



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:18 PM BST

PDB ID : 1BFM
Title : HISTONE B FROM METHANOTHERMUS FERVIDUS
Authors : Starich, M.R.; Sandman, K.; Reeve, J.N.; Summers, M.F.
Deposited on : 1995-09-28

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

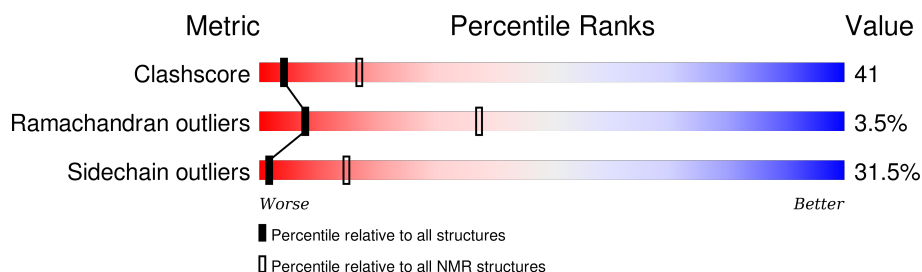
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	69	
1	B	69	

2 Ensemble composition and analysis

This entry contains 33 models. Model 12 is the overall representative, medoid model (most similar to other models).

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:3-A:67, B:3-B:67 (130)	0.60	12

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2238 atoms, of which 1164 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HISTONE B.

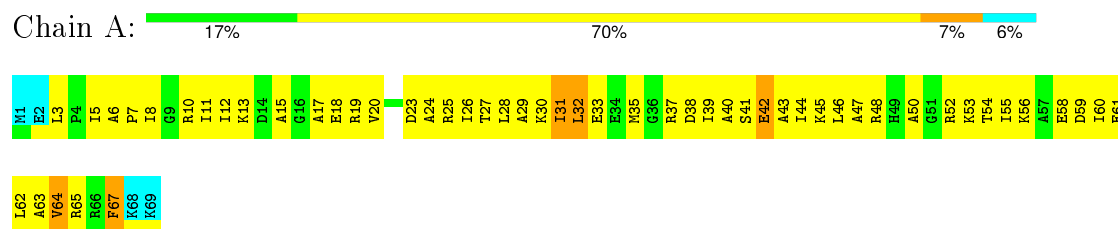
Mol	Chain	Residues	Atoms						Trace
1	A	69	Total	C	H	N	O	S	0
			1119	335	582	102	98	2	
1	B	69	Total	C	H	N	O	S	0
			1119	335	582	102	98	2	

4 Residue-property plots [i](#)

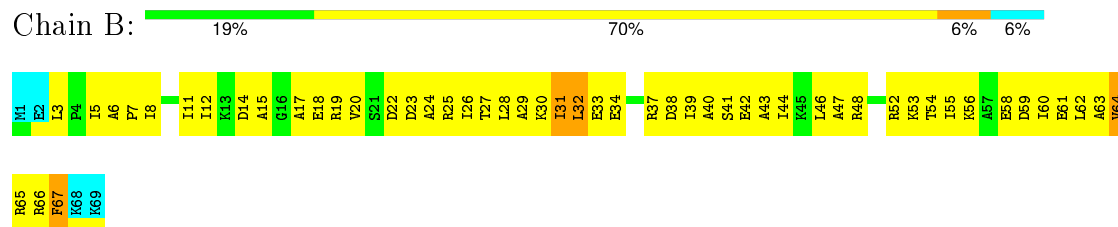
4.1 Average score per residue in the NMR ensemble

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: HISTONE B



• Molecule 1: HISTONE B

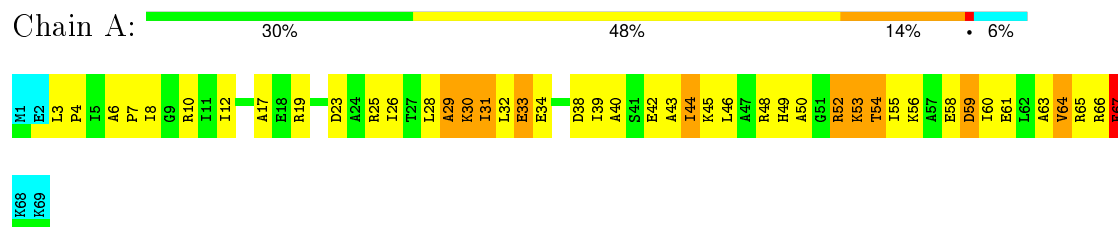


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: HISTONE B



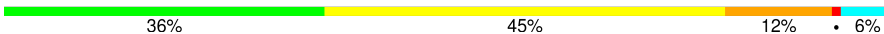
- Molecule 1: HISTONE B

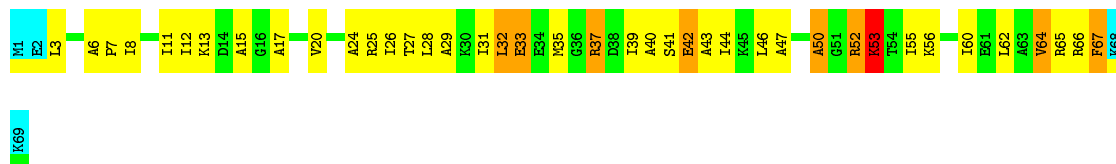
Chain B: 



4.2.2 Score per residue for model 2

- Molecule 1: HISTONE B

Chain A: 



- Molecule 1: HISTONE B

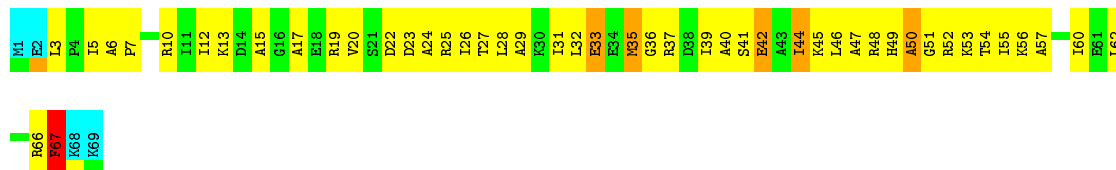
Chain B: 



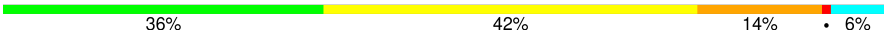
4.2.3 Score per residue for model 3

- Molecule 1: HISTONE B

Chain A: 



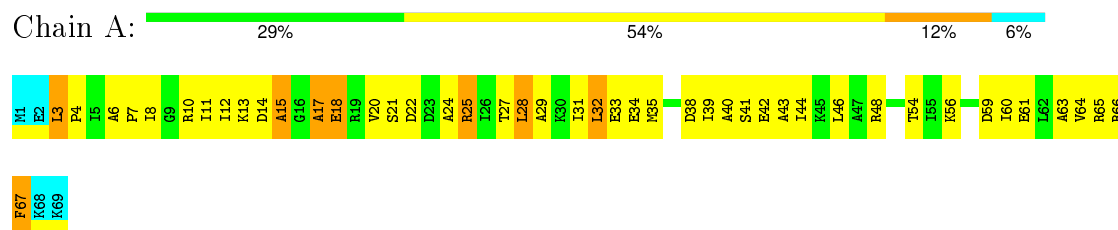
- Molecule 1: HISTONE B

Chain B: 

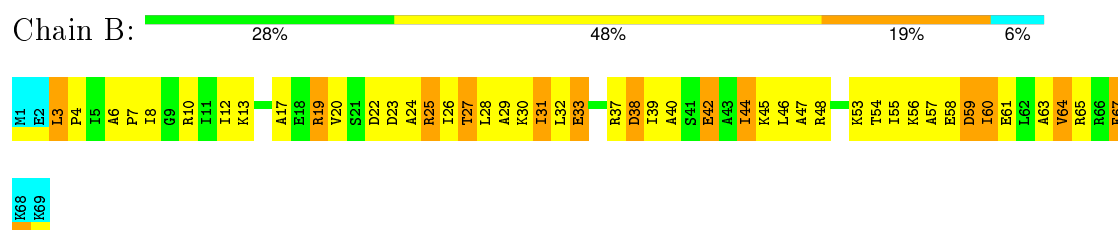


4.2.4 Score per residue for model 4

- Molecule 1: HISTONE B

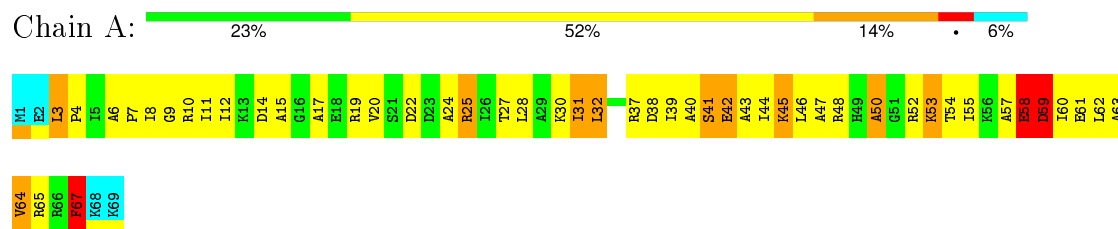


- Molecule 1: HISTONE B

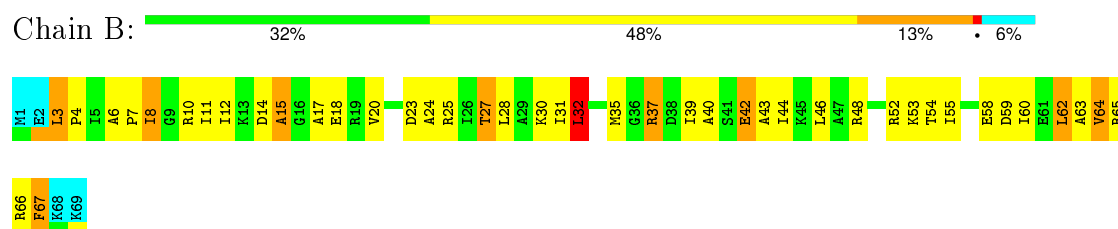


4.2.5 Score per residue for model 5

- Molecule 1: HISTONE B

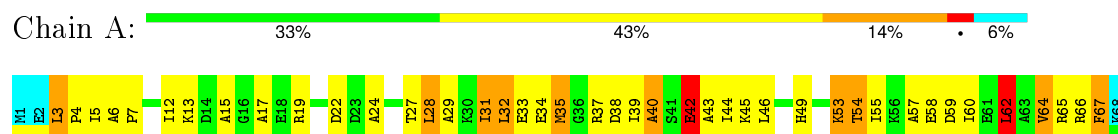


- Molecule 1: HISTONE B




4.2.6 Score per residue for model 6

- Molecule 1: HISTONE B



K69

- Molecule 1: HISTONE B

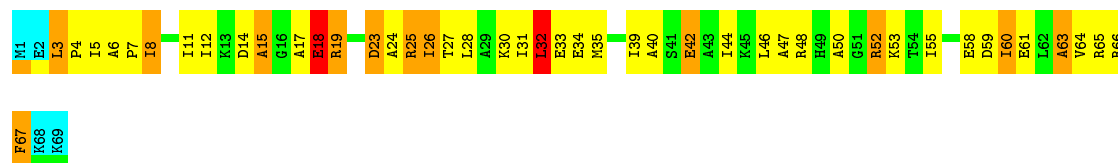
Chain B: 



4.2.7 Score per residue for model 7

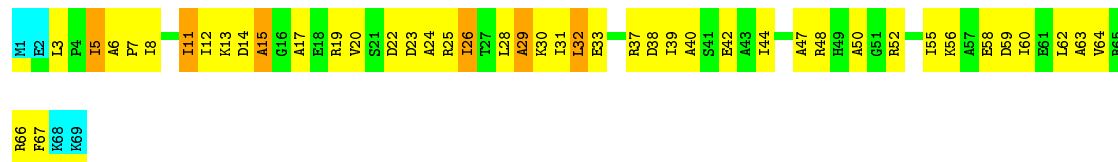
- Molecule 1: HISTONE B

Chain A: 



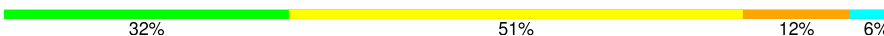
- Molecule 1: HISTONE B

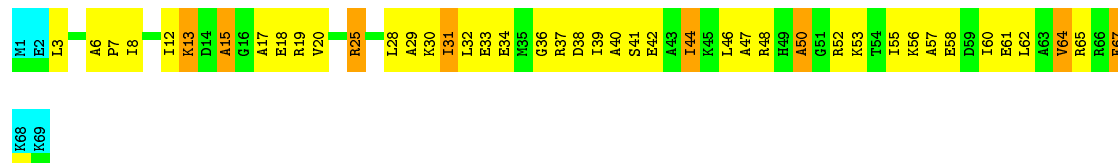
Chain B: 



4.2.8 Score per residue for model 8

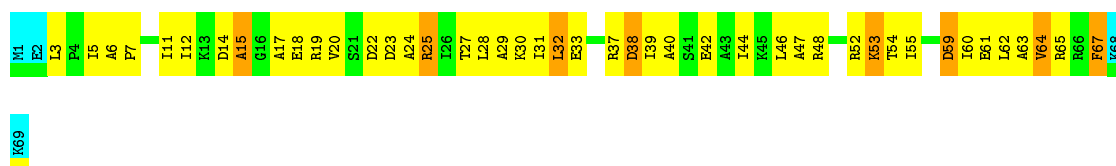
- Molecule 1: HISTONE B

Chain A: 



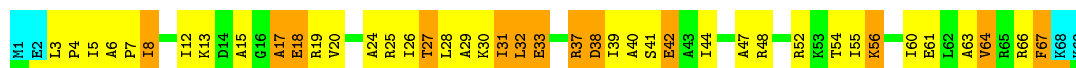
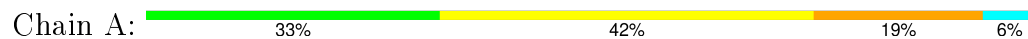
- Molecule 1: HISTONE B

Chain B: 

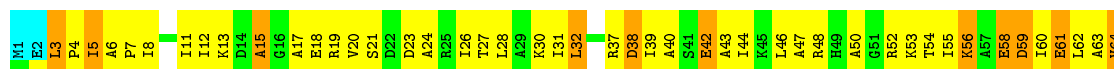
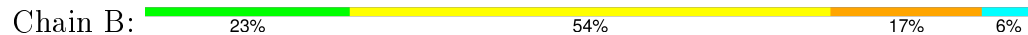


4.2.9 Score per residue for model 9

- Molecule 1: HISTONE B

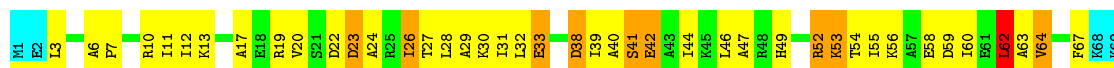
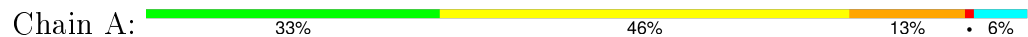


- Molecule 1: HISTONE B

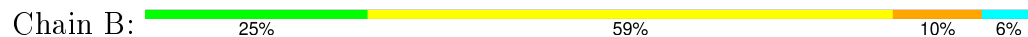


4.2.10 Score per residue for model 10

- Molecule 1: HISTONE B

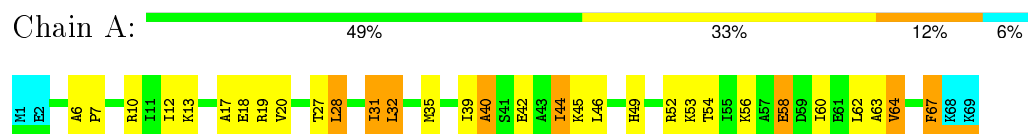


- Molecule 1: HISTONE B

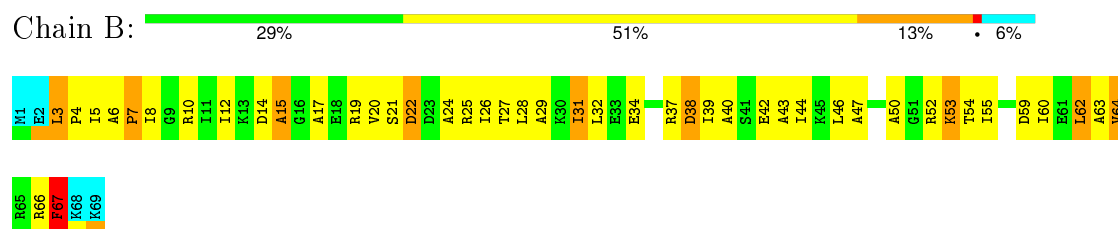


4.2.11 Score per residue for model 11

- Molecule 1: HISTONE B

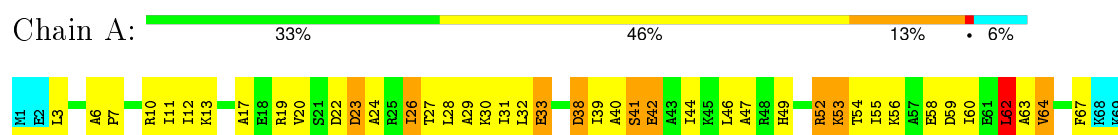


- Molecule 1: HISTONE B

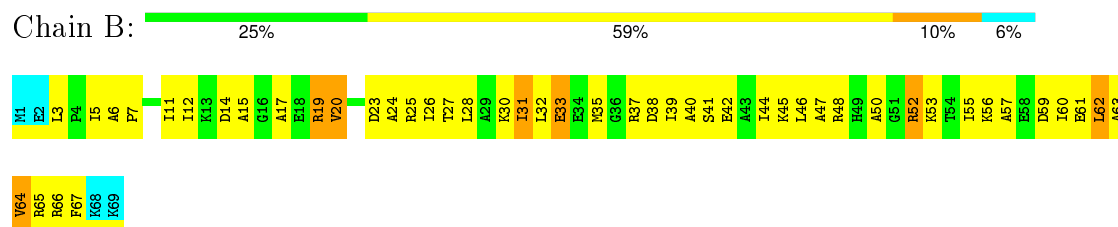


4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: HISTONE B

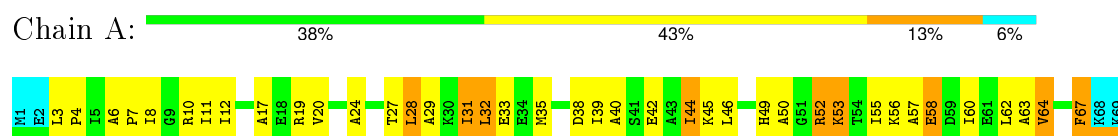


- Molecule 1: HISTONE B

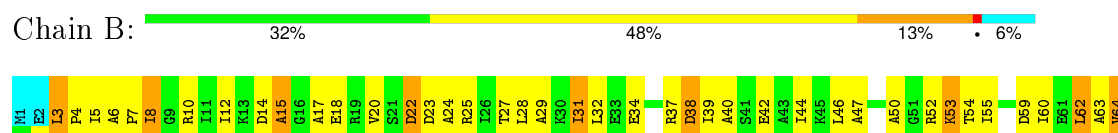


4.2.13 Score per residue for model 13

- Molecule 1: HISTONE B



- Molecule 1: HISTONE B



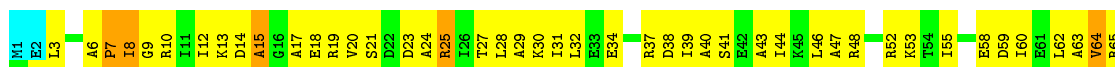


4.2.14 Score per residue for model 14

- Molecule 1: HISTONE B



- Molecule 1: HISTONE B

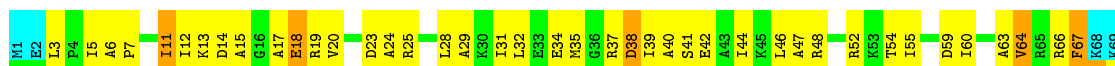


4.2.15 Score per residue for model 15

- Molecule 1: HISTONE B



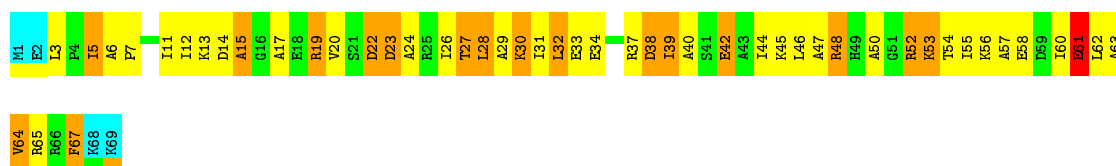
- Molecule 1: HISTONE B



4.2.16 Score per residue for model 16

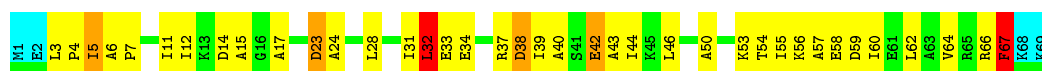
- Molecule 1: HISTONE B





- Molecule 1: HISTONE B

Chain B: 39% 46% 6% 6%



4.2.17 Score per residue for model 17

- Molecule 1: HISTONE B

Chain A: 28% 52% 13% 6%



- Molecule 1: HISTONE B

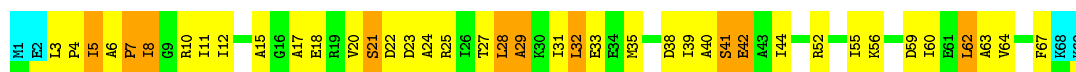
Chain B: 30% 54% 10% 6%



4.2.18 Score per residue for model 18

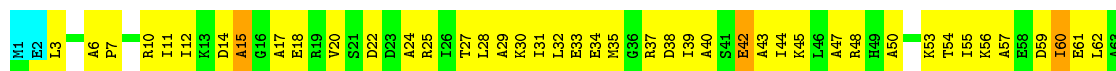
- Molecule 1: HISTONE B

Chain A: 36% 43% 14% 6%



- Molecule 1: HISTONE B

Chain B: 28% 59% 6% 6%



4.2.19 Score per residue for model 19

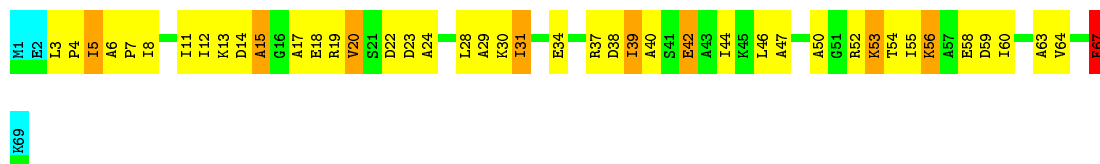
• Molecule 1: HISTONE B

Chain A: 30% 48% 14% • 6%



• Molecule 1: HISTONE B

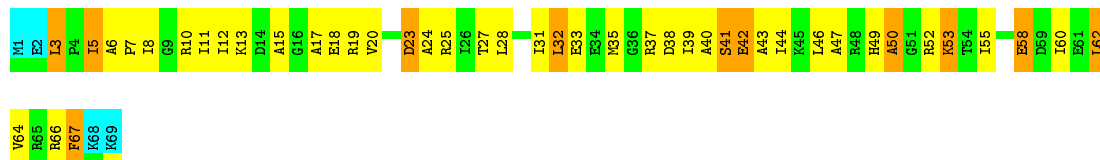
Chain B: 32% 49% 12% • 6%



4.2.20 Score per residue for model 20

• Molecule 1: HISTONE B

Chain A: 30% 48% 16% 6%



• Molecule 1: HISTONE B

Chain B: 32% 51% 12% 6%



4.2.21 Score per residue for model 21

• Molecule 1: HISTONE B

Chain A: 30% 49% 14% 6%



• Molecule 1: HISTONE B

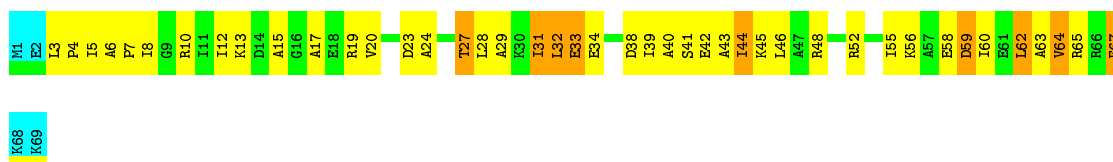
Chain B: 38% 43% 12% • 6%



4.2.22 Score per residue for model 22

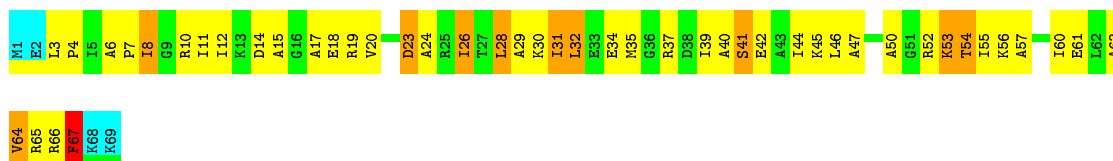
- Molecule 1: HISTONE B

Chain A: 32% 49% 13% 6%



- Molecule 1: HISTONE B

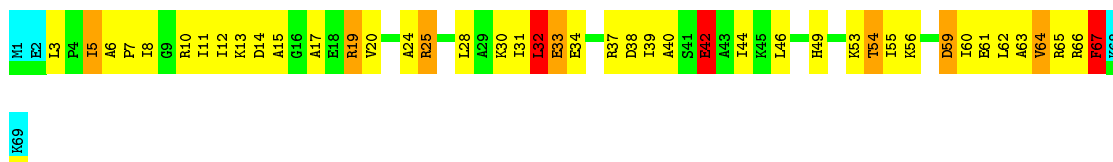
Chain B: 26% 52% 14% 6%



4.2.23 Score per residue for model 23

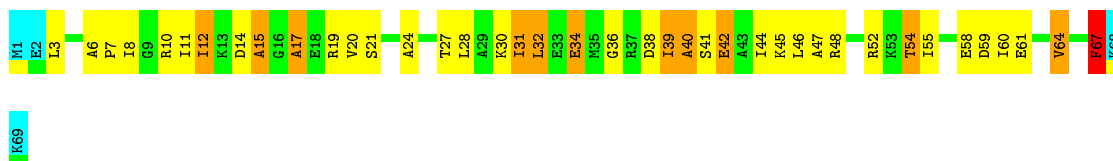
- Molecule 1: HISTONE B

Chain A: 32% 48% 10% 6%



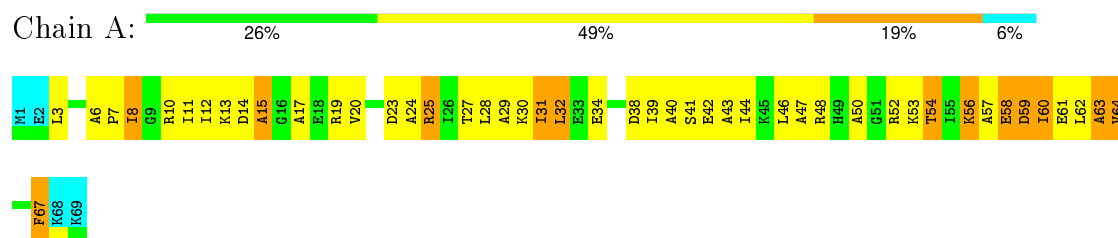
- Molecule 1: HISTONE B

Chain B: 36% 41% 16% 6%

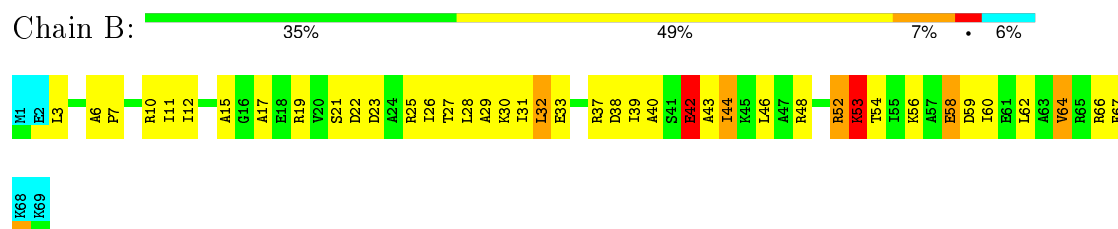


4.2.24 Score per residue for model 24

- Molecule 1: HISTONE B

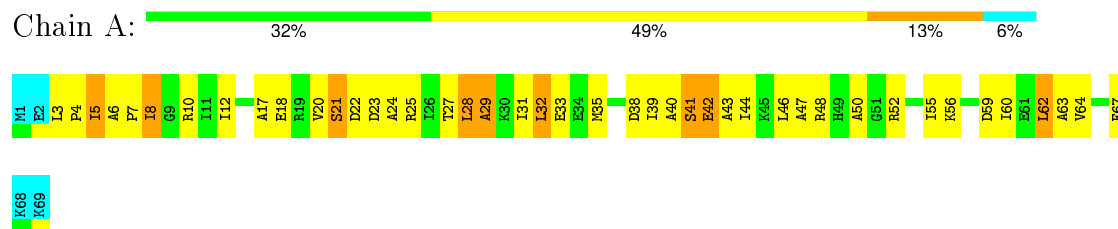


- Molecule 1: HISTONE B

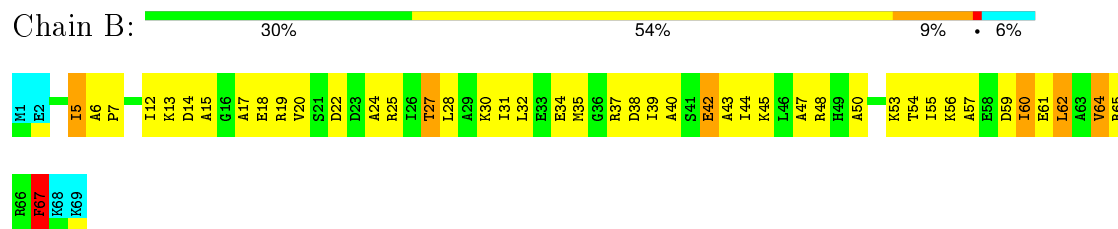


4.2.25 Score per residue for model 25

- Molecule 1: HISTONE B



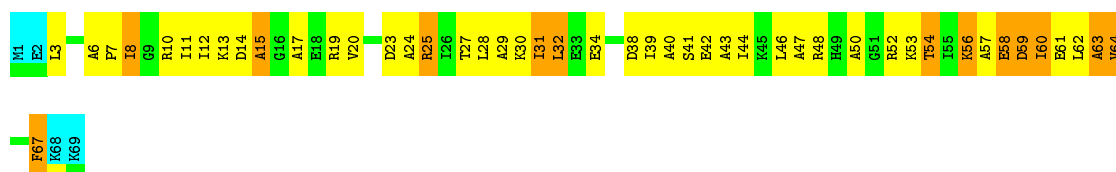
- Molecule 1: HISTONE B



4.2.26 Score per residue for model 26

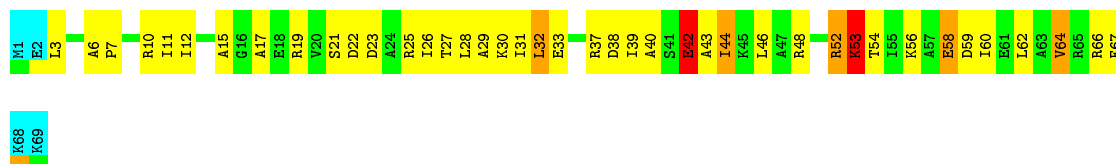
- Molecule 1: HISTONE B





- Molecule 1: HISTONE B

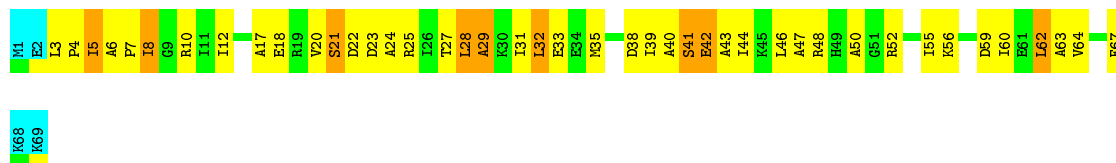
Chain B: 35% 49% 7% 6%



4.2.27 Score per residue for model 27

- Molecule 1: HISTONE B

Chain A: 32% 49% 13% 6%



- Molecule 1: HISTONE B

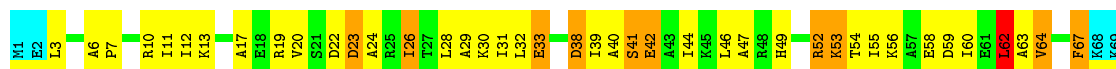
Chain B: 30% 54% 9% 6%



4.2.28 Score per residue for model 28

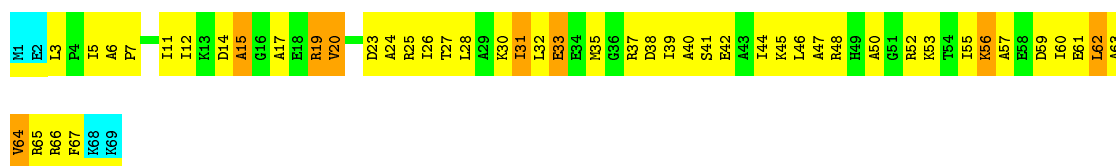
- Molecule 1: HISTONE B

Chain A: 35% 43% 14% 6%



- Molecule 1: HISTONE B

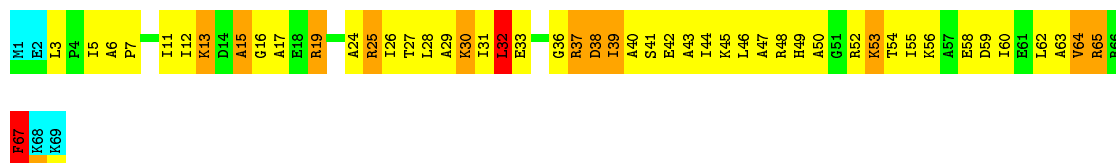
Chain B: 25% 58% 12% 6%



4.2.29 Score per residue for model 29

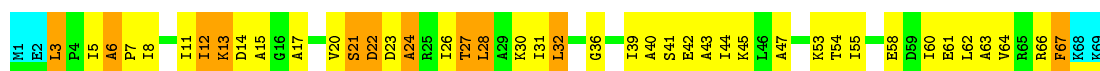
- Molecule 1: HISTONE B

Chain A: 23% 52% 16% 6%



- Molecule 1: HISTONE B

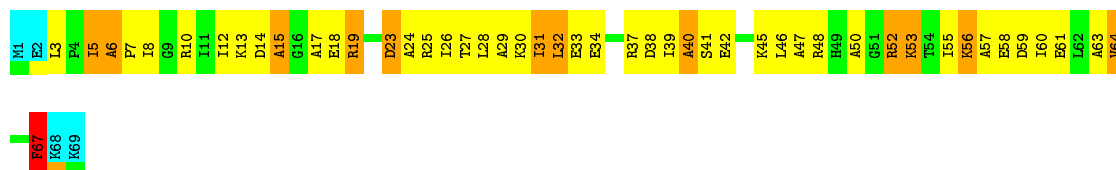
Chain B: 33% 45% 16% 6%



4.2.30 Score per residue for model 30

- Molecule 1: HISTONE B

Chain A: 25% 51% 17% 6%



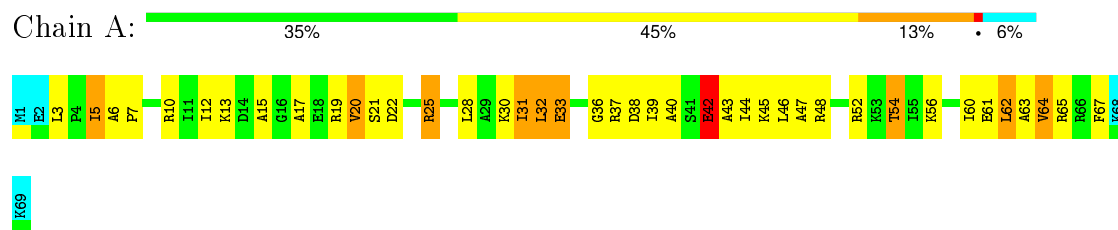
- Molecule 1: HISTONE B

Chain B: 38% 46% 10% 6%

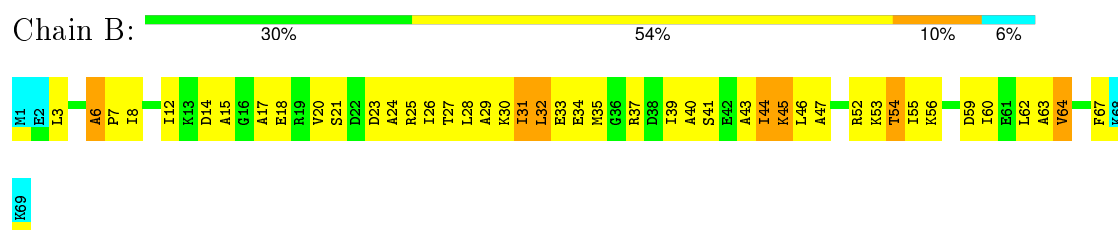


4.2.31 Score per residue for model 31

- Molecule 1: HISTONE B

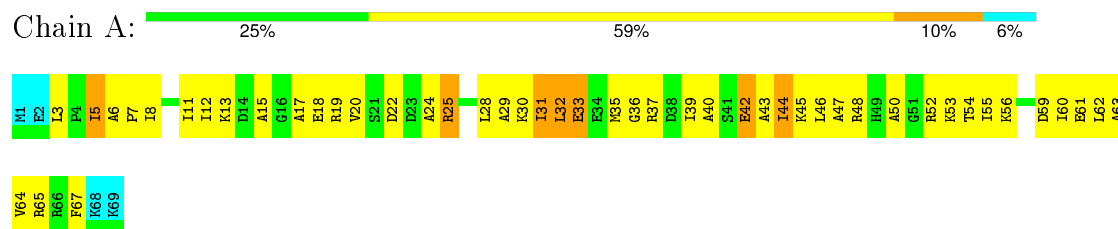


- Molecule 1: HISTONE B

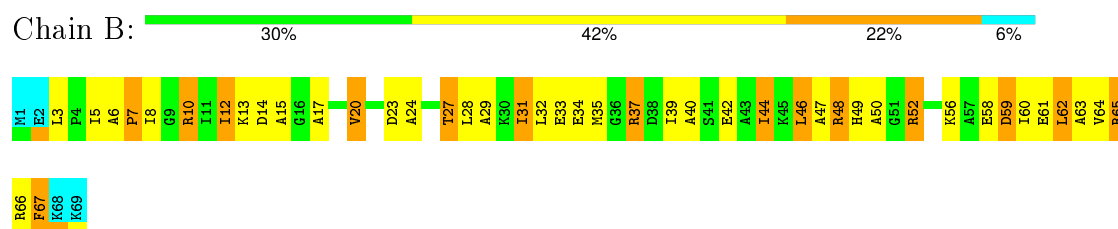


4.2.32 Score per residue for model 32

- Molecule 1: HISTONE B

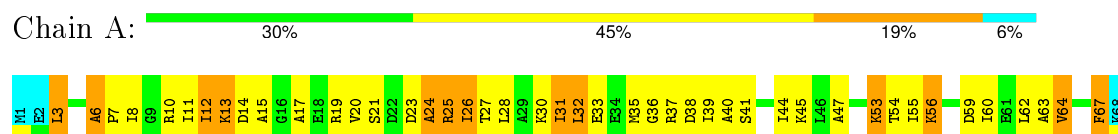


- Molecule 1: HISTONE B



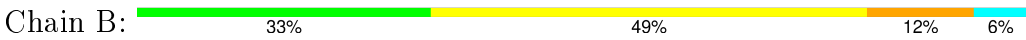
4.2.33 Score per residue for model 33

- Molecule 1: HISTONE B



K69

● Molecule 1: HISTONE B



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 33 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

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

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.58±0.00	0±0/505 (0.0±0.0%)	0.97±0.01	1±0/677 (0.1±0.1%)
1	B	0.58±0.00	0±0/505 (0.0±0.0%)	0.96±0.01	1±0/677 (0.1±0.0%)
All	All	0.58	0/33330 (0.0%)	0.97	57/44682 (0.1%)

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	3.6±2.0
1	B	0.0±0.0	3.7±1.7
All	All	0	239

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	67	PHE	CB-CG-CD2	-7.95	115.23	120.80	23	11
1	B	67	PHE	CB-CG-CD1	-6.82	116.03	120.80	19	20
1	A	67	PHE	CB-CG-CD1	-6.26	116.42	120.80	32	12
1	A	67	PHE	CB-CG-CD2	-6.06	116.56	120.80	14	14

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	14	ASP	Mainchain	26
1	B	15	ALA	Mainchain	18

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Mol	Chain	Res	Type	Group	Models (Total)
1	B	29	ALA	Mainchain	15
1	A	14	ASP	Mainchain	10
1	A	32	LEU	Mainchain	10
1	A	15	ALA	Mainchain	10
1	A	29	ALA	Mainchain	10
1	B	62	LEU	Mainchain	9
1	A	42	GLU	Mainchain	9
1	A	62	LEU	Mainchain	8
1	B	27	THR	Mainchain	7
1	A	63	ALA	Mainchain	7
1	B	32	LEU	Mainchain	7
1	A	50	ALA	Mainchain	7
1	B	61	GLU	Mainchain	7
1	A	28	LEU	Mainchain	7
1	A	8	ILE	Mainchain	6
1	B	8	ILE	Mainchain	6
1	B	13	LYS	Mainchain	4
1	A	35	MET	Mainchain	4
1	A	13	LYS	Mainchain	4
1	A	27	THR	Mainchain	4
1	A	40	ALA	Mainchain	4
1	A	58	GLU	Mainchain	3
1	A	61	GLU	Mainchain	3
1	B	28	LEU	Mainchain	3
1	B	67	PHE	Sidechain	2
1	B	7	PRO	Mainchain	2
1	B	42	GLU	Mainchain	2
1	B	22	ASP	Mainchain	2
1	B	39	ILE	Mainchain	2
1	B	53	LYS	Mainchain	2
1	A	39	ILE	Mainchain	2
1	A	67	PHE	Mainchain	2
1	A	33	GLU	Mainchain	1
1	B	34	GLU	Mainchain	1
1	B	63	ALA	Mainchain	1
1	A	9	GLY	Mainchain	1
1	A	59	ASP	Mainchain	1
1	B	33	GLU	Mainchain	1
1	B	40	ALA	Mainchain	1
1	A	37	ARG	Mainchain	1
1	A	7	PRO	Mainchain	1
1	B	43	ALA	Mainchain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	48	ARG	Mainchain	1
1	B	48	ARG	Mainchain	1
1	A	45	LYS	Mainchain	1
1	B	12	ILE	Mainchain	1
1	A	34	GLU	Mainchain	1

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	501	539	538	62±8
1	B	501	539	538	62±6
All	All	33066	35574	35508	2843

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HD23	1:B:32:LEU:HD23	1.08	1.22	29	8
1:A:31:ILE:HD13	1:B:64:VAL:HG21	1.03	1.17	7	7
1:A:64:VAL:HG21	1:B:31:ILE:HD13	1.03	1.20	4	8
1:A:3:LEU:HD21	1:B:11:ILE:HD11	1.02	1.30	29	4
1:A:64:VAL:HG21	1:B:31:ILE:HG21	0.96	1.37	19	22
1:A:27:THR:HG22	1:B:60:ILE:HG22	0.95	1.35	18	5
1:A:60:ILE:HG22	1:B:27:THR:HG22	0.94	1.38	26	5
1:A:17:ALA:HB2	1:B:44:ILE:HD11	0.91	1.42	29	27
1:A:40:ALA:HB2	1:B:12:ILE:HD12	0.91	1.41	5	26
1:A:20:VAL:HG21	1:A:25:ARG:NH2	0.86	1.84	2	1
1:A:12:ILE:HG22	1:A:17:ALA:HB2	0.86	1.45	4	12
1:A:31:ILE:HG21	1:B:64:VAL:HG21	0.85	1.48	13	26
1:A:11:ILE:HD11	1:B:3:LEU:HD21	0.84	1.46	19	12
1:A:55:ILE:HD12	1:B:20:VAL:HG22	0.84	1.48	23	6
1:A:3:LEU:CB	1:A:29:ALA:HB1	0.83	2.04	6	6
1:A:60:ILE:CG2	1:B:28:LEU:HD13	0.83	2.04	14	7
1:A:3:LEU:HB2	1:A:29:ALA:HB1	0.83	1.48	13	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:12:ILE:HG22	1:B:17:ALA:HB2	0.82	1.51	23	17
1:A:32:LEU:HD23	1:B:32:LEU:CD2	0.81	2.04	33	4
1:B:12:ILE:HG21	1:B:25:ARG:NH2	0.81	1.88	5	1
1:A:44:ILE:HD11	1:B:17:ALA:HB2	0.81	1.51	18	24
1:B:3:LEU:HB3	1:B:8:ILE:HD12	0.81	1.53	3	1
1:A:64:VAL:CG2	1:B:31:ILE:HD13	0.81	2.06	4	4
1:B:55:ILE:HG23	1:B:59:ASP:HB3	0.81	1.52	9	5
1:A:28:LEU:HD12	1:A:31:ILE:CG2	0.81	2.06	15	2
1:A:17:ALA:CA	1:B:44:ILE:HD11	0.81	2.05	26	5
1:A:36:GLY:HA2	1:B:32:LEU:HD11	0.80	1.53	3	4
1:B:12:ILE:HD11	1:B:28:LEU:HD23	0.80	1.51	6	9
1:B:46:LEU:HD22	1:B:62:LEU:HD23	0.79	1.51	8	5
1:A:24:ALA:HB2	1:B:56:LYS:CA	0.79	2.06	4	5
1:B:39:ILE:HD13	1:B:64:VAL:HG23	0.79	1.52	17	13
1:A:28:LEU:HD13	1:B:60:ILE:HG23	0.79	1.54	20	15
1:A:47:ALA:HB2	1:A:55:ILE:HD13	0.79	1.53	10	11
1:B:12:ILE:HG22	1:B:17:ALA:CB	0.79	2.07	23	3
1:A:60:ILE:HG23	1:B:28:LEU:HD13	0.79	1.54	27	20
1:A:31:ILE:HG12	1:B:64:VAL:HG11	0.79	1.54	32	4
1:A:44:ILE:HG12	1:A:55:ILE:HD11	0.79	1.55	5	1
1:A:24:ALA:HB2	1:B:56:LYS:HA	0.78	1.54	2	4
1:A:5:ILE:HD13	1:A:25:ARG:NH2	0.78	1.93	7	1
1:A:3:LEU:HD13	1:A:33:GLU:CG	0.78	2.08	18	6
1:A:20:VAL:HG22	1:B:55:ILE:CG1	0.78	2.07	21	2
1:A:55:ILE:HG13	1:B:20:VAL:HG22	0.78	1.55	3	2
1:A:31:ILE:HD13	1:B:64:VAL:CG2	0.78	2.07	7	1
1:A:3:LEU:HD13	1:A:33:GLU:CB	0.77	2.09	1	1
1:A:39:ILE:HG21	1:A:64:VAL:HG23	0.77	1.53	27	18
1:A:28:LEU:HD11	1:B:39:ILE:HB	0.77	1.55	28	11
1:A:3:LEU:HD21	1:B:11:ILE:CD1	0.77	2.09	29	3
1:A:27:THR:CG2	1:B:60:ILE:HG22	0.77	2.10	18	5
1:A:32:LEU:HD12	1:B:32:LEU:HD23	0.77	1.54	7	1
1:A:60:ILE:HG13	1:B:28:LEU:HD22	0.76	1.57	16	5
1:A:11:ILE:HG23	1:B:37:ARG:HG3	0.76	1.57	4	5
1:A:40:ALA:HB1	1:B:12:ILE:HG23	0.76	1.56	1	29
1:A:32:LEU:HD21	1:B:39:ILE:HD12	0.76	1.56	30	3
1:A:44:ILE:HD11	1:B:17:ALA:CA	0.76	2.11	32	10
1:A:32:LEU:HD11	1:B:39:ILE:HD12	0.76	1.56	19	2
1:A:12:ILE:HG23	1:B:40:ALA:HB1	0.75	1.58	8	27
1:B:3:LEU:HB3	1:B:8:ILE:HD11	0.75	1.56	13	10
1:A:64:VAL:HG21	1:B:31:ILE:CD1	0.75	2.08	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ALA:HB2	1:B:12:ILE:CD1	0.75	2.11	5	29
1:A:17:ALA:HA	1:B:44:ILE:HD11	0.75	1.58	26	2
1:B:12:ILE:HD11	1:B:28:LEU:CD2	0.75	2.12	6	4
1:A:56:LYS:CA	1:B:24:ALA:HB2	0.75	2.12	33	5
1:A:44:ILE:HD11	1:B:17:ALA:N	0.75	1.96	21	8
1:A:60:ILE:HD12	1:B:28:LEU:HD21	0.75	1.58	22	7
1:A:3:LEU:HD13	1:A:33:GLU:HB3	0.74	1.57	1	4
1:A:28:LEU:HD22	1:B:60:ILE:HG13	0.74	1.58	8	6
1:A:3:LEU:HB2	1:A:8:ILE:HD11	0.74	1.59	33	5
1:A:28:LEU:HD22	1:B:60:ILE:CG2	0.74	2.13	13	3
1:A:3:LEU:CB	1:A:8:ILE:HD11	0.74	2.11	5	7
1:B:3:LEU:CB	1:B:8:ILE:HD11	0.74	2.12	13	11
1:A:32:LEU:HD12	1:B:32:LEU:HB3	0.74	1.58	2	4
1:B:17:ALA:HB1	1:B:20:VAL:CG2	0.74	2.13	17	2
1:B:39:ILE:HD13	1:B:64:VAL:CG2	0.73	2.12	17	15
1:A:60:ILE:HD12	1:B:28:LEU:CD2	0.73	2.13	20	5
1:A:47:ALA:CB	1:A:55:ILE:HD13	0.73	2.12	17	6
1:A:24:ALA:HB1	1:B:60:ILE:CG1	0.73	2.13	29	12
1:A:60:ILE:CG2	1:B:28:LEU:HD22	0.73	2.13	22	8
1:A:11:ILE:HD11	1:B:3:LEU:CD2	0.73	2.13	19	13
1:A:55:ILE:CG2	1:B:20:VAL:HG13	0.73	2.13	14	2
1:A:61:GLU:CG	1:B:31:ILE:HD11	0.73	2.14	26	2
1:A:17:ALA:N	1:B:44:ILE:HD11	0.73	1.98	31	5
1:A:32:LEU:HD12	1:B:32:LEU:CB	0.73	2.14	2	2
1:A:43:ALA:HB1	1:A:59:ASP:CG	0.73	2.04	5	1
1:B:20:VAL:HG11	1:B:25:ARG:CZ	0.73	2.14	5	1
1:A:15:ALA:HB1	1:B:41:SER:CB	0.72	2.14	6	2
1:A:20:VAL:HG22	1:B:55:ILE:HB	0.72	1.60	16	5
1:A:60:ILE:CG2	1:B:27:THR:HG22	0.72	2.12	26	10
1:A:11:ILE:HD11	1:B:3:LEU:HD22	0.72	1.61	2	3
1:A:19:ARG:NH2	1:B:44:ILE:HG23	0.72	2.00	16	1
1:B:27:THR:O	1:B:31:ILE:HD12	0.72	1.83	33	11
1:A:31:ILE:HD12	1:B:60:ILE:HG22	0.72	1.62	19	4
1:A:55:ILE:HB	1:B:20:VAL:HG13	0.72	1.62	17	11
1:A:12:ILE:HD12	1:B:40:ALA:HB2	0.72	1.60	4	26
1:A:39:ILE:HD13	1:A:64:VAL:HG23	0.72	1.61	6	12
1:A:39:ILE:HD13	1:A:64:VAL:CG2	0.71	2.15	6	13
1:A:32:LEU:O	1:B:32:LEU:HD21	0.71	1.84	30	12
1:A:60:ILE:HG23	1:B:28:LEU:HD22	0.71	1.60	33	5
1:A:32:LEU:HD21	1:B:32:LEU:O	0.71	1.84	31	13
1:A:27:THR:O	1:A:31:ILE:HD12	0.71	1.85	16	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:ILE:HG23	1:B:63:ALA:O	0.71	1.85	32	2
1:A:39:ILE:HG23	1:A:63:ALA:O	0.71	1.85	31	1
1:A:57:ALA:HA	1:B:27:THR:HG21	0.71	1.63	3	3
1:A:8:ILE:HA	1:A:11:ILE:HD12	0.71	1.62	2	3
1:B:28:LEU:O	1:B:32:LEU:HD12	0.71	1.85	21	4
1:A:15:ALA:HB1	1:B:41:SER:OG	0.71	1.86	21	3
1:A:24:ALA:HB1	1:B:55:ILE:HG22	0.71	1.61	21	6
1:A:15:ALA:HB1	1:B:41:SER:HB3	0.71	1.60	20	1
1:B:55:ILE:HG23	1:B:59:ASP:HB2	0.71	1.63	5	2
1:A:61:GLU:HG2	1:B:31:ILE:HD11	0.71	1.59	26	2
1:B:55:ILE:HG23	1:B:59:ASP:CB	0.71	2.15	9	7
1:A:20:VAL:CG1	1:A:24:ALA:HB3	0.71	2.16	33	11
1:A:20:VAL:HG22	1:B:55:ILE:HD12	0.71	1.61	18	10
1:A:23:ASP:HB3	1:B:57:ALA:HB2	0.70	1.62	30	1
1:A:47:ALA:O	1:A:50:ALA:HB3	0.70	1.85	7	17
1:A:39:ILE:HB	1:B:28:LEU:HD11	0.70	1.63	8	13
1:A:3:LEU:CD2	1:B:11:ILE:HD11	0.70	2.14	29	4
1:A:39:ILE:HG12	1:A:64:VAL:HG23	0.70	1.63	8	3
1:A:55:ILE:HG23	1:A:59:ASP:CG	0.70	2.07	5	1
1:A:20:VAL:HG21	1:A:25:ARG:CD	0.70	2.16	31	1
1:A:60:ILE:CG2	1:B:31:ILE:HD13	0.70	2.16	30	3
1:A:32:LEU:HD23	1:B:32:LEU:HB3	0.70	1.63	18	10
1:A:33:GLU:O	1:B:11:ILE:HD12	0.70	1.87	15	1
1:A:32:LEU:HD13	1:B:32:LEU:HG	0.70	1.61	6	2
1:A:3:LEU:HB3	1:A:8:ILE:HD11	0.69	1.62	32	14
1:A:3:LEU:HD13	1:A:33:GLU:HG2	0.69	1.63	27	3
1:B:3:LEU:CB	1:B:8:ILE:HD12	0.69	2.17	3	1
1:B:3:LEU:HD21	1:B:33:GLU:CG	0.69	2.17	31	1
1:A:12:ILE:HD11	1:A:28:LEU:HD23	0.69	1.63	3	12
1:A:24:ALA:CB	1:B:55:ILE:HG22	0.69	2.17	18	8
1:A:43:ALA:HA	1:A:46:LEU:HD12	0.69	1.64	14	6
1:A:60:ILE:CG1	1:B:28:LEU:HD22	0.69	2.18	9	6
1:A:32:LEU:CD2	1:B:32:LEU:HD23	0.69	2.17	31	5
1:A:56:LYS:HA	1:B:24:ALA:HB2	0.69	1.64	33	4
1:B:46:LEU:CD2	1:B:62:LEU:HD23	0.69	2.17	8	2
1:A:24:ALA:O	1:A:27:THR:HG22	0.69	1.86	5	1
1:B:39:ILE:HD13	1:B:64:VAL:HG22	0.69	1.63	7	1
1:A:5:ILE:HG21	1:A:26:ILE:HG12	0.69	1.65	3	1
1:B:28:LEU:HA	1:B:31:ILE:HD12	0.68	1.66	18	9
1:A:12:ILE:O	1:A:17:ALA:HB3	0.68	1.89	29	2
1:A:41:SER:OG	1:B:15:ALA:HB1	0.68	1.88	10	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ILE:CD1	1:A:28:LEU:HD23	0.68	2.19	3	9
1:B:47:ALA:HB2	1:B:55:ILE:HG12	0.68	1.62	4	4
1:A:54:THR:HG23	1:B:19:ARG:O	0.68	1.88	1	3
1:A:11:ILE:CD1	1:B:3:LEU:HD21	0.68	2.18	19	5
1:A:40:ALA:HB2	1:B:12:ILE:HD13	0.68	1.63	11	5
1:A:11:ILE:HG22	1:A:12:ILE:HD13	0.67	1.64	33	5
1:A:44:ILE:HD11	1:B:17:ALA:HA	0.67	1.66	32	5
1:A:54:THR:HG23	1:B:19:ARG:HG3	0.67	1.65	9	1
1:A:46:LEU:HD22	1:A:62:LEU:CD2	0.67	2.19	21	1
1:B:28:LEU:HD12	1:B:32:LEU:HD11	0.67	1.66	17	7
1:B:47:ALA:HB2	1:B:55:ILE:CD1	0.67	2.19	31	4
1:A:55:ILE:HG23	1:A:59:ASP:OD2	0.67	1.88	5	1
1:B:17:ALA:HB1	1:B:20:VAL:HG22	0.67	1.66	22	2
1:A:28:LEU:HD22	1:B:60:ILE:CG1	0.67	2.19	1	6
1:A:22:ASP:O	1:A:26:ILE:HD12	0.67	1.90	16	3
1:B:46:LEU:HD22	1:B:59:ASP:OD1	0.67	1.88	32	1
1:B:26:ILE:O	1:B:26:ILE:HD13	0.67	1.90	22	2
1:A:42:GLU:C	1:A:46:LEU:HD12	0.67	2.11	30	5
1:A:60:ILE:HG12	1:B:28:LEU:HD13	0.66	1.64	26	2
1:A:11:ILE:HG23	1:B:37:ARG:HG2	0.66	1.66	32	1
1:B:57:ALA:HB1	1:B:61:GLU:OE2	0.66	1.90	17	1
1:A:55:ILE:HD12	1:B:20:VAL:CG2	0.66	2.19	23	1
1:A:42:GLU:O	1:A:46:LEU:HD13	0.66	1.91	32	17
1:A:43:ALA:HB1	1:A:59:ASP:OD2	0.66	1.91	5	1
1:A:46:LEU:HD22	1:A:62:LEU:HD23	0.66	1.68	21	1
1:A:20:VAL:HG13	1:B:55:ILE:HB	0.65	1.67	21	5
1:A:32:LEU:HD11	1:B:32:LEU:O	0.65	1.90	7	5
1:B:26:ILE:HD13	1:B:26:ILE:O	0.65	1.92	7	2
1:B:12:ILE:O	1:B:15:ALA:HB3	0.65	1.90	14	28
1:A:6:ALA:HB3	1:A:7:PRO:HD3	0.65	1.69	1	33
1:B:42:GLU:C	1:B:46:LEU:HD12	0.65	2.12	33	5
1:A:15:ALA:HB1	1:B:41:SER:HB2	0.65	1.66	6	3
1:B:39:ILE:HG21	1:B:64:VAL:HG23	0.65	1.69	17	18
1:A:58:GLU:O	1:A:62:LEU:HD23	0.65	1.91	11	4
1:A:28:LEU:HA	1:A:31:ILE:HD12	0.65	1.68	26	3
1:A:3:LEU:HD13	1:A:33:GLU:HB2	0.65	1.69	14	4
1:A:55:ILE:CD1	1:B:20:VAL:HG22	0.65	2.22	23	2
1:B:8:ILE:HA	1:B:11:ILE:HD12	0.64	1.67	22	3
1:B:6:ALA:HB3	1:B:7:PRO:HD3	0.64	1.69	2	33
1:A:31:ILE:HD13	1:B:60:ILE:CG2	0.64	2.22	2	5
1:A:27:THR:C	1:A:31:ILE:HD12	0.64	2.13	9	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ALA:HB2	1:A:55:ILE:CD1	0.64	2.22	9	7
1:A:23:ASP:O	1:A:26:ILE:HG22	0.64	1.92	10	3
1:A:41:SER:CA	1:B:15:ALA:HB1	0.64	2.22	15	1
1:A:26:ILE:HD13	1:A:26:ILE:O	0.64	1.91	7	1
1:A:3:LEU:HD11	1:B:11:ILE:HD11	0.64	1.70	20	2
1:B:43:ALA:HA	1:B:46:LEU:HD12	0.64	1.67	30	7
1:A:20:VAL:HG13	1:A:24:ALA:HB3	0.64	1.70	26	6
1:A:56:LYS:C	1:B:24:ALA:HB2	0.64	2.14	21	5
1:A:39:ILE:CG2	1:A:64:VAL:HG23	0.63	2.22	27	23
1:A:3:LEU:HB3	1:A:29:ALA:HB1	0.63	1.69	6	1
1:B:5:ILE:HD12	1:B:25:ARG:HD2	0.63	1.70	15	1
1:A:28:LEU:CD2	1:B:60:ILE:HD12	0.63	2.23	13	2
1:A:60:ILE:HG22	1:B:27:THR:CG2	0.63	2.21	26	2
1:A:60:ILE:HG21	1:B:27:THR:HB	0.63	1.70	33	1
1:A:27:THR:HG22	1:B:60:ILE:CG2	0.63	2.23	3	9
1:A:55:ILE:HG23	1:A:59:ASP:HB2	0.63	1.70	23	2
1:B:60:ILE:O	1:B:64:VAL:HG23	0.63	1.93	29	5
1:A:23:ASP:HB2	1:B:57:ALA:HB2	0.63	1.69	16	1
1:B:3:LEU:HD21	1:B:33:GLU:HG2	0.63	1.70	31	1
1:A:60:ILE:HG23	1:B:28:LEU:CD2	0.63	2.23	33	5
1:A:20:VAL:HG12	1:A:24:ALA:HB3	0.63	1.71	33	4
1:B:12:ILE:CD1	1:B:28:LEU:HD23	0.63	2.24	15	9
1:A:55:ILE:CG2	1:B:20:VAL:HG12	0.63	2.24	28	3
1:A:5:ILE:HD13	1:A:25:ARG:NH1	0.63	2.08	3	1
1:A:20:VAL:HG21	1:A:25:ARG:HD2	0.63	1.68	31	1
1:B:28:LEU:HD12	1:B:32:LEU:CD1	0.62	2.24	17	5
1:A:12:ILE:O	1:A:15:ALA:HB3	0.62	1.94	16	21
1:A:26:ILE:O	1:A:29:ALA:HB3	0.62	1.94	9	3
1:B:46:LEU:HD21	1:B:66:ARG:NH2	0.62	2.07	1	1
1:A:33:GLU:HG2	1:B:11:ILE:HD13	0.62	1.70	8	1
1:A:44:ILE:CG1	1:A:55:ILE:HD11	0.62	2.22	5	1
1:A:17:ALA:HB2	1:B:44:ILE:CD1	0.62	2.25	14	22
1:A:3:LEU:HD11	1:A:33:GLU:HB2	0.62	1.71	16	2
1:B:12:ILE:HG21	1:B:20:VAL:HG21	0.62	1.72	11	1
1:A:28:LEU:HD12	1:A:31:ILE:HG21	0.62	1.69	15	2
1:A:28:LEU:HD12	1:A:31:ILE:HG22	0.62	1.70	15	2
1:B:31:ILE:HG22	1:B:32:LEU:HD12	0.62	1.70	27	3
1:A:32:LEU:HD21	1:B:39:ILE:CD1	0.61	2.25	30	2
1:B:11:ILE:HG22	1:B:12:ILE:HD13	0.61	1.72	7	2
1:A:12:ILE:HG22	1:A:17:ALA:CB	0.61	2.25	4	1
1:A:55:ILE:HG22	1:B:24:ALA:HB1	0.61	1.71	30	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ILE:HD12	1:B:32:LEU:HD11	0.61	1.71	4	7
1:B:47:ALA:O	1:B:50:ALA:HB3	0.61	1.95	32	14
1:A:28:LEU:HD22	1:B:60:ILE:HG21	0.61	1.70	5	3
1:A:32:LEU:HD13	1:B:32:LEU:CG	0.61	2.25	6	1
1:B:12:ILE:O	1:B:17:ALA:HB3	0.61	1.96	32	2
1:A:28:LEU:HD21	1:B:60:ILE:HD12	0.61	1.71	13	3
1:A:58:GLU:O	1:A:62:LEU:HD12	0.61	1.95	10	4
1:A:32:LEU:HD12	1:B:32:LEU:CD2	0.61	2.25	7	1
1:A:60:ILE:CG1	1:B:24:ALA:HB1	0.61	2.26	3	10
1:A:58:GLU:O	1:A:62:LEU:HD13	0.61	1.95	22	3
1:A:62:LEU:N	1:A:62:LEU:HD23	0.61	2.11	31	1
1:A:19:ARG:HH22	1:B:44:ILE:HG23	0.61	1.55	16	1
1:A:42:GLU:HB3	1:A:63:ALA:HB1	0.61	1.72	15	8
1:B:39:ILE:CG1	1:B:64:VAL:HG23	0.60	2.26	6	12
1:B:26:ILE:O	1:B:29:ALA:HB3	0.60	1.97	33	7
1:A:64:VAL:HG21	1:B:31:ILE:CG2	0.60	2.26	31	1
1:A:12:ILE:HG23	1:B:40:ALA:CB	0.60	2.27	9	31
1:A:32:LEU:HD11	1:B:36:GLY:CA	0.60	2.25	29	2
1:A:60:ILE:CG1	1:B:28:LEU:HD13	0.60	2.27	26	3
1:A:3:LEU:HD21	1:A:33:GLU:OE2	0.60	1.96	15	1
1:B:58:GLU:O	1:B:62:LEU:HD22	0.60	1.97	32	1
1:A:31:ILE:HD13	1:B:60:ILE:HG22	0.60	1.74	6	2
1:A:54:THR:HG22	1:A:55:ILE:O	0.60	1.97	32	5
1:A:27:THR:HG23	1:B:60:ILE:HG21	0.60	1.71	5	1
1:A:3:LEU:HD21	1:A:33:GLU:HG3	0.59	1.74	17	1
1:A:5:ILE:HG22	1:A:25:ARG:NH1	0.59	2.12	32	1
1:A:37:ARG:NE	1:B:11:ILE:HG23	0.59	2.11	19	1
1:A:31:ILE:HD11	1:B:61:GLU:CG	0.59	2.27	29	1
1:A:41:SER:CB	1:B:15:ALA:HB1	0.59	2.28	15	2
1:B:58:GLU:C	1:B:62:LEU:HD23	0.59	2.17	29	1
1:A:60:ILE:O	1:A:64:VAL:HG23	0.59	1.96	26	4
1:A:64:VAL:HG11	1:B:31:ILE:HD13	0.59	1.72	16	1
1:B:20:VAL:CG1	1:B:24:ALA:HB3	0.59	2.27	7	6
1:A:60:ILE:CG2	1:B:31:ILE:HD12	0.58	2.28	16	1
1:B:5:ILE:HD12	1:B:25:ARG:HD3	0.58	1.75	13	2
1:A:55:ILE:CB	1:B:20:VAL:HG13	0.58	2.28	14	2
1:A:28:LEU:HD12	1:A:32:LEU:CD1	0.58	2.27	11	2
1:B:3:LEU:HD12	1:B:29:ALA:O	0.58	1.99	6	1
1:B:39:ILE:CD1	1:B:64:VAL:HG23	0.58	2.28	1	13
1:A:31:ILE:HD11	1:B:61:GLU:HG2	0.58	1.74	29	2
1:A:41:SER:HB2	1:B:15:ALA:HB1	0.58	1.74	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:LEU:HB2	1:B:8:ILE:HD11	0.58	1.75	5	9
1:A:21:SER:HA	1:B:54:THR:HG21	0.58	1.76	33	1
1:A:31:ILE:CD1	1:B:60:ILE:HG22	0.58	2.27	19	8
1:B:58:GLU:C	1:B:62:LEU:HD12	0.58	2.18	14	1
1:B:47:ALA:HB2	1:B:55:ILE:HD13	0.58	1.75	31	6
1:B:12:ILE:HG21	1:B:25:ARG:CZ	0.58	2.27	5	1
1:A:60:ILE:HG22	1:B:31:ILE:CD1	0.58	2.28	19	5
1:A:55:ILE:HB	1:B:20:VAL:HG12	0.58	1.75	19	5
1:A:61:GLU:C	1:A:62:LEU:HD23	0.58	2.20	31	1
1:B:27:THR:HG22	1:B:31:ILE:HD11	0.58	1.75	4	8
1:B:46:LEU:HD22	1:B:62:LEU:HG	0.57	1.75	11	2
1:B:46:LEU:HD21	1:B:66:ARG:HH21	0.57	1.59	1	1
1:A:36:GLY:CA	1:B:32:LEU:HD11	0.57	2.28	3	2
1:A:57:ALA:CA	1:B:27:THR:HG21	0.57	2.29	26	2
1:B:20:VAL:HG11	1:B:25:ARG:NH2	0.57	2.15	5	1
1:A:55:ILE:HG23	1:A:59:ASP:OD1	0.57	1.99	5	1
1:A:17:ALA:HB1	1:A:20:VAL:HG23	0.57	1.76	5	1
1:B:21:SER:O	1:B:24:ALA:HB3	0.57	2.00	23	2
1:A:32:LEU:O	1:B:32:LEU:HD22	0.57	1.98	22	1
1:A:40:ALA:CB	1:B:12:ILE:HG23	0.57	2.30	7	28
1:A:60:ILE:HG13	1:B:24:ALA:HB1	0.57	1.76	3	11
1:A:20:VAL:HG22	1:B:55:ILE:HG13	0.57	1.76	15	2
1:A:39:ILE:CG1	1:A:64:VAL:HG23	0.57	2.29	8	8
1:A:28:LEU:CD1	1:B:39:ILE:HG21	0.57	2.30	33	4
1:A:28:LEU:HD13	1:B:60:ILE:HG13	0.57	1.75	3	2
1:A:47:ALA:HB1	1:A:53:LYS:HB3	0.57	1.74	30	1
1:B:64:VAL:HG22	1:B:67:PHE:CZ	0.57	2.35	23	1
1:B:46:LEU:HD11	1:B:63:ALA:HA	0.56	1.75	11	10
1:B:5:ILE:HD12	1:B:25:ARG:CD	0.56	2.30	13	2
1:B:28:LEU:HD12	1:B:32:LEU:HD12	0.56	1.76	33	2
1:A:46:LEU:HD22	1:A:63:ALA:HB2	0.56	1.76	26	12
1:B:50:ALA:HB1	1:B:53:LYS:NZ	0.56	2.16	16	1
1:A:5:ILE:HD13	1:A:25:ARG:HH22	0.56	1.59	7	1
1:A:17:ALA:HB1	1:A:20:VAL:CG2	0.56	2.30	21	5
1:B:5:ILE:HG21	1:B:25:ARG:HE	0.56	1.60	21	1
1:A:6:ALA:HB3	1:A:7:PRO:CD	0.56	2.31	10	33
1:A:55:ILE:HG22	1:B:20:VAL:HG13	0.56	1.78	14	1
1:B:6:ALA:HB3	1:B:7:PRO:CD	0.56	2.31	23	33
1:A:3:LEU:HD21	1:A:33:GLU:CD	0.56	2.21	16	1
1:A:60:ILE:HG21	1:B:28:LEU:HD22	0.55	1.77	10	8
1:B:27:THR:C	1:B:31:ILE:HD12	0.55	2.21	14	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:HD22	1:B:60:ILE:HG23	0.55	1.78	13	2
1:A:17:ALA:N	1:B:44:ILE:HD13	0.55	2.16	6	7
1:A:55:ILE:HB	1:B:20:VAL:HG22	0.55	1.77	21	4
1:A:27:THR:HG22	1:A:31:ILE:CD1	0.55	2.31	33	6
1:A:28:LEU:HD11	1:B:39:ILE:CB	0.55	2.30	10	6
1:A:31:ILE:HD13	1:B:60:ILE:HG21	0.55	1.78	2	1
1:A:39:ILE:HD13	1:A:64:VAL:HG22	0.55	1.79	32	5
1:A:8:ILE:HD11	1:A:29:ALA:HA	0.55	1.76	30	3
1:B:40:ALA:C	1:B:44:ILE:HD12	0.55	2.21	2	12
1:A:5:ILE:HG23	1:A:26:ILE:CD1	0.55	2.31	29	1
1:A:43:ALA:HA	1:A:46:LEU:HD22	0.55	1.79	26	4
1:A:36:GLY:CA	1:B:32:LEU:HD21	0.55	2.32	8	1
1:B:46:LEU:HD11	1:B:62:LEU:O	0.54	2.02	30	1
1:B:26:ILE:HG22	1:B:30:LYS:HD2	0.54	1.78	9	1
1:B:43:ALA:O	1:B:55:ILE:HD12	0.54	2.00	33	1
1:A:8:ILE:HD11	1:A:29:ALA:CA	0.54	2.31	30	3
1:B:20:VAL:HG11	1:B:25:ARG:NE	0.54	2.17	5	1
1:B:3:LEU:HD21	1:B:33:GLU:OE1	0.54	2.03	6	2
1:A:5:ILE:HD13	1:A:5:ILE:H	0.54	1.62	32	7
1:A:44:ILE:HD13	1:B:17:ALA:N	0.54	2.17	16	8
1:A:32:LEU:C	1:B:32:LEU:HD21	0.54	2.23	30	2
1:A:24:ALA:HB2	1:B:55:ILE:C	0.54	2.22	18	5
1:A:50:ALA:HB1	1:A:52:ARG:HB2	0.54	1.80	13	1
1:B:3:LEU:HD11	1:B:33:GLU:OE1	0.54	2.02	6	1
1:A:27:THR:HG22	1:A:31:ILE:HD11	0.54	1.80	26	8
1:A:28:LEU:HD11	1:B:39:ILE:HG21	0.54	1.80	33	2
1:B:42:GLU:HB3	1:B:63:ALA:HB1	0.54	1.79	3	6
1:B:39:ILE:CG2	1:B:64:VAL:HG23	0.54	2.33	15	24
1:A:3:LEU:HD13	1:A:33:GLU:HG3	0.54	1.78	28	3
1:A:28:LEU:O	1:A:32:LEU:HD23	0.54	2.03	2	1
1:A:44:ILE:HD11	1:B:17:ALA:CB	0.53	2.30	18	7
1:B:58:GLU:O	1:B:62:LEU:HD13	0.53	2.01	9	2
1:A:59:ASP:O	1:A:63:ALA:HB2	0.53	2.03	33	2
1:A:3:LEU:CD1	1:A:33:GLU:HB2	0.53	2.33	22	3
1:A:31:ILE:HG22	1:A:32:LEU:HD22	0.53	1.79	4	2
1:B:24:ALA:O	1:B:27:THR:HG22	0.53	2.02	14	1
1:A:60:ILE:HG22	1:B:31:ILE:HD12	0.53	1.80	5	1
1:B:43:ALA:N	1:B:63:ALA:HB2	0.53	2.18	31	4
1:A:31:ILE:HD13	1:B:60:ILE:HG23	0.53	1.80	18	5
1:A:32:LEU:HD11	1:B:36:GLY:HA2	0.53	1.79	29	1
1:B:39:ILE:HG23	1:B:67:PHE:HE2	0.53	1.64	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LEU:O	1:A:62:LEU:HD13	0.53	2.04	27	2
1:A:3:LEU:N	1:A:3:LEU:HD23	0.53	2.18	7	1
1:A:62:LEU:HD13	1:A:62:LEU:O	0.53	2.04	25	1
1:B:43:ALA:HB1	1:B:55:ILE:CG2	0.53	2.34	30	1
1:A:44:ILE:O	1:A:47:ALA:HB3	0.53	2.04	2	3
1:A:5:ILE:HG22	1:A:25:ARG:HB3	0.53	1.78	15	1
1:A:3:LEU:HD12	1:A:29:ALA:O	0.53	2.04	32	1
1:A:57:ALA:HB2	1:B:23:ASP:HB3	0.53	1.81	6	5
1:B:3:LEU:HD12	1:B:8:ILE:HD11	0.53	1.79	33	1
1:B:58:GLU:O	1:B:62:LEU:HG	0.53	2.03	26	3
1:B:8:ILE:HG22	1:B:25:ARG:HH12	0.53	1.64	14	1
1:B:3:LEU:HB2	1:B:29:ALA:HB1	0.52	1.81	1	1
1:A:47:ALA:HB1	1:A:53:LYS:CB	0.52	2.34	30	1
1:A:44:ILE:HA	1:A:55:ILE:HD11	0.52	1.81	23	1
1:A:23:ASP:HA	1:A:26:ILE:HG22	0.52	1.81	19	3
1:A:44:ILE:CD1	1:B:17:ALA:HB2	0.52	2.33	4	8
1:A:24:ALA:HB2	1:B:56:LYS:N	0.52	2.19	4	6
1:A:8:ILE:CD1	1:A:29:ALA:HB2	0.52	2.35	30	3
1:A:39:ILE:CD1	1:A:64:VAL:HG23	0.52	2.34	11	9
1:A:40:ALA:C	1:A:44:ILE:HD12	0.52	2.25	29	1
1:B:22:ASP:O	1:B:26:ILE:HD12	0.52	2.05	1	3
1:B:20:VAL:HG12	1:B:21:SER:N	0.52	2.20	23	2
1:A:11:ILE:HG22	1:A:12:ILE:CD1	0.52	2.33	33	2
1:B:53:LYS:O	1:B:54:THR:HG22	0.52	2.04	21	4
1:A:57:ALA:HB2	1:B:23:ASP:CB	0.52	2.34	6	2
1:B:20:VAL:HG21	1:B:25:ARG:NH2	0.52	2.20	4	1
1:B:39:ILE:HG12	1:B:64:VAL:HG23	0.52	1.82	8	6
1:A:27:THR:HG22	1:B:60:ILE:HG21	0.52	1.82	2	2
1:A:24:ALA:HB2	1:B:55:ILE:O	0.52	2.05	3	1
1:B:35:MET:CG	1:B:39:ILE:HD11	0.52	2.35	6	1
1:B:12:ILE:HD11	1:B:28:LEU:HG	0.52	1.81	31	3
1:B:36:GLY:HA2	1:B:39:ILE:HD12	0.52	1.81	23	1
1:A:11:ILE:HG23	1:B:37:ARG:CG	0.52	2.34	4	1
1:B:23:ASP:HA	1:B:26:ILE:HG22	0.52	1.82	22	2
1:A:60:ILE:HG12	1:B:28:LEU:HD21	0.52	1.80	31	1
1:A:60:ILE:HG21	1:B:28:LEU:N	0.51	2.20	11	6
1:A:52:ARG:NE	1:A:53:LYS:H	0.51	2.04	2	1
1:B:17:ALA:HB1	1:B:20:VAL:HG21	0.51	1.83	15	2
1:A:12:ILE:CD1	1:B:40:ALA:HB2	0.51	2.35	5	30
1:B:5:ILE:HD13	1:B:5:ILE:H	0.51	1.65	7	5
1:B:5:ILE:HD13	1:B:25:ARG:CZ	0.51	2.36	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:N	1:B:60:ILE:HG21	0.51	2.20	19	8
1:A:24:ALA:HB1	1:B:60:ILE:HG13	0.51	1.82	22	4
1:A:20:VAL:HG11	1:A:25:ARG:HH21	0.51	1.65	14	1
1:B:42:GLU:O	1:B:46:LEU:HG	0.51	2.06	30	1
1:A:24:ALA:HB1	1:B:60:ILE:HG12	0.51	1.82	29	1
1:A:17:ALA:CB	1:B:44:ILE:HD11	0.51	2.32	22	2
1:A:28:LEU:HD13	1:B:60:ILE:CG2	0.51	2.30	20	1
1:B:46:LEU:HD22	1:B:62:LEU:CD2	0.50	2.36	17	4
1:A:54:THR:HG22	1:A:55:ILE:N	0.50	2.21	33	1
1:A:33:GLU:HG3	1:B:11:ILE:HD12	0.50	1.82	16	2
1:A:20:VAL:HG22	1:B:55:ILE:HG12	0.50	1.82	21	1
1:B:54:THR:HG22	1:B:55:ILE:O	0.50	2.07	16	2
1:B:4:PRO:HG2	1:B:7:PRO:HG2	0.50	1.82	19	1
1:A:8:ILE:HD11	1:A:29:ALA:CB	0.50	2.37	30	3
1:A:55:ILE:HG22	1:B:24:ALA:CB	0.50	2.36	5	1
1:A:28:LEU:HD22	1:B:60:ILE:HG12	0.50	1.83	4	1
1:B:47:ALA:CB	1:B:55:ILE:HD13	0.50	2.37	15	4
1:A:3:LEU:N	1:A:3:LEU:HD12	0.50	2.22	30	3
1:B:39:ILE:HG23	1:B:67:PHE:CE2	0.50	2.42	19	1
1:A:3:LEU:HD11	1:B:11:ILE:CD1	0.50	2.37	20	1
1:A:4:PRO:HG2	1:A:7:PRO:HG2	0.50	1.84	22	4
1:B:46:LEU:HD11	1:B:62:LEU:C	0.50	2.27	30	1
1:A:3:LEU:HD21	1:A:33:GLU:HB2	0.50	1.84	6	1
1:B:5:ILE:HD13	1:B:25:ARG:NE	0.50	2.22	8	2
1:A:39:ILE:CG2	1:B:28:LEU:HD11	0.49	2.37	21	9
1:A:20:VAL:HG13	1:A:24:ALA:CB	0.49	2.37	27	5
1:B:5:ILE:H	1:B:5:ILE:HD13	0.49	1.67	9	4
1:A:60:ILE:HG21	1:B:27:THR:CB	0.49	2.37	33	1
1:A:39:ILE:HG21	1:B:28:LEU:CD1	0.49	2.37	21	8
1:A:3:LEU:HD12	1:A:3:LEU:N	0.49	2.22	20	1
1:B:20:VAL:HG21	1:B:25:ARG:HG3	0.49	1.83	31	1
1:A:23:ASP:HB3	1:A:26:ILE:HB	0.49	1.85	33	1
1:A:39:ILE:CB	1:B:28:LEU:HD11	0.49	2.34	8	7
1:B:58:GLU:O	1:B:62:LEU:HD12	0.49	2.07	14	1
1:A:32:LEU:CD1	1:B:32:LEU:HD23	0.49	2.37	20	2
1:B:47:ALA:HB2	1:B:55:ILE:HG13	0.49	1.83	22	1
1:B:20:VAL:HG21	1:B:25:ARG:HH21	0.49	1.67	4	1
1:A:42:GLU:O	1:A:46:LEU:HD12	0.49	2.07	30	2
1:A:28:LEU:HD13	1:B:60:ILE:CG1	0.49	2.37	3	1
1:A:46:LEU:HD11	1:A:63:ALA:HA	0.49	1.83	14	3
1:A:3:LEU:HD11	1:A:33:GLU:HB3	0.49	1.83	31	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ARG:O	1:B:54:THR:HG23	0.49	2.07	15	1
1:A:4:PRO:HB2	1:A:7:PRO:HG2	0.49	1.85	14	3
1:B:20:VAL:HG12	1:B:24:ALA:HB3	0.49	1.83	11	2
1:A:27:THR:HG22	1:A:31:ILE:HD12	0.49	1.83	33	2
1:A:24:ALA:HB2	1:B:56:LYS:C	0.49	2.28	9	3
1:A:43:ALA:HB2	1:A:60:ILE:HG13	0.49	1.84	31	1
1:B:4:PRO:HB2	1:B:7:PRO:HD2	0.49	1.83	4	6
1:A:3:LEU:CD1	1:B:11:ILE:HD11	0.49	2.38	1	5
1:B:3:LEU:HG	1:B:33:GLU:HB3	0.49	1.84	7	1
1:A:33:GLU:HG2	1:B:11:ILE:HD12	0.48	1.85	10	3
1:A:47:ALA:HB1	1:A:52:ARG:O	0.48	2.08	31	1
1:B:4:PRO:HB2	1:B:7:PRO:HG2	0.48	1.84	2	1
1:A:43:ALA:CA	1:A:63:ALA:HB2	0.48	2.38	29	2
1:A:60:ILE:HG22	1:B:31:ILE:HD13	0.48	1.85	32	1
1:A:64:VAL:HA	1:A:67:PHE:CE1	0.48	2.44	1	4
1:A:27:THR:HG21	1:B:57:ALA:HA	0.48	1.85	18	4
1:A:8:ILE:HG13	1:A:29:ALA:HB2	0.48	1.83	30	1
1:A:28:LEU:HD13	1:B:60:ILE:HG12	0.48	1.85	27	3
1:B:5:ILE:N	1:B:5:ILE:HD13	0.48	2.23	21	1
1:A:39:ILE:HG21	1:B:28:LEU:HD11	0.48	1.86	4	7
1:A:33:GLU:HB2	1:A:37:ARG:NH2	0.48	2.24	19	1
1:B:35:MET:HG2	1:B:39:ILE:HD11	0.48	1.84	15	1
1:A:55:ILE:CG1	1:B:20:VAL:HG22	0.48	2.38	17	2
1:B:3:LEU:HD11	1:B:33:GLU:HB2	0.48	1.86	2	5
1:A:54:THR:HG21	1:B:21:SER:OG	0.48	2.09	29	1
1:A:32:LEU:HD12	1:B:32:LEU:CG	0.48	2.39	2	2
1:B:42:GLU:O	1:B:46:LEU:HD12	0.48	2.09	16	6
1:B:6:ALA:N	1:B:7:PRO:HD2	0.48	2.23	8	2
1:A:54:THR:HG21	1:B:21:SER:HB2	0.48	1.85	11	2
1:B:3:LEU:HD23	1:B:3:LEU:N	0.48	2.24	9	4
1:A:4:PRO:HB2	1:A:7:PRO:HD2	0.48	1.84	27	7
1:B:41:SER:HA	1:B:44:ILE:HD12	0.47	1.85	20	1
1:B:3:LEU:CD1	1:B:33:GLU:HB2	0.47	2.39	30	2
1:B:12:ILE:C	1:B:17:ALA:HB3	0.47	2.29	23	1
1:B:27:THR:HG22	1:B:31:ILE:HD13	0.47	1.85	31	1
1:A:12:ILE:HD13	1:B:40:ALA:HB2	0.47	1.87	30	2
1:B:44:ILE:O	1:B:47:ALA:HB3	0.47	2.09	22	3
1:B:5:ILE:CD1	1:B:5:ILE:H	0.47	2.22	21	1
1:A:20:VAL:HG12	1:A:21:SER:N	0.47	2.24	4	1
1:B:58:GLU:HA	1:B:62:LEU:HD23	0.47	1.86	29	1
1:A:60:ILE:CG2	1:B:27:THR:HG23	0.47	2.40	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ILE:HB	1:A:25:ARG:NH2	0.47	2.23	23	1
1:A:20:VAL:HG12	1:A:24:ALA:CB	0.47	2.38	33	1
1:B:44:ILE:HG12	1:B:55:ILE:HD13	0.47	1.86	3	1
1:A:20:VAL:HG22	1:B:55:ILE:CB	0.47	2.34	16	1
1:A:20:VAL:HG22	1:B:55:ILE:HD13	0.47	1.84	16	1
1:A:8:ILE:CG1	1:A:29:ALA:HB2	0.47	2.39	30	1
1:B:42:GLU:HG3	1:B:67:PHE:CZ	0.47	2.45	33	2
1:B:39:ILE:HG12	1:B:67:PHE:CE2	0.47	2.45	23	5
1:A:58:GLU:OE2	1:A:62:LEU:HD11	0.47	2.10	26	2
1:A:60:ILE:HG21	1:B:27:THR:HG23	0.47	1.86	14	1
1:A:11:ILE:HG23	1:B:37:ARG:HD2	0.47	1.86	5	1
1:A:17:ALA:HB1	1:A:20:VAL:HG21	0.47	1.86	21	1
1:A:3:LEU:HG	1:A:33:GLU:HB2	0.47	1.85	33	3
1:A:21:SER:HB2	1:B:54:THR:HG23	0.47	1.86	27	3
1:A:56:LYS:N	1:B:24:ALA:HB2	0.47	2.25	33	2
1:B:54:THR:HG22	1:B:55:ILE:N	0.47	2.25	2	4
1:B:58:GLU:CA	1:B:62:LEU:HD23	0.47	2.40	29	1
1:B:5:ILE:HG21	1:B:26:ILE:CG1	0.47	2.40	29	1
1:A:6:ALA:N	1:A:7:PRO:HD2	0.46	2.24	19	2
1:A:39:ILE:HG21	1:A:64:VAL:CG2	0.46	2.35	27	2
1:A:31:ILE:HG21	1:B:64:VAL:CG2	0.46	2.39	29	2
1:A:43:ALA:O	1:A:47:ALA:HB2	0.46	2.10	20	1
1:A:39:ILE:HG12	1:A:67:PHE:CE2	0.46	2.45	4	6
1:A:42:GLU:HG3	1:A:67:PHE:CZ	0.46	2.46	2	1
1:A:39:ILE:O	1:A:63:ALA:HB1	0.46	2.10	11	1
1:B:31:ILE:N	1:B:31:ILE:HD12	0.46	2.26	31	2
1:A:3:LEU:O	1:A:29:ALA:HB1	0.46	2.10	29	1
1:A:20:VAL:HG13	1:B:55:ILE:CG2	0.46	2.41	16	2
1:A:39:ILE:HA	1:A:42:GLU:HB2	0.46	1.87	23	2
1:A:12:ILE:CD1	1:A:28:LEU:HD21	0.46	2.41	19	1
1:A:47:ALA:C	1:A:50:ALA:HB3	0.46	2.31	20	1
1:B:4:PRO:CD	1:B:7:PRO:HG2	0.46	2.40	3	1
1:B:43:ALA:HB1	1:B:55:ILE:HG21	0.46	1.87	30	1
1:A:32:LEU:CG	1:B:32:LEU:HD23	0.46	2.39	31	1
1:A:39:ILE:HG12	1:A:67:PHE:CZ	0.46	2.46	1	5
1:A:30:LYS:NZ	1:A:30:LYS:HB3	0.46	2.26	29	1
1:A:32:LEU:HB3	1:B:32:LEU:HD23	0.46	1.88	10	3
1:A:46:LEU:O	1:A:50:ALA:HB2	0.46	2.09	3	1
1:A:38:ASP:HB3	1:A:67:PHE:CE2	0.46	2.45	33	1
1:A:60:ILE:HB	1:B:27:THR:HG21	0.46	1.88	31	2
1:A:28:LEU:CA	1:A:31:ILE:HD12	0.46	2.38	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:ILE:HA	1:B:67:PHE:CE2	0.46	2.46	7	6
1:A:39:ILE:HA	1:A:67:PHE:CE2	0.46	2.46	26	4
1:A:28:LEU:O	1:A:32:LEU:HD12	0.46	2.11	8	1
1:A:46:LEU:HD21	1:A:66:ARG:CD	0.46	2.41	3	1
1:A:42:GLU:HG2	1:A:67:PHE:CE1	0.46	2.46	5	2
1:A:42:GLU:HG2	1:A:67:PHE:CZ	0.46	2.46	10	6
1:A:38:ASP:HB3	1:A:67:PHE:CZ	0.45	2.45	23	8
1:B:18:GLU:HG3	1:B:19:ARG:N	0.45	2.26	27	2
1:A:5:ILE:HG21	1:A:25:ARG:HG3	0.45	1.88	29	1
1:B:44:ILE:HA	1:B:55:ILE:HD11	0.45	1.88	20	1
1:A:54:THR:HG22	1:B:21:SER:HB3	0.45	1.88	31	1
1:A:20:VAL:HG12	1:A:21:SER:H	0.45	1.69	4	1
1:A:4:PRO:HB2	1:A:7:PRO:CG	0.45	2.42	6	3
1:B:3:LEU:HD12	1:B:29:ALA:HA	0.45	1.88	1	1
1:A:26:ILE:HA	1:A:29:ALA:HB3	0.45	1.88	1	1
1:A:32:LEU:HD11	1:B:36:GLY:N	0.45	2.26	3	1
1:A:57:ALA:O	1:B:27:THR:HG21	0.45	2.10	26	2
1:B:39:ILE:CG2	1:B:63:ALA:HB3	0.45	2.41	14	1
1:B:47:ALA:HB2	1:B:55:ILE:CG1	0.45	2.37	4	1
1:A:20:VAL:HG13	1:B:55:ILE:CB	0.45	2.41	4	1
1:A:3:LEU:HD21	1:A:33:GLU:HG2	0.45	1.88	33	1
1:A:39:ILE:HD12	1:B:32:LEU:CD1	0.45	2.41	26	2
1:B:39:ILE:CG1	1:B:67:PHE:CE2	0.45	3.00	14	1
1:A:60:ILE:N	1:A:60:ILE:CD1	0.45	2.80	30	2
1:A:19:ARG:CD	1:A:19:ARG:N	0.45	2.80	16	1
1:A:13:LYS:HD3	1:A:18:GLU:HB2	0.45	1.86	4	1
1:A:3:LEU:HD12	1:B:11:ILE:HD11	0.45	1.89	1	1
1:B:57:ALA:O	1:B:61:GLU:HB2	0.45	2.12	4	6
1:A:30:LYS:O	1:A:34:GLU:HB2	0.45	2.12	17	4
1:A:54:THR:HG22	1:B:21:SER:N	0.45	2.27	17	1
1:A:54:THR:CG2	1:B:21:SER:N	0.45	2.80	26	2
1:A:64:VAL:HG21	1:B:31:ILE:HG12	0.45	1.88	32	1
1:A:48:ARG:CD	1:A:52:ARG:NH1	0.45	2.80	16	1
1:B:20:VAL:CG1	1:B:21:SER:N	0.45	2.80	23	1
1:A:28:LEU:HB2	1:B:60:ILE:HG23	0.45	1.86	32	1
1:A:32:LEU:HA	1:B:32:LEU:CD2	0.45	2.42	5	1
1:B:64:VAL:CG2	1:B:67:PHE:CZ	0.45	3.00	23	1
1:B:38:ASP:HB3	1:B:67:PHE:CZ	0.45	2.46	15	7
1:A:5:ILE:H	1:A:5:ILE:HD13	0.45	1.72	23	4
1:A:29:ALA:O	1:A:33:GLU:HB2	0.45	2.11	18	3
1:B:22:ASP:CA	1:B:25:ARG:NH1	0.45	2.80	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ARG:N	1:B:11:ILE:CG2	0.45	2.80	15	1
1:A:3:LEU:N	1:A:3:LEU:CD2	0.45	2.80	6	1
1:A:31:ILE:HD12	1:B:60:ILE:CG2	0.45	2.42	3	2
1:A:64:VAL:CG1	1:A:65:ARG:N	0.45	2.80	29	2
1:B:54:THR:CG2	1:B:55:ILE:N	0.45	2.80	2	4
1:B:22:ASP:HA	1:B:25:ARG:NH1	0.45	2.27	7	2
1:B:35:MET:HG3	1:B:39:ILE:HD11	0.45	1.87	6	1
1:A:54:THR:CG2	1:A:55:ILE:N	0.45	2.80	33	1
1:A:58:GLU:HA	1:A:61:GLU:HB2	0.45	1.88	1	1
1:B:60:ILE:N	1:B:60:ILE:CD1	0.45	2.80	8	3
1:B:44:ILE:HG12	1:B:55:ILE:HD11	0.45	1.88	14	1
1:B:5:ILE:CD1	1:B:25:ARG:NH2	0.45	2.80	2	1
1:A:9:GLY:HA3	1:A:25:ARG:NH1	0.45	2.27	21	1
1:A:52:ARG:NE	1:A:53:LYS:N	0.44	2.64	2	1
1:B:42:GLU:HG2	1:B:67:PHE:CE1	0.44	2.47	6	2
1:B:20:VAL:HB	1:B:24:ALA:HB3	0.44	1.89	10	3
1:B:27:THR:HG22	1:B:31:ILE:CD1	0.44	2.41	23	4
1:B:39:ILE:CG1	1:B:67:PHE:CZ	0.44	3.00	8	1
1:B:26:ILE:N	1:B:26:ILE:CD1	0.44	2.80	26	1
1:A:46:LEU:HD11	1:A:63:ALA:CA	0.44	2.42	14	1
1:B:26:ILE:CD1	1:B:26:ILE:N	0.44	2.80	24	1
1:B:20:VAL:CG2	1:B:25:ARG:NH2	0.44	2.80	4	1
1:A:44:ILE:CD1	1:B:17:ALA:N	0.44	2.80	17	1
1:A:3:LEU:HG	1:A:33:GLU:HB3	0.44	1.88	19	2
1:B:38:ASP:HB3	1:B:67:PHE:CE2	0.44	2.48	8	4
1:B:46:LEU:CD1	1:B:63:ALA:N	0.44	2.80	14	3
1:B:39:ILE:HG12	1:B:67:PHE:CE1	0.44	2.48	18	3
1:A:31:ILE:CG2	1:B:64:VAL:HG21	0.44	2.34	13	1
1:A:39:ILE:CG1	1:A:67:PHE:CE2	0.44	3.00	4	2
1:B:42:GLU:HG2	1:B:67:PHE:HB3	0.44	1.90	27	3
1:B:20:VAL:HG12	1:B:21:SER:H	0.44	1.73	14	2
1:A:56:LYS:HG3	1:A:59:ASP:HB2	0.44	1.88	26	2
1:A:42:GLU:CG	1:A:67:PHE:CE1	0.44	3.00	5	1
1:A:54:THR:HG22	1:A:56:LYS:NZ	0.44	2.27	3	1
1:A:32:LEU:HD11	1:B:39:ILE:CD1	0.44	2.43	23	2
1:A:40:ALA:CB	1:B:12:ILE:HD12	0.44	2.32	22	1
1:B:39:ILE:HG12	1:B:67:PHE:CZ	0.44	2.48	8	4
1:B:5:ILE:HD13	1:B:25:ARG:HE	0.44	1.73	8	1
1:A:5:ILE:HD12	1:A:5:ILE:C	0.44	2.33	7	2
1:A:57:ALA:O	1:A:61:GLU:HB2	0.44	2.13	30	2
1:A:27:THR:CG2	1:B:60:ILE:HG21	0.44	2.43	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:LEU:CG	1:B:33:GLU:HB3	0.44	2.43	7	1
1:B:42:GLU:HG3	1:B:67:PHE:CE1	0.44	2.47	33	2
1:B:4:PRO:HB2	1:B:7:PRO:CD	0.44	2.43	19	4
1:A:37:ARG:N	1:B:11:ILE:HG22	0.44	2.28	29	1
1:B:29:ALA:O	1:B:33:GLU:HB2	0.44	2.12	3	1
1:A:8:ILE:CG2	1:A:25:ARG:NH2	0.44	2.81	23	1
1:B:39:ILE:HG21	1:B:64:VAL:CG2	0.44	2.41	17	2
1:A:60:ILE:HG21	1:B:27:THR:HG22	0.44	1.90	20	2
1:B:22:ASP:HB3	1:B:25:ARG:NH1	0.44	2.28	20	1
1:A:43:ALA:HA	1:A:46:LEU:HB2	0.43	1.90	32	5
1:A:24:ALA:HA	1:B:60:ILE:HG13	0.43	1.89	21	4
1:A:60:ILE:HG13	1:B:24:ALA:CB	0.43	2.43	15	6
1:B:48:ARG:HB2	1:B:52:ARG:NE	0.43	2.28	32	1
1:B:20:VAL:HG13	1:B:24:ALA:HB3	0.43	1.89	31	1
1:B:43:ALA:HB2	1:B:60:ILE:HG13	0.43	1.90	18	3
1:A:60:ILE:N	1:A:60:ILE:HD12	0.43	2.28	30	2
1:B:58:GLU:O	1:B:62:LEU:HD23	0.43	2.12	29	1
1:A:41:SER:N	1:B:15:ALA:HB1	0.43	2.27	15	1
1:A:42:GLU:HG3	1:A:67:PHE:CE2	0.43	2.48	30	1
1:A:44:ILE:HG12	1:A:55:ILE:CD1	0.43	2.43	23	1
1:B:30:LYS:O	1:B:34:GLU:HB2	0.43	2.12	23	3
1:A:60:ILE:HG13	1:B:24:ALA:HA	0.43	1.91	22	2
1:B:35:MET:HB3	1:B:39:ILE:HD11	0.43	1.89	18	3
1:A:5:ILE:HG23	1:A:26:ILE:HD11	0.43	1.89	29	1
1:B:3:LEU:HD21	1:B:33:GLU:HG3	0.43	1.90	30	1
1:A:20:VAL:HG13	1:B:55:ILE:HG22	0.43	1.88	16	1
1:A:20:VAL:HG21	1:A:25:ARG:HH22	0.43	1.64	2	1
1:A:20:VAL:HG12	1:A:25:ARG:HG3	0.43	1.88	18	3
1:A:55:ILE:CB	1:B:20:VAL:HG12	0.43	2.43	10	3
1:B:31:ILE:HG23	1:B:35:MET:HE3	0.43	1.88	32	1
1:A:12:ILE:HD12	1:A:28:LEU:CD2	0.43	2.44	23	1
1:B:47:ALA:HB3	1:B:55:ILE:CD1	0.43	2.43	2	1
1:A:5:ILE:HG21	1:A:25:ARG:HD3	0.43	1.90	19	1
1:A:44:ILE:HD13	1:B:17:ALA:CA	0.43	2.43	10	5
1:A:28:LEU:HD13	1:B:39:ILE:HG21	0.43	1.91	32	1
1:B:3:LEU:HB2	1:B:8:ILE:CD1	0.43	2.44	5	2
1:A:55:ILE:HB	1:B:20:VAL:CG1	0.43	2.44	10	4
1:A:8:ILE:HD12	1:A:29:ALA:CB	0.43	2.44	15	1
1:A:31:ILE:HG12	1:B:64:VAL:HG21	0.43	1.90	16	1
1:A:3:LEU:HD21	1:A:33:GLU:CG	0.43	2.43	33	1
1:A:60:ILE:HG21	1:B:31:ILE:HD13	0.43	1.88	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:ILE:CD1	1:B:60:ILE:N	0.43	2.82	2	1
1:A:32:LEU:HD11	1:B:36:GLY:HA3	0.43	1.90	33	1
1:A:4:PRO:HB2	1:A:7:PRO:CD	0.43	2.43	18	5
1:B:39:ILE:HG22	1:B:63:ALA:HB3	0.43	1.91	14	1
1:B:43:ALA:CA	1:B:63:ALA:HB2	0.43	2.44	9	2
1:A:4:PRO:HG2	1:A:7:PRO:HG3	0.43	1.91	4	1
1:A:22:ASP:HB3	1:A:25:ARG:NH2	0.43	2.29	4	1
1:B:26:ILE:CD1	1:B:30:LYS:HD3	0.43	2.43	3	1
1:A:5:ILE:HD12	1:A:6:ALA:N	0.43	2.29	7	1
1:A:20:VAL:HG12	1:A:25:ARG:CG	0.43	2.43	18	1
1:A:21:SER:HB2	1:B:54:THR:CG2	0.43	2.44	4	1
1:A:60:ILE:HG21	1:B:27:THR:CG2	0.43	2.43	14	3
1:A:5:ILE:CG2	1:A:25:ARG:HB3	0.43	2.44	15	1
1:A:8:ILE:HD13	1:A:29:ALA:HA	0.43	1.91	8	1
1:A:3:LEU:CG	1:A:33:GLU:HB3	0.42	2.45	19	1
1:A:25:ARG:HH21	1:A:28:LEU:HD23	0.42	1.74	8	1
1:A:8:ILE:HG22	1:A:25:ARG:NH1	0.42	2.29	14	1
1:A:43:ALA:HB2	1:A:63:ALA:HB2	0.42	1.90	22	1
1:A:60:ILE:HG12	1:B:28:LEU:HD22	0.42	1.89	29	1
1:B:4:PRO:HD2	1:B:7:PRO:HG2	0.42	1.90	3	1
1:B:26:ILE:N	1:B:26:ILE:HD12	0.42	2.28	26	1
1:A:20:VAL:CG2	1:B:55:ILE:HD13	0.42	2.44	16	1
1:B:26:ILE:HD12	1:B:26:ILE:N	0.42	2.28	24	1
1:B:28:LEU:CA	1:B:31:ILE:HD12	0.42	2.41	27	4
1:A:5:ILE:CG2	1:A:26:ILE:HG12	0.42	2.43	30	1
1:A:44:ILE:HD13	1:B:17:ALA:HA	0.42	1.90	6	1
1:A:12:ILE:C	1:A:17:ALA:HB3	0.42	2.34	4	1
1:A:38:ASP:CB	1:A:67:PHE:CE2	0.42	3.03	33	1
1:B:40:ALA:O	1:B:44:ILE:HD12	0.42	2.15	29	1
1:A:42:GLU:HG3	1:A:67:PHE:CE1	0.42	2.49	26	2
1:A:8:ILE:HD11	1:A:29:ALA:HB2	0.42	1.90	30	3
1:A:17:ALA:N	1:B:44:ILE:CD1	0.42	2.80	4	1
1:A:5:ILE:HB	1:A:25:ARG:CB	0.42	2.44	15	2
1:A:28:LEU:HD11	1:B:39:ILE:CG2	0.42	2.45	33	2
1:A:54:THR:HB	1:B:21:SER:HB2	0.42	1.91	33	1
1:A:43:ALA:HB1	1:A:59:ASP:HB3	0.42	1.89	29	1
1:A:46:LEU:CD1	1:A:63:ALA:N	0.42	2.83	14	1
1:B:10:ARG:HD3	1:B:10:ARG:N	0.42	2.29	32	1
1:A:4:PRO:HG2	1:A:7:PRO:CG	0.42	2.45	4	3
1:B:17:ALA:CB	1:B:20:VAL:HG22	0.42	2.40	22	1
1:B:5:ILE:HD12	1:B:25:ARG:NH2	0.42	2.30	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASP:HB3	1:A:26:ILE:CG2	0.42	2.44	33	1
1:A:43:ALA:O	1:A:55:ILE:HD12	0.42	2.14	32	1
1:A:3:LEU:CD1	1:A:33:GLU:HG3	0.42	2.45	22	1
1:B:44:ILE:HG12	1:B:55:ILE:CD1	0.42	2.45	8	2
1:B:5:ILE:HB	1:B:25:ARG:HB3	0.42	1.90	10	3
1:A:24:ALA:CB	1:B:60:ILE:HG13	0.42	2.45	20	2
1:A:38:ASP:O	1:A:42:GLU:HB2	0.42	2.15	20	5
1:B:5:ILE:CG2	1:B:26:ILE:HD13	0.42	2.45	10	3
1:B:38:ASP:O	1:B:42:GLU:HB2	0.42	2.15	9	5
1:A:55:ILE:CB	1:B:20:VAL:HG22	0.42	2.44	23	1
1:A:12:ILE:HB	1:A:25:ARG:NH1	0.41	2.29	33	1
1:B:4:PRO:HG2	1:B:7:PRO:CG	0.41	2.45	22	6
1:B:64:VAL:CG1	1:B:65:ARG:N	0.41	2.83	30	1
1:A:5:ILE:HA	1:A:25:ARG:NH2	0.41	2.29	32	1
1:A:9:GLY:HA2	1:A:25:ARG:HG2	0.41	1.92	5	1
1:B:5:ILE:CG2	1:B:26:ILE:HG13	0.41	2.44	9	1
1:A:53:LYS:HG2	1:A:54:THR:N	0.41	2.30	6	1
1:A:32:LEU:CD1	1:B:39:ILE:HD12	0.41	2.38	19	2
1:B:6:ALA:H	1:B:7:PRO:HD2	0.41	1.74	29	3
1:B:52:ARG:HA	1:B:52:ARG:NE	0.41	2.31	14	1
1:A:38:ASP:HB3	1:A:67:PHE:CE1	0.41	2.50	9	1
1:A:46:LEU:CD1	1:A:63:ALA:HA	0.41	2.45	21	2
1:A:46:LEU:CD2	1:A:63:ALA:N	0.41	2.83	10	3
1:A:52:ARG:HB3	1:A:52:ARG:CZ	0.41	2.46	10	2
1:A:52:ARG:CZ	1:A:52:ARG:HB3	0.41	2.46	12	1
1:A:27:THR:HG21	1:B:57:ALA:CA	0.41	2.45	2	1
1:B:5:ILE:N	1:B:5:ILE:CD1	0.41	2.83	21	1
1:B:20:VAL:HG21	1:B:25:ARG:HE	0.41	1.75	30	1
1:B:31:ILE:HG23	1:B:35:MET:CE	0.41	2.45	32	1
1:B:65:ARG:NH1	1:B:65:ARG:HB3	0.41	2.30	32	1
1:A:55:ILE:HG21	1:B:25:ARG:HH22	0.41	1.76	5	1
1:A:52:ARG:CD	1:A:53:LYS:N	0.41	2.83	2	1
1:B:46:LEU:CD1	1:B:63:ALA:HA	0.41	2.45	10	6
1:B:39:ILE:HG13	1:B:67:PHE:CE2	0.41	2.50	8	1
1:A:12:ILE:HG23	1:B:44:ILE:HD11	0.41	1.92	3	1
1:B:64:VAL:HA	1:B:67:PHE:CD2	0.41	2.51	3	1
1:A:46:LEU:HD23	1:A:59:ASP:O	0.41	2.16	26	2
1:B:43:ALA:N	1:B:63:ALA:CB	0.41	2.84	31	1
1:B:64:VAL:HA	1:B:67:PHE:CD1	0.41	2.50	27	4
1:A:42:GLU:O	1:A:46:LEU:HG	0.41	2.15	20	1
1:A:44:ILE:CG2	1:A:45:LYS:N	0.41	2.84	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LEU:N	1:A:62:LEU:CD2	0.41	2.80	31	1
1:A:39:ILE:HG12	1:A:67:PHE:CE1	0.41	2.51	13	2
1:A:28:LEU:HG	1:A:32:LEU:CD1	0.41	2.46	18	3
1:B:5:ILE:HG21	1:B:26:ILE:HG13	0.41	1.92	29	1
1:A:3:LEU:CD1	1:A:3:LEU:N	0.41	2.84	20	1
1:A:5:ILE:HG13	1:A:25:ARG:HD3	0.41	1.92	20	1
1:B:37:ARG:O	1:B:40:ALA:HB3	0.41	2.16	15	1
1:A:33:GLU:HG2	1:B:11:ILE:CD1	0.41	2.45	8	1
1:A:20:VAL:HG22	1:B:55:ILE:CD1	0.41	2.45	3	1
1:A:21:SER:HB3	1:B:54:THR:CG2	0.41	2.46	31	1
1:A:46:LEU:CD2	1:A:63:ALA:HA	0.41	2.46	19	1
1:B:42:GLU:HG2	1:B:67:PHE:CB	0.41	2.46	27	3
1:A:54:THR:HB	1:A:56:LYS:NZ	0.41	2.30	28	3
1:B:12:ILE:HD12	1:B:28:LEU:HD23	0.41	1.92	15	1
1:A:33:GLU:HG3	1:B:11:ILE:CD1	0.41	2.46	15	1
1:A:41:SER:O	1:A:44:ILE:HG22	0.41	2.15	22	2
1:B:44:ILE:CG1	1:B:55:ILE:HD13	0.41	2.46	3	1
1:A:55:ILE:CG2	1:A:60:ILE:HD11	0.41	2.46	14	1
1:B:8:ILE:HD13	1:B:29:ALA:HA	0.41	1.92	7	1
1:A:37:ARG:HD3	1:B:15:ALA:HA	0.41	1.92	2	1
1:A:24:ALA:CA	1:B:60:ILE:HG13	0.41	2.46	21	2
1:A:6:ALA:H	1:A:7:PRO:HD2	0.41	1.76	30	2
1:A:5:ILE:HG13	1:A:25:ARG:NE	0.41	2.31	19	1
1:A:8:ILE:HD12	1:A:29:ALA:HB2	0.41	1.93	15	1
1:B:43:ALA:HA	1:B:46:LEU:HB2	0.41	1.92	26	2
1:A:18:GLU:HG3	1:A:19:ARG:NH1	0.41	2.31	7	1
1:A:30:LYS:HB3	1:A:30:LYS:NZ	0.41	2.31	31	1
1:A:11:ILE:HD13	1:B:33:GLU:HG2	0.41	1.93	4	1
1:A:23:ASP:OD1	1:B:57:ALA:HB2	0.40	2.16	20	1
1:A:43:ALA:CB	1:A:60:ILE:HD12	0.40	2.46	26	2
1:A:8:ILE:HB	1:A:25:ARG:HG3	0.40	1.93	26	2
1:A:40:ALA:HB1	1:B:12:ILE:CG2	0.40	2.40	14	1
1:B:9:GLY:HA2	1:B:25:ARG:NH1	0.40	2.30	14	1
1:A:27:THR:HG21	1:B:57:ALA:O	0.40	2.16	16	1
1:A:57:ALA:N	1:B:23:ASP:HB3	0.40	2.31	6	1
1:B:5:ILE:HG21	1:B:25:ARG:NE	0.40	2.30	21	1
1:B:3:LEU:CG	1:B:33:GLU:HB2	0.40	2.46	8	1
1:B:12:ILE:HG13	1:B:25:ARG:NH2	0.40	2.31	14	1
1:A:32:LEU:HD21	1:B:32:LEU:C	0.40	2.36	16	1
1:B:39:ILE:O	1:B:63:ALA:HB1	0.40	2.17	31	1
1:A:3:LEU:CG	1:A:33:GLU:HB2	0.40	2.46	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ILE:HG13	1:B:24:ALA:CA	0.40	2.45	11	2
1:B:22:ASP:HA	1:B:25:ARG:NE	0.40	2.32	13	1
1:A:3:LEU:N	1:A:3:LEU:CD1	0.40	2.84	26	2
1:B:48:ARG:HD2	1:B:49:HIS:N	0.40	2.31	32	1
1:B:44:ILE:CG2	1:B:45:LYS:N	0.40	2.84	31	1
1:A:57:ALA:C	1:B:27:THR:HG21	0.40	2.37	26	2
1:A:60:ILE:CG2	1:B:27:THR:CG2	0.40	3.00	14	1
1:A:64:VAL:CG2	1:B:31:ILE:HG21	0.40	2.47	32	1
1:A:60:ILE:HG12	1:B:24:ALA:HB1	0.40	1.94	5	1
1:B:42:GLU:CB	1:B:67:PHE:CZ	0.40	3.05	16	1
1:A:37:ARG:O	1:A:40:ALA:HB3	0.40	2.16	9	1
1:A:44:ILE:CD1	1:B:17:ALA:HA	0.40	2.47	6	1
1:B:28:LEU:HG	1:B:32:LEU:CD1	0.40	2.47	11	1
1:B:12:ILE:CD1	1:B:28:LEU:CD2	0.40	3.00	18	1
1:B:38:ASP:HB3	1:B:67:PHE:CD2	0.40	2.51	18	1
1:A:23:ASP:CB	1:A:26:ILE:CG2	0.40	3.00	33	1
1:A:28:LEU:CD2	1:B:60:ILE:HG23	0.40	2.46	13	1
1:A:40:ALA:CB	1:B:12:ILE:HG12	0.40	2.46	1	1
1:A:31:ILE:CD1	1:B:60:ILE:CG2	0.40	3.00	1	1
1:B:3:LEU:HG	1:B:33:GLU:HB2	0.40	1.94	8	1
1:A:5:ILE:HG21	1:A:26:ILE:CG1	0.40	2.40	3	1
1:B:6:ALA:CB	1:B:7:PRO:CD	0.40	3.00	16	1
1:A:32:LEU:CD1	1:B:32:LEU:CG	0.40	3.00	7	1
1:B:22:ASP:HA	1:B:25:ARG:CZ	0.40	2.47	7	1
1:A:44:ILE:CG1	1:A:55:ILE:CD1	0.40	3.00	23	1
1:A:60:ILE:CG1	1:B:24:ALA:CB	0.40	3.00	11	1
1:A:46:LEU:HD21	1:A:63:ALA:N	0.40	2.32	11	1
1:A:57:ALA:N	1:B:24:ALA:HB2	0.40	2.31	21	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	65/69 (94%)	54±3 (84±5%)	8±3 (13±5%)	2±2 (3±2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	65/69 (94%)	56±3 (86±5%)	7±3 (11±4%)	2±1 (4±2%)	8	37
All	All	4290/4554 (94%)	3636 (85%)	503 (12%)	151 (4%)	8	37

All 38 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	31	ILE	17
1	A	31	ILE	14
1	B	52	ARG	13
1	A	53	LYS	12
1	B	53	LYS	10
1	A	52	ARG	10
1	B	19	ARG	7
1	B	54	THR	7
1	A	54	THR	6
1	A	19	ARG	6
1	A	18	GLU	5
1	B	18	GLU	5
1	A	64	VAL	4
1	B	64	VAL	4
1	B	12	ILE	2
1	A	8	ILE	2
1	B	11	ILE	2
1	A	17	ALA	2
1	A	51	GLY	2
1	A	6	ALA	2
1	B	6	ALA	2
1	A	11	ILE	1
1	B	36	GLY	1
1	A	3	LEU	1
1	A	62	LEU	1
1	A	60	ILE	1
1	A	24	ALA	1
1	A	36	GLY	1
1	B	23	ASP	1
1	A	12	ILE	1
1	B	22	ASP	1
1	B	7	PRO	1
1	B	24	ALA	1
1	A	22	ASP	1
1	B	20	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	5	ILE	1
1	A	16	GLY	1
1	B	17	ALA	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	50/54 (93%)	34±2 (67±5%)	16±2 (33±5%)	1	13
1	B	50/54 (93%)	35±3 (70±6%)	15±3 (30±6%)	2	17
All	All	3300/3564 (93%)	2260 (68%)	1040 (32%)	2	15

All 81 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	59	ASP	28
1	B	42	GLU	26
1	A	19	ARG	24
1	B	64	VAL	23
1	B	48	ARG	22
1	B	30	LYS	22
1	B	38	ASP	22
1	B	37	ARG	22
1	A	53	LYS	22
1	B	53	LYS	22
1	A	10	ARG	22
1	A	59	ASP	22
1	A	42	GLU	21
1	A	52	ARG	21
1	A	56	LYS	21
1	A	48	ARG	20
1	A	38	ASP	20
1	A	64	VAL	20
1	A	30	LYS	19
1	A	13	LYS	19
1	B	19	ARG	19

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Mol	Chain	Res	Type	Models (Total)
1	B	23	ASP	18
1	A	32	LEU	18
1	B	66	ARG	18
1	A	23	ASP	17
1	A	25	ARG	17
1	B	65	ARG	17
1	A	41	SER	17
1	A	45	LYS	16
1	B	34	GLU	16
1	A	65	ARG	16
1	B	56	LYS	15
1	B	52	ARG	15
1	B	10	ARG	15
1	A	37	ARG	14
1	B	45	LYS	14
1	A	62	LEU	13
1	A	5	ILE	13
1	A	33	GLU	13
1	A	35	MET	13
1	A	49	HIS	12
1	B	33	GLU	12
1	A	66	ARG	12
1	A	18	GLU	12
1	B	13	LYS	12
1	B	22	ASP	12
1	B	32	LEU	12
1	A	67	PHE	12
1	A	22	ASP	11
1	B	41	SER	10
1	B	67	PHE	10
1	A	44	ILE	10
1	B	5	ILE	10
1	B	58	GLU	10
1	B	18	GLU	10
1	A	58	GLU	9
1	B	25	ARG	9
1	A	61	GLU	8
1	B	3	LEU	8
1	A	34	GLU	7
1	B	62	LEU	7
1	B	61	GLU	6
1	B	35	MET	6

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Mol	Chain	Res	Type	Models (Total)
1	A	3	LEU	6
1	A	26	ILE	5
1	B	20	VAL	5
1	B	26	ILE	5
1	B	44	ILE	5
1	B	60	ILE	5
1	A	31	ILE	4
1	B	54	THR	4
1	B	28	LEU	4
1	A	54	THR	4
1	A	21	SER	3
1	A	28	LEU	3
1	B	27	THR	2
1	A	60	ILE	2
1	B	8	ILE	1
1	B	46	LEU	1
1	A	20	VAL	1
1	B	21	SER	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided