LEU:HD13	0.59	2.26	13	1
1:A:108:ILE:O	1:A:108:ILE:HG23	0.59	1.97	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:VAL:HG21	1:A:120:SER:O	0.59	1.97	1	4
1:A:73:ILE:HD11	1:B:43:LEU:HD13	0.59	1.74	15	6
1:B:38:ILE:HG23	1:B:38:ILE:O	0.59	1.97	20	3
1:A:137:ALA:HB1	1:B:133:HIS:CD2	0.59	2.33	5	1
1:A:95:THR:HG23	1:A:109:PRO:HB3	0.59	1.74	19	1
1:A:40:LEU:C	1:A:40:LEU:HD12	0.59	2.16	9	1
1:B:40:LEU:CG	1:B:44:LEU:HD22	0.59	2.26	18	1
1:A:90:VAL:HG23	1:A:124:THR:O	0.59	1.98	4	13
1:B:45:ILE:HG21	1:B:51:THR:HG21	0.59	1.73	7	3
1:A:132:ILE:O	1:A:132:ILE:HG22	0.59	1.97	3	7
1:B:124:THR:C	1:B:125:LEU:HD22	0.59	2.17	10	3
1:B:90:VAL:HG23	1:B:124:THR:O	0.59	1.97	4	13
1:A:130:VAL:O	1:A:130:VAL:HG22	0.59	1.97	13	9
1:B:96:VAL:H	1:B:108:ILE:HD12	0.59	1.56	16	1
1:A:71:LEU:HD13	1:A:71:LEU:C	0.59	2.18	3	5
1:A:45:ILE:HG21	1:A:51:THR:HG21	0.59	1.73	7	3
1:A:45:ILE:CG2	1:A:51:THR:HG21	0.59	2.27	7	2
1:B:87:ILE:O	1:B:87:ILE:HG23	0.59	1.98	16	9
1:A:132:ILE:HG22	1:A:132:ILE:O	0.59	1.97	8	9
1:A:40:LEU:HD13	1:B:45:ILE:HG13	0.58	1.73	9	1
1:B:131:VAL:O	1:B:132:ILE:HD12	0.58	1.98	8	4
1:B:71:LEU:HD13	1:B:71:LEU:C	0.58	2.18	3	6
1:A:130:VAL:HG22	1:A:130:VAL:O	0.58	1.97	3	9
1:B:72:LEU:HD13	1:B:132:ILE:HG23	0.58	1.74	3	1
1:B:45:ILE:CG2	1:B:51:THR:HG21	0.58	2.28	7	2
1:A:54:VAL:CG1	1:A:72:LEU:HD23	0.58	2.28	3	1
1:A:45:ILE:HG13	1:B:40:LEU:HD13	0.58	1.74	9	1
1:A:85:ILE:HD13	1:A:85:ILE:C	0.58	2.19	10	4
1:A:72:LEU:HD13	1:A:132:ILE:HG23	0.58	1.74	3	1
1:A:131:VAL:O	1:A:132:ILE:HD12	0.58	1.98	8	3
1:B:64:GLY:HA2	1:B:96:VAL:HG11	0.58	1.74	18	1
1:B:99:LEU:H	1:B:99:LEU:HD23	0.58	1.59	13	5
1:B:85:ILE:C	1:B:85:ILE:HD13	0.58	2.19	10	2
1:A:40:LEU:HG	1:A:44:LEU:HD22	0.58	1.76	18	1
1:A:75:ASP:CB	1:A:131:VAL:HG12	0.58	2.28	3	4
1:B:108:ILE:HD13	1:B:108:ILE:C	0.58	2.19	8	2
1:A:64:GLY:C	1:A:96:VAL:HG11	0.58	2.18	3	2
1:B:54:VAL:CG1	1:B:72:LEU:HD23	0.58	2.28	3	1
1:A:99:LEU:HD23	1:A:99:LEU:H	0.58	1.59	2	8
1:A:87:ILE:O	1:A:87:ILE:HG23	0.57	1.98	16	8
1:A:71:LEU:C	1:A:71:LEU:HD13	0.57	2.19	11	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:HD22	1:B:45:ILE:HD12	0.57	1.76	6	1
1:A:74:VAL:HG23	1:A:131:VAL:O	0.57	1.99	12	8
1:A:108:ILE:HD11	1:A:115:SER:N	0.57	2.13	15	5
1:A:131:VAL:HG21	1:A:133:HIS:CE1	0.57	2.35	7	6
1:A:135:VAL:CG2	1:B:135:VAL:HG22	0.57	2.27	3	1
1:A:40:LEU:HA	1:A:43:LEU:HD23	0.57	1.77	8	4
1:B:130:VAL:HG22	1:B:130:VAL:O	0.57	1.98	9	9
1:A:108:ILE:HG23	1:A:108:ILE:O	0.57	1.98	19	5
1:A:105:VAL:HG22	1:A:119:ILE:HB	0.57	1.77	20	2
1:B:40:LEU:HA	1:B:43:LEU:HD23	0.57	1.77	8	4
1:A:71:LEU:HD11	1:B:44:LEU:HD11	0.57	1.76	18	5
1:A:43:LEU:HD13	1:B:73:ILE:HD11	0.57	1.74	15	6
1:B:59:ASP:HA	1:B:62:ILE:HD11	0.57	1.76	3	5
1:A:38:ILE:HG23	1:B:53:PHE:HE2	0.57	1.59	6	1
1:B:74:VAL:HG23	1:B:131:VAL:O	0.57	1.99	12	8
1:A:88:ALA:HB3	1:A:95:THR:HG1	0.57	1.60	10	3
1:B:82:HIS:NE2	1:B:101:LEU:HD11	0.57	2.15	9	1
1:B:71:LEU:C	1:B:71:LEU:HD13	0.56	2.21	19	8
1:B:107:LEU:HD13	1:B:119:ILE:CD1	0.56	2.15	11	2
1:B:131:VAL:HG21	1:B:133:HIS:CE1	0.56	2.35	7	6
1:A:45:ILE:HD12	1:B:40:LEU:HG	0.56	1.76	20	2
1:B:75:ASP:CB	1:B:131:VAL:HG12	0.56	2.29	3	3
1:A:38:ILE:O	1:A:38:ILE:HG23	0.56	1.99	4	3
1:A:99:LEU:HD13	1:A:107:LEU:CD1	0.56	2.30	16	3
1:B:101:LEU:HD12	1:B:102:ARG:N	0.56	2.15	9	1
1:A:40:LEU:HG	1:B:45:ILE:HD12	0.56	1.77	20	2
1:A:107:LEU:HB2	1:A:119:ILE:HD11	0.56	1.77	13	3
1:A:59:ASP:HA	1:A:62:ILE:HD11	0.56	1.76	3	6
1:A:62:ILE:HD12	1:A:111:ASN:CB	0.56	2.30	7	1
1:A:45:ILE:HD12	1:B:40:LEU:HD22	0.56	1.75	6	1
1:A:117:ILE:HG23	1:A:117:ILE:O	0.56	2.00	7	4
1:B:99:LEU:HD13	1:B:107:LEU:CD1	0.56	2.31	15	5
1:B:52:TYR:HB2	1:B:74:VAL:HG13	0.56	1.77	20	1
1:B:85:ILE:HD13	1:B:85:ILE:C	0.56	2.20	3	3
1:B:117:ILE:O	1:B:117:ILE:HG23	0.56	2.00	14	4
1:B:95:THR:HG21	1:B:107:LEU:HD21	0.56	1.77	4	2
1:B:40:LEU:HG	1:B:44:LEU:HD22	0.56	1.77	18	1
1:A:44:LEU:HD11	1:B:71:LEU:HD11	0.56	1.76	18	5
1:B:99:LEU:HD23	1:B:99:LEU:H	0.56	1.61	20	10
1:B:63:ASP:CG	1:B:108:ILE:HD11	0.56	2.21	13	1
1:A:108:ILE:HD13	1:A:115:SER:C	0.55	2.21	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:HG12	1:A:51:THR:HG21	0.55	1.78	19	1
1:B:105:VAL:HG11	1:B:119:ILE:O	0.55	2.01	14	1
1:A:78:ILE:HD13	1:A:130:VAL:HG11	0.55	1.77	13	1
1:B:45:ILE:HG12	1:B:51:THR:HG21	0.55	1.78	19	1
1:A:52:TYR:HB2	1:A:74:VAL:HG13	0.55	1.77	20	1
1:B:64:GLY:C	1:B:96:VAL:HG11	0.55	2.22	19	2
1:B:72:LEU:C	1:B:72:LEU:HD23	0.55	2.21	7	4
1:B:78:ILE:HD13	1:B:130:VAL:HG11	0.55	1.78	13	1
1:A:45:ILE:CD1	1:B:40:LEU:HD11	0.55	2.25	7	2
1:B:80:ALA:HB1	1:B:86:VAL:CG1	0.55	2.32	15	6
1:B:65:GLY:O	1:B:72:LEU:HD12	0.55	2.02	19	2
1:A:43:LEU:HD12	1:A:43:LEU:N	0.55	2.17	10	2
1:B:101:LEU:HD12	1:B:101:LEU:C	0.55	2.22	9	1
1:A:101:LEU:HD13	1:A:125:LEU:HB3	0.55	1.77	13	2
1:B:38:ILE:H	1:B:38:ILE:HD13	0.55	1.61	9	1
1:A:72:LEU:HD23	1:A:72:LEU:C	0.55	2.21	7	6
1:B:38:ILE:O	1:B:38:ILE:HG23	0.55	2.02	6	3
1:B:105:VAL:HG11	1:B:122:GLU:H	0.55	1.62	17	4
1:B:43:LEU:N	1:B:43:LEU:HD12	0.55	2.17	10	2
1:B:62:ILE:HD12	1:B:111:ASN:CB	0.54	2.32	7	2
1:B:87:ILE:HG23	1:B:87:ILE:O	0.54	2.02	10	9
1:A:65:GLY:C	1:A:72:LEU:HD23	0.54	2.23	20	1
1:A:40:LEU:HD12	1:B:45:ILE:CD1	0.54	2.28	2	1
1:A:82:HIS:CE1	1:A:101:LEU:CD1	0.54	2.91	7	1
1:A:38:ILE:CG1	1:A:40:LEU:HD23	0.54	2.32	1	1
1:A:80:ALA:HB1	1:A:86:VAL:CG1	0.54	2.32	15	4
1:A:96:VAL:H	1:A:108:ILE:HD12	0.54	1.61	11	2
1:B:134:VAL:HG23	1:B:134:VAL:O	0.54	2.03	3	1
1:B:102:ARG:HB2	1:B:103:PRO:HD3	0.54	1.80	8	2
1:A:135:VAL:HG22	1:B:135:VAL:CG2	0.54	2.27	3	1
1:A:87:ILE:HG23	1:A:87:ILE:O	0.54	2.03	20	10
1:B:105:VAL:HG11	1:B:122:GLU:CB	0.54	2.32	5	1
1:B:65:GLY:C	1:B:72:LEU:HD23	0.54	2.23	20	1
1:A:65:GLY:O	1:A:72:LEU:HD12	0.54	2.03	19	2
1:B:82:HIS:CE1	1:B:101:LEU:CD1	0.54	2.90	9	1
1:B:43:LEU:CD1	1:B:44:LEU:CD1	0.54	2.86	7	5
1:B:72:LEU:HD11	1:B:131:VAL:CG2	0.54	2.33	20	1
1:B:99:LEU:CD1	1:B:101:LEU:HD11	0.54	2.32	14	3
1:A:47:HIS:N	1:A:47:HIS:CD2	0.54	2.76	17	1
1:B:45:ILE:HD12	1:B:51:THR:HG21	0.54	1.78	15	1
1:B:61:MET:CG	1:B:96:VAL:HG21	0.53	2.33	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:95:THR:HG21	1:B:107:LEU:CD1	0.53	2.25	5	1
1:B:54:VAL:HG12	1:B:72:LEU:HG	0.53	1.80	3	1
1:B:96:VAL:N	1:B:108:ILE:HD12	0.53	2.18	16	1
1:B:105:VAL:HG11	1:B:122:GLU:CA	0.53	2.32	20	2
1:B:99:LEU:HD21	1:B:127:VAL:CG2	0.53	2.34	13	1
1:B:88:ALA:HB3	1:B:95:THR:HG1	0.53	1.62	19	1
1:A:43:LEU:CD1	1:A:44:LEU:CD1	0.53	2.86	7	5
1:A:56:ALA:HB1	1:A:66:ILE:CA	0.53	2.34	18	8
1:B:108:ILE:HD11	1:B:115:SER:N	0.53	2.19	5	3
1:B:105:VAL:HG11	1:B:122:GLU:HB2	0.53	1.80	5	2
1:A:43:LEU:CD1	1:B:53:PHE:CD2	0.53	2.92	19	1
1:B:56:ALA:HB1	1:B:66:ILE:CA	0.53	2.34	18	8
1:B:134:VAL:O	1:B:134:VAL:HG23	0.53	2.03	19	2
1:A:119:ILE:HG21	1:A:125:LEU:HD21	0.53	1.80	1	1
1:B:105:VAL:HG23	1:B:118:THR:OG1	0.53	2.02	16	2
1:A:71:LEU:HD11	1:A:73:ILE:CD1	0.53	2.33	3	2
1:A:72:LEU:HD11	1:A:131:VAL:CG2	0.53	2.33	20	1
1:B:74:VAL:HG13	1:B:74:VAL:O	0.53	2.04	17	1
1:A:134:VAL:O	1:A:134:VAL:HG23	0.53	2.03	19	2
1:B:71:LEU:HD11	1:B:73:ILE:CD1	0.53	2.33	3	2
1:A:102:ARG:CB	1:A:103:PRO:HD3	0.53	2.34	11	19
1:A:133:HIS:NE2	1:B:135:VAL:HG12	0.53	2.19	2	1
1:A:73:ILE:CD1	1:B:44:LEU:HD21	0.53	2.34	7	1
1:A:119:ILE:HG21	1:A:125:LEU:HD23	0.53	1.80	11	2
1:A:74:VAL:O	1:A:74:VAL:HG13	0.53	2.04	17	1
1:A:45:ILE:HD12	1:A:51:THR:HG21	0.53	1.78	15	1
1:A:53:PHE:CD2	1:B:43:LEU:CD1	0.53	2.92	19	1
1:A:40:LEU:HA	1:A:43:LEU:HD11	0.53	1.81	10	2
1:A:44:LEU:HD21	1:B:73:ILE:CD1	0.52	2.34	7	1
1:A:54:VAL:HG12	1:A:72:LEU:HG	0.52	1.80	3	1
1:B:90:VAL:HG21	1:B:125:LEU:HD21	0.52	1.79	8	1
1:B:105:VAL:HG11	1:B:122:GLU:N	0.52	2.18	15	5
1:A:97:LYS:HD2	1:A:108:ILE:HG23	0.52	1.81	6	2
1:B:72:LEU:HD23	1:B:72:LEU:C	0.52	2.25	14	7
1:A:105:VAL:HG21	1:A:122:GLU:CA	0.52	2.33	10	1
1:A:52:TYR:CB	1:A:74:VAL:HG13	0.52	2.35	20	8
1:A:72:LEU:C	1:A:72:LEU:HD13	0.52	2.24	17	3
1:A:40:LEU:HD11	1:B:45:ILE:CD1	0.52	2.25	7	2
1:B:102:ARG:CB	1:B:103:PRO:HD3	0.52	2.35	11	19
1:B:105:VAL:HG21	1:B:119:ILE:O	0.52	2.04	9	1
1:A:40:LEU:HD12	1:A:40:LEU:C	0.52	2.25	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:LEU:C	1:B:40:LEU:HD12	0.52	2.25	13	2
1:B:71:LEU:HD13	1:B:71:LEU:O	0.52	2.05	15	1
1:A:102:ARG:N	1:A:103:PRO:CD	0.52	2.72	13	1
1:B:40:LEU:O	1:B:40:LEU:HD13	0.52	2.05	10	1
1:A:97:LYS:HG2	1:A:108:ILE:HG23	0.52	1.82	16	2
1:A:114:TYR:CD2	1:A:114:TYR:O	0.52	2.63	13	7
1:B:40:LEU:HA	1:B:43:LEU:HD11	0.52	1.80	10	2
1:A:102:ARG:CB	1:A:103:PRO:CD	0.52	2.87	11	19
1:B:63:ASP:O	1:B:85:ILE:HD11	0.52	2.05	20	1
1:A:73:ILE:HD11	1:B:43:LEU:HD11	0.52	1.81	4	2
1:A:99:LEU:H	1:A:99:LEU:HD23	0.52	1.63	15	5
1:A:108:ILE:HD13	1:A:108:ILE:C	0.52	2.24	18	1
1:A:135:VAL:HG12	1:B:133:HIS:NE2	0.52	2.19	2	1
1:A:72:LEU:C	1:A:72:LEU:HD23	0.52	2.25	19	5
1:B:72:LEU:C	1:B:72:LEU:HD13	0.52	2.24	17	4
1:A:63:ASP:O	1:A:85:ILE:HD11	0.52	2.05	20	1
1:B:108:ILE:HD13	1:B:115:SER:C	0.51	2.26	5	5
1:A:101:LEU:HD11	1:A:125:LEU:HB3	0.51	1.82	11	2
1:A:90:VAL:HG21	1:A:125:LEU:HD21	0.51	1.80	8	1
1:B:47:HIS:N	1:B:47:HIS:CD2	0.51	2.76	17	1
1:B:85:ILE:O	1:B:85:ILE:CG2	0.51	2.59	11	9
1:B:101:LEU:HD11	1:B:125:LEU:HB3	0.51	1.81	11	1
1:B:38:ILE:N	1:B:38:ILE:HD13	0.51	2.20	9	1
1:A:134:VAL:HG23	1:A:134:VAL:O	0.51	2.04	1	1
1:B:119:ILE:HG21	1:B:125:LEU:HD23	0.51	1.83	11	4
1:A:85:ILE:CG2	1:A:85:ILE:O	0.51	2.59	11	4
1:A:100:GLN:C	1:A:101:LEU:HD23	0.51	2.25	20	4
1:B:52:TYR:CB	1:B:74:VAL:HG13	0.51	2.35	20	7
1:B:102:ARG:CB	1:B:103:PRO:CD	0.51	2.89	11	18
1:A:102:ARG:HB2	1:A:103:PRO:HD3	0.51	1.81	10	2
1:A:40:LEU:HD11	1:A:44:LEU:HD22	0.51	1.81	8	2
1:B:108:ILE:HD13	1:B:116:PRO:N	0.51	2.21	2	1
1:B:105:VAL:HG12	1:B:119:ILE:HB	0.51	1.83	7	1
1:B:114:TYR:CD2	1:B:114:TYR:O	0.51	2.64	14	6
1:B:86:VAL:HG21	1:B:127:VAL:HG21	0.51	1.83	11	3
1:B:109:PRO:O	1:B:110:MET:CB	0.51	2.58	11	11
1:B:102:ARG:N	1:B:103:PRO:CD	0.51	2.74	14	3
1:B:72:LEU:HD12	1:B:72:LEU:C	0.51	2.26	3	1
1:A:43:LEU:HD11	1:B:73:ILE:CD1	0.51	2.36	12	3
1:B:90:VAL:CB	1:B:125:LEU:HD22	0.51	2.36	5	3
1:A:95:THR:HG23	1:A:109:PRO:CB	0.51	2.35	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:85:ILE:HG21	1:B:132:ILE:HD12	0.50	1.83	20	1
1:A:102:ARG:HB2	1:A:103:PRO:CD	0.50	2.36	10	1
1:B:94:PHE:O	1:B:95:THR:HG23	0.50	2.06	1	1
1:A:72:LEU:HD12	1:A:72:LEU:C	0.50	2.26	3	1
1:A:85:ILE:HD13	1:A:85:ILE:O	0.50	2.06	3	1
1:A:62:ILE:HD12	1:A:111:ASN:HB2	0.50	1.83	7	1
1:A:73:ILE:CD1	1:B:43:LEU:HD11	0.50	2.36	12	3
1:A:105:VAL:HG11	1:A:122:GLU:CB	0.50	2.37	5	1
1:B:100:GLN:C	1:B:101:LEU:HD23	0.50	2.26	16	6
1:B:114:TYR:O	1:B:114:TYR:CD2	0.50	2.65	10	7
1:A:45:ILE:HD12	1:B:40:LEU:HD21	0.50	1.84	16	2
1:B:52:TYR:HB3	1:B:74:VAL:HG13	0.50	1.83	17	1
1:A:52:TYR:HB3	1:A:74:VAL:HG13	0.50	1.83	17	1
1:A:107:LEU:HG	1:A:108:ILE:HG22	0.50	1.84	13	1
1:A:43:LEU:HD11	1:B:73:ILE:HD11	0.50	1.82	4	2
1:A:39:ASP:O	1:A:41:ASN:N	0.50	2.45	2	1
1:A:71:LEU:HD11	1:B:44:LEU:CD1	0.50	2.36	6	5
1:A:119:ILE:HG21	1:A:125:LEU:CD2	0.50	2.37	1	3
1:A:139:ARG:CB	1:B:131:VAL:HG23	0.50	2.37	5	1
1:A:40:LEU:HD13	1:A:40:LEU:O	0.50	2.05	10	1
1:B:118:THR:HG23	1:B:118:THR:O	0.50	2.06	7	1
1:B:87:ILE:HG22	1:B:129:GLY:O	0.50	2.07	20	1
1:B:39:ASP:O	1:B:41:ASN:N	0.50	2.45	2	1
1:B:43:LEU:HG	1:B:44:LEU:HD13	0.50	1.84	7	4
1:A:90:VAL:CB	1:A:125:LEU:HD22	0.50	2.36	5	3
1:A:85:ILE:HG21	1:A:132:ILE:HD12	0.50	1.82	20	1
1:A:71:LEU:HD13	1:A:71:LEU:O	0.50	2.05	15	1
1:A:114:TYR:O	1:A:114:TYR:CD2	0.50	2.65	9	8
1:A:87:ILE:HG22	1:A:129:GLY:O	0.50	2.07	20	1
1:A:72:LEU:N	1:A:72:LEU:CD2	0.50	2.74	11	1
1:A:137:ALA:CB	1:B:133:HIS:CE1	0.50	2.94	11	2
1:A:44:LEU:HD23	1:B:44:LEU:CB	0.49	2.37	13	6
1:B:80:ALA:HA	1:B:130:VAL:HG23	0.49	1.84	4	3
1:A:72:LEU:HD21	1:A:132:ILE:HG22	0.49	1.84	17	1
1:A:44:LEU:HD11	1:B:135:VAL:HG21	0.49	1.83	11	1
1:A:133:HIS:CE1	1:B:137:ALA:CB	0.49	2.95	11	2
1:A:45:ILE:CD1	1:B:40:LEU:HD12	0.49	2.28	2	1
1:A:44:LEU:CD1	1:B:71:LEU:HD11	0.49	2.36	6	5
1:B:107:LEU:HD21	1:B:125:LEU:HD12	0.49	1.84	7	1
1:A:137:ALA:CB	1:B:133:HIS:CD2	0.49	2.95	8	4
1:A:41:ASN:HB2	1:B:40:LEU:HD21	0.49	1.84	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:114:TYR:O	1:B:114:TYR:CD1	0.49	2.65	4	1
1:A:86:VAL:HG21	1:A:127:VAL:HG21	0.49	1.83	11	2
1:B:85:ILE:HD13	1:B:85:ILE:O	0.49	2.08	3	2
1:A:63:ASP:OD1	1:A:64:GLY:N	0.49	2.44	5	17
1:A:44:LEU:CB	1:B:44:LEU:HD23	0.49	2.37	13	6
1:A:133:HIS:CD2	1:B:137:ALA:CB	0.49	2.95	8	4
1:A:82:HIS:CE1	1:A:101:LEU:CG	0.49	2.95	7	1
1:B:107:LEU:CD1	1:B:119:ILE:HD11	0.49	2.18	11	1
1:A:101:LEU:HD12	1:A:101:LEU:C	0.49	2.27	7	1
1:B:117:ILE:HG23	1:B:117:ILE:O	0.49	2.07	6	3
1:A:85:ILE:HD13	1:B:138:MET:CG	0.49	2.38	14	1
1:B:102:ARG:HB2	1:B:103:PRO:CD	0.49	2.36	8	1
1:A:114:TYR:CD1	1:A:114:TYR:O	0.49	2.66	17	2
1:A:131:VAL:HG23	1:B:139:ARG:CB	0.49	2.37	5	1
1:A:97:LYS:N	1:A:97:LYS:CE	0.49	2.75	20	1
1:B:40:LEU:HD12	1:B:44:LEU:HD22	0.49	1.81	8	1
1:A:43:LEU:HG	1:A:44:LEU:HD13	0.49	1.84	7	4
1:A:50:ALA:HB1	1:A:77:ALA:CB	0.49	2.36	12	2
1:B:106:GLN:C	1:B:107:LEU:HD12	0.49	2.26	7	1
1:B:50:ALA:HB1	1:B:77:ALA:CB	0.49	2.36	12	2
1:A:137:ALA:N	1:B:133:HIS:CD2	0.49	2.81	2	1
1:A:80:ALA:HA	1:A:130:VAL:HG23	0.48	1.85	4	3
1:A:54:VAL:CG1	1:A:72:LEU:CD1	0.48	2.91	11	1
1:B:117:ILE:HD13	1:B:118:THR:N	0.48	2.23	15	1
1:A:107:LEU:HB3	1:A:117:ILE:HG23	0.48	1.83	13	1
1:A:56:ALA:HB1	1:A:66:ILE:HA	0.48	1.85	18	2
1:B:119:ILE:HG22	1:B:120:SER:N	0.48	2.23	7	14
1:B:108:ILE:O	1:B:108:ILE:CG2	0.48	2.61	14	2
1:A:82:HIS:CE1	1:A:101:LEU:HG	0.48	2.43	7	1
1:A:45:ILE:CD1	1:B:40:LEU:CD1	0.48	2.91	19	2
1:A:131:VAL:HG23	1:B:139:ARG:HB2	0.48	1.84	18	4
1:B:43:LEU:HD12	1:B:44:LEU:N	0.48	2.23	9	2
1:B:72:LEU:HD21	1:B:132:ILE:HG22	0.48	1.85	17	1
1:B:72:LEU:CD2	1:B:72:LEU:N	0.48	2.75	11	1
1:A:43:LEU:HD11	1:B:53:PHE:CB	0.48	2.38	15	1
1:A:40:LEU:HD21	1:B:41:ASN:HB2	0.48	1.84	13	1
1:A:40:LEU:HD13	1:A:40:LEU:C	0.48	2.29	10	1
1:A:38:ILE:HG23	1:B:53:PHE:CE2	0.48	2.42	6	1
1:B:114:TYR:CD1	1:B:114:TYR:N	0.48	2.82	8	1
1:A:133:HIS:CD2	1:B:137:ALA:N	0.48	2.81	2	1
1:A:85:ILE:HG22	1:B:139:ARG:C	0.48	2.29	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LEU:HD13	1:A:72:LEU:C	0.48	2.28	10	1
1:A:86:VAL:HG21	1:A:127:VAL:CG2	0.48	2.38	9	3
1:A:45:ILE:HG22	1:A:46:GLN:N	0.48	2.24	13	6
1:B:40:LEU:C	1:B:40:LEU:HD13	0.48	2.29	10	1
1:B:56:ALA:HB1	1:B:66:ILE:HA	0.48	1.85	18	2
1:A:40:LEU:HD21	1:B:45:ILE:HD12	0.48	1.84	16	2
1:B:119:ILE:HG21	1:B:125:LEU:CD2	0.48	2.39	9	2
1:B:75:ASP:CB	1:B:131:VAL:CG1	0.48	2.92	3	2
1:B:73:ILE:O	1:B:131:VAL:HG13	0.48	2.09	19	1
1:A:52:TYR:CB	1:A:74:VAL:CG1	0.48	2.92	20	3
1:B:63:ASP:OD1	1:B:64:GLY:N	0.48	2.47	5	17
1:B:114:TYR:CG	1:B:114:TYR:O	0.48	2.67	11	4
1:B:38:ILE:CD1	1:B:38:ILE:N	0.48	2.77	9	1
1:B:45:ILE:HG22	1:B:46:GLN:N	0.48	2.24	6	6
1:B:108:ILE:CD1	1:B:108:ILE:O	0.48	2.62	8	2
1:B:114:TYR:O	1:B:114:TYR:CG	0.48	2.66	9	5
1:B:54:VAL:CG1	1:B:72:LEU:CD1	0.48	2.91	11	1
1:A:75:ASP:CB	1:A:131:VAL:CG1	0.48	2.92	3	2
1:A:45:ILE:HD12	1:B:40:LEU:CD2	0.48	2.39	16	1
1:A:139:ARG:C	1:B:85:ILE:HG22	0.48	2.29	7	3
1:A:95:THR:HG21	1:A:107:LEU:HD21	0.48	1.85	6	3
1:A:95:THR:HG21	1:A:107:LEU:HG	0.48	1.86	19	1
1:A:95:THR:OG1	1:A:107:LEU:HD21	0.48	2.09	3	2
1:A:43:LEU:HD12	1:A:44:LEU:N	0.48	2.24	9	2
1:A:73:ILE:CD1	1:B:43:LEU:CD1	0.47	2.92	4	5
1:B:119:ILE:HG21	1:B:125:LEU:HD21	0.47	1.84	1	1
1:A:71:LEU:CD1	1:B:44:LEU:CD1	0.47	2.91	16	7
1:A:44:LEU:CD1	1:B:71:LEU:CD1	0.47	2.91	16	8
1:A:108:ILE:O	1:A:108:ILE:HD13	0.47	2.08	5	1
1:B:43:LEU:CD1	1:B:44:LEU:N	0.47	2.77	9	2
1:A:71:LEU:HD21	1:B:43:LEU:HD21	0.47	1.85	4	1
1:B:99:LEU:HD22	1:B:127:VAL:HG22	0.47	1.85	9	1
1:B:84:ASP:N	1:B:98:LYS:CG	0.47	2.76	18	1
1:B:52:TYR:CB	1:B:74:VAL:CG1	0.47	2.92	20	3
1:A:80:ALA:CB	1:A:86:VAL:CG1	0.47	2.92	14	5
1:A:40:LEU:CD1	1:A:44:LEU:HD21	0.47	2.39	14	1
1:B:40:LEU:CD1	1:B:44:LEU:HD21	0.47	2.39	14	1
1:B:95:THR:HG21	1:B:107:LEU:HD12	0.47	1.85	8	1
1:A:139:ARG:HB2	1:B:131:VAL:HG23	0.47	1.85	18	2
1:B:86:VAL:HG21	1:B:127:VAL:CG2	0.47	2.39	9	3
1:A:105:VAL:CG1	1:A:105:VAL:O	0.47	2.63	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:105:VAL:CG1	1:B:105:VAL:O	0.47	2.62	14	1
1:B:80:ALA:CB	1:B:86:VAL:CG1	0.47	2.92	14	4
1:B:46:GLN:O	1:B:47:HIS:CG	0.47	2.68	13	1
1:A:73:ILE:O	1:A:131:VAL:HG13	0.47	2.09	19	1
1:A:43:LEU:CD1	1:A:44:LEU:N	0.47	2.78	10	2
1:A:64:GLY:CA	1:A:96:VAL:CG1	0.47	2.91	18	1
1:A:78:ILE:HG22	1:A:79:THR:N	0.47	2.25	7	8
1:A:40:LEU:CD1	1:B:40:LEU:CD1	0.47	2.92	6	2
1:A:108:ILE:CD1	1:A:115:SER:N	0.47	2.78	4	5
1:A:137:ALA:CB	1:B:133:HIS:NE2	0.47	2.78	16	3
1:A:63:ASP:HB3	1:A:110:MET:HB2	0.47	1.87	5	2
1:A:40:LEU:HD13	1:B:41:ASN:HB2	0.47	1.83	5	1
1:A:95:THR:HG21	1:A:107:LEU:CG	0.47	2.39	19	1
1:A:40:LEU:CD2	1:B:45:ILE:HD12	0.47	2.39	16	1
1:B:40:LEU:CD1	1:B:44:LEU:CD2	0.47	2.93	14	4
1:A:40:LEU:CD1	1:B:45:ILE:CD1	0.47	2.92	14	2
1:B:65:GLY:HA3	1:B:134:VAL:HG22	0.47	1.86	15	1
1:A:119:ILE:HG22	1:A:120:SER:N	0.47	2.24	8	17
1:A:109:PRO:O	1:A:110:MET:CB	0.47	2.61	11	9
1:B:114:TYR:CD2	1:B:115:SER:O	0.47	2.68	18	3
1:A:43:LEU:CD1	1:B:73:ILE:CD1	0.47	2.92	4	5
1:B:93:GLU:O	1:B:94:PHE:CG	0.47	2.68	1	1
1:A:93:GLU:O	1:A:94:PHE:CD1	0.47	2.68	19	3
1:A:40:LEU:CD2	1:B:41:ASN:CB	0.47	2.92	13	1
1:B:78:ILE:HG22	1:B:79:THR:N	0.47	2.25	7	7
1:B:86:VAL:CG2	1:B:99:LEU:HD22	0.47	2.39	6	1
1:A:133:HIS:NE2	1:B:137:ALA:CB	0.47	2.78	6	4
1:A:43:LEU:CD2	1:B:71:LEU:HD11	0.47	2.38	20	2
1:A:135:VAL:HG21	1:B:44:LEU:HD11	0.47	1.86	11	1
1:A:53:PHE:CB	1:B:43:LEU:HD11	0.47	2.39	15	1
1:A:54:VAL:CG1	1:A:72:LEU:CD2	0.47	2.93	3	1
1:A:131:VAL:HG22	1:A:132:ILE:N	0.47	2.25	17	15
1:A:114:TYR:CD2	1:A:115:SER:O	0.47	2.68	7	1
1:A:86:VAL:CG2	1:A:127:VAL:HG11	0.47	2.40	11	1
1:A:99:LEU:N	1:A:99:LEU:HD23	0.47	2.25	11	1
1:A:90:VAL:CG2	1:A:125:LEU:HD21	0.47	2.40	8	1
1:A:99:LEU:CB	1:A:107:LEU:CD1	0.47	2.92	8	2
1:A:62:ILE:CD1	1:A:111:ASN:ND2	0.47	2.78	12	1
1:A:40:LEU:CB	1:B:45:ILE:CD1	0.47	2.93	6	1
1:A:87:ILE:HD12	1:A:95:THR:O	0.47	2.10	11	2
1:B:108:ILE:CD1	1:B:115:SER:N	0.47	2.77	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ILE:CD1	1:A:94:PHE:CE2	0.47	2.97	5	1
1:A:114:TYR:CG	1:A:114:TYR:O	0.47	2.68	13	3
1:B:40:LEU:HD11	1:B:44:LEU:HD22	0.47	1.86	18	2
1:A:114:TYR:O	1:A:114:TYR:CD1	0.47	2.68	12	1
1:A:44:LEU:HD13	1:A:44:LEU:N	0.46	2.25	15	2
1:A:46:GLN:O	1:A:47:HIS:CG	0.46	2.68	13	1
1:B:82:HIS:CE1	1:B:101:LEU:HG	0.46	2.45	9	1
1:A:41:ASN:CA	1:B:40:LEU:HD22	0.46	2.37	18	1
1:A:114:TYR:O	1:A:114:TYR:CG	0.46	2.68	9	8
1:A:40:LEU:CD1	1:A:44:LEU:CD2	0.46	2.93	14	4
1:B:47:HIS:O	1:B:47:HIS:CD2	0.46	2.68	17	1
1:B:86:VAL:CG2	1:B:127:VAL:HG11	0.46	2.40	11	1
1:B:44:LEU:HD13	1:B:44:LEU:N	0.46	2.25	15	1
1:A:41:ASN:CB	1:B:40:LEU:CD2	0.46	2.92	13	1
1:B:64:GLY:O	1:B:134:VAL:HG21	0.46	2.10	12	1
1:A:46:GLN:O	1:A:47:HIS:CD2	0.46	2.68	3	2
1:B:46:GLN:O	1:B:47:HIS:CD2	0.46	2.68	3	2
1:A:64:GLY:O	1:A:134:VAL:HG21	0.46	2.10	12	1
1:A:40:LEU:HD12	1:A:44:LEU:HD22	0.46	1.81	8	2
1:A:52:TYR:O	1:A:74:VAL:CG1	0.46	2.64	4	19
1:B:96:VAL:HG12	1:B:97:LYS:H	0.46	1.70	14	2
1:B:90:VAL:CG2	1:B:125:LEU:HD21	0.46	2.40	8	1
1:A:137:ALA:N	1:B:133:HIS:NE2	0.46	2.64	2	1
1:B:119:ILE:CG2	1:B:120:SER:N	0.46	2.79	14	2
1:A:86:VAL:HA	1:A:132:ILE:HD11	0.46	1.87	7	1
1:A:38:ILE:HG12	1:A:40:LEU:HD23	0.46	1.87	9	2
1:B:54:VAL:CG1	1:B:72:LEU:CD2	0.46	2.93	3	1
1:A:131:VAL:CG2	1:A:133:HIS:CE1	0.46	2.99	3	4
1:A:65:GLY:HA3	1:A:134:VAL:HG22	0.46	1.85	15	1
1:B:62:ILE:HD12	1:B:111:ASN:HB2	0.46	1.87	7	1
1:B:131:VAL:HG22	1:B:132:ILE:N	0.46	2.26	6	15
1:A:105:VAL:HG12	1:A:119:ILE:HD13	0.46	1.86	3	2
1:B:95:THR:CG2	1:B:107:LEU:HD11	0.46	2.30	5	1
1:A:63:ASP:OD2	1:A:110:MET:N	0.46	2.49	20	2
1:B:93:GLU:O	1:B:94:PHE:CD1	0.46	2.69	12	2
1:A:72:LEU:CD2	1:A:132:ILE:HG23	0.46	2.41	16	1
1:A:135:VAL:CG1	1:B:135:VAL:HG22	0.46	2.39	18	1
1:A:133:HIS:NE2	1:B:137:ALA:N	0.46	2.64	2	1
1:A:75:ASP:O	1:A:129:GLY:CA	0.46	2.64	19	17
1:A:131:VAL:CG2	1:A:133:HIS:NE2	0.46	2.79	14	2
1:A:47:HIS:O	1:A:47:HIS:CD2	0.46	2.68	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ILE:HG22	1:A:72:LEU:HB2	0.46	1.88	20	1
1:B:66:ILE:HG22	1:B:72:LEU:HB2	0.46	1.87	20	1
1:A:43:LEU:CG	1:A:44:LEU:HD13	0.46	2.41	8	3
1:B:131:VAL:CG2	1:B:133:HIS:CE1	0.46	2.99	3	4
1:A:45:ILE:CD1	1:B:40:LEU:CB	0.46	2.94	6	1
1:B:131:VAL:CG2	1:B:133:HIS:NE2	0.46	2.79	14	2
1:A:108:ILE:O	1:A:108:ILE:CD1	0.46	2.64	14	1
1:A:71:LEU:HD11	1:B:43:LEU:CD2	0.46	2.38	20	2
1:B:108:ILE:O	1:B:108:ILE:CD1	0.46	2.64	18	1
1:B:86:VAL:HA	1:B:132:ILE:HD11	0.45	1.87	7	1
1:B:118:THR:O	1:B:118:THR:HG23	0.45	2.10	14	1
1:B:80:ALA:HB3	1:B:127:VAL:HG11	0.45	1.88	4	1
1:B:72:LEU:CD2	1:B:132:ILE:HG23	0.45	2.41	16	1
1:A:53:PHE:CZ	1:B:43:LEU:HD22	0.45	2.46	7	1
1:B:75:ASP:O	1:B:129:GLY:CA	0.45	2.64	19	17
1:B:107:LEU:HB2	1:B:119:ILE:HD11	0.45	1.87	1	1
1:B:43:LEU:CG	1:B:44:LEU:HD13	0.45	2.41	7	4
1:B:84:ASP:O	1:B:86:VAL:N	0.45	2.50	19	8
1:B:132:ILE:CG1	1:B:132:ILE:O	0.45	2.64	20	1
1:A:95:THR:HG21	1:A:107:LEU:CD2	0.45	2.41	11	3
1:A:118:THR:HG23	1:A:118:THR:O	0.45	2.12	11	1
1:A:86:VAL:HA	1:A:132:ILE:HD13	0.45	1.89	8	1
1:A:99:LEU:HD12	1:A:101:LEU:HD11	0.45	1.87	2	1
1:B:63:ASP:OD1	1:B:63:ASP:N	0.45	2.49	20	3
1:A:117:ILE:O	1:A:117:ILE:HG23	0.45	2.10	12	2
1:A:53:PHE:HE2	1:B:38:ILE:HG23	0.45	1.71	18	1
1:B:66:ILE:CD1	1:B:66:ILE:O	0.45	2.64	18	8
1:A:47:HIS:CD2	1:A:51:THR:OG1	0.45	2.69	17	1
1:A:41:ASN:HB2	1:B:40:LEU:HD13	0.45	1.84	5	1
1:A:40:LEU:HD13	1:A:43:LEU:HD12	0.45	1.88	14	1
1:B:62:ILE:HG23	1:B:67:SER:CB	0.45	2.41	3	1
1:B:52:TYR:O	1:B:74:VAL:CG1	0.45	2.65	19	18
1:A:66:ILE:O	1:A:66:ILE:CD1	0.45	2.65	18	5
1:B:74:VAL:HA	1:B:131:VAL:HG23	0.45	1.89	20	1
1:A:90:VAL:CG2	1:A:125:LEU:CD2	0.45	2.94	8	1
1:B:99:LEU:N	1:B:99:LEU:HD23	0.45	2.27	7	4
1:A:94:PHE:O	1:A:95:THR:HG23	0.45	2.12	7	1
1:B:47:HIS:CD2	1:B:51:THR:OG1	0.45	2.69	17	1
1:A:64:GLY:O	1:A:96:VAL:CG1	0.45	2.64	19	2
1:A:43:LEU:HD22	1:B:53:PHE:CZ	0.45	2.46	7	1
1:B:101:LEU:CD1	1:B:125:LEU:O	0.45	2.65	7	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:66:ILE:CG1	1:B:66:ILE:O	0.45	2.65	7	6
1:A:87:ILE:HD12	1:A:96:VAL:HG22	0.45	1.88	15	2
1:B:105:VAL:O	1:B:105:VAL:CG1	0.45	2.65	18	1
1:A:66:ILE:O	1:A:66:ILE:CG1	0.45	2.65	7	11
1:B:96:VAL:HG12	1:B:97:LYS:N	0.45	2.27	7	1
1:A:104:THR:HG22	1:A:105:VAL:N	0.45	2.27	15	2
1:B:99:LEU:HD11	1:B:127:VAL:HG23	0.45	1.89	10	1
1:A:74:VAL:HA	1:A:131:VAL:HG23	0.44	1.89	20	1
1:A:85:ILE:CD1	1:A:85:ILE:O	0.44	2.66	8	2
1:A:43:LEU:HD21	1:B:71:LEU:HD21	0.44	1.89	4	1
1:B:99:LEU:CD2	1:B:127:VAL:CG2	0.44	2.94	9	1
1:B:106:GLN:CA	1:B:119:ILE:HD12	0.44	2.42	18	1
1:A:40:LEU:CD1	1:A:41:ASN:N	0.44	2.75	3	2
1:B:95:THR:HG23	1:B:109:PRO:CG	0.44	2.41	5	1
1:A:132:ILE:CG1	1:A:132:ILE:O	0.44	2.64	20	1
1:A:73:ILE:HG13	1:B:44:LEU:HD21	0.44	1.89	9	1
1:A:82:HIS:CD2	1:A:102:ARG:HD3	0.44	2.47	16	1
1:B:62:ILE:CD1	1:B:111:ASN:ND2	0.44	2.79	12	1
1:A:110:MET:O	1:A:112:SER:N	0.44	2.50	11	1
1:A:82:HIS:NE2	1:A:101:LEU:CD1	0.44	2.78	7	1
1:A:108:ILE:CG2	1:A:108:ILE:O	0.44	2.66	7	1
1:B:52:TYR:O	1:B:74:VAL:N	0.44	2.50	19	5
1:B:40:LEU:CD1	1:B:41:ASN:N	0.44	2.79	6	2
1:A:105:VAL:O	1:A:105:VAL:CG1	0.44	2.65	10	1
1:A:52:TYR:O	1:A:74:VAL:N	0.44	2.50	19	6
1:A:73:ILE:HB	1:A:133:HIS:CB	0.44	2.43	20	1
1:B:73:ILE:HB	1:B:133:HIS:CB	0.44	2.43	20	1
1:A:43:LEU:C	1:A:43:LEU:CD1	0.44	2.86	11	1
1:A:41:ASN:O	1:A:45:ILE:HD12	0.44	2.12	10	1
1:A:101:LEU:CD1	1:A:125:LEU:O	0.44	2.65	2	8
1:A:71:LEU:HD12	1:B:44:LEU:HD12	0.44	1.90	17	1
1:B:99:LEU:HD23	1:B:99:LEU:N	0.44	2.28	13	6
1:B:90:VAL:CG2	1:B:125:LEU:CD2	0.44	2.95	8	1
1:B:108:ILE:CG2	1:B:108:ILE:O	0.44	2.66	9	1
1:B:110:MET:SD	1:B:113:ALA:HB3	0.44	2.53	9	1
1:A:40:LEU:HD22	1:B:41:ASN:CA	0.44	2.37	18	1
1:B:115:SER:HB3	1:B:116:PRO:HD2	0.44	1.90	7	2
1:B:66:ILE:O	1:B:66:ILE:CG1	0.44	2.66	20	11
1:A:84:ASP:O	1:A:86:VAL:N	0.44	2.51	19	6
1:A:39:ASP:O	1:A:43:LEU:N	0.44	2.51	5	5
1:A:108:ILE:CD1	1:A:108:ILE:O	0.44	2.63	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:HD13	1:A:43:LEU:CD1	0.44	2.42	14	1
1:A:59:ASP:O	1:A:111:ASN:ND2	0.44	2.51	5	2
1:A:99:LEU:HD23	1:A:99:LEU:N	0.44	2.28	2	5
1:B:46:GLN:C	1:B:47:HIS:CG	0.44	2.92	10	4
1:B:41:ASN:O	1:B:45:ILE:CG1	0.44	2.66	10	1
1:B:110:MET:SD	1:B:114:TYR:CE2	0.44	3.11	16	1
1:A:95:THR:OG1	1:A:109:PRO:CG	0.44	2.66	2	1
1:B:62:ILE:CG1	1:B:111:ASN:OD1	0.44	2.66	8	2
1:A:138:MET:CG	1:B:85:ILE:HD13	0.44	2.43	14	1
1:B:96:VAL:O	1:B:97:LYS:CB	0.44	2.64	14	6
1:B:39:ASP:O	1:B:43:LEU:N	0.44	2.51	5	3
1:A:132:ILE:HG12	1:A:132:ILE:O	0.44	2.11	20	1
1:B:132:ILE:HG12	1:B:132:ILE:O	0.44	2.11	20	1
1:B:98:LYS:CG	1:B:98:LYS:O	0.44	2.65	11	1
1:B:78:ILE:CD1	1:B:130:VAL:HG11	0.44	2.43	13	1
1:A:108:ILE:CG1	1:A:108:ILE:O	0.44	2.66	16	1
1:A:66:ILE:CD1	1:A:66:ILE:O	0.44	2.66	15	8
1:A:120:SER:O	1:A:122:GLU:N	0.44	2.51	14	5
1:A:99:LEU:CD1	1:A:101:LEU:HD11	0.44	2.43	12	2
1:A:59:ASP:O	1:A:62:ILE:HD11	0.44	2.13	15	2
1:A:44:LEU:HD23	1:B:44:LEU:CG	0.44	2.43	13	3
1:B:56:ALA:HB3	1:B:70:ASP:O	0.44	2.13	13	1
1:A:97:LYS:CG	1:A:107:LEU:HD12	0.43	2.43	14	1
1:B:64:GLY:CA	1:B:96:VAL:CG1	0.43	2.92	18	2
1:B:97:LYS:CB	1:B:109:PRO:HD2	0.43	2.43	19	1
1:B:86:VAL:HA	1:B:132:ILE:HD13	0.43	1.89	8	1
1:B:85:ILE:O	1:B:85:ILE:CD1	0.43	2.66	8	1
1:B:82:HIS:CE1	1:B:101:LEU:CG	0.43	3.01	9	1
1:A:88:ALA:HB3	1:A:95:THR:HG22	0.43	1.81	2	1
1:A:105:VAL:O	1:A:105:VAL:CG2	0.43	2.67	15	5
1:A:73:ILE:HD12	1:B:43:LEU:HD11	0.43	1.90	17	1
1:A:80:ALA:HB3	1:A:127:VAL:HG11	0.43	1.88	4	1
1:B:90:VAL:CG2	1:B:124:THR:O	0.43	2.67	7	7
1:A:63:ASP:OD1	1:A:63:ASP:N	0.43	2.47	20	3
1:B:64:GLY:O	1:B:134:VAL:CG1	0.43	2.66	1	1
1:A:62:ILE:CD1	1:A:111:ASN:OD1	0.43	2.67	1	1
1:B:85:ILE:CD1	1:B:85:ILE:O	0.43	2.65	3	2
1:A:75:ASP:OD2	1:A:131:VAL:CG1	0.43	2.66	10	1
1:B:61:MET:O	1:B:66:ILE:CG1	0.43	2.67	9	2
1:A:66:ILE:CG1	1:A:66:ILE:O	0.43	2.67	10	6
1:A:40:LEU:CD2	1:B:45:ILE:HD11	0.43	2.42	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:CG1	1:A:111:ASN:OD1	0.43	2.66	1	1
1:A:110:MET:SD	1:A:110:MET:N	0.43	2.92	20	1
1:A:41:ASN:CA	1:B:40:LEU:HD21	0.43	2.43	13	1
1:B:60:SER:O	1:B:110:MET:CG	0.43	2.66	19	1
1:B:41:ASN:O	1:B:45:ILE:HD12	0.43	2.12	10	1
1:A:41:ASN:O	1:A:45:ILE:CG1	0.43	2.66	10	1
1:A:108:ILE:HD13	1:A:116:PRO:CA	0.43	2.44	2	1
1:B:85:ILE:C	1:B:86:VAL:HG13	0.43	2.34	7	2
1:B:117:ILE:O	1:B:117:ILE:CG2	0.43	2.66	15	2
1:B:85:ILE:CD1	1:B:85:ILE:C	0.43	2.86	11	1
1:A:132:ILE:N	1:A:132:ILE:CD1	0.43	2.77	19	1
1:A:88:ALA:HB3	1:A:95:THR:HB	0.43	1.89	19	1
1:A:105:VAL:CG2	1:A:105:VAL:O	0.43	2.67	4	3
1:A:46:GLN:C	1:A:47:HIS:CG	0.43	2.92	15	4
1:B:95:THR:CG2	1:B:109:PRO:CG	0.43	2.96	3	1
1:A:62:ILE:HG23	1:A:67:SER:CB	0.43	2.43	3	1
1:A:66:ILE:C	1:A:66:ILE:HD12	0.43	2.34	3	1
1:A:97:LYS:CD	1:A:108:ILE:HG23	0.43	2.44	3	1
1:A:107:LEU:CD2	1:A:119:ILE:HD11	0.43	2.30	14	1
1:B:105:VAL:O	1:B:105:VAL:CG2	0.43	2.67	15	4
1:B:85:ILE:C	1:B:85:ILE:CD1	0.43	2.86	15	2
1:A:40:LEU:HD21	1:B:44:LEU:CB	0.43	2.44	18	1
1:A:96:VAL:HG12	1:A:97:LYS:N	0.43	2.29	7	1
1:B:104:THR:HG22	1:B:105:VAL:N	0.43	2.28	16	4
1:B:85:ILE:O	1:B:132:ILE:CD1	0.43	2.67	7	2
1:A:107:LEU:O	1:A:108:ILE:C	0.43	2.57	13	2
1:A:40:LEU:HD21	1:B:41:ASN:CA	0.43	2.42	13	1
1:B:66:ILE:C	1:B:66:ILE:HD12	0.43	2.34	3	1
1:B:75:ASP:OD2	1:B:131:VAL:CG1	0.43	2.66	10	1
1:B:56:ALA:CB	1:B:70:ASP:OD1	0.43	2.67	18	6
1:A:43:LEU:HG	1:A:44:LEU:N	0.43	2.29	6	1
1:A:82:HIS:CE1	1:A:101:LEU:HB2	0.43	2.49	12	7
1:A:43:LEU:CD1	1:A:44:LEU:HD13	0.43	2.44	5	1
1:B:45:ILE:CG2	1:B:51:THR:OG1	0.43	2.67	11	2
1:A:85:ILE:C	1:A:85:ILE:CD1	0.43	2.86	11	2
1:B:110:MET:O	1:B:110:MET:CE	0.43	2.67	15	1
1:B:45:ILE:CG1	1:B:51:THR:HG21	0.43	2.44	19	1
1:A:44:LEU:HD21	1:B:73:ILE:HG13	0.43	1.89	9	1
1:A:45:ILE:O	1:A:46:GLN:CG	0.42	2.67	8	6
1:B:45:ILE:O	1:B:46:GLN:CG	0.42	2.67	5	6
1:A:90:VAL:CG2	1:A:124:THR:O	0.42	2.67	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:SER:O	1:B:68:ASP:C	0.42	2.57	15	4
1:A:45:ILE:HD11	1:B:40:LEU:CD2	0.42	2.42	1	1
1:B:63:ASP:CB	1:B:110:MET:HB2	0.42	2.44	1	1
1:B:62:ILE:CD1	1:B:111:ASN:OD1	0.42	2.67	1	2
1:A:71:LEU:HD22	1:A:71:LEU:C	0.42	2.34	5	1
1:A:105:VAL:HG11	1:A:122:GLU:CA	0.42	2.43	16	2
1:A:60:SER:O	1:A:111:ASN:N	0.42	2.52	20	2
1:B:109:PRO:O	1:B:110:MET:CG	0.42	2.67	11	2
1:A:67:SER:O	1:A:68:ASP:C	0.42	2.57	15	3
1:A:44:LEU:CG	1:B:44:LEU:HD23	0.42	2.44	13	3
1:A:56:ALA:HB3	1:A:70:ASP:O	0.42	2.14	13	1
1:A:44:LEU:HD12	1:B:135:VAL:HG21	0.42	1.90	2	1
1:A:107:LEU:HD21	1:A:109:PRO:HG3	0.42	1.89	2	1
1:B:120:SER:O	1:B:122:GLU:N	0.42	2.52	7	4
1:B:96:VAL:O	1:B:97:LYS:HB3	0.42	2.14	7	1
1:B:66:ILE:O	1:B:66:ILE:CD1	0.42	2.67	5	9
1:B:82:HIS:CE1	1:B:101:LEU:HB2	0.42	2.49	18	7
1:A:133:HIS:CD2	1:B:137:ALA:HA	0.42	2.50	20	4
1:A:137:ALA:HA	1:B:133:HIS:CD2	0.42	2.49	20	4
1:A:84:ASP:O	1:A:86:VAL:HG13	0.42	2.14	20	1
1:A:45:ILE:CG2	1:A:46:GLN:N	0.42	2.82	13	1
1:B:71:LEU:CD1	1:B:73:ILE:CD1	0.42	2.97	3	1
1:A:132:ILE:O	1:A:132:ILE:CG2	0.42	2.67	8	3
1:B:95:THR:OG1	1:B:107:LEU:HD21	0.42	2.14	12	1
1:B:40:LEU:HD13	1:B:43:LEU:CD1	0.42	2.44	14	1
1:B:56:ALA:HB2	1:B:66:ILE:HG22	0.42	1.91	14	1
1:B:38:ILE:CG1	1:B:38:ILE:O	0.42	2.67	4	2
1:B:45:ILE:HG22	1:B:46:GLN:H	0.42	1.74	20	1
1:A:97:LYS:NZ	1:A:107:LEU:HD11	0.42	2.29	20	1
1:A:85:ILE:CD1	1:A:85:ILE:C	0.42	2.86	15	1
1:A:40:LEU:O	1:A:43:LEU:CD1	0.42	2.67	13	2
1:B:114:TYR:N	1:B:114:TYR:CD1	0.42	2.87	13	2
1:A:61:MET:CB	1:A:66:ILE:HD11	0.42	2.44	4	1
1:B:82:HIS:NE2	1:B:101:LEU:CD1	0.42	2.83	9	1
1:A:102:ARG:HB3	1:A:103:PRO:HD3	0.42	1.91	9	1
1:A:40:LEU:HD21	1:B:44:LEU:HB2	0.42	1.92	18	1
1:A:135:VAL:HG21	1:B:44:LEU:HD12	0.42	1.91	2	1
1:A:85:ILE:O	1:A:132:ILE:CD1	0.42	2.67	7	2
1:A:85:ILE:C	1:A:86:VAL:HG13	0.42	2.34	7	2
1:B:115:SER:CB	1:B:116:PRO:CD	0.42	2.97	7	2
1:B:86:VAL:HB	1:B:127:VAL:HG11	0.42	1.91	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:130:VAL:O	1:B:130:VAL:CG2	0.42	2.68	3	2
1:B:59:ASP:O	1:B:62:ILE:HD11	0.42	2.14	20	1
1:A:45:ILE:HG23	1:A:51:THR:CG2	0.42	2.39	15	2
1:A:85:ILE:O	1:A:85:ILE:HD13	0.42	2.13	10	1
1:A:41:ASN:HB2	1:A:45:ILE:HD12	0.42	1.91	10	1
1:B:87:ILE:CG2	1:B:87:ILE:O	0.42	2.68	16	2
1:B:87:ILE:HD12	1:B:95:THR:O	0.42	2.14	6	1
1:B:40:LEU:HD13	1:B:43:LEU:HD12	0.42	1.90	14	1
1:A:44:LEU:HD12	1:B:71:LEU:HD12	0.42	1.90	17	1
1:A:56:ALA:CB	1:A:70:ASP:OD2	0.42	2.67	11	5
1:A:85:ILE:O	1:A:85:ILE:CG2	0.42	2.68	9	3
1:B:59:ASP:O	1:B:62:ILE:CD1	0.42	2.67	20	1
1:A:59:ASP:O	1:A:62:ILE:CD1	0.42	2.68	20	2
1:B:40:LEU:HD12	1:B:40:LEU:O	0.42	2.15	13	1
1:B:105:VAL:HG12	1:B:119:ILE:HD13	0.42	1.90	3	1
1:A:136:LYS:C	1:B:133:HIS:CD2	0.42	2.93	2	1
1:A:56:ALA:CB	1:A:70:ASP:OD1	0.42	2.67	18	6
1:A:97:LYS:CD	1:A:108:ILE:O	0.42	2.68	6	2
1:B:132:ILE:CG2	1:B:132:ILE:O	0.42	2.67	8	3
1:B:52:TYR:CB	1:B:74:VAL:O	0.42	2.68	17	1
1:A:137:ALA:CA	1:B:133:HIS:CD2	0.42	3.03	5	2
1:B:84:ASP:O	1:B:86:VAL:HG13	0.42	2.13	20	1
1:A:114:TYR:CD1	1:A:114:TYR:N	0.42	2.88	11	1
1:A:75:ASP:OD2	1:A:131:VAL:HG11	0.42	2.15	15	1
1:A:71:LEU:CD1	1:A:73:ILE:CD1	0.42	2.97	3	1
1:A:40:LEU:CD2	1:B:45:ILE:CD1	0.42	2.92	8	1
1:B:73:ILE:O	1:B:133:HIS:N	0.42	2.53	16	1
1:B:110:MET:CE	1:B:110:MET:O	0.42	2.68	12	1
1:B:130:VAL:HG13	1:B:131:VAL:N	0.42	2.30	7	1
1:A:130:VAL:HG13	1:A:131:VAL:N	0.42	2.30	7	1
1:A:99:LEU:HD22	1:A:127:VAL:HG22	0.42	1.90	7	1
1:A:86:VAL:HB	1:A:127:VAL:HG11	0.42	1.91	1	3
1:B:98:LYS:O	1:B:108:ILE:CG2	0.42	2.68	1	2
1:A:64:GLY:O	1:A:134:VAL:CG1	0.42	2.67	1	1
1:B:43:LEU:CD1	1:B:44:LEU:HD13	0.42	2.44	5	1
1:A:78:ILE:HB	1:A:130:VAL:HG11	0.42	1.92	13	1
1:A:139:ARG:O	1:B:132:ILE:HD13	0.42	2.15	19	1
1:B:52:TYR:O	1:B:74:VAL:O	0.42	2.38	12	1
1:B:108:ILE:HD13	1:B:116:PRO:CA	0.42	2.44	2	1
1:A:43:LEU:HD22	1:B:53:PHE:CE1	0.42	2.50	7	1
1:B:107:LEU:O	1:B:108:ILE:C	0.42	2.57	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:MET:O	1:A:66:ILE:CG1	0.42	2.67	7	1
1:A:63:ASP:CB	1:A:110:MET:HB2	0.42	2.45	1	1
1:B:44:LEU:N	1:B:44:LEU:HD13	0.42	2.30	17	1
1:B:102:ARG:N	1:B:103:PRO:HD2	0.42	2.30	2	2
1:B:55:LYS:CE	1:B:70:ASP:O	0.42	2.68	2	5
1:A:55:LYS:HG2	1:A:71:LEU:HD23	0.42	1.91	11	1
1:B:45:ILE:HG23	1:B:51:THR:CG2	0.42	2.39	15	1
1:A:40:LEU:CD2	1:B:41:ASN:HB2	0.42	2.45	13	1
1:B:40:LEU:O	1:B:43:LEU:CD1	0.42	2.68	13	2
1:B:45:ILE:CG2	1:B:46:GLN:N	0.42	2.82	13	1
1:A:45:ILE:CG1	1:A:51:THR:HG21	0.42	2.44	19	1
1:B:88:ALA:HB2	1:B:99:LEU:HD13	0.42	1.91	19	1
1:B:107:LEU:HD21	1:B:109:PRO:HG3	0.42	1.92	3	1
1:A:110:MET:O	1:A:110:MET:CE	0.42	2.68	3	1
1:B:41:ASN:HB2	1:B:45:ILE:HD12	0.42	1.91	10	1
1:A:137:ALA:HB2	1:B:133:HIS:CD2	0.42	2.50	8	1
1:A:99:LEU:HA	1:A:107:LEU:HD12	0.42	1.91	9	1
1:A:96:VAL:O	1:A:97:LYS:CB	0.42	2.68	17	5
1:B:43:LEU:HG	1:B:44:LEU:N	0.42	2.29	6	1
1:A:63:ASP:HB2	1:A:110:MET:HE2	0.42	1.92	1	1
1:B:107:LEU:O	1:B:108:ILE:O	0.42	2.38	14	3
1:A:63:ASP:OD1	1:A:96:VAL:O	0.42	2.38	11	4
1:B:74:VAL:CG1	1:B:74:VAL:O	0.42	2.68	17	1
1:B:56:ALA:CB	1:B:70:ASP:OD2	0.42	2.68	11	5
1:B:53:PHE:CD1	1:B:53:PHE:N	0.42	2.88	20	1
1:B:60:SER:O	1:B:111:ASN:N	0.42	2.53	20	2
1:A:71:LEU:O	1:A:135:VAL:N	0.42	2.53	11	1
1:B:117:ILE:C	1:B:117:ILE:HD13	0.42	2.35	15	1
1:A:130:VAL:CG2	1:A:130:VAL:O	0.42	2.67	3	2
1:A:44:LEU:N	1:A:44:LEU:HD22	0.42	2.30	4	1
1:B:86:VAL:HA	1:B:132:ILE:CD1	0.42	2.45	18	1
1:B:108:ILE:C	1:B:108:ILE:CD1	0.42	2.88	18	1
1:B:98:LYS:O	1:B:98:LYS:CG	0.42	2.68	12	1
1:A:56:ALA:HB2	1:A:66:ILE:HG22	0.42	1.91	14	1
1:A:52:TYR:N	1:A:74:VAL:O	0.42	2.53	16	2
1:A:43:LEU:HD23	1:B:71:LEU:HD21	0.42	1.92	13	1
1:A:85:ILE:O	1:A:85:ILE:CD1	0.42	2.68	10	1
1:A:133:HIS:CD2	1:B:136:LYS:C	0.42	2.93	2	1
1:A:118:THR:O	1:A:118:THR:HG23	0.41	2.14	7	1
1:A:133:HIS:CD2	1:B:137:ALA:CA	0.41	3.03	5	2
1:A:51:THR:HG23	1:A:74:VAL:O	0.41	2.15	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LYS:CG	1:A:108:ILE:O	0.41	2.68	18	1
1:A:99:LEU:CD2	1:A:127:VAL:CG2	0.41	2.96	7	1
1:A:55:LYS:CE	1:A:70:ASP:O	0.41	2.68	2	6
1:B:105:VAL:CG2	1:B:105:VAL:O	0.41	2.67	17	1
1:A:52:TYR:CB	1:A:74:VAL:O	0.41	2.68	17	1
1:B:63:ASP:OD1	1:B:96:VAL:O	0.41	2.38	3	4
1:B:108:ILE:HD13	1:B:109:PRO:C	0.41	2.35	11	1
1:A:45:ILE:CG2	1:A:51:THR:OG1	0.41	2.69	18	2
1:A:59:ASP:OD1	1:A:59:ASP:N	0.41	2.53	8	3
1:A:40:LEU:HD12	1:A:40:LEU:O	0.41	2.15	13	1
1:A:43:LEU:HD21	1:B:71:LEU:CD1	0.41	2.37	3	1
1:A:95:THR:CG2	1:A:109:PRO:HG3	0.41	2.45	8	1
1:B:90:VAL:CG1	1:B:93:GLU:HB2	0.41	2.45	8	1
1:B:61:MET:CB	1:B:66:ILE:HD11	0.41	2.45	4	1
1:A:53:PHE:CE1	1:B:43:LEU:HD22	0.41	2.50	7	1
1:A:73:ILE:HD11	1:B:44:LEU:HD21	0.41	1.91	7	1
1:B:95:THR:CG2	1:B:107:LEU:HD21	0.41	2.44	6	1
1:B:59:ASP:OD1	1:B:59:ASP:N	0.41	2.53	16	2
1:B:59:ASP:C	1:B:62:ILE:HD11	0.41	2.36	20	1
1:B:78:ILE:HB	1:B:130:VAL:HG11	0.41	1.92	13	1
1:A:98:LYS:CG	1:A:98:LYS:O	0.41	2.68	8	1
1:B:44:LEU:H	1:B:44:LEU:HD22	0.41	1.75	4	1
1:A:132:ILE:CG2	1:A:132:ILE:O	0.41	2.68	9	1
1:A:64:GLY:O	1:A:134:VAL:CG2	0.41	2.68	18	1
1:B:59:ASP:O	1:B:111:ASN:ND2	0.41	2.53	1	1
1:B:94:PHE:O	1:B:95:THR:CG2	0.41	2.68	1	1
1:A:41:ASN:OD1	1:A:42:GLN:N	0.41	2.54	2	4
1:B:39:ASP:OD1	1:B:41:ASN:ND2	0.41	2.53	17	2
1:A:96:VAL:HG13	1:A:131:VAL:HG13	0.41	1.91	20	1
1:B:43:LEU:C	1:B:43:LEU:CD1	0.41	2.86	11	1
1:B:95:THR:HB	1:B:108:ILE:HG21	0.41	1.91	13	1
1:B:38:ILE:O	1:B:38:ILE:CG1	0.41	2.68	19	1
1:A:108:ILE:HD11	1:A:114:TYR:C	0.41	2.36	4	1
1:A:73:ILE:O	1:A:133:HIS:N	0.41	2.53	16	2
1:B:64:GLY:O	1:B:134:VAL:CG2	0.41	2.67	18	1
1:A:52:TYR:O	1:A:74:VAL:O	0.41	2.38	12	1
1:B:115:SER:CB	1:B:116:PRO:HD2	0.41	2.46	7	2
1:A:38:ILE:O	1:A:38:ILE:CG1	0.41	2.68	7	2
1:B:99:LEU:HD12	1:B:101:LEU:HD11	0.41	1.93	14	1
1:B:59:ASP:N	1:B:59:ASP:OD1	0.41	2.53	11	1
1:A:71:LEU:HD21	1:B:43:LEU:HD23	0.41	1.93	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:130:VAL:CG2	1:B:130:VAL:O	0.41	2.69	9	1
1:A:40:LEU:HD11	1:B:41:ASN:HA	0.41	1.93	2	1
1:A:39:ASP:OD2	1:A:43:LEU:N	0.41	2.53	2	1
1:B:63:ASP:OD1	1:B:97:LYS:N	0.41	2.53	2	1
1:A:52:TYR:HB3	1:A:74:VAL:CG1	0.41	2.45	5	2
1:A:39:ASP:OD1	1:A:41:ASN:ND2	0.41	2.53	1	2
1:A:67:SER:N	1:A:70:ASP:OD1	0.41	2.53	1	1
1:A:88:ALA:N	1:A:95:THR:O	0.41	2.54	15	2
1:B:59:ASP:HA	1:B:62:ILE:CD1	0.41	2.46	5	1
1:A:59:ASP:C	1:A:62:ILE:HD11	0.41	2.36	15	2
1:A:78:ILE:CD1	1:A:130:VAL:HG11	0.41	2.43	13	1
1:B:63:ASP:OD2	1:B:108:ILE:CD1	0.41	2.66	16	1
1:A:44:LEU:CB	1:B:40:LEU:HD21	0.41	2.45	18	1
1:A:63:ASP:OD1	1:A:97:LYS:N	0.41	2.54	2	1
1:A:108:ILE:HD11	1:A:114:TYR:CA	0.41	2.46	6	1
1:A:74:VAL:O	1:A:74:VAL:CG1	0.41	2.68	17	1
1:A:59:ASP:N	1:A:59:ASP:OD1	0.41	2.54	17	1
1:A:87:ILE:O	1:A:87:ILE:CG2	0.41	2.68	5	1
1:A:90:VAL:CG1	1:A:93:GLU:HB2	0.41	2.46	20	3
1:A:43:LEU:HG	1:B:53:PHE:CD1	0.41	2.51	11	1
1:A:111:ASN:O	1:A:113:ALA:N	0.41	2.54	11	1
1:A:132:ILE:HD13	1:B:139:ARG:O	0.41	2.16	19	1
1:A:53:PHE:HB3	1:A:73:ILE:CD1	0.41	2.46	3	1
1:B:71:LEU:CD1	1:B:73:ILE:HD11	0.41	2.43	3	1
1:A:120:SER:CB	1:A:123:ASP:OD2	0.41	2.69	4	1
1:A:44:LEU:HD21	1:B:73:ILE:HD11	0.41	1.91	7	1
1:B:85:ILE:CG2	1:B:85:ILE:O	0.41	2.67	7	2
1:B:132:ILE:O	1:B:132:ILE:CG2	0.41	2.68	14	1
1:B:41:ASN:OD1	1:B:42:GLN:N	0.41	2.54	20	3
1:A:130:VAL:O	1:A:130:VAL:CG2	0.41	2.68	9	2
1:A:45:ILE:HG22	1:A:46:GLN:H	0.41	1.74	20	1
1:A:39:ASP:O	1:A:40:LEU:C	0.41	2.59	2	1
1:B:43:LEU:HB3	1:B:44:LEU:HD22	0.41	1.92	2	1
1:A:134:VAL:HG12	1:B:136:LYS:O	0.41	2.15	7	1
1:B:56:ALA:CB	1:B:66:ILE:HA	0.41	2.46	2	4
1:B:39:ASP:OD2	1:B:42:GLN:CB	0.41	2.69	1	1
1:A:56:ALA:CB	1:A:66:ILE:HA	0.41	2.45	5	3
1:B:52:TYR:N	1:B:74:VAL:O	0.41	2.54	5	1
1:B:87:ILE:O	1:B:87:ILE:CG2	0.41	2.68	5	1
1:B:64:GLY:HA2	1:B:96:VAL:CG1	0.41	2.46	20	1
1:B:131:VAL:O	1:B:131:VAL:HG22	0.41	2.16	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:55:LYS:HG2	1:B:71:LEU:HD23	0.41	1.91	11	1
1:A:86:VAL:CG2	1:A:127:VAL:HG21	0.41	2.46	11	1
1:A:41:ASN:HB2	1:B:40:LEU:CD2	0.41	2.45	13	1
1:A:98:LYS:O	1:A:98:LYS:CG	0.41	2.68	10	1
1:A:95:THR:CG2	1:A:109:PRO:CG	0.41	2.98	8	1
1:B:51:THR:HG23	1:B:74:VAL:O	0.41	2.15	4	1
1:A:44:LEU:H	1:A:44:LEU:HD22	0.41	1.76	4	1
1:A:100:GLN:OE1	1:A:103:PRO:CG	0.41	2.69	9	1
1:A:108:ILE:O	1:A:108:ILE:HG13	0.41	2.16	16	1
1:A:82:HIS:CD2	1:A:102:ARG:CD	0.41	3.04	16	1
1:B:109:PRO:HG3	1:B:114:TYR:CZ	0.41	2.50	18	1
1:A:95:THR:OG1	1:A:109:PRO:CB	0.41	2.69	2	1
1:A:136:LYS:O	1:B:134:VAL:HG12	0.41	2.15	7	1
1:A:108:ILE:CD1	1:A:108:ILE:C	0.41	2.88	1	1
1:B:75:ASP:OD2	1:B:131:VAL:HG11	0.41	2.15	15	1
1:B:107:LEU:HB3	1:B:117:ILE:CG2	0.41	2.46	9	1
1:A:85:ILE:HG12	1:A:96:VAL:CG1	0.41	2.46	18	1
1:A:135:VAL:HG22	1:B:135:VAL:CG1	0.41	2.39	18	1
1:B:39:ASP:OD2	1:B:43:LEU:N	0.41	2.53	2	1
1:A:108:ILE:HD13	1:A:110:MET:N	0.40	2.31	7	1
1:B:52:TYR:HB3	1:B:74:VAL:CG1	0.40	2.45	5	2
1:A:60:SER:O	1:A:61:MET:CG	0.40	2.69	14	1
1:A:47:HIS:CG	1:A:50:ALA:HB3	0.40	2.51	17	1
1:A:119:ILE:CG2	1:A:120:SER:N	0.40	2.84	10	2
1:A:65:GLY:CA	1:A:96:VAL:HG11	0.40	2.46	19	1
1:A:133:HIS:CD2	1:B:137:ALA:HB2	0.40	2.50	8	1
1:A:86:VAL:HA	1:A:132:ILE:CD1	0.40	2.45	18	1
1:B:96:VAL:O	1:B:97:LYS:CG	0.40	2.69	1	1
1:A:40:LEU:HA	1:A:43:LEU:CB	0.40	2.46	14	1
1:A:59:ASP:HA	1:A:62:ILE:CD1	0.40	2.46	4	2
1:A:40:LEU:HD21	1:B:41:ASN:HA	0.40	1.93	13	1
1:A:47:HIS:ND1	1:A:75:ASP:OD1	0.40	2.54	3	1
1:A:87:ILE:CG2	1:A:87:ILE:O	0.40	2.70	10	1
1:B:39:ASP:O	1:B:40:LEU:C	0.40	2.58	2	1
1:A:54:VAL:O	1:A:54:VAL:HG13	0.40	2.16	7	1
1:A:131:VAL:HG22	1:A:131:VAL:O	0.40	2.16	20	1
1:A:96:VAL:HG13	1:A:131:VAL:CG1	0.40	2.46	20	1
1:A:130:VAL:CG1	1:B:139:ARG:HA	0.40	2.46	20	1
1:B:97:LYS:HB2	1:B:108:ILE:CB	0.40	2.47	11	1
1:A:43:LEU:CD2	1:A:43:LEU:C	0.40	2.86	3	1
1:A:40:LEU:HG	1:B:45:ILE:CD1	0.40	2.47	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:ASN:O	1:B:45:ILE:HB	0.40	2.17	10	1
1:B:108:ILE:O	1:B:108:ILE:HG13	0.40	2.16	10	1
1:A:75:ASP:N	1:A:75:ASP:OD1	0.40	2.54	4	1
1:B:44:LEU:N	1:B:44:LEU:HD22	0.40	2.30	4	1
1:A:93:GLU:O	1:A:94:PHE:CG	0.40	2.74	18	1
1:A:41:ASN:HA	1:B:40:LEU:HD11	0.40	1.92	2	1
1:B:107:LEU:O	1:B:117:ILE:HG22	0.40	2.16	14	1
1:A:85:ILE:CD1	1:B:138:MET:HG2	0.40	2.46	14	1
1:B:47:HIS:CG	1:B:50:ALA:HB3	0.40	2.50	17	1
1:A:139:ARG:HA	1:B:130:VAL:CG1	0.40	2.46	20	1
1:A:53:PHE:CD1	1:B:43:LEU:HG	0.40	2.51	11	1
1:B:43:LEU:CD1	1:B:43:LEU:N	0.40	2.84	10	1
1:A:39:ASP:OD2	1:A:42:GLN:CB	0.40	2.69	4	1
1:B:54:VAL:HG13	1:B:54:VAL:O	0.40	2.16	7	1
1:A:64:GLY:HA3	1:A:96:VAL:CG1	0.40	2.47	6	1
1:A:76:SER:HB2	1:A:128:PHE:CD2	0.40	2.52	1	1
1:A:43:LEU:HD11	1:B:73:ILE:HD12	0.40	1.92	17	1
1:B:71:LEU:CD1	1:B:71:LEU:C	0.40	2.90	3	1
1:B:53:PHE:HB3	1:B:73:ILE:CD1	0.40	2.46	3	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	101/115 (88%)	70±3 (69±3%)	21±3 (21±3%)	10±2 (10±2%)	2	11
1	B	101/115 (88%)	70±3 (69±3%)	21±3 (21±3%)	10±3 (10±3%)	1	10
All	All	4040/4600 (88%)	2792 (69%)	849 (21%)	399 (10%)	2	10

All 61 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	77	ALA	20
1	B	77	ALA	20

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Mol	Chain	Res	Type	Models (Total)
1	A	68	ASP	13
1	B	68	ASP	13
1	A	80	ALA	13
1	B	120	SER	13
1	B	80	ALA	13
1	A	120	SER	12
1	B	85	ILE	11
1	A	85	ILE	11
1	B	132	ILE	11
1	B	109	PRO	10
1	A	132	ILE	10
1	A	59	ASP	10
1	A	109	PRO	10
1	B	59	ASP	9
1	A	46	GLN	9
1	B	123	ASP	9
1	B	46	GLN	9
1	A	38	ILE	9
1	A	123	ASP	9
1	B	111	ASN	8
1	B	45	ILE	8
1	A	130	VAL	8
1	B	38	ILE	8
1	A	45	ILE	8
1	B	130	VAL	8
1	A	69	GLY	7
1	B	69	GLY	7
1	B	65	GLY	6
1	A	121	SER	6
1	B	121	SER	5
1	B	110	MET	5
1	A	65	GLY	5
1	A	111	ASN	5
1	B	108	ILE	5
1	B	49	SER	4
1	A	49	SER	4
1	B	96	VAL	4
1	A	40	LEU	3
1	B	113	ALA	3
1	A	64	GLY	3
1	A	96	VAL	3
1	B	64	GLY	3

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Mol	Chain	Res	Type	Models (Total)
1	B	112	SER	3
1	B	40	LEU	3
1	A	119	ILE	2
1	B	61	MET	2
1	B	115	SER	2
1	B	97	LYS	2
1	A	61	MET	2
1	A	112	SER	2
1	A	97	LYS	2
1	A	108	ILE	2
1	A	48	PRO	1
1	A	113	ALA	1
1	B	50	ALA	1
1	B	48	PRO	1
1	A	50	ALA	1
1	B	119	ILE	1
1	A	110	MET	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	87/97 (90%)	69±3 (80±3%)	18±3 (20±3%)	4	35
1	B	87/97 (90%)	70±4 (80±4%)	17±4 (20±4%)	5	36
All	All	3480/3880 (90%)	2786 (80%)	694 (20%)	5	36

All 101 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	55	LYS	20
1	B	43	LEU	20
1	B	55	LYS	20
1	A	43	LEU	20
1	B	52	TYR	17
1	A	102	ARG	17
1	A	52	TYR	17

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Mol	Chain	Res	Type	Models (Total)
1	B	102	ARG	15
1	A	87	ILE	14
1	A	97	LYS	14
1	B	87	ILE	14
1	A	110	MET	14
1	B	110	MET	13
1	B	98	LYS	13
1	B	44	LEU	13
1	A	44	LEU	13
1	B	125	LEU	11
1	B	108	ILE	11
1	B	138	MET	11
1	A	108	ILE	11
1	A	138	MET	11
1	A	40	LEU	11
1	B	97	LYS	11
1	A	125	LEU	11
1	B	40	LEU	11
1	A	98	LYS	10
1	B	61	MET	10
1	B	139	ARG	10
1	A	61	MET	10
1	A	139	ARG	10
1	B	133	HIS	9
1	A	123	ASP	9
1	B	136	LYS	9
1	A	133	HIS	9
1	B	123	ASP	9
1	A	136	LYS	9
1	A	107	LEU	8
1	B	121	SER	8
1	A	128	PHE	8
1	A	121	SER	8
1	B	128	PHE	8
1	A	42	GLN	7
1	A	38	ILE	7
1	B	42	GLN	7
1	B	38	ILE	7
1	B	117	ILE	6
1	B	122	GLU	6
1	B	120	SER	6
1	A	122	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	120	SER	6
1	B	85	ILE	5
1	A	85	ILE	5
1	A	46	GLN	5
1	B	100	GLN	5
1	B	46	GLN	5
1	B	96	VAL	5
1	A	96	VAL	4
1	A	93	GLU	4
1	A	100	GLN	4
1	A	67	SER	4
1	B	60	SER	4
1	B	49	SER	4
1	B	57	SER	4
1	A	49	SER	4
1	A	57	SER	4
1	A	60	SER	4
1	A	117	ILE	4
1	B	67	SER	4
1	B	93	GLU	3
1	A	94	PHE	3
1	B	71	LEU	3
1	B	72	LEU	3
1	A	71	LEU	3
1	A	72	LEU	3
1	A	111	ASN	3
1	B	94	PHE	3
1	B	95	THR	2
1	B	84	ASP	2
1	B	75	ASP	2
1	A	75	ASP	2
1	A	95	THR	2
1	B	106	GLN	2
1	A	68	ASP	2
1	B	115	SER	2
1	B	68	ASP	2
1	B	111	ASN	2
1	A	104	THR	2
1	A	84	ASP	2
1	A	45	ILE	1
1	B	132	ILE	1
1	A	106	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	91	ASP	1
1	B	91	ASP	1
1	A	115	SER	1
1	A	131	VAL	1
1	B	107	LEU	1
1	A	132	ILE	1
1	B	104	THR	1
1	A	47	HIS	1
1	B	45	ILE	1
1	B	47	HIS	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 66% for the well-defined parts and 63% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5022

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	1958
Number of shifts mapped to atoms	1958
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
$^{13}\text{C}_\alpha$	216	0.03 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	190	0.49 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	212	-1.41 ± 0.30	Should be applied

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 66%, i.e. 1536 atoms were assigned a chemical shift out of a possible 2342. 14 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	778/1004 (77%)	386/400 (96%)	198/408 (49%)	194/196 (99%)
Sidechain	736/1210 (61%)	408/694 (59%)	328/484 (68%)	0/32 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	22/128 (17%)	22/70 (31%)	0/52 (0%)	0/6 (0%)
Overall	1536/2342 (66%)	816/1164 (70%)	526/944 (56%)	194/234 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 1670 atoms were assigned a chemical shift out of a possible 2654. 14 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	854/1126 (76%)	426/448 (95%)	216/460 (47%)	212/218 (97%)
Sidechain	792/1366 (58%)	440/788 (56%)	352/538 (65%)	0/40 (0%)
Aromatic	24/162 (15%)	24/88 (27%)	0/68 (0%)	0/6 (0%)
Overall	1670/2654 (63%)	890/1324 (67%)	568/1066 (53%)	212/264 (80%)

7.1.4 Statistically unusual chemical shifts ⓘ

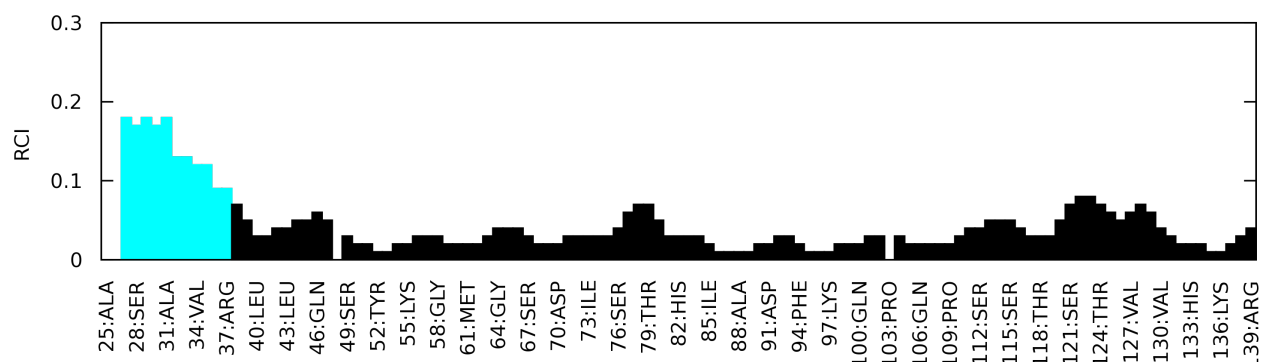
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	95	THR	CB	30.16	78.10 – 61.30	-23.5
1	A	95	THR	CB	30.16	78.10 – 61.30	-23.5

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:

