



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:30 PM UTC

PDB ID : 1EXE / pdb_00001exe
Title : SOLUTION STRUCTURE OF A MUTANT OF TRANSCRIPTION FACTOR 1.
Authors : Liu, W.; Vu, H.M.; Geiduschek, E.P.; Kearns, D.R.
Deposited on : 2000-05-02

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

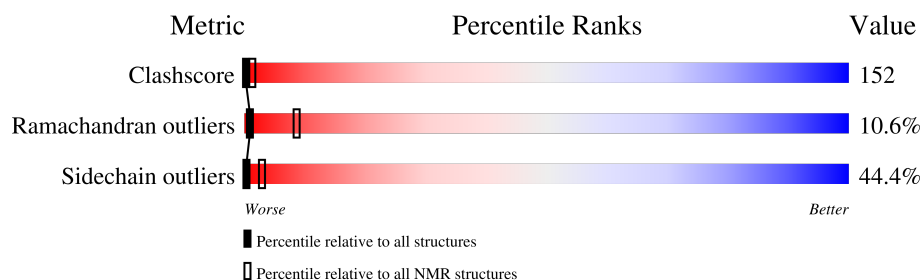
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	99	
1	B	99	

2 Ensemble composition and analysis

This entry contains 23 models. Model 12 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:1-A:54, A:75-A:95, B:1-B:54, B:75-B:97 (152)	0.91	12

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3090 atoms, of which 1590 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TRANSCRIPTION FACTOR 1.

Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1545	476	795	127	145	2	
1	B	99	Total	C	H	N	O	S	0
			1545	476	795	127	145	2	

There are 4 discrepancies between the modelled and reference sequences:

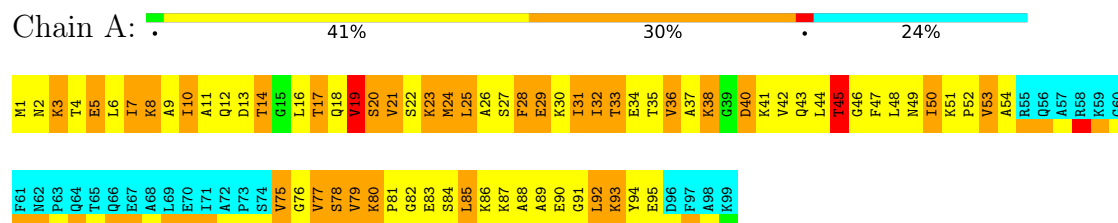
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	GLU	engineered mutation	UNP P04445
A	32	ILE	THR	engineered mutation	UNP P04445
B	15	GLY	GLU	engineered mutation	UNP P04445
B	32	ILE	THR	engineered mutation	UNP P04445

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

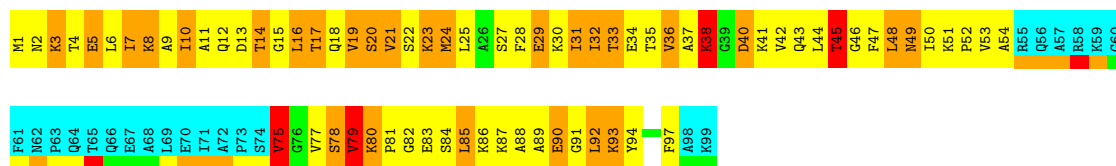
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

• Molecule 1: TRANSCRIPTION FACTOR 1



- Molecule 1: TRANSCRIPTION FACTOR 1

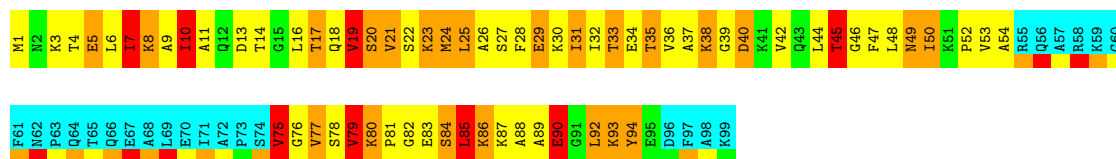
Chain B: 5% 41% 27% • 22%



4.2.2 Score per residue for model 2

- Molecule 1: TRANSCRIPTION FACTOR 1

Chain A: 8% 36% 23% 8% 24%



- Molecule 1: TRANSCRIPTION FACTOR 1

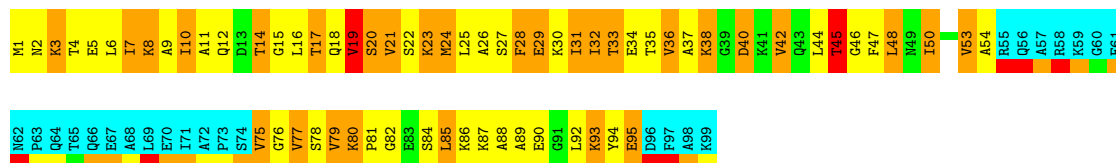
Chain B: 6% 37% 29% 5% 22%



4.2.3 Score per residue for model 3

- Molecule 1: TRANSCRIPTION FACTOR 1

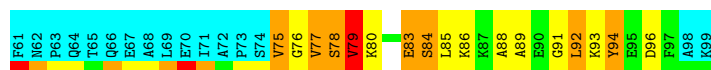
Chain A: 9% 35% 29% • 24%



- Molecule 1: TRANSCRIPTION FACTOR 1

Chain B: 9% 41% 23% • 22%



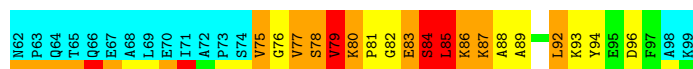


4.2.4 Score per residue for model 4

- Molecule 1: TRANSCRIPTION FACTOR 1



- Molecule 1: TRANSCRIPTION FACTOR 1

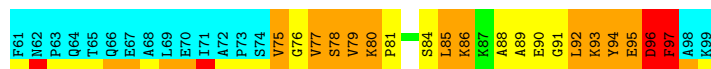


4.2.5 Score per residue for model 5

- Molecule 1: TRANSCRIPTION FACTOR 1



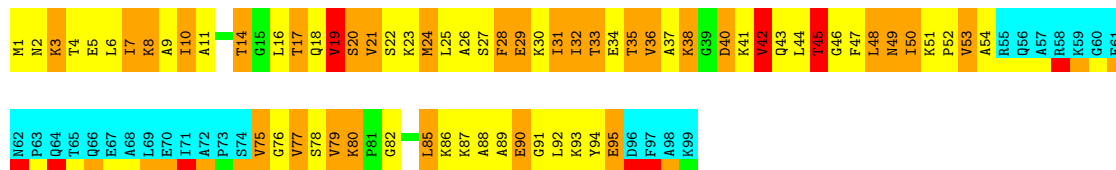
- Molecule 1: TRANSCRIPTION FACTOR 1



4.2.6 Score per residue for model 6

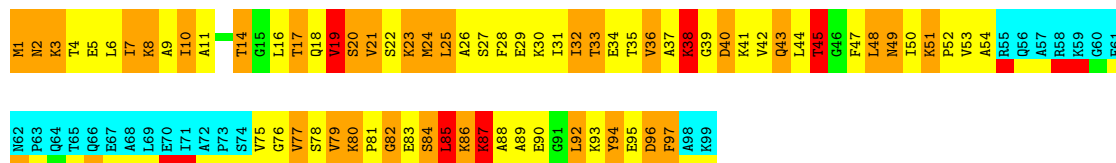
• Molecule 1: TRANSCRIPTION FACTOR 1

Chain A: 7% 36% 29% 5% 24%



• Molecule 1: TRANSCRIPTION FACTOR 1

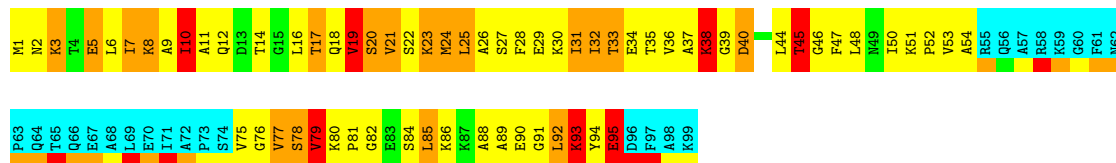
Chain B: 5% 36% 31% 5% 22%



4.2.7 Score per residue for model 7

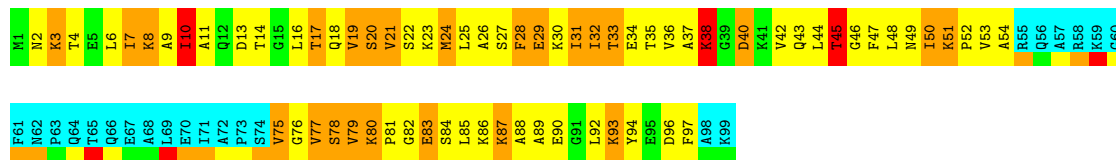
• Molecule 1: TRANSCRIPTION FACTOR 1

Chain A: 9% 41% 18% 7% 24%



• Molecule 1: TRANSCRIPTION FACTOR 1

Chain B: 8% 42% 24% 5% 22%



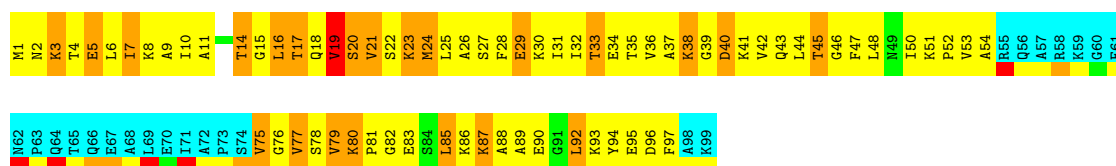
4.2.8 Score per residue for model 8

• Molecule 1: TRANSCRIPTION FACTOR 1

Chain A: 9% 38% 22% 6% 24%

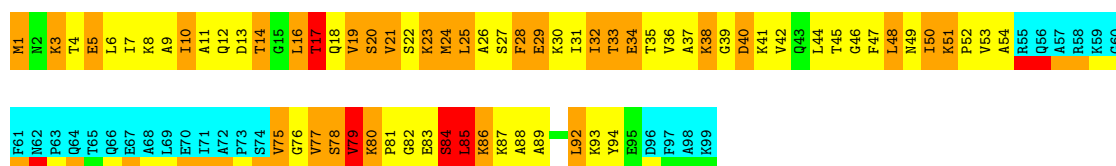


• Molecule 1: TRANSCRIPTION FACTOR 1

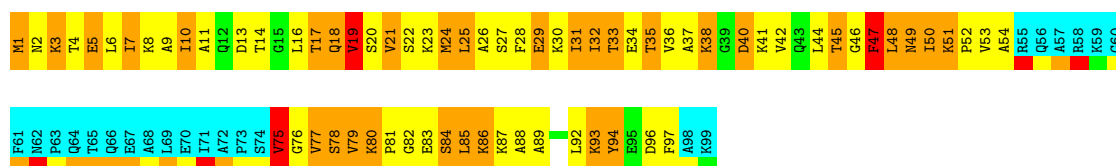


4.2.9 Score per residue for model 9

• Molecule 1: TRANSCRIPTION FACTOR 1

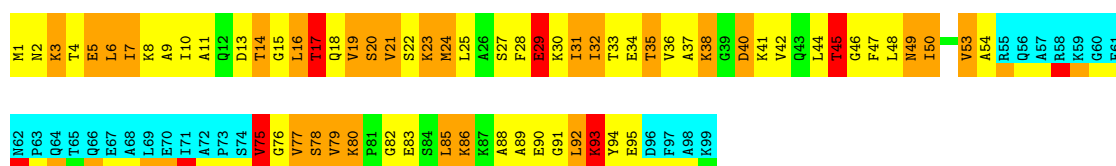


• Molecule 1: TRANSCRIPTION FACTOR 1

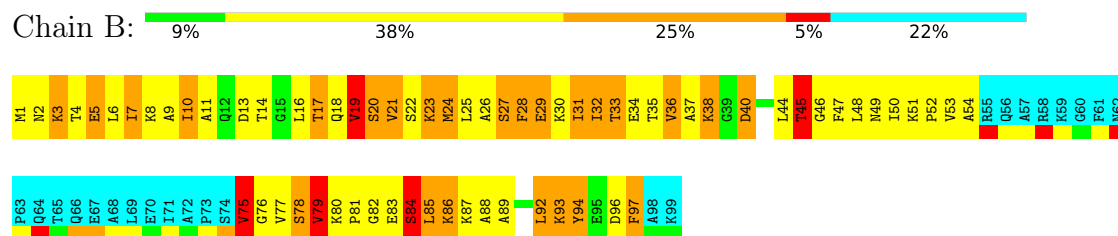


4.2.10 Score per residue for model 10

• Molecule 1: TRANSCRIPTION FACTOR 1

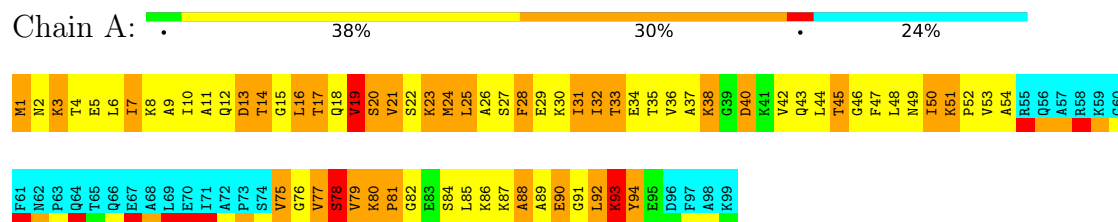


• Molecule 1: TRANSCRIPTION FACTOR 1

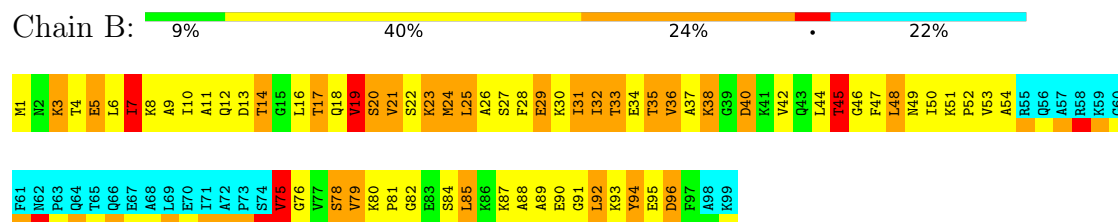


4.2.11 Score per residue for model 11

- Molecule 1: TRANSCRIPTION FACTOR 1

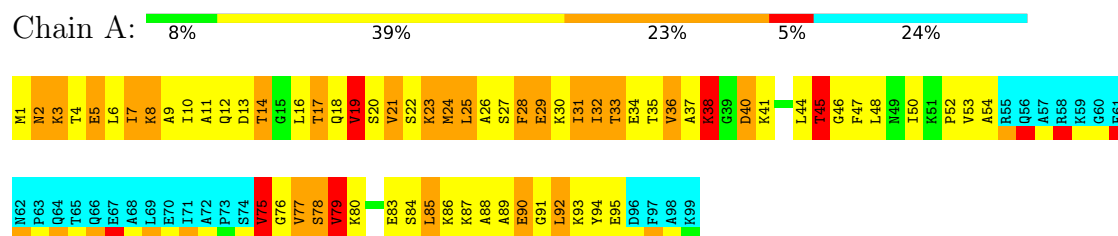


- Molecule 1: TRANSCRIPTION FACTOR 1

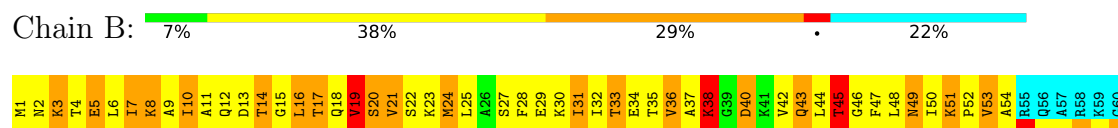


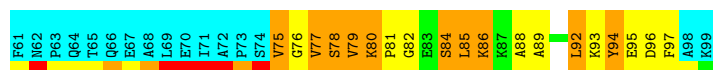
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: TRANSCRIPTION FACTOR 1



- Molecule 1: TRANSCRIPTION FACTOR 1





4.2.13 Score per residue for model 13

- Molecule 1: TRANSCRIPTION FACTOR 1

Chain A: 6% 40% 25% • 24%



- Molecule 1: TRANSCRIPTION FACTOR 1

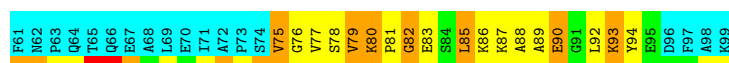
Chain B: 7% 40% 27% • 22%



4.2.14 Score per residue for model 14

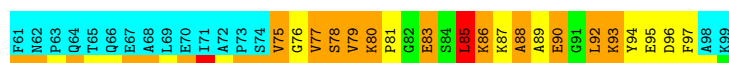
- Molecule 1: TRANSCRIPTION FACTOR 1

Chain A: 6% 38% 30% • 24%



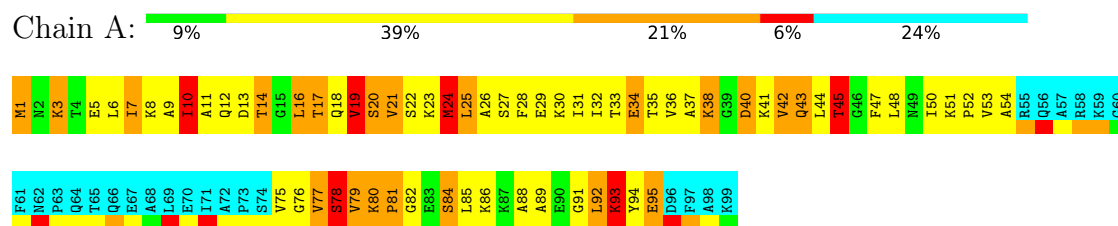
- Molecule 1: TRANSCRIPTION FACTOR 1

Chain B: 7% 35% 32% • 22%

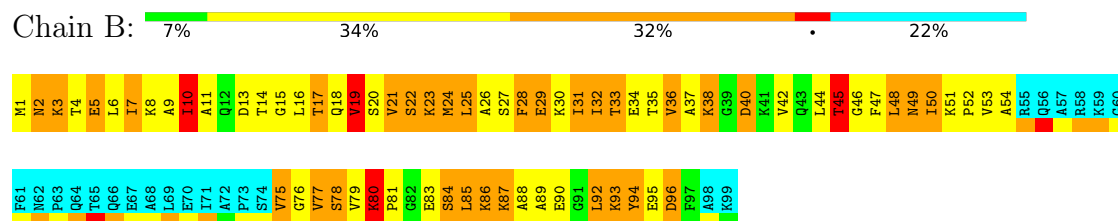


4.2.15 Score per residue for model 15

• Molecule 1: TRANSCRIPTION FACTOR 1

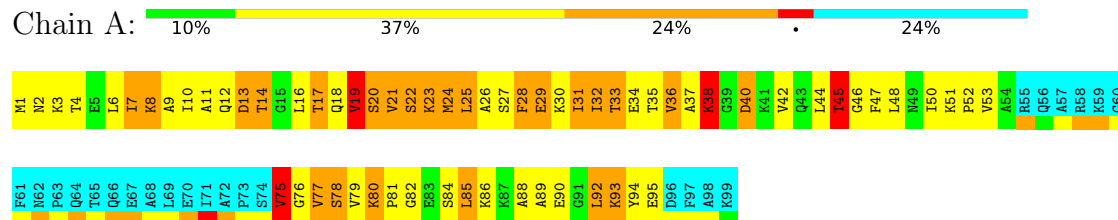


• Molecule 1: TRANSCRIPTION FACTOR 1

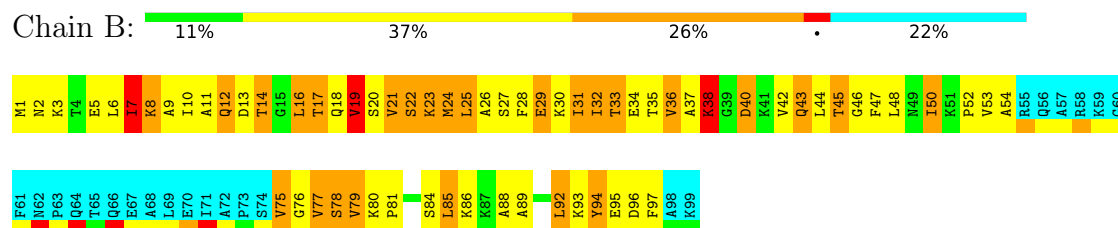


4.2.16 Score per residue for model 16

• Molecule 1: TRANSCRIPTION FACTOR 1



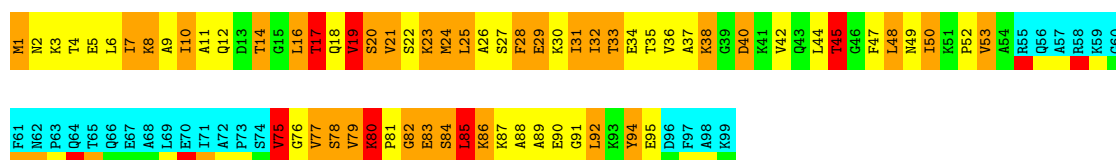
• Molecule 1: TRANSCRIPTION FACTOR 1



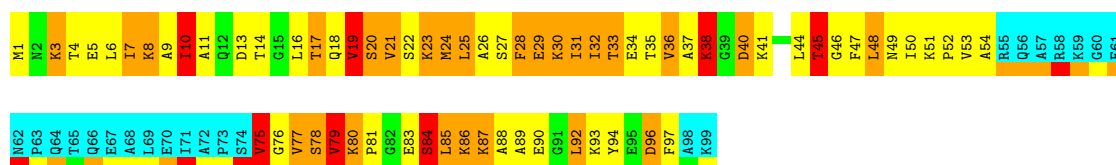
4.2.17 Score per residue for model 17

• Molecule 1: TRANSCRIPTION FACTOR 1



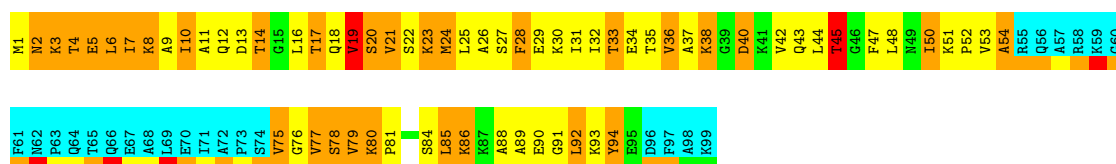


• Molecule 1: TRANSCRIPTION FACTOR 1

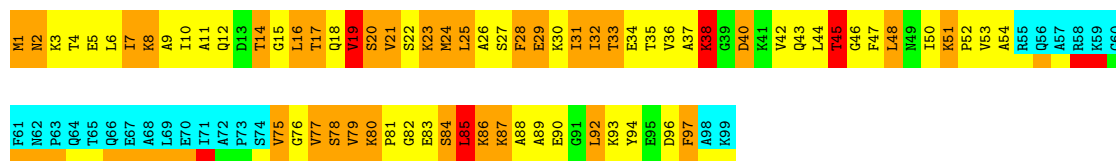


4.2.18 Score per residue for model 18

• Molecule 1: TRANSCRIPTION FACTOR 1

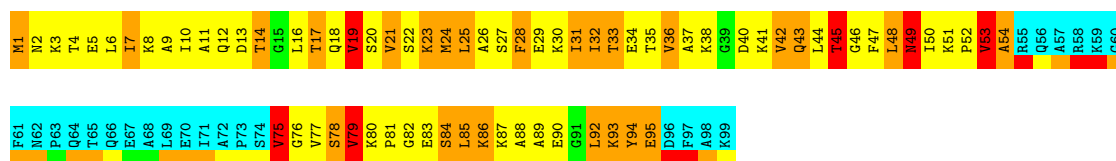
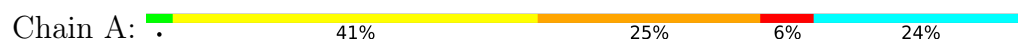


• Molecule 1: TRANSCRIPTION FACTOR 1

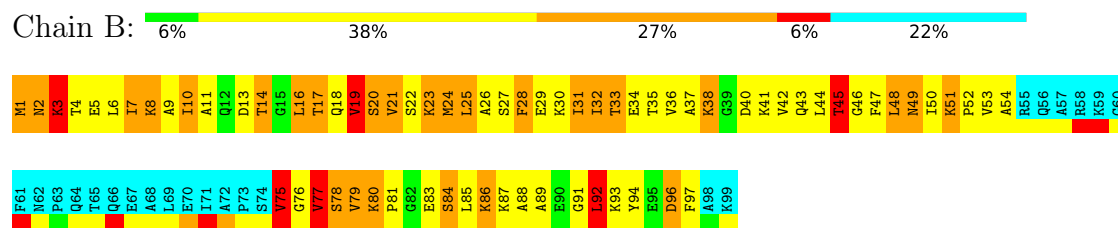


4.2.19 Score per residue for model 19

• Molecule 1: TRANSCRIPTION FACTOR 1

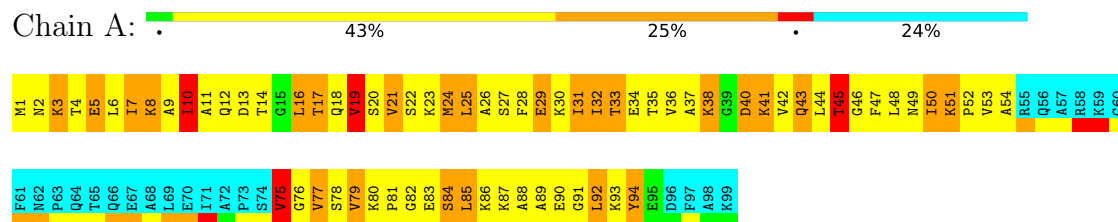


• Molecule 1: TRANSCRIPTION FACTOR 1

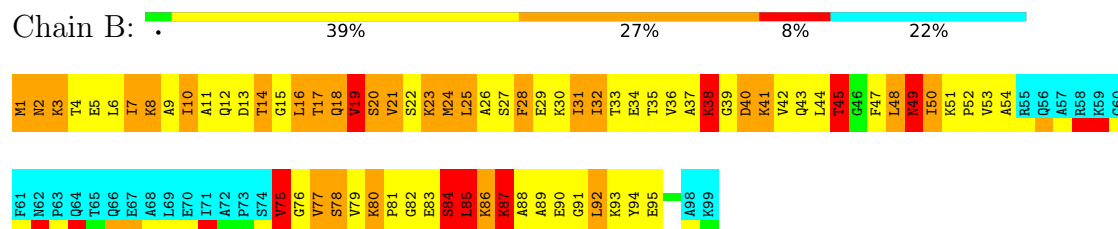


4.2.20 Score per residue for model 20

- Molecule 1: TRANSCRIPTION FACTOR 1

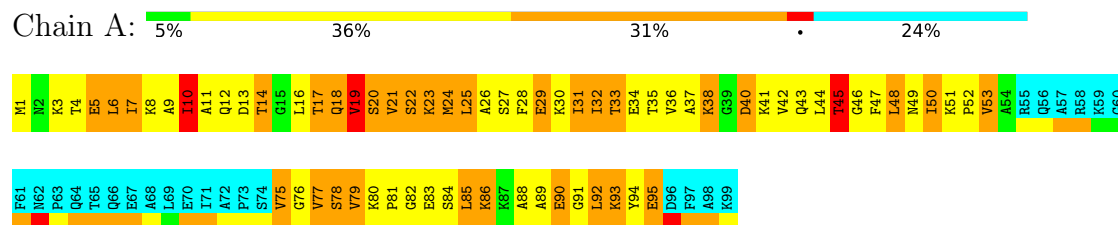


- Molecule 1: TRANSCRIPTION FACTOR 1

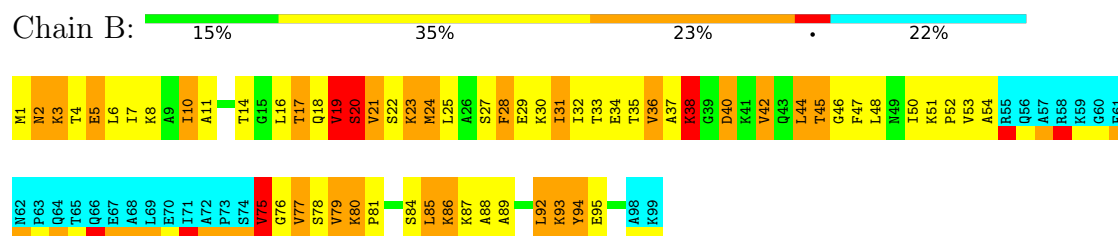


4.2.21 Score per residue for model 21

- Molecule 1: TRANSCRIPTION FACTOR 1

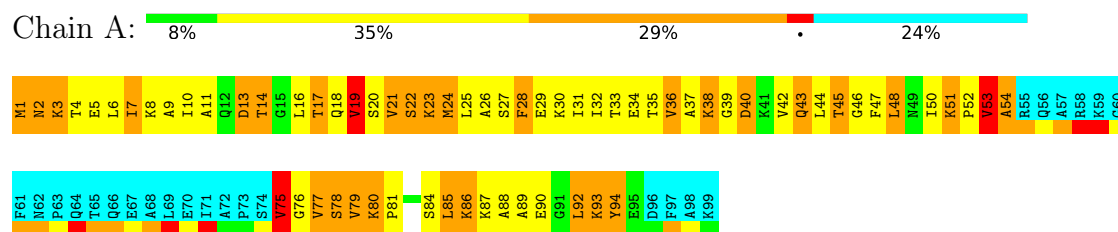


- Molecule 1: TRANSCRIPTION FACTOR 1

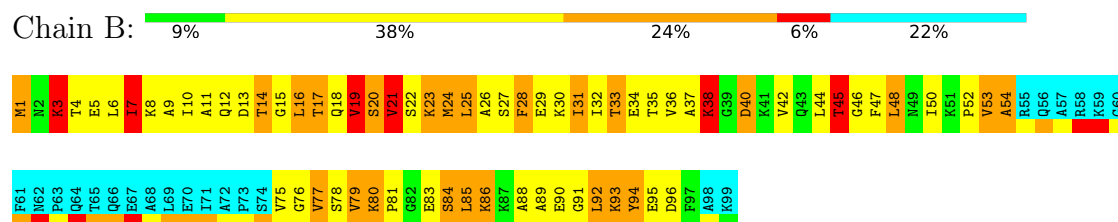


4.2.22 Score per residue for model 22

• Molecule 1: TRANSCRIPTION FACTOR 1

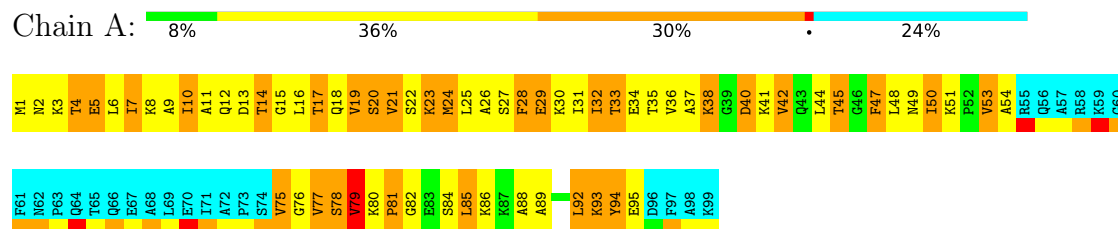


• Molecule 1: TRANSCRIPTION FACTOR 1

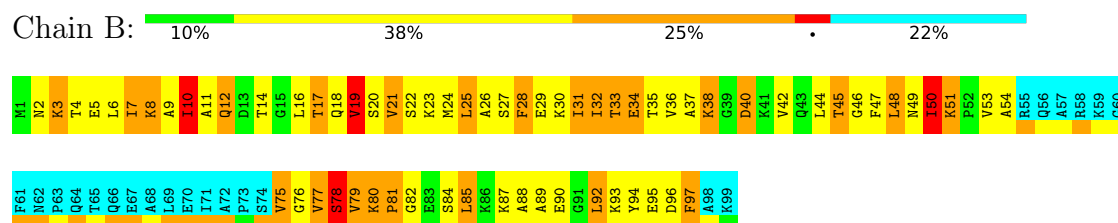


4.2.23 Score per residue for model 23

• Molecule 1: TRANSCRIPTION FACTOR 1



• Molecule 1: TRANSCRIPTION FACTOR 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Distance geometry, simulated annealing, molecular dynamics*.

Of the 50 calculated structures, 23 were deposited, based on the following criterion: *structures with acceptable covalent geometry, 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	structure solution	3
X-PLOR	refinement	3

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	1.43±0.02	0±0/564 (0.0± 0.1%)	1.60±0.04	3±2/758 (0.4± 0.2%)
1	B	1.42±0.01	0±0/584 (0.0± 0.0%)	1.61±0.04	4±2/785 (0.5± 0.3%)
All	All	1.42	4/26404 (0.0%)	1.61	144/35489 (0.4%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	82	GLY	N-CA	6.67	1.49	1.44	14	2
1	B	75	VAL	N-CA	5.34	1.53	1.46	1	1
1	A	86	LYS	C-N	-5.13	1.27	1.33	17	1

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	A	42	VAL	N-CA-CB	-7.64	104.65	112.06	6	1
1	A	86	LYS	N-CA-C	-7.33	103.29	111.28	4	5
1	B	86	LYS	N-CA-C	-6.87	103.79	111.28	2	8
1	A	33	THR	N-CA-CB	-6.60	100.50	110.07	4	1
1	B	75	VAL	N-CA-CB	-6.51	104.92	112.34	17	1
1	A	10	ILE	N-CA-C	-6.41	106.30	111.81	7	5
1	A	86	LYS	N-CA-CB	-6.39	100.48	110.06	17	6
1	B	86	LYS	N-CA-CB	-6.28	100.89	110.12	2	9
1	B	38	LYS	N-CA-C	-6.26	105.80	113.50	21	15
1	B	87	LYS	N-CA-CB	-6.20	101.00	110.12	6	8
1	A	90	GLU	N-CA-C	-6.11	104.73	111.82	2	7
1	A	87	LYS	N-CA-C	-5.97	104.86	111.36	9	3
1	A	93	LYS	N-CA-CB	-5.76	104.88	111.79	20	1
1	B	48	LEU	N-CA-CB	-5.76	102.09	111.24	23	1
1	A	38	LYS	N-CA-C	-5.72	105.13	111.71	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	MET	N-CA-CB	-5.70	101.73	110.12	15	2
1	B	7	ILE	N-CA-CB	-5.68	104.66	110.62	22	5
1	B	24	MET	N-CA-CB	-5.63	101.83	110.16	12	5
1	B	37	ALA	N-CA-CB	-5.60	102.83	110.56	14	1
1	A	49	ASN	N-CA-CB	-5.59	103.71	110.53	19	2
1	B	10	ILE	N-CA-C	-5.58	107.01	111.81	2	6
1	A	87	LYS	N-CA-CB	-5.55	101.97	110.12	17	3
1	B	79	VAL	N-CA-CB	-5.54	102.09	111.23	1	1
1	B	18	GLN	N-CA-C	-5.54	106.11	112.86	13	4
1	A	29	GLU	N-CA-C	-5.53	106.38	113.23	4	2
1	A	18	GLN	N-CA-C	-5.49	106.16	112.86	21	1
1	A	53	VAL	N-CA-CB	-5.49	105.21	112.34	17	5
1	B	90	GLU	N-CA-C	-5.42	105.47	111.71	18	2
1	A	79	VAL	N-CA-CB	-5.41	102.30	111.23	9	3
1	B	87	LYS	N-CA-C	-5.35	105.53	111.36	2	5
1	B	50	ILE	N-CA-CB	-5.33	104.41	112.35	23	1
1	B	49	ASN	N-CA-CB	-5.33	102.74	111.74	20	1
1	B	53	VAL	N-CA-CB	-5.22	105.56	112.34	12	2
1	A	50	ILE	N-CA-CB	-5.21	104.50	110.49	8	2
1	A	13	ASP	N-CA-C	-5.20	105.69	111.36	16	3
1	B	88	ALA	N-CA-C	-5.14	105.67	111.28	14	1
1	B	17	THR	N-CA-CB	-5.13	103.56	110.95	4	1
1	B	97	PHE	N-CA-C	-5.09	99.96	110.80	5	1
1	B	85	LEU	N-CA-CB	-5.06	102.73	110.33	14	1
1	B	20	SER	N-CA-C	-5.05	105.43	112.30	21	1
1	A	88	ALA	N-CA-C	-5.05	105.86	111.36	11	1
1	B	13	ASP	N-CA-C	-5.04	106.39	112.54	22	2
1	A	7	ILE	N-CA-CB	-5.01	105.16	110.62	1	2
1	A	32	ILE	N-CA-C	-5.01	105.61	110.42	4	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	559	608	608	228±18
1	B	578	621	621	229±19
All	All	26151	28267	28266	8284

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 152.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:SER:O	1:A:86:LYS:N	1.34	1.59	9	3
1:B:84:SER:O	1:B:86:LYS:N	1.33	1.58	4	6
1:A:30:LYS:O	1:A:34:GLU:HB2	1.31	1.23	19	21
1:B:30:LYS:O	1:B:34:GLU:HB2	1.28	1.26	20	22
1:B:30:LYS:O	1:B:34:GLU:HB3	1.20	1.35	23	1
1:A:30:LYS:O	1:A:34:GLU:HB3	1.20	1.35	9	2
1:A:94:TYR:O	1:A:95:GLU:C	1.14	1.90	15	2
1:B:30:LYS:O	1:B:34:GLU:CB	1.14	1.95	9	23
1:A:89:ALA:N	1:B:37:ALA:HB1	1.12	1.58	14	4
1:B:85:LEU:O	1:B:88:ALA:N	1.12	1.82	6	9
1:A:16:LEU:HD13	1:B:19:VAL:HG23	1.12	1.17	11	11
1:A:84:SER:O	1:A:85:LEU:C	1.12	1.89	4	3
1:A:30:LYS:O	1:A:34:GLU:CB	1.11	1.97	19	22
1:A:16:LEU:HD11	1:B:19:VAL:HG23	1.11	1.18	15	7
1:A:20:SER:O	1:A:22:SER:N	1.11	1.84	13	23
1:B:84:SER:O	1:B:85:LEU:C	1.09	1.94	20	6
1:B:20:SER:O	1:B:22:SER:N	1.09	1.85	3	23
1:A:36:VAL:HG11	1:A:77:VAL:HG23	1.08	1.21	13	2
1:A:19:VAL:HG11	1:B:19:VAL:HG11	1.07	1.24	14	23
1:A:32:ILE:HG22	1:B:85:LEU:HD21	1.07	1.25	15	1
1:A:36:VAL:HG21	1:A:77:VAL:HG23	1.06	1.21	14	4
1:B:84:SER:C	1:B:86:LYS:N	1.06	2.11	20	6
1:B:14:THR:HG22	1:B:16:LEU:CD1	1.05	1.81	11	7
1:B:36:VAL:HG23	1:B:50:ILE:HD12	1.05	1.26	19	2
1:B:36:VAL:HG21	1:B:77:VAL:HG23	1.05	1.24	21	4
1:A:75:VAL:HG11	1:B:89:ALA:HB3	1.05	1.17	7	3
1:A:14:THR:HG22	1:A:16:LEU:CD1	1.05	1.82	19	13
1:A:85:LEU:HD23	1:B:36:VAL:HG11	1.04	1.22	17	2
1:A:84:SER:C	1:A:86:LYS:N	1.03	2.09	4	3
1:A:85:LEU:HD13	1:B:77:VAL:HG21	1.03	1.28	13	3
1:A:88:ALA:C	1:B:37:ALA:HB1	1.03	1.79	2	14
1:A:85:LEU:HD21	1:B:36:VAL:HG11	1.03	1.20	15	1
1:B:48:LEU:HD13	1:B:80:LYS:HG2	1.03	1.18	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:96:ASP:O	1:B:97:PHE:C	1.02	2.02	5	1
1:A:14:THR:HG22	1:A:16:LEU:HD11	1.01	1.28	11	16
1:A:19:VAL:HG23	1:B:16:LEU:CD1	1.01	1.86	12	11
1:A:42:VAL:HG13	1:B:6:LEU:HD11	1.01	1.33	3	9
1:A:16:LEU:CD1	1:B:19:VAL:HG23	1.00	1.86	5	14
1:A:19:VAL:HG23	1:B:16:LEU:HD11	1.00	1.04	19	7
1:A:92:LEU:HD21	1:B:75:VAL:HG21	0.99	1.30	8	5
1:A:20:SER:O	1:A:23:LYS:N	0.99	1.95	21	23
1:B:20:SER:O	1:B:23:LYS:N	0.98	1.97	5	23
1:B:84:SER:C	1:B:85:LEU:HD22	0.97	1.84	18	1
1:B:30:LYS:O	1:B:34:GLU:CG	0.97	2.12	4	22
1:A:25:LEU:HD12	1:A:25:LEU:C	0.96	1.83	20	6
1:A:37:ALA:HB2	1:B:88:ALA:HB1	0.96	1.32	14	10
1:A:83:GLU:O	1:A:85:LEU:N	0.96	1.98	19	6
1:A:36:VAL:HG21	1:A:77:VAL:HG22	0.96	1.36	4	1
1:A:36:VAL:HG21	1:B:85:LEU:HD22	0.96	1.34	19	4
1:B:10:ILE:O	1:B:14:THR:OG1	0.96	1.84	7	23
1:B:84:SER:C	1:B:86:LYS:H	0.96	1.67	6	6
1:A:31:ILE:HD13	1:B:9:ALA:HB1	0.95	1.38	2	8
1:A:89:ALA:HB3	1:B:75:VAL:HG11	0.95	1.33	14	5
1:A:85:LEU:HD12	1:B:36:VAL:HG21	0.95	1.38	9	1
1:B:83:GLU:O	1:B:85:LEU:N	0.95	2.00	17	9
1:A:85:LEU:HD11	1:B:36:VAL:HG12	0.95	1.34	19	2
1:A:53:VAL:O	1:A:75:VAL:HG22	0.95	1.62	22	2
1:B:49:ASN:O	1:B:79:VAL:O	0.94	1.83	15	3
1:A:89:ALA:CB	1:B:75:VAL:HG11	0.94	1.92	12	7
1:A:77:VAL:HG11	1:B:85:LEU:HD13	0.94	1.35	10	2
1:B:14:THR:HG22	1:B:16:LEU:HD11	0.94	1.38	13	10
1:B:50:ILE:HA	1:B:79:VAL:HG21	0.94	1.36	19	3
1:A:75:VAL:HG11	1:B:89:ALA:CB	0.94	1.91	23	4
1:B:25:LEU:C	1:B:25:LEU:HD12	0.94	1.87	20	6
1:A:7:ILE:HG23	1:A:21:VAL:HB	0.94	1.38	9	5
1:A:32:ILE:HG21	1:B:47:PHE:CE1	0.94	1.98	15	14
1:A:78:SER:O	1:A:79:VAL:HG23	0.94	1.63	21	3
1:A:77:VAL:HG11	1:B:84:SER:O	0.93	1.63	2	1
1:B:10:ILE:HG21	1:B:24:MET:HE1	0.93	1.38	14	2
1:A:32:ILE:HD13	1:A:42:VAL:HG11	0.93	1.37	4	1
1:A:10:ILE:O	1:A:14:THR:OG1	0.93	1.84	20	23
1:A:44:LEU:HD12	1:A:48:LEU:CB	0.93	1.94	17	22
1:A:31:ILE:HA	1:A:34:GLU:CG	0.93	1.94	9	2
1:A:36:VAL:HG21	1:B:85:LEU:HD12	0.92	1.39	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:ALA:HB1	1:B:75:VAL:HG11	0.92	1.38	22	7
1:A:48:LEU:CD1	1:B:48:LEU:HD11	0.92	1.95	9	2
1:A:48:LEU:HD11	1:B:48:LEU:HD11	0.91	1.40	9	2
1:A:7:ILE:CD1	1:A:25:LEU:HD23	0.91	1.95	20	2
1:B:7:ILE:CD1	1:B:25:LEU:HD23	0.91	1.95	23	3
1:A:47:PHE:CE1	1:B:32:ILE:HG21	0.90	2.01	12	15
1:A:75:VAL:HB	1:B:94:TYR:CD2	0.90	2.01	5	2
1:A:85:LEU:HD11	1:B:36:VAL:CG1	0.90	1.94	19	2
1:A:91:GLY:C	1:A:92:LEU:HD23	0.90	1.91	17	2
1:A:85:LEU:HD12	1:B:33:THR:OG1	0.90	1.66	2	2
1:A:19:VAL:HG23	1:B:16:LEU:HD13	0.89	1.43	8	11
1:B:53:VAL:HG22	1:B:76:GLY:O	0.89	1.67	2	18
1:B:44:LEU:HD12	1:B:48:LEU:CB	0.89	1.97	17	21
1:B:36:VAL:HG23	1:B:42:VAL:HG12	0.89	1.41	6	2
1:A:14:THR:CG2	1:A:16:LEU:HD11	0.89	1.97	11	4
1:B:85:LEU:HD12	1:B:85:LEU:C	0.89	1.90	23	1
1:A:89:ALA:HB1	1:B:75:VAL:CG1	0.88	1.98	7	9
1:A:19:VAL:O	1:B:16:LEU:HD22	0.88	1.68	17	14
1:A:75:VAL:HB	1:B:89:ALA:HB1	0.88	1.43	15	3
1:A:89:ALA:HB1	1:B:75:VAL:HG21	0.88	1.44	11	2
1:A:14:THR:HG22	1:B:20:SER:HB2	0.88	1.44	20	9
1:A:84:SER:C	1:A:86:LYS:H	0.88	1.72	9	3
1:A:75:VAL:HG21	1:B:92:LEU:HD21	0.88	1.42	19	3
1:A:92:LEU:HD12	1:A:92:LEU:O	0.88	1.67	21	12
1:A:89:ALA:HB1	1:B:75:VAL:HG12	0.88	1.45	7	4
1:A:85:LEU:HD23	1:B:36:VAL:CG1	0.87	1.99	17	1
1:A:36:VAL:HG21	1:A:77:VAL:CG2	0.87	1.98	14	4
1:A:85:LEU:HD13	1:B:33:THR:O	0.87	1.70	19	2
1:A:7:ILE:HG22	1:A:8:LYS:CE	0.87	1.98	9	1
1:A:85:LEU:HD12	1:B:36:VAL:CG2	0.86	1.99	9	1
1:B:3:LYS:O	1:B:25:LEU:HD22	0.86	1.69	9	2
1:A:36:VAL:HG11	1:B:85:LEU:HD23	0.86	1.47	18	1
1:B:96:ASP:OD1	1:B:96:ASP:N	0.86	2.06	5	1
1:B:78:SER:O	1:B:79:VAL:HG23	0.86	1.71	13	1
1:B:1:MET:HE2	1:B:6:LEU:HD23	0.86	1.47	11	3
1:A:30:LYS:O	1:A:34:GLU:CG	0.86	2.24	10	21
1:A:16:LEU:HD22	1:B:19:VAL:O	0.86	1.71	2	12
1:B:35:THR:HG21	1:B:42:VAL:HG23	0.85	1.48	11	3
1:A:77:VAL:HG11	1:B:81:PRO:HB3	0.85	1.48	8	1
1:A:36:VAL:CG2	1:B:85:LEU:HD13	0.85	2.01	23	1
1:B:44:LEU:HD12	1:B:48:LEU:HB2	0.85	1.48	8	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:VAL:CG2	1:B:16:LEU:HD11	0.85	1.97	19	7
1:A:54:ALA:HA	1:A:75:VAL:CA	0.85	2.01	14	4
1:A:44:LEU:HD22	1:B:28:PHE:CE1	0.85	2.07	5	10
1:A:85:LEU:HD13	1:B:77:VAL:CG1	0.85	2.02	7	2
1:A:42:VAL:HG22	1:B:1:MET:HB2	0.85	1.46	9	3
1:A:37:ALA:HB1	1:B:88:ALA:O	0.85	1.69	18	14
1:B:89:ALA:HA	1:B:92:LEU:HD23	0.85	1.43	17	20
1:A:16:LEU:HD13	1:B:19:VAL:CG2	0.85	2.01	16	16
1:A:36:VAL:HG21	1:B:85:LEU:HD13	0.85	1.48	23	1
1:A:20:SER:HB2	1:B:14:THR:HG22	0.84	1.50	17	12
1:B:85:LEU:HD12	1:B:85:LEU:O	0.84	1.71	23	1
1:B:34:GLU:O	1:B:38:LYS:N	0.84	2.10	14	19
1:B:54:ALA:HA	1:B:75:VAL:N	0.84	1.86	7	4
1:A:20:SER:HB3	1:B:16:LEU:HD21	0.84	1.47	19	3
1:A:77:VAL:HG21	1:B:85:LEU:CB	0.84	2.02	3	7
1:A:85:LEU:CB	1:B:77:VAL:HG21	0.84	2.03	18	11
1:A:75:VAL:HB	1:B:94:TYR:CE2	0.84	2.08	5	2
1:A:6:LEU:HD11	1:B:42:VAL:HG13	0.84	1.46	15	7
1:A:84:SER:C	1:A:85:LEU:HD22	0.84	1.97	2	2
1:A:32:ILE:CD1	1:A:42:VAL:HG11	0.84	2.02	4	1
1:A:35:THR:HG21	1:A:42:VAL:HG23	0.84	1.48	14	4
1:B:47:PHE:CD1	1:B:85:LEU:HD21	0.84	2.08	16	6
1:A:14:THR:HG22	1:B:20:SER:OG	0.84	1.71	7	1
1:A:85:LEU:CD2	1:B:36:VAL:HG11	0.83	2.03	15	4
1:A:37:ALA:HB2	1:B:88:ALA:O	0.83	1.72	9	9
1:B:7:ILE:HG23	1:B:21:VAL:HB	0.83	1.51	11	10
1:A:16:LEU:HD21	1:B:20:SER:HB3	0.83	1.47	4	6
1:A:8:LYS:HA	1:A:11:ALA:HB3	0.83	1.50	15	23
1:A:50:ILE:HG22	1:A:79:VAL:CG2	0.83	2.03	6	3
1:A:54:ALA:HB2	1:A:75:VAL:HG23	0.83	1.49	3	1
1:A:35:THR:HG23	1:A:40:ASP:CB	0.83	2.04	10	16
1:B:7:ILE:HG13	1:B:25:LEU:HD12	0.83	1.48	5	9
1:A:85:LEU:HB3	1:A:88:ALA:HB3	0.82	1.51	13	2
1:A:77:VAL:HG21	1:B:85:LEU:CD1	0.82	2.03	20	2
1:B:1:MET:HE2	1:B:6:LEU:CD2	0.82	2.04	21	3
1:A:28:PHE:O	1:A:31:ILE:HG13	0.82	1.74	15	22
1:A:24:MET:HB3	1:B:14:THR:HG21	0.82	1.51	11	2
1:B:35:THR:HG21	1:B:42:VAL:HG13	0.82	1.52	8	2
1:A:4:THR:O	1:A:7:ILE:HB	0.82	1.75	9	6
1:A:47:PHE:CD2	1:A:48:LEU:HD23	0.82	2.09	17	3
1:A:32:ILE:HG22	1:B:85:LEU:CD2	0.82	2.03	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:7:ILE:HG21	1:B:25:LEU:HD22	0.82	1.49	18	1
1:A:19:VAL:CG2	1:B:16:LEU:HD13	0.82	2.05	11	16
1:A:75:VAL:CG1	1:B:89:ALA:HB1	0.82	2.05	19	8
1:A:85:LEU:N	1:A:85:LEU:HD22	0.82	1.90	17	2
1:A:92:LEU:HD23	1:B:37:ALA:C	0.82	2.00	3	3
1:A:85:LEU:HD22	1:B:36:VAL:HG21	0.82	1.51	13	1
1:A:21:VAL:HA	1:A:24:MET:HE2	0.81	1.52	17	20
1:A:37:ALA:HB2	1:B:88:ALA:CB	0.81	2.05	14	10
1:A:42:VAL:HG13	1:A:50:ILE:HB	0.81	1.52	8	3
1:B:92:LEU:O	1:B:92:LEU:HD12	0.81	1.74	14	20
1:B:48:LEU:HD23	1:B:80:LYS:O	0.81	1.75	12	10
1:B:36:VAL:CG2	1:B:50:ILE:HD12	0.81	2.04	14	2
1:A:9:ALA:CB	1:B:31:ILE:HD13	0.81	2.04	10	12
1:A:88:ALA:O	1:B:37:ALA:HB1	0.81	1.74	19	15
1:B:36:VAL:CG2	1:B:50:ILE:HG22	0.81	2.05	2	1
1:B:10:ILE:C	1:B:14:THR:HG1	0.81	1.81	13	5
1:A:14:THR:HG22	1:A:16:LEU:HD13	0.81	1.53	21	7
1:A:80:LYS:CB	1:A:81:PRO:HD3	0.81	2.06	4	2
1:A:44:LEU:HD12	1:A:48:LEU:HB2	0.80	1.51	1	15
1:A:92:LEU:HG	1:B:36:VAL:O	0.80	1.76	4	1
1:A:50:ILE:HD11	1:B:48:LEU:HD11	0.80	1.53	8	2
1:A:33:THR:O	1:B:88:ALA:HB1	0.80	1.76	17	7
1:A:89:ALA:HA	1:A:92:LEU:HD23	0.80	1.53	18	12
1:B:14:THR:HG22	1:B:16:LEU:HD13	0.80	1.52	6	5
1:A:44:LEU:HD12	1:A:48:LEU:HB3	0.80	1.53	20	11
1:A:2:ASN:C	1:A:6:LEU:HD12	0.80	2.01	6	8
1:B:19:VAL:HG22	1:B:20:SER:H	0.80	1.35	10	18
1:A:53:VAL:O	1:A:75:VAL:HG23	0.80	1.76	6	2
1:A:53:VAL:HG22	1:A:76:GLY:O	0.80	1.76	9	20
1:A:85:LEU:O	1:A:85:LEU:HD12	0.80	1.77	6	2
1:B:36:VAL:HG21	1:B:50:ILE:HG22	0.80	1.52	2	3
1:A:85:LEU:O	1:A:89:ALA:N	0.79	2.15	17	9
1:A:93:LYS:O	1:A:94:TYR:C	0.79	2.22	19	16
1:B:47:PHE:CD2	1:B:48:LEU:HD23	0.79	2.13	6	1
1:A:84:SER:C	1:B:77:VAL:HG11	0.79	2.03	9	2
1:A:47:PHE:CD1	1:A:85:LEU:HD21	0.79	2.12	12	5
1:B:31:ILE:HA	1:B:34:GLU:HG2	0.79	1.53	23	1
1:B:29:GLU:O	1:B:33:THR:OG1	0.79	2.01	13	1
1:B:91:GLY:C	1:B:92:LEU:HD23	0.79	2.00	13	2
1:A:20:SER:OG	1:A:24:MET:N	0.79	2.14	5	8
1:A:85:LEU:HD13	1:B:77:VAL:CG2	0.79	2.08	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:LEU:HD13	1:B:80:LYS:CG	0.79	2.05	20	1
1:B:2:ASN:C	1:B:6:LEU:HD12	0.79	2.03	1	4
1:A:77:VAL:CG2	1:B:85:LEU:HD22	0.79	2.07	7	4
1:B:14:THR:HG22	1:B:16:LEU:CD2	0.79	2.08	16	6
1:B:48:LEU:HD13	1:B:80:LYS:CB	0.79	2.08	9	2
1:A:33:THR:HA	1:B:85:LEU:HD23	0.79	1.53	17	9
1:B:31:ILE:O	1:B:34:GLU:HG3	0.79	1.78	23	1
1:B:32:ILE:HD13	1:B:42:VAL:HG21	0.79	1.54	3	1
1:A:85:LEU:CG	1:B:77:VAL:HG21	0.79	2.08	8	4
1:A:92:LEU:CD1	1:B:75:VAL:HG21	0.79	2.07	4	2
1:A:48:LEU:HD23	1:A:80:LYS:O	0.78	1.77	16	13
1:B:44:LEU:HD12	1:B:48:LEU:HB3	0.78	1.55	3	12
1:A:20:SER:OG	1:B:16:LEU:HD11	0.78	1.78	9	8
1:B:78:SER:C	1:B:79:VAL:HG12	0.78	2.03	17	3
1:A:43:GLN:O	1:A:44:LEU:HD23	0.78	1.78	11	3
1:B:28:PHE:O	1:B:31:ILE:HG13	0.78	1.77	23	22
1:A:19:VAL:C	1:B:16:LEU:HD22	0.78	2.04	6	6
1:A:44:LEU:O	1:A:46:GLY:N	0.78	2.15	11	16
1:B:85:LEU:N	1:B:85:LEU:HD12	0.78	1.93	17	2
1:A:31:ILE:HD13	1:B:9:ALA:CB	0.78	2.09	16	8
1:A:20:SER:HB2	1:B:14:THR:HG21	0.78	1.55	4	3
1:B:93:LYS:O	1:B:94:TYR:C	0.78	2.23	5	16
1:A:77:VAL:HG11	1:B:85:LEU:HB2	0.78	1.55	17	4
1:A:85:LEU:HD22	1:B:77:VAL:CG2	0.78	2.09	15	4
1:A:6:LEU:HD11	1:B:42:VAL:CG1	0.78	2.08	2	7
1:B:8:LYS:HA	1:B:11:ALA:HB3	0.78	1.53	13	23
1:A:48:LEU:HD13	1:B:48:LEU:HD13	0.78	1.56	22	1
1:A:42:VAL:CG1	1:B:6:LEU:HD11	0.77	2.09	4	6
1:A:54:ALA:HB1	1:B:96:ASP:HB3	0.77	1.54	5	1
1:A:48:LEU:HD12	1:A:80:LYS:O	0.77	1.79	7	1
1:A:28:PHE:HB2	1:B:10:ILE:HD11	0.77	1.55	9	5
1:B:35:THR:HG21	1:B:42:VAL:CG1	0.77	2.08	8	2
1:A:50:ILE:HD12	1:A:79:VAL:HG22	0.77	1.57	16	3
1:A:1:MET:HE2	1:A:6:LEU:CD2	0.77	2.10	12	5
1:B:78:SER:O	1:B:79:VAL:HG13	0.77	1.79	12	1
1:B:49:ASN:N	1:B:80:LYS:O	0.77	2.17	20	2
1:A:36:VAL:HG13	1:A:52:PRO:HB3	0.77	1.55	18	10
1:A:16:LEU:HD22	1:B:19:VAL:C	0.77	2.04	21	8
1:B:7:ILE:HD12	1:B:25:LEU:HD23	0.77	1.55	23	3
1:A:27:SER:O	1:A:31:ILE:HG23	0.77	1.80	15	5
1:A:76:GLY:O	1:A:78:SER:N	0.77	2.17	2	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:ALA:O	1:B:37:ALA:CA	0.77	2.32	4	2
1:B:94:TYR:CD1	1:B:94:TYR:C	0.77	2.61	15	6
1:B:31:ILE:HA	1:B:34:GLU:CG	0.77	2.10	23	1
1:A:53:VAL:O	1:A:75:VAL:HA	0.77	1.79	14	2
1:B:53:VAL:O	1:B:75:VAL:HG22	0.77	1.77	5	1
1:B:77:VAL:HG13	1:B:77:VAL:O	0.77	1.78	17	7
1:A:3:LYS:CG	1:A:25:LEU:HD13	0.76	2.10	13	1
1:A:9:ALA:HB1	1:B:31:ILE:HD13	0.76	1.55	9	12
1:B:54:ALA:HA	1:B:75:VAL:HA	0.76	1.57	11	5
1:A:42:VAL:HG23	1:B:6:LEU:HD11	0.76	1.57	5	1
1:A:92:LEU:HD21	1:B:75:VAL:CG2	0.76	2.11	8	3
1:A:3:LYS:HG2	1:A:25:LEU:HD13	0.76	1.58	13	3
1:A:77:VAL:HG21	1:B:84:SER:CA	0.76	2.09	6	1
1:A:19:VAL:HG22	1:A:20:SER:N	0.76	1.95	18	23
1:B:7:ILE:CG2	1:B:25:LEU:HD22	0.76	2.10	18	2
1:A:36:VAL:HG21	1:B:85:LEU:CD2	0.76	2.11	19	3
1:B:48:LEU:HD13	1:B:80:LYS:HB3	0.76	1.58	9	2
1:B:42:VAL:HG22	1:B:50:ILE:CG1	0.76	2.09	21	1
1:B:21:VAL:HA	1:B:24:MET:HE2	0.76	1.58	9	12
1:A:85:LEU:HD22	1:B:33:THR:OG1	0.76	1.81	9	2
1:A:85:LEU:CD1	1:B:77:VAL:HG21	0.76	2.11	13	3
1:A:50:ILE:CD1	1:A:79:VAL:HG23	0.76	2.10	15	6
1:B:11:ALA:HB2	1:B:21:VAL:HG11	0.76	1.55	22	5
1:A:89:ALA:HB2	1:B:36:VAL:CG1	0.76	2.11	11	1
1:A:78:SER:O	1:A:79:VAL:HG13	0.76	1.79	23	1
1:B:19:VAL:HG22	1:B:20:SER:N	0.76	1.95	10	23
1:B:20:SER:OG	1:B:24:MET:N	0.76	2.19	2	10
1:A:85:LEU:HB3	1:B:77:VAL:HG21	0.76	1.57	14	8
1:A:19:VAL:HG23	1:B:16:LEU:HB2	0.75	1.55	6	6
1:A:18:GLN:O	1:A:19:VAL:C	0.75	2.28	13	23
1:B:25:LEU:HG	1:B:26:ALA:N	0.75	1.95	6	4
1:A:75:VAL:HG12	1:B:89:ALA:HB1	0.75	1.56	19	4
1:A:37:ALA:HB1	1:B:88:ALA:C	0.75	2.06	1	7
1:A:37:ALA:HA	1:B:92:LEU:HB3	0.75	1.58	10	18
1:B:50:ILE:HG22	1:B:79:VAL:CG2	0.75	2.12	21	2
1:A:92:LEU:CD2	1:B:75:VAL:HG21	0.75	2.10	8	2
1:A:36:VAL:HG11	1:A:77:VAL:HG22	0.75	1.58	17	2
1:A:28:PHE:O	1:A:32:ILE:CG1	0.75	2.34	23	23
1:A:42:VAL:CG2	1:B:6:LEU:HD11	0.75	2.10	16	4
1:A:35:THR:HG21	1:A:42:VAL:CG2	0.75	2.11	14	4
1:B:95:GLU:O	1:B:97:PHE:N	0.75	2.20	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:THR:OG1	1:B:85:LEU:HD12	0.75	1.82	18	2
1:A:77:VAL:HG21	1:B:85:LEU:CG	0.75	2.11	14	4
1:A:48:LEU:HD21	1:B:50:ILE:HD11	0.75	1.57	23	4
1:A:91:GLY:HA3	1:B:37:ALA:HB1	0.74	1.59	4	2
1:B:48:LEU:HD22	1:B:80:LYS:CB	0.74	2.11	20	1
1:A:14:THR:HG21	1:B:24:MET:HB3	0.74	1.58	19	6
1:A:89:ALA:CA	1:A:92:LEU:HD23	0.74	2.12	23	6
1:A:50:ILE:HD11	1:A:79:VAL:HG23	0.74	1.59	15	1
1:A:92:LEU:HD23	1:A:92:LEU:N	0.74	1.96	17	2
1:B:36:VAL:HG13	1:B:52:PRO:CG	0.74	2.12	19	4
1:A:92:LEU:HD13	1:B:75:VAL:HG21	0.74	1.58	4	1
1:A:44:LEU:HD22	1:B:3:LYS:HD2	0.74	1.57	23	1
1:A:42:VAL:HG23	1:A:50:ILE:HD11	0.74	1.59	9	1
1:A:19:VAL:HG22	1:A:20:SER:H	0.74	1.42	18	14
1:A:85:LEU:HD13	1:A:85:LEU:H	0.74	1.42	2	2
1:A:75:VAL:CG2	1:B:92:LEU:HD21	0.74	2.13	19	1
1:B:35:THR:HG23	1:B:40:ASP:CB	0.74	2.12	11	12
1:A:7:ILE:HD12	1:A:25:LEU:HD23	0.74	1.59	20	2
1:B:43:GLN:O	1:B:44:LEU:HD23	0.74	1.83	6	5
1:A:16:LEU:HD11	1:B:19:VAL:CG2	0.74	2.06	4	5
1:A:3:LYS:O	1:A:25:LEU:HD22	0.74	1.82	17	2
1:B:20:SER:O	1:B:21:VAL:C	0.74	2.31	6	23
1:A:85:LEU:HD22	1:B:36:VAL:HG11	0.74	1.60	5	4
1:A:16:LEU:HB2	1:B:19:VAL:HG23	0.74	1.59	8	9
1:B:85:LEU:O	1:B:89:ALA:N	0.73	2.21	18	10
1:A:50:ILE:CD1	1:A:79:VAL:HG22	0.73	2.11	21	3
1:A:35:THR:HG22	1:A:40:ASP:CB	0.73	2.13	19	2
1:A:47:PHE:CD2	1:B:29:GLU:HG3	0.73	2.18	7	7
1:A:89:ALA:CA	1:B:37:ALA:HB1	0.73	2.12	14	3
1:B:89:ALA:CA	1:B:92:LEU:HD23	0.73	2.12	14	11
1:A:29:GLU:HG3	1:B:47:PHE:CD1	0.73	2.18	7	4
1:A:49:ASN:C	1:A:79:VAL:HG23	0.73	2.07	20	4
1:A:42:VAL:HG12	1:B:1:MET:CB	0.73	2.13	20	2
1:A:77:VAL:HG21	1:B:84:SER:HA	0.73	1.57	6	1
1:B:50:ILE:HD13	1:B:79:VAL:HB	0.73	1.61	18	5
1:A:14:THR:HB	1:A:16:LEU:HD12	0.73	1.58	1	4
1:A:20:SER:O	1:A:21:VAL:C	0.73	2.32	4	23
1:A:37:ALA:CB	1:B:88:ALA:O	0.73	2.36	9	16
1:A:35:THR:HG21	1:A:42:VAL:HG13	0.73	1.60	15	2
1:B:36:VAL:O	1:B:52:PRO:HG3	0.72	1.84	14	7
1:A:14:THR:HG22	1:B:20:SER:HG	0.72	1.42	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:HE2	1:A:6:LEU:HD23	0.72	1.58	22	3
1:A:6:LEU:HD11	1:B:42:VAL:HG21	0.72	1.60	13	1
1:B:18:GLN:O	1:B:19:VAL:C	0.72	2.32	23	23
1:B:36:VAL:HG23	1:B:50:ILE:CD1	0.72	2.13	19	1
1:A:19:VAL:CG1	1:B:19:VAL:HG11	0.72	2.11	14	16
1:B:36:VAL:HG22	1:B:52:PRO:HD3	0.72	1.60	5	5
1:A:48:LEU:HD22	1:A:82:GLY:HA2	0.72	1.60	4	1
1:A:75:VAL:HG12	1:B:89:ALA:CB	0.72	2.14	17	12
1:B:85:LEU:HB3	1:B:88:ALA:HB3	0.72	1.61	15	6
1:A:35:THR:C	1:A:40:ASP:HB2	0.72	2.09	19	2
1:A:85:LEU:CB	1:A:88:ALA:HB3	0.72	2.14	4	3
1:B:86:LYS:O	1:B:89:ALA:HB3	0.72	1.85	14	7
1:A:47:PHE:CG	1:A:85:LEU:HD23	0.72	2.19	8	1
1:A:88:ALA:O	1:B:37:ALA:HB2	0.72	1.84	4	4
1:A:50:ILE:HG22	1:A:79:VAL:HG23	0.72	1.60	6	2
1:B:54:ALA:HA	1:B:75:VAL:CA	0.72	2.14	11	3
1:A:42:VAL:HG11	1:B:6:LEU:CD1	0.72	2.15	9	1
1:A:50:ILE:HG23	1:A:79:VAL:HG22	0.72	1.61	16	1
1:A:47:PHE:O	1:A:82:GLY:CA	0.72	2.38	1	5
1:A:7:ILE:HG22	1:A:25:LEU:HD23	0.72	1.59	11	1
1:B:35:THR:HG22	1:B:40:ASP:CB	0.72	2.14	13	1
1:A:36:VAL:CG2	1:B:85:LEU:HD12	0.72	2.13	2	1
1:A:91:GLY:CA	1:B:37:ALA:HB1	0.72	2.15	4	2
1:A:89:ALA:HB1	1:B:75:VAL:HB	0.72	1.62	13	4
1:A:50:ILE:CG1	1:A:79:VAL:HG22	0.72	2.15	21	2
1:B:85:LEU:N	1:B:85:LEU:HD13	0.71	1.98	18	2
1:A:77:VAL:HG11	1:B:84:SER:CB	0.71	2.15	18	1
1:A:89:ALA:CB	1:B:75:VAL:HG12	0.71	2.15	4	4
1:A:54:ALA:HB1	1:B:96:ASP:CB	0.71	2.15	5	1
1:A:85:LEU:HG	1:B:77:VAL:HG21	0.71	1.62	8	1
1:A:82:GLY:O	1:A:83:GLU:C	0.71	2.33	4	3
1:A:42:VAL:HG12	1:B:1:MET:CG	0.71	2.15	18	1
1:A:19:VAL:HG11	1:B:19:VAL:CG1	0.71	2.14	2	22
1:B:47:PHE:O	1:B:82:GLY:N	0.71	2.23	6	8
1:A:7:ILE:HG13	1:A:25:LEU:HD12	0.71	1.62	15	3
1:A:14:THR:HG22	1:B:20:SER:CB	0.71	2.15	20	3
1:A:19:VAL:HB	1:B:19:VAL:HB	0.71	1.60	2	22
1:A:47:PHE:CE2	1:B:32:ILE:HG21	0.71	2.21	4	5
1:B:83:GLU:O	1:B:86:LYS:N	0.71	2.24	6	6
1:A:31:ILE:O	1:A:34:GLU:HG3	0.71	1.84	15	1
1:B:83:GLU:O	1:B:84:SER:C	0.71	2.34	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:THR:O	1:B:7:ILE:HG13	0.71	1.86	21	9
1:A:1:MET:HB3	1:B:42:VAL:HG22	0.71	1.61	11	2
1:B:32:ILE:O	1:B:36:VAL:HG22	0.71	1.85	22	1
1:A:54:ALA:HA	1:A:75:VAL:HA	0.71	1.62	14	8
1:B:85:LEU:HD13	1:B:85:LEU:H	0.71	1.45	18	2
1:A:6:LEU:HD11	1:B:42:VAL:CG2	0.71	2.15	20	2
1:A:53:VAL:O	1:A:76:GLY:N	0.71	2.23	3	18
1:A:93:LYS:O	1:A:93:LYS:CG	0.71	2.37	19	2
1:A:14:THR:CG2	1:B:20:SER:HB2	0.70	2.16	5	11
1:A:10:ILE:C	1:A:14:THR:HG1	0.70	1.91	20	4
1:B:28:PHE:O	1:B:32:ILE:CG1	0.70	2.39	19	22
1:A:48:LEU:HD13	1:B:48:LEU:CD1	0.70	2.16	22	3
1:B:6:LEU:O	1:B:9:ALA:HB3	0.70	1.85	22	21
1:A:42:VAL:HG21	1:B:6:LEU:HD11	0.70	1.62	16	1
1:B:16:LEU:HD12	1:B:17:THR:N	0.70	2.01	19	1
1:A:42:VAL:CG2	1:B:6:LEU:HD21	0.70	2.16	5	1
1:A:50:ILE:HA	1:A:79:VAL:CB	0.70	2.16	9	3
1:A:77:VAL:HG13	1:A:77:VAL:O	0.70	1.86	15	8
1:A:85:LEU:HD23	1:B:33:THR:HA	0.70	1.62	12	6
1:A:92:LEU:HD12	1:A:93:LYS:HB2	0.70	1.61	11	2
1:A:19:VAL:CG2	1:B:14:THR:HG21	0.70	2.17	19	1
1:A:50:ILE:HD13	1:A:79:VAL:HB	0.70	1.63	22	2
1:B:3:LYS:HD3	1:B:25:LEU:HD11	0.70	1.62	9	2
1:A:77:VAL:HG12	1:A:79:VAL:CG1	0.70	2.16	19	2
1:A:77:VAL:HG12	1:A:77:VAL:O	0.70	1.86	4	1
1:A:89:ALA:HB1	1:B:75:VAL:CG2	0.70	2.17	11	1
1:A:31:ILE:HA	1:A:34:GLU:HG2	0.69	1.64	15	2
1:A:36:VAL:O	1:A:52:PRO:HG3	0.69	1.87	1	3
1:A:88:ALA:O	1:B:37:ALA:CB	0.69	2.41	4	8
1:A:92:LEU:CG	1:B:36:VAL:O	0.69	2.40	4	1
1:B:42:VAL:HG12	1:B:50:ILE:HG22	0.69	1.63	20	1
1:A:44:LEU:HD12	1:A:48:LEU:HD12	0.69	1.64	1	2
1:A:77:VAL:HG21	1:B:85:LEU:HD13	0.69	1.65	20	4
1:A:92:LEU:HD12	1:B:38:LYS:N	0.69	2.01	17	2
1:A:4:THR:O	1:A:7:ILE:HG13	0.69	1.87	18	13
1:A:28:PHE:CZ	1:B:44:LEU:HD22	0.69	2.23	17	3
1:A:44:LEU:CD1	1:A:48:LEU:HD12	0.69	2.17	1	4
1:B:16:LEU:HD12	1:B:16:LEU:N	0.69	2.02	8	7
1:B:10:ILE:O	1:B:14:THR:HG23	0.69	1.88	9	5
1:B:85:LEU:HD23	1:B:85:LEU:O	0.69	1.86	7	1
1:B:80:LYS:H	1:B:81:PRO:HD2	0.69	1.45	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD11	1:B:20:SER:OG	0.69	1.88	20	3
1:B:34:GLU:O	1:B:38:LYS:HB2	0.69	1.88	2	15
1:B:7:ILE:HG22	1:B:25:LEU:HD23	0.69	1.63	19	1
1:A:36:VAL:HG11	1:A:77:VAL:CG2	0.69	2.18	17	4
1:B:7:ILE:HA	1:B:25:LEU:HD12	0.69	1.63	21	2
1:A:92:LEU:HD12	1:A:92:LEU:C	0.69	2.13	1	6
1:B:14:THR:C	1:B:16:LEU:HD12	0.69	2.13	10	14
1:A:75:VAL:HG12	1:B:89:ALA:HB2	0.69	1.65	10	4
1:A:85:LEU:HD13	1:B:77:VAL:HG11	0.69	1.64	7	2
1:B:36:VAL:HG11	1:B:77:VAL:HG23	0.69	1.63	3	3
1:B:50:ILE:HG23	1:B:79:VAL:HG12	0.69	1.63	12	1
1:A:35:THR:HG21	1:B:1:MET:SD	0.69	2.28	21	3
1:A:6:LEU:O	1:A:9:ALA:HB3	0.69	1.88	13	23
1:A:42:VAL:HG22	1:B:1:MET:CB	0.69	2.16	9	1
1:A:3:LYS:O	1:A:25:LEU:HD12	0.69	1.88	15	1
1:A:85:LEU:HD22	1:B:33:THR:HA	0.69	1.63	19	1
1:A:29:GLU:O	1:A:33:THR:HB	0.68	1.87	4	8
1:B:44:LEU:N	1:B:48:LEU:O	0.68	2.25	6	3
1:A:17:THR:HG21	1:B:17:THR:CG2	0.68	2.19	15	17
1:A:38:LYS:N	1:B:92:LEU:HD12	0.68	2.03	7	3
1:B:36:VAL:HG13	1:B:52:PRO:HB3	0.68	1.63	5	8
1:A:33:THR:HA	1:B:85:LEU:HD13	0.68	1.64	4	1
1:B:48:LEU:HD22	1:B:80:LYS:HB3	0.68	1.63	20	3
1:A:29:GLU:HG2	1:B:45:THR:HG22	0.68	1.65	8	6
1:A:77:VAL:HG21	1:B:85:LEU:HB3	0.68	1.64	3	7
1:A:17:THR:HG21	1:B:17:THR:HG21	0.68	1.66	13	14
1:A:50:ILE:HG22	1:A:79:VAL:HG12	0.68	1.66	23	1
1:A:20:SER:HB2	1:B:14:THR:CG2	0.68	2.18	8	7
1:A:49:ASN:O	1:A:79:VAL:HA	0.68	1.88	2	5
1:A:49:ASN:O	1:A:79:VAL:HB	0.68	1.89	19	3
1:A:36:VAL:HG22	1:A:52:PRO:HB3	0.68	1.63	16	2
1:A:28:PHE:HA	1:A:31:ILE:CG1	0.68	2.18	4	23
1:B:28:PHE:HA	1:B:31:ILE:CG1	0.68	2.19	21	22
1:A:47:PHE:CD1	1:B:29:GLU:HG3	0.68	2.23	1	5
1:B:27:SER:O	1:B:31:ILE:HG23	0.68	1.88	23	7
1:A:7:ILE:HG21	1:A:25:LEU:CD2	0.68	2.18	19	3
1:B:27:SER:O	1:B:31:ILE:N	0.68	2.27	9	21
1:A:92:LEU:HD12	1:B:37:ALA:C	0.68	2.13	20	2
1:A:34:GLU:O	1:A:38:LYS:N	0.68	2.27	21	18
1:B:7:ILE:HG22	1:B:25:LEU:HD22	0.68	1.66	6	1
1:A:35:THR:HG22	1:A:40:ASP:HB2	0.68	1.64	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:50:ILE:CG1	1:B:79:VAL:HG22	0.68	2.19	13	1
1:A:37:ALA:O	1:B:92:LEU:HB2	0.67	1.89	7	3
1:B:44:LEU:O	1:B:46:GLY:N	0.67	2.27	8	21
1:B:48:LEU:CD1	1:B:80:LYS:HG2	0.67	2.11	20	1
1:A:48:LEU:HD11	1:B:50:ILE:CD1	0.67	2.19	23	1
1:A:14:THR:CG2	1:A:16:LEU:CD1	0.67	2.70	19	10
1:A:77:VAL:HG12	1:A:79:VAL:HG12	0.67	1.66	8	2
1:A:77:VAL:HG21	1:B:85:LEU:HB2	0.67	1.65	13	5
1:B:14:THR:HG22	1:B:16:LEU:HD21	0.67	1.66	22	7
1:B:93:LYS:O	1:B:93:LYS:CG	0.67	2.43	5	1
1:B:7:ILE:HG22	1:B:25:LEU:CD2	0.67	2.19	6	2
1:A:83:GLU:O	1:A:84:SER:C	0.67	2.37	19	6
1:A:35:THR:HG21	1:A:42:VAL:CG1	0.67	2.19	15	2
1:B:7:ILE:HG12	1:B:21:VAL:O	0.67	1.89	17	10
1:A:92:LEU:HB3	1:B:37:ALA:HA	0.67	1.65	9	10
1:A:50:ILE:HA	1:A:79:VAL:HB	0.67	1.66	9	3
1:B:25:LEU:C	1:B:25:LEU:CD1	0.67	2.62	20	5
1:B:42:VAL:HG22	1:B:50:ILE:HG22	0.67	1.67	23	1
1:A:21:VAL:HA	1:A:24:MET:CE	0.67	2.17	17	18
1:A:37:ALA:CB	1:B:88:ALA:C	0.67	2.68	18	11
1:B:11:ALA:HB2	1:B:21:VAL:CG1	0.67	2.20	22	3
1:B:85:LEU:C	1:B:85:LEU:CD1	0.67	2.66	23	1
1:A:32:ILE:O	1:A:36:VAL:HG22	0.67	1.90	23	2
1:A:35:THR:HG22	1:A:40:ASP:CA	0.67	2.20	19	2
1:A:47:PHE:CZ	1:B:32:ILE:HG21	0.67	2.25	22	14
1:A:24:MET:HB3	1:B:10:ILE:HG23	0.67	1.66	2	8
1:A:85:LEU:HB3	1:B:77:VAL:HG11	0.67	1.65	5	2
1:A:42:VAL:HG11	1:B:6:LEU:HD11	0.67	1.66	9	3
1:A:3:LYS:HA	1:A:25:LEU:HD11	0.67	1.66	11	1
1:A:42:VAL:HG12	1:B:1:MET:SD	0.67	2.30	18	1
1:A:20:SER:C	1:A:22:SER:N	0.66	2.53	13	23
1:B:50:ILE:HD12	1:B:79:VAL:HG12	0.66	1.66	12	2
1:B:42:VAL:HG23	1:B:50:ILE:HB	0.66	1.65	8	1
1:B:85:LEU:HD12	1:B:85:LEU:H	0.66	1.46	10	2
1:A:1:MET:HE2	1:A:6:LEU:HG	0.66	1.66	21	2
1:A:92:LEU:HB3	1:B:37:ALA:O	0.66	1.90	2	13
1:A:92:LEU:HD23	1:B:37:ALA:O	0.66	1.90	3	2
1:A:85:LEU:HB3	1:A:88:ALA:CB	0.66	2.21	4	1
1:B:35:THR:HG21	1:B:42:VAL:CG2	0.66	2.20	11	4
1:B:35:THR:HG22	1:B:40:ASP:HB2	0.66	1.65	13	1
1:A:7:ILE:N	1:A:25:LEU:HD12	0.66	2.06	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:HG21	1:A:50:ILE:HG22	0.66	1.68	1	2
1:A:25:LEU:C	1:A:25:LEU:CD1	0.66	2.59	20	6
1:A:85:LEU:HD22	1:B:36:VAL:CG1	0.66	2.21	14	1
1:B:42:VAL:HG22	1:B:50:ILE:HG12	0.66	1.66	21	1
1:B:3:LYS:HB3	1:B:25:LEU:HD13	0.66	1.66	23	1
1:B:36:VAL:HG22	1:B:52:PRO:CD	0.66	2.20	11	5
1:A:7:ILE:HA	1:A:25:LEU:HD12	0.66	1.67	22	6
1:B:36:VAL:CG2	1:B:42:VAL:HG12	0.66	2.20	6	1
1:A:19:VAL:HG13	1:A:20:SER:H	0.66	1.49	23	13
1:A:14:THR:HG21	1:B:19:VAL:CG2	0.66	2.21	9	5
1:A:14:THR:HG22	1:A:16:LEU:HD21	0.66	1.66	9	6
1:A:50:ILE:N	1:A:79:VAL:HG23	0.66	2.06	20	1
1:A:10:ILE:O	1:A:14:THR:CB	0.66	2.44	11	23
1:A:16:LEU:HD11	1:B:20:SER:CB	0.66	2.20	20	4
1:A:16:LEU:HD21	1:B:20:SER:CB	0.66	2.21	13	4
1:A:77:VAL:HG11	1:B:85:LEU:HD12	0.66	1.66	20	1
1:B:48:LEU:HD22	1:B:80:LYS:CG	0.66	2.21	20	1
1:A:86:LYS:O	1:A:89:ALA:HB3	0.66	1.91	15	11
1:A:81:PRO:HB2	1:B:77:VAL:HG11	0.66	1.68	2	1
1:A:85:LEU:N	1:A:85:LEU:HD13	0.66	2.05	2	2
1:A:35:THR:HG22	1:A:40:ASP:O	0.66	1.90	21	3
1:B:50:ILE:HD13	1:B:79:VAL:HG21	0.66	1.66	1	1
1:B:20:SER:C	1:B:22:SER:N	0.65	2.53	18	23
1:A:89:ALA:N	1:B:37:ALA:CB	0.65	2.52	14	3
1:A:16:LEU:HD13	1:B:19:VAL:HG22	0.65	1.67	3	11
1:A:88:ALA:HB1	1:B:36:VAL:HB	0.65	1.65	4	2
1:A:29:GLU:HG3	1:B:47:PHE:CD2	0.65	2.26	21	6
1:A:48:LEU:CD1	1:B:48:LEU:HD13	0.65	2.21	22	3
1:A:31:ILE:CD1	1:B:6:LEU:HD23	0.65	2.20	23	5
1:A:1:MET:SD	1:B:35:THR:HG21	0.65	2.31	2	4
1:A:36:VAL:HG21	1:A:77:VAL:HG13	0.65	1.66	17	1
1:A:81:PRO:HB3	1:B:77:VAL:HG12	0.65	1.67	20	1
1:A:47:PHE:HA	1:A:82:GLY:HA2	0.65	1.66	11	2
1:B:14:THR:CG2	1:B:16:LEU:CD1	0.65	2.72	3	7
1:B:16:LEU:HD12	1:B:16:LEU:H	0.65	1.52	6	10
1:A:45:THR:HG22	1:B:29:GLU:HG2	0.65	1.68	11	6
1:A:77:VAL:CG2	1:B:85:LEU:HD21	0.65	2.21	18	2
1:A:7:ILE:HD11	1:A:21:VAL:C	0.65	2.16	17	1
1:A:33:THR:OG1	1:B:85:LEU:HB2	0.65	1.92	23	1
1:A:32:ILE:HG21	1:B:47:PHE:CZ	0.65	2.27	2	16
1:B:49:ASN:O	1:B:50:ILE:HD13	0.65	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD12	1:A:47:PHE:CE1	0.65	2.26	8	8
1:A:75:VAL:HG13	1:A:77:VAL:HG23	0.65	1.66	6	1
1:A:85:LEU:H	1:A:85:LEU:HD23	0.65	1.51	9	1
1:A:25:LEU:HG	1:A:26:ALA:N	0.65	2.06	19	5
1:A:47:PHE:HD1	1:A:85:LEU:HD11	0.65	1.52	13	1
1:B:7:ILE:N	1:B:25:LEU:HD12	0.65	2.07	14	4
1:B:36:VAL:HG13	1:B:52:PRO:HG3	0.65	1.68	2	4
1:A:28:PHE:CE1	1:B:44:LEU:HD22	0.65	2.27	3	11
1:A:88:ALA:CB	1:B:33:THR:O	0.65	2.44	4	3
1:B:84:SER:O	1:B:86:LYS:CA	0.65	2.44	4	6
1:B:47:PHE:O	1:B:48:LEU:HD22	0.65	1.91	6	1
1:A:47:PHE:HD2	1:A:48:LEU:HD23	0.65	1.50	17	2
1:A:50:ILE:HD13	1:A:79:VAL:HG23	0.65	1.68	4	4
1:A:88:ALA:C	1:B:37:ALA:CB	0.65	2.70	15	17
1:B:10:ILE:O	1:B:14:THR:CB	0.65	2.44	3	22
1:A:84:SER:O	1:A:86:LYS:CA	0.65	2.45	4	3
1:A:16:LEU:N	1:A:16:LEU:HD12	0.65	2.07	5	2
1:A:75:VAL:HG23	1:B:94:TYR:CD1	0.65	2.27	19	1
1:B:19:VAL:HG13	1:B:20:SER:H	0.65	1.52	1	11
1:A:93:LYS:CG	1:A:93:LYS:O	0.65	2.45	7	4
1:A:6:LEU:HD11	1:B:42:VAL:HG22	0.65	1.68	20	1
1:A:88:ALA:C	1:B:37:ALA:HB2	0.64	2.17	11	8
1:A:16:LEU:H	1:A:16:LEU:HD12	0.64	1.51	3	12
1:A:24:MET:O	1:B:10:ILE:HD11	0.64	1.91	7	2
1:A:85:LEU:HB2	1:B:77:VAL:HG11	0.64	1.69	20	4
1:A:2:ASN:O	1:A:6:LEU:HD12	0.64	1.91	5	5
1:A:75:VAL:HB	1:B:94:TYR:CG	0.64	2.27	14	1
1:A:7:ILE:HG21	1:A:25:LEU:HD22	0.64	1.69	19	2
1:B:36:VAL:HG21	1:B:77:VAL:CG2	0.64	2.14	21	1
1:A:35:THR:HG23	1:A:40:ASP:HB2	0.64	1.68	9	16
1:B:29:GLU:O	1:B:33:THR:HB	0.64	1.93	2	10
1:B:47:PHE:CE2	1:B:48:LEU:HG	0.64	2.28	8	4
1:A:54:ALA:HA	1:A:75:VAL:N	0.64	2.08	5	3
1:B:80:LYS:HB2	1:B:81:PRO:HD2	0.64	1.67	2	6
1:A:75:VAL:CB	1:B:89:ALA:HB1	0.64	2.22	15	4
1:B:47:PHE:O	1:B:85:LEU:HD11	0.64	1.91	13	1
1:B:15:GLY:O	1:B:16:LEU:C	0.64	2.41	20	7
1:A:13:ASP:OD2	1:B:31:ILE:HG21	0.64	1.92	14	4
1:B:14:THR:CA	1:B:16:LEU:HD12	0.64	2.22	10	8
1:A:54:ALA:CA	1:A:75:VAL:HA	0.64	2.23	14	4
1:B:33:THR:O	1:B:36:VAL:HG23	0.64	1.93	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:44:LEU:HD12	1:B:47:PHE:CE1	0.64	2.28	4	6
1:A:35:THR:HG23	1:A:40:ASP:HB3	0.64	1.68	6	10
1:A:6:LEU:HD23	1:B:31:ILE:CD1	0.64	2.23	6	4
1:A:34:GLU:O	1:A:37:ALA:HB3	0.64	1.91	14	1
1:B:44:LEU:HD13	1:B:47:PHE:CE1	0.64	2.27	23	1
1:A:44:LEU:HD22	1:B:28:PHE:CZ	0.64	2.27	15	4
1:A:20:SER:HB3	1:B:16:LEU:CD1	0.64	2.22	2	3
1:B:47:PHE:O	1:B:82:GLY:CA	0.64	2.46	6	1
1:B:4:THR:O	1:B:7:ILE:CG1	0.64	2.46	14	9
1:B:82:GLY:O	1:B:83:GLU:C	0.64	2.41	6	1
1:B:7:ILE:HD11	1:B:21:VAL:O	0.64	1.92	20	3
1:A:84:SER:HB3	1:A:86:LYS:HB2	0.63	1.70	17	3
1:A:92:LEU:CD2	1:B:36:VAL:O	0.63	2.47	4	1
1:A:84:SER:O	1:B:77:VAL:HG21	0.63	1.93	9	1
1:A:28:PHE:CE1	1:A:32:ILE:HG13	0.63	2.28	18	7
1:B:92:LEU:HD23	1:B:92:LEU:N	0.63	2.05	13	2
1:B:50:ILE:CD1	1:B:79:VAL:HG12	0.63	2.24	12	2
1:B:49:ASN:C	1:B:79:VAL:HG23	0.63	2.19	1	1
1:A:4:THR:O	1:A:7:ILE:CG1	0.63	2.47	4	13
1:B:94:TYR:CE1	1:B:96:ASP:OD1	0.63	2.51	5	1
1:A:20:SER:HB3	1:A:23:LYS:CB	0.63	2.23	22	9
1:B:28:PHE:CE2	1:B:32:ILE:HD11	0.63	2.27	13	12
1:A:82:GLY:O	1:A:85:LEU:HD12	0.63	1.94	20	3
1:A:24:MET:HE3	1:A:25:LEU:N	0.63	2.09	11	1
1:A:42:VAL:HG23	1:A:50:ILE:HB	0.63	1.70	15	2
1:B:78:SER:O	1:B:79:VAL:CG1	0.63	2.46	12	1
1:A:85:LEU:HD21	1:B:36:VAL:HG21	0.63	1.69	11	1
1:B:88:ALA:O	1:B:92:LEU:HG	0.63	1.94	1	3
1:A:85:LEU:HB2	1:B:77:VAL:HG21	0.63	1.70	3	6
1:A:28:PHE:CZ	1:B:44:LEU:HD13	0.63	2.29	14	6
1:A:37:ALA:CB	1:B:88:ALA:HB1	0.63	2.24	18	6
1:A:77:VAL:HG11	1:B:81:PRO:CB	0.63	2.24	8	1
1:B:47:PHE:C	1:B:82:GLY:HA3	0.63	2.18	23	1
1:B:7:ILE:HG22	1:B:8:LYS:N	0.63	2.08	15	11
1:B:53:VAL:O	1:B:76:GLY:N	0.63	2.32	16	20
1:A:88:ALA:HA	1:B:37:ALA:HB2	0.63	1.70	4	1
1:A:75:VAL:CG1	1:B:89:ALA:HB3	0.63	2.11	7	2
1:A:49:ASN:O	1:A:79:VAL:CB	0.63	2.46	19	3
1:A:25:LEU:HD12	1:A:25:LEU:O	0.63	1.93	11	2
1:B:35:THR:HG22	1:B:40:ASP:CA	0.63	2.24	13	1
1:A:77:VAL:HG11	1:B:85:LEU:CB	0.63	2.24	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:7:ILE:HG22	1:B:25:LEU:HD12	0.63	1.71	12	3
1:B:76:GLY:O	1:B:78:SER:N	0.63	2.31	4	17
1:B:14:THR:HG22	1:B:16:LEU:CG	0.63	2.24	19	3
1:B:10:ILE:HG22	1:B:21:VAL:HG12	0.63	1.71	19	3
1:A:50:ILE:N	1:A:50:ILE:HD13	0.63	2.08	21	2
1:A:53:VAL:HG22	1:A:76:GLY:HA3	0.63	1.70	23	1
1:A:27:SER:O	1:A:31:ILE:N	0.62	2.31	9	21
1:A:94:TYR:CD1	1:B:75:VAL:N	0.62	2.67	9	12
1:A:42:VAL:HG12	1:B:1:MET:HB2	0.62	1.71	22	2
1:A:28:PHE:CE2	1:A:32:ILE:HD11	0.62	2.30	6	11
1:A:48:LEU:HD22	1:A:82:GLY:CA	0.62	2.24	4	1
1:B:49:ASN:N	1:B:81:PRO:HG2	0.62	2.09	6	1
1:A:85:LEU:O	1:A:88:ALA:HB3	0.62	1.94	4	3
1:A:89:ALA:HB2	1:B:75:VAL:HG12	0.62	1.70	4	2
1:B:47:PHE:O	1:B:81:PRO:HA	0.62	1.95	10	13
1:A:75:VAL:CG1	1:A:77:VAL:HG23	0.62	2.24	6	1
1:A:94:TYR:CD1	1:B:75:VAL:O	0.62	2.52	1	1
1:A:78:SER:C	1:A:79:VAL:HG12	0.62	2.20	7	5
1:A:42:VAL:HB	1:B:6:LEU:HD11	0.62	1.71	15	2
1:A:7:ILE:HD11	1:A:25:LEU:HD23	0.62	1.69	20	1
1:B:42:VAL:HG22	1:B:50:ILE:CG2	0.62	2.25	23	1
1:B:28:PHE:O	1:B:32:ILE:HG12	0.62	1.94	22	10
1:B:94:TYR:O	1:B:97:PHE:N	0.62	2.30	5	1
1:A:7:ILE:HG22	1:A:8:LYS:HE3	0.62	1.69	9	1
1:A:40:ASP:OD1	1:A:50:ILE:HG22	0.62	1.94	19	1
1:B:28:PHE:HA	1:B:31:ILE:HG12	0.62	1.70	23	6
1:B:21:VAL:HA	1:B:24:MET:CE	0.62	2.25	20	14
1:B:47:PHE:CD1	1:B:85:LEU:HD12	0.62	2.29	11	1
1:A:78:SER:O	1:A:79:VAL:CG2	0.62	2.47	14	3
1:A:54:ALA:HB2	1:B:97:PHE:HB3	0.62	1.72	23	5
1:A:14:THR:C	1:A:16:LEU:HD12	0.62	2.19	2	10
1:A:36:VAL:HG11	1:B:85:LEU:HD22	0.62	1.72	5	2
1:B:78:SER:C	1:B:79:VAL:CG1	0.62	2.72	17	4
1:B:49:ASN:O	1:B:79:VAL:HB	0.62	1.95	2	4
1:B:20:SER:CB	1:B:23:LYS:HG2	0.62	2.24	2	1
1:B:28:PHE:CE1	1:B:29:GLU:HG3	0.62	2.29	14	1
1:A:92:LEU:HD12	1:A:93:LYS:HB3	0.61	1.71	3	1
1:B:85:LEU:N	1:B:85:LEU:CD1	0.61	2.63	10	3
1:B:28:PHE:O	1:B:32:ILE:HD13	0.61	1.95	12	1
1:B:42:VAL:HB	1:B:50:ILE:CG1	0.61	2.25	19	1
1:A:47:PHE:O	1:A:82:GLY:N	0.61	2.33	4	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:VAL:HG11	1:B:81:PRO:HD3	0.61	1.71	11	3
1:A:33:THR:OG1	1:B:85:LEU:HD22	0.61	1.95	2	2
1:A:85:LEU:CD1	1:B:36:VAL:HG21	0.61	2.25	4	1
1:B:28:PHE:CD1	1:B:29:GLU:N	0.61	2.68	18	7
1:A:10:ILE:HD11	1:B:28:PHE:N	0.61	2.10	21	2
1:A:94:TYR:CD2	1:B:75:VAL:HB	0.61	2.30	10	1
1:A:3:LYS:O	1:A:25:LEU:HD13	0.61	1.95	17	1
1:A:75:VAL:H	1:B:89:ALA:HB1	0.61	1.55	2	1
1:A:83:GLU:C	1:A:85:LEU:N	0.61	2.58	17	6
1:B:77:VAL:HG22	1:B:77:VAL:O	0.61	1.94	14	7
1:A:53:VAL:HG22	1:A:76:GLY:CA	0.61	2.25	23	1
1:B:10:ILE:O	1:B:14:THR:CG2	0.61	2.48	9	5
1:B:75:VAL:CG1	1:B:77:VAL:HG23	0.61	2.24	9	2
1:A:4:THR:O	1:A:7:ILE:HG12	0.61	1.96	13	2
1:A:7:ILE:HG13	1:A:8:LYS:N	0.61	2.10	4	13
1:A:29:GLU:HG2	1:B:47:PHE:CE1	0.61	2.30	3	2
1:A:36:VAL:HG22	1:A:52:PRO:HD3	0.61	1.71	5	4
1:A:50:ILE:HD13	1:A:79:VAL:HG21	0.61	1.70	19	2
1:A:24:MET:HG2	1:B:14:THR:HG22	0.61	1.72	9	4
1:A:31:ILE:O	1:A:35:THR:N	0.61	2.29	4	11
1:A:77:VAL:HG21	1:B:84:SER:C	0.61	2.20	6	1
1:A:36:VAL:HG22	1:A:52:PRO:CD	0.61	2.25	8	2
1:A:7:ILE:HG22	1:A:25:LEU:CD2	0.61	2.26	11	1
1:B:11:ALA:CB	1:B:21:VAL:HG11	0.61	2.26	14	3
1:A:14:THR:HG22	1:B:20:SER:HB3	0.61	1.72	2	3
1:A:77:VAL:HG21	1:B:85:LEU:CD2	0.61	2.26	14	2
1:A:28:PHE:HE2	1:B:44:LEU:HD22	0.61	1.56	4	7
1:A:20:SER:HB2	1:A:23:LYS:HB2	0.61	1.73	12	6
1:B:4:THR:O	1:B:7:ILE:HB	0.61	1.96	22	12
1:A:16:LEU:HD21	1:B:20:SER:OG	0.61	1.95	20	3
1:B:44:LEU:HB3	1:B:47:PHE:CE2	0.61	2.31	9	2
1:A:7:ILE:HG22	1:A:8:LYS:N	0.61	2.11	7	6
1:A:44:LEU:HD22	1:B:28:PHE:HE1	0.61	1.56	7	5
1:A:35:THR:CG2	1:A:42:VAL:HG23	0.61	2.25	17	2
1:A:21:VAL:CA	1:A:24:MET:HE2	0.61	2.25	17	1
1:A:7:ILE:HG12	1:A:21:VAL:O	0.61	1.96	1	5
1:A:79:VAL:HG11	1:B:81:PRO:CD	0.61	2.26	11	2
1:A:89:ALA:CB	1:B:75:VAL:CG1	0.61	2.79	15	8
1:B:77:VAL:O	1:B:78:SER:O	0.61	2.19	9	3
1:A:7:ILE:CG2	1:A:25:LEU:HD23	0.61	2.25	11	1
1:A:36:VAL:CG1	1:A:77:VAL:HG22	0.61	2.26	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:27:SER:O	1:B:31:ILE:CG1	0.60	2.48	6	15
1:B:24:MET:HE3	1:B:25:LEU:HD23	0.60	1.72	17	10
1:B:20:SER:HB2	1:B:23:LYS:HB2	0.60	1.73	7	3
1:A:11:ALA:HB2	1:A:21:VAL:HG11	0.60	1.71	4	4
1:B:1:MET:HE2	1:B:6:LEU:HG	0.60	1.73	3	5
1:A:44:LEU:HD13	1:B:28:PHE:CZ	0.60	2.30	22	7
1:B:50:ILE:N	1:B:50:ILE:CD1	0.60	2.63	13	2
1:A:31:ILE:HA	1:A:34:GLU:HG3	0.60	1.73	9	1
1:A:48:LEU:CG	1:B:48:LEU:HD11	0.60	2.26	9	1
1:A:77:VAL:HG12	1:B:84:SER:C	0.60	2.21	15	1
1:A:77:VAL:HG21	1:B:84:SER:O	0.60	1.97	10	1
1:A:79:VAL:CG2	1:A:80:LYS:N	0.60	2.64	9	14
1:A:32:ILE:HG21	1:B:47:PHE:CE2	0.60	2.31	10	4
1:B:80:LYS:CB	1:B:81:PRO:HD3	0.60	2.26	6	1
1:A:86:LYS:HG3	1:B:77:VAL:HG12	0.60	1.74	10	1
1:A:89:ALA:CB	1:B:75:VAL:HG21	0.60	2.24	11	1
1:B:25:LEU:HD23	1:B:28:PHE:CD2	0.60	2.30	21	1
1:A:77:VAL:CG2	1:B:85:LEU:HD12	0.60	2.26	9	1
1:A:77:VAL:CG1	1:B:85:LEU:HD13	0.60	2.20	10	1
1:A:35:THR:HG22	1:A:40:ASP:HA	0.60	1.72	20	2
1:A:28:PHE:CE2	1:A:29:GLU:HG3	0.60	2.31	9	7
1:B:23:LYS:O	1:B:27:SER:CB	0.60	2.50	2	14
1:A:47:PHE:O	1:A:81:PRO:HA	0.60	1.97	13	10
1:A:36:VAL:HG11	1:B:85:LEU:CD2	0.60	2.23	18	2
1:A:81:PRO:CB	1:B:77:VAL:HG12	0.60	2.27	20	1
1:B:53:VAL:HG22	1:B:76:GLY:CA	0.60	2.27	5	3
1:A:31:ILE:O	1:A:35:THR:OG1	0.60	2.20	19	5
1:B:78:SER:O	1:B:79:VAL:CG2	0.60	2.48	13	1
1:A:19:VAL:CG2	1:A:20:SER:N	0.60	2.65	18	15
1:B:50:ILE:HG13	1:B:79:VAL:HG22	0.60	1.72	13	1
1:A:50:ILE:CD1	1:A:50:ILE:N	0.60	2.64	21	3
1:A:92:LEU:O	1:A:93:LYS:CB	0.60	2.50	15	14
1:B:7:ILE:HG13	1:B:8:LYS:N	0.60	2.11	14	9
1:B:7:ILE:HD13	1:B:21:VAL:CG2	0.60	2.27	8	6
1:A:85:LEU:CG	1:B:33:THR:HA	0.60	2.27	17	3
1:B:19:VAL:CG2	1:B:20:SER:N	0.60	2.63	10	16
1:A:85:LEU:CD2	1:B:36:VAL:HG21	0.60	2.24	13	1
1:A:16:LEU:HD13	1:B:19:VAL:C	0.60	2.22	20	1
1:B:31:ILE:O	1:B:35:THR:CB	0.59	2.50	9	17
1:B:50:ILE:HA	1:B:79:VAL:HB	0.59	1.74	1	2
1:B:79:VAL:CG2	1:B:80:LYS:N	0.59	2.65	17	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD11	1:B:50:ILE:HD11	0.59	1.73	3	2
1:A:31:ILE:HD12	1:B:6:LEU:HD23	0.59	1.73	5	1
1:B:92:LEU:O	1:B:93:LYS:CG	0.59	2.50	14	2
1:A:42:VAL:HG12	1:A:42:VAL:O	0.59	1.97	6	1
1:B:16:LEU:HD12	1:B:17:THR:H	0.59	1.57	19	1
1:B:33:THR:HA	1:B:36:VAL:CG2	0.59	2.27	23	2
1:B:1:MET:CE	1:B:6:LEU:HD23	0.59	2.24	11	3
1:B:20:SER:HB3	1:B:23:LYS:CB	0.59	2.27	6	9
1:A:37:ALA:HB2	1:B:88:ALA:C	0.59	2.22	19	11
1:A:94:TYR:CE1	1:B:75:VAL:N	0.59	2.71	6	4
1:A:80:LYS:HB2	1:A:81:PRO:HD3	0.59	1.75	4	1
1:A:47:PHE:CE2	1:B:29:GLU:HG3	0.59	2.32	10	8
1:B:7:ILE:HD11	1:B:21:VAL:C	0.59	2.22	9	1
1:A:20:SER:HB2	1:B:16:LEU:HD21	0.59	1.74	16	1
1:A:94:TYR:CE1	1:B:75:VAL:O	0.59	2.55	1	2
1:A:77:VAL:CG2	1:B:85:LEU:HD13	0.59	2.26	5	4
1:B:36:VAL:HG13	1:B:52:PRO:CB	0.59	2.27	5	4
1:B:21:VAL:O	1:B:25:LEU:HD23	0.59	1.97	18	1
1:A:3:LYS:HD2	1:A:25:LEU:HD13	0.59	1.72	20	1
1:B:28:PHE:CE1	1:B:32:ILE:HG13	0.59	2.32	3	6
1:B:7:ILE:CG2	1:B:25:LEU:CD2	0.59	2.80	6	2
1:B:85:LEU:N	1:B:85:LEU:HD22	0.59	2.12	6	1
1:A:80:LYS:CB	1:A:81:PRO:CD	0.59	2.80	4	4
1:B:20:SER:OG	1:B:23:LYS:CB	0.59	2.51	15	9
1:A:19:VAL:HG22	1:B:16:LEU:HD13	0.59	1.72	3	12
1:A:85:LEU:O	1:A:88:ALA:N	0.59	2.35	13	5
1:A:33:THR:HA	1:B:85:LEU:HG	0.59	1.73	18	3
1:A:75:VAL:CB	1:B:94:TYR:CD2	0.59	2.83	5	2
1:A:14:THR:HG21	1:B:24:MET:HG3	0.59	1.74	7	1
1:A:25:LEU:HA	1:A:28:PHE:HB3	0.59	1.74	9	17
1:B:80:LYS:N	1:B:81:PRO:HD2	0.59	2.13	20	3
1:B:4:THR:O	1:B:7:ILE:HG23	0.59	1.97	18	3
1:A:84:SER:CB	1:A:86:LYS:HB2	0.59	2.28	17	4
1:A:29:GLU:O	1:A:33:THR:CB	0.59	2.50	4	2
1:B:47:PHE:CE1	1:B:48:LEU:HG	0.59	2.33	9	9
1:A:42:VAL:HG13	1:B:1:MET:HB3	0.59	1.73	9	1
1:A:50:ILE:CD1	1:A:79:VAL:HG13	0.59	2.28	16	1
1:A:92:LEU:HD12	1:B:38:LYS:CA	0.59	2.27	17	1
1:A:92:LEU:HB2	1:B:37:ALA:O	0.59	1.98	20	2
1:A:15:GLY:O	1:A:16:LEU:C	0.59	2.45	11	3
1:A:20:SER:CB	1:B:14:THR:HG22	0.59	2.24	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:50:ILE:HD12	1:B:79:VAL:CG1	0.59	2.28	12	2
1:B:50:ILE:CD1	1:B:79:VAL:HG22	0.59	2.27	13	1
1:A:77:VAL:HG21	1:B:85:LEU:HG	0.59	1.73	14	4
1:B:85:LEU:O	1:B:88:ALA:HB3	0.59	1.97	2	7
1:A:85:LEU:HD12	1:B:77:VAL:HG23	0.59	1.75	4	1
1:A:88:ALA:CA	1:B:37:ALA:HB2	0.59	2.28	4	2
1:A:25:LEU:HD12	1:A:26:ALA:N	0.59	2.13	13	2
1:A:1:MET:HG3	1:B:42:VAL:HG23	0.59	1.75	22	1
1:A:44:LEU:HD12	1:A:48:LEU:CD1	0.58	2.27	15	3
1:B:83:GLU:C	1:B:85:LEU:N	0.58	2.61	17	9
1:A:7:ILE:HB	1:A:21:VAL:C	0.58	2.23	4	11
1:A:10:ILE:HG22	1:A:21:VAL:HG12	0.58	1.74	23	8
1:A:20:SER:HB3	1:B:14:THR:CG2	0.58	2.28	19	3
1:B:21:VAL:HA	1:B:24:MET:SD	0.58	2.38	16	13
1:A:44:LEU:O	1:A:45:THR:C	0.58	2.44	23	22
1:A:85:LEU:CD2	1:B:77:VAL:HG22	0.58	2.28	1	1
1:A:92:LEU:CB	1:B:37:ALA:O	0.58	2.50	23	12
1:B:42:VAL:HG13	1:B:50:ILE:HB	0.58	1.73	22	2
1:B:28:PHE:CD2	1:B:32:ILE:HD11	0.58	2.33	12	1
1:A:88:ALA:O	1:A:92:LEU:HG	0.58	1.98	17	2
1:B:42:VAL:HG12	1:B:50:ILE:CG2	0.58	2.29	20	1
1:B:31:ILE:O	1:B:35:THR:N	0.58	2.37	9	8
1:B:92:LEU:O	1:B:93:LYS:CB	0.58	2.51	14	4
1:B:47:PHE:O	1:B:82:GLY:HA2	0.58	1.98	6	1
1:B:47:PHE:CD2	1:B:85:LEU:HD21	0.58	2.33	12	1
1:A:1:MET:CB	1:B:42:VAL:HG22	0.58	2.28	11	3
1:B:35:THR:HG23	1:B:40:ASP:HB2	0.58	1.74	11	10
1:B:44:LEU:O	1:B:45:THR:C	0.58	2.46	15	20
1:B:36:VAL:HG23	1:B:42:VAL:CG1	0.58	2.24	6	1
1:A:30:LYS:O	1:A:34:GLU:HG3	0.58	1.97	10	18
1:A:34:GLU:O	1:A:38:LYS:HB2	0.58	1.99	5	7
1:A:54:ALA:HB2	1:B:97:PHE:CB	0.58	2.29	1	1
1:A:7:ILE:HD13	1:A:21:VAL:CG2	0.58	2.27	18	7
1:B:85:LEU:HD22	1:B:85:LEU:N	0.58	2.12	18	1
1:A:17:THR:HG22	1:A:19:VAL:H	0.58	1.58	13	15
1:A:20:SER:OG	1:A:23:LYS:HB2	0.58	1.98	17	8
1:A:24:MET:HE3	1:A:25:LEU:HD23	0.58	1.75	1	5
1:B:3:LYS:O	1:B:7:ILE:CG2	0.58	2.52	10	8
1:B:30:LYS:O	1:B:34:GLU:HG3	0.58	1.94	13	20
1:B:79:VAL:HG22	1:B:80:LYS:N	0.58	2.14	1	10
1:A:88:ALA:O	1:B:37:ALA:HA	0.58	1.98	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:VAL:HG11	1:B:84:SER:HB2	0.58	1.75	18	1
1:A:78:SER:C	1:A:79:VAL:HG22	0.58	2.23	23	1
1:A:28:PHE:CD2	1:A:29:GLU:HG3	0.58	2.34	4	5
1:A:31:ILE:O	1:A:35:THR:CB	0.58	2.52	19	14
1:B:80:LYS:HB3	1:B:81:PRO:HD3	0.58	1.75	6	1
1:B:48:LEU:C	1:B:80:LYS:HD2	0.58	2.24	15	2
1:B:50:ILE:HG23	1:B:79:VAL:HB	0.58	1.74	17	1
1:B:7:ILE:CG2	1:B:25:LEU:HD23	0.58	2.29	19	1
1:B:2:ASN:O	1:B:6:LEU:HD12	0.58	1.99	1	2
1:A:37:ALA:O	1:B:92:LEU:CB	0.58	2.52	16	11
1:A:85:LEU:C	1:A:88:ALA:H	0.58	2.06	4	3
1:A:44:LEU:HD13	1:B:28:PHE:CE2	0.58	2.34	8	1
1:B:49:ASN:C	1:B:80:LYS:HA	0.58	2.24	20	3
1:A:50:ILE:HD12	1:A:79:VAL:CG2	0.58	2.28	16	1
1:A:50:ILE:HG23	1:A:79:VAL:CG2	0.58	2.29	16	1
1:B:75:VAL:HG12	1:B:77:VAL:HG23	0.58	1.74	20	1
1:B:50:ILE:HG13	1:B:79:VAL:HG23	0.58	1.76	23	1
1:A:37:ALA:C	1:B:92:LEU:HD12	0.58	2.24	13	3
1:A:44:LEU:CD1	1:A:48:LEU:HB2	0.58	2.27	1	8
1:B:35:THR:HG22	1:B:40:ASP:O	0.58	1.99	23	6
1:A:14:THR:HB	1:B:19:VAL:CG2	0.58	2.28	2	2
1:A:28:PHE:O	1:A:32:ILE:HG12	0.57	1.99	22	13
1:A:44:LEU:HB3	1:A:47:PHE:CE1	0.57	2.34	17	6
1:A:29:GLU:HG3	1:B:47:PHE:CE2	0.57	2.33	5	7
1:A:37:ALA:HA	1:B:89:ALA:HA	0.57	1.76	13	3
1:A:10:ILE:HD11	1:B:28:PHE:HB2	0.57	1.77	2	1
1:A:42:VAL:HG21	1:B:6:LEU:HD21	0.57	1.74	5	3
1:A:76:GLY:O	1:A:77:VAL:C	0.57	2.46	6	2
1:A:36:VAL:HG13	1:B:88:ALA:HB1	0.57	1.74	20	1
1:A:77:VAL:CG1	1:B:84:SER:OG	0.57	2.52	2	2
1:A:77:VAL:HG11	1:B:85:LEU:CD1	0.57	2.22	10	1
1:A:20:SER:CB	1:B:16:LEU:HD11	0.57	2.29	17	5
1:A:52:PRO:CB	1:A:75:VAL:HG21	0.57	2.29	6	1
1:A:77:VAL:HG12	1:B:84:SER:HA	0.57	1.76	15	1
1:A:94:TYR:HA	1:B:75:VAL:CG2	0.57	2.29	7	1
1:A:77:VAL:HG21	1:B:85:LEU:HD12	0.57	1.76	9	1
1:A:85:LEU:HD23	1:B:33:THR:CA	0.57	2.29	22	2
1:B:3:LYS:HA	1:B:25:LEU:HD11	0.57	1.74	19	1
1:B:77:VAL:O	1:B:77:VAL:HG12	0.57	1.98	19	1
1:B:48:LEU:CB	1:B:80:LYS:HG3	0.57	2.29	20	1
1:A:20:SER:HB3	1:B:14:THR:HG22	0.57	1.76	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:95:GLU:C	1:B:97:PHE:N	0.57	2.61	5	1
1:A:47:PHE:O	1:A:85:LEU:HD11	0.57	1.99	23	1
1:A:20:SER:C	1:A:24:MET:HG3	0.57	2.25	21	16
1:A:14:THR:CG2	1:B:20:SER:OG	0.57	2.53	16	7
1:A:77:VAL:HG23	1:B:85:LEU:HD22	0.57	1.76	7	1
1:A:36:VAL:HG13	1:A:52:PRO:CB	0.57	2.26	18	1
1:A:20:SER:CB	1:A:23:LYS:HB2	0.57	2.29	9	9
1:A:88:ALA:CB	1:B:37:ALA:CB	0.57	2.82	2	4
1:B:85:LEU:CB	1:B:88:ALA:HB3	0.57	2.30	4	5
1:B:28:PHE:CD1	1:B:32:ILE:HG13	0.57	2.34	23	6
1:A:28:PHE:CE1	1:A:32:ILE:CD1	0.57	2.88	9	4
1:A:47:PHE:CE1	1:A:48:LEU:HG	0.57	2.34	12	8
1:A:47:PHE:CD2	1:A:85:LEU:HD21	0.57	2.35	23	1
1:A:92:LEU:HG	1:A:93:LYS:N	0.57	2.15	7	4
1:A:92:LEU:O	1:A:92:LEU:CD1	0.57	2.48	21	8
1:A:92:LEU:N	1:A:92:LEU:CD2	0.57	2.64	17	1
1:A:77:VAL:HG11	1:B:84:SER:C	0.56	2.25	20	2
1:A:28:PHE:CD1	1:A:29:GLU:N	0.56	2.73	13	7
1:A:85:LEU:N	1:A:85:LEU:HD23	0.56	2.14	9	1
1:A:36:VAL:CG2	1:B:85:LEU:HD22	0.56	2.29	10	1
1:B:51:LYS:O	1:B:78:SER:N	0.56	2.38	14	9
1:B:3:LYS:NZ	1:B:25:LEU:O	0.56	2.38	13	2
1:A:75:VAL:CG1	1:B:94:TYR:CD2	0.56	2.88	14	1
1:B:49:ASN:H	1:B:80:LYS:C	0.56	2.07	20	2
1:A:36:VAL:HG21	1:A:77:VAL:CG1	0.56	2.30	17	1
1:B:10:ILE:O	1:B:14:THR:N	0.56	2.38	21	10
1:B:14:THR:HB	1:B:16:LEU:HD12	0.56	1.75	17	7
1:B:50:ILE:N	1:B:79:VAL:HG11	0.56	2.15	19	3
1:A:77:VAL:HG21	1:B:85:LEU:HD22	0.56	1.77	22	3
1:A:7:ILE:HD13	1:A:21:VAL:HG23	0.56	1.76	18	6
1:B:53:VAL:HG22	1:B:76:GLY:HA3	0.56	1.75	5	3
1:A:29:GLU:HG3	1:B:47:PHE:CE1	0.56	2.36	6	3
1:A:7:ILE:HD12	1:A:21:VAL:C	0.56	2.25	16	1
1:B:51:LYS:N	1:B:79:VAL:CG1	0.56	2.69	2	3
1:B:14:THR:CG2	1:B:16:LEU:HD11	0.56	2.30	8	5
1:A:27:SER:O	1:A:31:ILE:HG13	0.56	2.00	21	8
1:A:75:VAL:CG1	1:B:89:ALA:HB2	0.56	2.30	6	1
1:A:7:ILE:CG2	1:A:21:VAL:HB	0.56	2.25	9	1
1:A:77:VAL:HG13	1:B:85:LEU:HD21	0.56	1.77	23	1
1:A:21:VAL:HA	1:A:24:MET:SD	0.56	2.40	18	9
1:A:28:PHE:CE1	1:A:32:ILE:HD11	0.56	2.36	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:VAL:HG22	1:A:80:LYS:N	0.56	2.15	11	14
1:A:28:PHE:CA	1:B:10:ILE:HD11	0.56	2.30	13	3
1:B:44:LEU:CD1	1:B:48:LEU:HD12	0.56	2.30	20	2
1:A:3:LYS:CE	1:A:29:GLU:HB2	0.56	2.30	9	5
1:B:10:ILE:HG21	1:B:24:MET:CE	0.56	2.23	14	2
1:B:7:ILE:CG2	1:B:25:LEU:HD12	0.56	2.31	12	1
1:B:21:VAL:O	1:B:25:LEU:HB3	0.56	2.01	18	1
1:A:19:VAL:CG2	1:B:14:THR:HB	0.56	2.30	2	9
1:A:24:MET:O	1:A:28:PHE:N	0.56	2.38	10	11
1:B:35:THR:O	1:B:38:LYS:N	0.56	2.38	17	9
1:A:86:LYS:HG3	1:B:77:VAL:HG23	0.56	1.78	6	2
1:A:75:VAL:HG11	1:B:89:ALA:HB1	0.56	1.76	8	3
1:B:14:THR:HG22	1:B:16:LEU:HG	0.56	1.76	19	1
1:A:37:ALA:C	1:B:92:LEU:HB3	0.56	2.25	19	11
1:A:75:VAL:N	1:B:89:ALA:HB1	0.56	2.15	2	2
1:A:34:GLU:O	1:A:38:LYS:HG2	0.56	2.01	21	2
1:A:53:VAL:C	1:A:75:VAL:HA	0.56	2.26	15	3
1:A:47:PHE:CD1	1:A:85:LEU:HD23	0.56	2.36	8	1
1:A:92:LEU:HD11	1:B:75:VAL:CG2	0.56	2.31	8	1
1:B:76:GLY:O	1:B:77:VAL:C	0.56	2.47	15	4
1:A:90:GLU:HA	1:A:94:TYR:CD1	0.56	2.35	11	1
1:B:53:VAL:HG13	1:B:78:SER:OG	0.56	2.01	19	1
1:A:6:LEU:HD23	1:B:31:ILE:HD12	0.56	1.78	4	2
1:B:47:PHE:CG	1:B:85:LEU:HD21	0.56	2.35	4	1
1:A:51:LYS:CG	1:A:78:SER:CB	0.56	2.83	6	1
1:A:53:VAL:CG2	1:A:76:GLY:HA3	0.56	2.31	23	2
1:A:88:ALA:HB1	1:B:33:THR:O	0.56	2.01	9	1
1:A:28:PHE:CZ	1:A:32:ILE:HD11	0.56	2.35	15	1
1:A:19:VAL:HG22	1:B:14:THR:HG21	0.56	1.77	19	1
1:A:3:LYS:O	1:A:7:ILE:HG13	0.56	2.01	9	4
1:A:75:VAL:HG12	1:B:94:TYR:CE2	0.56	2.36	14	1
1:A:7:ILE:CD1	1:A:21:VAL:O	0.55	2.54	15	8
1:A:47:PHE:CE1	1:B:32:ILE:CG2	0.55	2.85	12	12
1:A:36:VAL:CG2	1:B:85:LEU:HD21	0.55	2.31	7	1
1:A:17:THR:CG2	1:B:17:THR:HG21	0.55	2.32	12	15
1:A:29:GLU:HG2	1:B:47:PHE:CE2	0.55	2.36	14	6
1:B:85:LEU:C	1:B:88:ALA:H	0.55	2.09	15	8
1:A:85:LEU:HD12	1:A:85:LEU:C	0.55	2.22	6	1
1:B:44:LEU:HB3	1:B:47:PHE:CE1	0.55	2.36	23	5
1:A:33:THR:HA	1:B:85:LEU:HD12	0.55	1.76	8	2
1:A:28:PHE:CB	1:B:10:ILE:HD11	0.55	2.31	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:VAL:O	1:A:77:VAL:HG22	0.55	2.01	5	8
1:A:92:LEU:O	1:A:93:LYS:HB3	0.55	1.99	6	2
1:B:3:LYS:HA	1:B:25:LEU:HD13	0.55	1.76	6	1
1:B:49:ASN:CB	1:B:81:PRO:CG	0.55	2.84	6	1
1:B:50:ILE:N	1:B:50:ILE:HD13	0.55	2.16	13	1
1:A:85:LEU:HD22	1:B:77:VAL:HG21	0.55	1.77	15	2
1:B:47:PHE:CD1	1:B:85:LEU:HD11	0.55	2.36	15	1
1:B:1:MET:HA	1:B:5:GLU:CB	0.55	2.30	8	11
1:B:20:SER:CB	1:B:23:LYS:HB2	0.55	2.31	20	10
1:B:25:LEU:HA	1:B:28:PHE:HB3	0.55	1.78	5	14
1:A:34:GLU:HA	1:A:37:ALA:HB3	0.55	1.79	14	2
1:A:85:LEU:HG	1:B:33:THR:HA	0.55	1.77	17	5
1:A:92:LEU:HB3	1:B:36:VAL:O	0.55	2.01	13	1
1:A:18:GLN:O	1:A:21:VAL:HG22	0.55	2.01	21	1
1:B:42:VAL:HG22	1:B:50:ILE:HG13	0.55	1.77	21	1
1:A:28:PHE:C	1:A:31:ILE:HG13	0.55	2.26	3	22
1:A:37:ALA:CA	1:B:92:LEU:HB3	0.55	2.30	4	12
1:A:28:PHE:CE2	1:A:32:ILE:CD1	0.55	2.90	8	10
1:A:51:LYS:O	1:A:51:LYS:HG3	0.55	2.01	9	7
1:B:92:LEU:O	1:B:92:LEU:CD1	0.55	2.55	10	8
1:B:49:ASN:N	1:B:80:LYS:HA	0.55	2.16	9	2
1:A:16:LEU:CD1	1:B:19:VAL:CG2	0.55	2.76	11	4
1:B:7:ILE:HD11	1:B:25:LEU:HD23	0.55	1.78	20	2
1:A:42:VAL:HG13	1:A:50:ILE:CB	0.55	2.27	8	1
1:A:50:ILE:CA	1:A:79:VAL:HB	0.55	2.31	9	3
1:A:89:ALA:HA	1:B:37:ALA:HA	0.55	1.77	20	3
1:A:50:ILE:N	1:A:50:ILE:HD12	0.55	2.16	15	1
1:B:21:VAL:O	1:B:24:MET:HE2	0.55	2.02	20	3
1:A:77:VAL:HG11	1:B:84:SER:CA	0.55	2.31	18	1
1:B:36:VAL:HG22	1:B:52:PRO:HB3	0.55	1.78	21	1
1:A:92:LEU:N	1:B:37:ALA:HA	0.55	2.17	4	2
1:A:36:VAL:HG21	1:B:85:LEU:HD21	0.55	1.78	7	1
1:A:49:ASN:CB	1:A:81:PRO:CG	0.55	2.85	17	1
1:A:53:VAL:O	1:A:53:VAL:HG23	0.55	2.01	11	18
1:B:28:PHE:CD1	1:B:28:PHE:C	0.55	2.84	23	9
1:A:14:THR:CA	1:A:16:LEU:HD12	0.55	2.32	7	2
1:B:11:ALA:HA	1:B:14:THR:OG1	0.55	2.02	23	9
1:B:25:LEU:CG	1:B:26:ALA:N	0.55	2.70	6	5
1:A:36:VAL:HG13	1:A:52:PRO:HG3	0.55	1.78	9	1
1:A:3:LYS:HE3	1:A:29:GLU:HB2	0.55	1.78	15	1
1:B:50:ILE:HA	1:B:79:VAL:HA	0.55	1.78	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:CD1	1:B:42:VAL:HG13	0.55	2.31	1	1
1:A:92:LEU:C	1:A:92:LEU:CD1	0.55	2.79	6	5
1:B:28:PHE:C	1:B:31:ILE:HG13	0.55	2.27	8	17
1:A:47:PHE:CD1	1:A:48:LEU:HG	0.55	2.36	20	12
1:A:45:THR:CG2	1:A:47:PHE:CE2	0.55	2.89	8	4
1:A:79:VAL:HG12	1:A:80:LYS:N	0.55	2.16	16	3
1:A:92:LEU:HD21	1:B:38:LYS:C	0.55	2.27	14	1
1:A:85:LEU:HB3	1:B:33:THR:OG1	0.55	2.02	19	1
1:B:3:LYS:NZ	1:B:29:GLU:HB2	0.55	2.17	23	1
1:B:51:LYS:N	1:B:79:VAL:HG11	0.54	2.17	2	3
1:A:28:PHE:CD1	1:A:29:GLU:HG3	0.54	2.37	11	3
1:A:77:VAL:HG21	1:B:85:LEU:HD21	0.54	1.77	14	2
1:A:92:LEU:HD12	1:B:37:ALA:HA	0.54	1.78	14	1
1:A:89:ALA:HB2	1:B:75:VAL:HG11	0.54	1.79	15	1
1:B:28:PHE:HA	1:B:31:ILE:HD12	0.54	1.79	18	1
1:A:27:SER:O	1:A:31:ILE:CG1	0.54	2.56	9	16
1:B:47:PHE:CD1	1:B:48:LEU:N	0.54	2.75	3	5
1:B:34:GLU:O	1:B:38:LYS:CB	0.54	2.55	14	4
1:B:77:VAL:O	1:B:77:VAL:CG1	0.54	2.51	17	2
1:B:90:GLU:HA	1:B:94:TYR:CB	0.54	2.32	13	1
1:B:42:VAL:CG2	1:B:50:ILE:HD11	0.54	2.31	14	2
1:A:31:ILE:HA	1:A:34:GLU:CB	0.54	2.32	15	1
1:A:3:LYS:O	1:A:7:ILE:CG2	0.54	2.55	5	14
1:A:75:VAL:CG1	1:B:89:ALA:CB	0.54	2.78	23	7
1:B:24:MET:HE1	1:B:25:LEU:HG	0.54	1.79	5	4
1:A:77:VAL:CG1	1:A:79:VAL:HG12	0.54	2.32	6	1
1:A:24:MET:HB3	1:B:14:THR:HG23	0.54	1.78	14	4
1:B:44:LEU:HD13	1:B:47:PHE:CZ	0.54	2.37	23	4
1:B:47:PHE:HB2	1:B:85:LEU:HD23	0.54	1.79	2	1
1:A:28:PHE:CE2	1:B:44:LEU:HD22	0.54	2.38	23	3
1:A:7:ILE:HG13	1:A:25:LEU:CD1	0.54	2.32	15	2
1:B:35:THR:HG23	1:B:40:ASP:HB3	0.54	1.78	11	5
1:B:7:ILE:CD1	1:B:21:VAL:O	0.54	2.56	23	13
1:A:28:PHE:O	1:A:32:ILE:N	0.54	2.37	8	14
1:B:85:LEU:O	1:B:88:ALA:CA	0.54	2.53	6	2
1:A:75:VAL:N	1:B:94:TYR:CE1	0.54	2.75	9	3
1:A:21:VAL:O	1:A:24:MET:HE2	0.54	2.03	17	2
1:A:33:THR:HA	1:B:85:LEU:CG	0.54	2.32	18	1
1:A:75:VAL:HG22	1:A:76:GLY:H	0.54	1.63	18	1
1:A:92:LEU:CD2	1:B:75:VAL:HG11	0.54	2.33	1	1
1:B:85:LEU:HD23	1:B:85:LEU:H	0.54	1.61	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:THR:HG21	1:B:19:VAL:HG22	0.54	1.79	15	3
1:B:16:LEU:CD1	1:B:16:LEU:N	0.54	2.70	12	5
1:A:20:SER:OG	1:B:14:THR:CG2	0.54	2.56	13	4
1:A:75:VAL:N	1:B:94:TYR:CD1	0.54	2.76	22	9
1:B:83:GLU:O	1:B:87:LYS:N	0.54	2.40	19	4
1:A:77:VAL:HG11	1:B:84:SER:HA	0.54	1.80	18	2
1:B:3:LYS:CE	1:B:29:GLU:HB2	0.54	2.33	23	4
1:A:24:MET:CB	1:B:10:ILE:HG23	0.54	2.32	14	1
1:B:49:ASN:H	1:B:80:LYS:CA	0.54	2.15	20	2
1:A:16:LEU:HD11	1:B:20:SER:HB2	0.54	1.79	2	2
1:A:42:VAL:HB	1:A:50:ILE:CG1	0.54	2.33	10	4
1:A:10:ILE:O	1:A:14:THR:N	0.54	2.37	7	4
1:A:29:GLU:HB3	1:B:45:THR:CG2	0.54	2.32	8	5
1:B:45:THR:HG23	1:B:47:PHE:CD2	0.54	2.37	15	7
1:A:77:VAL:O	1:A:77:VAL:CG1	0.54	2.55	4	2
1:A:16:LEU:CD1	1:A:16:LEU:N	0.54	2.71	5	2
1:A:8:LYS:CE	1:A:8:LYS:N	0.54	2.70	9	1
1:B:48:LEU:HD12	1:B:49:ASN:H	0.54	1.63	23	1
1:A:14:THR:CB	1:A:16:LEU:HD12	0.54	2.33	1	2
1:B:27:SER:O	1:B:31:ILE:HG13	0.54	2.02	17	10
1:B:90:GLU:HA	1:B:94:TYR:HB2	0.54	1.78	14	2
1:B:28:PHE:CE1	1:B:32:ILE:HD11	0.54	2.38	8	3
1:B:47:PHE:O	1:B:81:PRO:C	0.54	2.51	6	1
1:A:75:VAL:HB	1:B:94:TYR:HB2	0.54	1.80	8	5
1:B:50:ILE:N	1:B:80:LYS:HD3	0.54	2.18	20	2
1:B:20:SER:C	1:B:24:MET:HG3	0.54	2.27	1	9
1:B:92:LEU:N	1:B:92:LEU:CD2	0.54	2.70	13	2
1:A:33:THR:HA	1:B:85:LEU:HD22	0.54	1.79	4	1
1:A:84:SER:O	1:A:88:ALA:HB2	0.54	2.03	15	1
1:B:5:GLU:O	1:B:8:LYS:HG3	0.54	2.03	21	2
1:B:7:ILE:CG1	1:B:21:VAL:O	0.53	2.56	9	11
1:B:7:ILE:HD11	1:B:22:SER:HA	0.53	1.80	3	4
1:A:17:THR:HG22	1:A:19:VAL:N	0.53	2.17	17	11
1:B:47:PHE:CD1	1:B:48:LEU:HG	0.53	2.38	5	7
1:A:85:LEU:HD21	1:B:32:ILE:HG22	0.53	1.80	8	1
1:A:19:VAL:CG1	1:B:19:VAL:CG1	0.53	2.85	2	16
1:B:20:SER:OG	1:B:23:LYS:HB2	0.53	2.02	13	4
1:B:49:ASN:C	1:B:79:VAL:HB	0.53	2.28	19	3
1:A:20:SER:HB3	1:A:24:MET:N	0.53	2.18	15	3
1:A:85:LEU:HD13	1:B:36:VAL:HG21	0.53	1.81	4	1
1:A:92:LEU:HD21	1:B:38:LYS:O	0.53	2.03	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:CB	1:A:47:PHE:CE1	0.53	2.91	11	4
1:B:17:THR:HG22	1:B:19:VAL:H	0.53	1.64	4	18
1:A:75:VAL:HG13	1:A:76:GLY:N	0.53	2.18	20	5
1:A:42:VAL:HG23	1:A:50:ILE:CD1	0.53	2.32	9	1
1:A:75:VAL:CG1	1:B:94:TYR:CE2	0.53	2.91	14	1
1:A:7:ILE:CG1	1:A:21:VAL:O	0.53	2.57	17	4
1:A:33:THR:O	1:B:88:ALA:CB	0.53	2.56	6	5
1:A:37:ALA:HB2	1:B:88:ALA:CA	0.53	2.33	6	5
1:B:53:VAL:O	1:B:53:VAL:HG23	0.53	2.03	18	16
1:A:19:VAL:CG2	1:B:16:LEU:CD1	0.53	2.80	4	6
1:B:53:VAL:CG2	1:B:76:GLY:HA3	0.53	2.33	5	3
1:B:78:SER:C	1:B:79:VAL:HG13	0.53	2.28	12	2
1:A:7:ILE:HD11	1:A:21:VAL:O	0.53	2.04	20	3
1:B:78:SER:O	1:B:79:VAL:HG12	0.53	2.03	17	1
1:A:42:VAL:HG22	1:B:6:LEU:HD11	0.53	1.81	23	1
1:A:28:PHE:HA	1:A:31:ILE:HG12	0.53	1.80	15	6
1:A:47:PHE:CD1	1:A:47:PHE:C	0.53	2.87	22	11
1:B:24:MET:HE3	1:B:25:LEU:N	0.53	2.18	19	3
1:B:76:GLY:C	1:B:77:VAL:HG23	0.53	2.28	7	1
1:B:45:THR:CG2	1:B:47:PHE:CD1	0.53	2.91	8	2
1:A:28:PHE:CE2	1:B:44:LEU:HD13	0.53	2.38	20	2
1:B:7:ILE:HG22	1:B:25:LEU:CD1	0.53	2.34	1	1
1:B:24:MET:HE3	1:B:25:LEU:CD2	0.53	2.33	7	5
1:A:48:LEU:CD2	1:A:80:LYS:O	0.53	2.57	21	3
1:A:32:ILE:CG2	1:B:47:PHE:CE1	0.53	2.92	21	10
1:A:31:ILE:HG21	1:B:13:ASP:OD2	0.53	2.04	19	3
1:B:27:SER:HA	1:B:30:LYS:HB3	0.53	1.80	9	4
1:A:92:LEU:HB3	1:B:37:ALA:CA	0.53	2.34	9	1
1:B:28:PHE:CD2	1:B:32:ILE:HG13	0.53	2.39	14	2
1:B:93:LYS:CG	1:B:93:LYS:O	0.53	2.57	14	1
1:A:79:VAL:HG12	1:B:81:PRO:HG3	0.53	1.79	20	1
1:B:44:LEU:C	1:B:45:THR:CG2	0.53	2.82	12	19
1:A:47:PHE:CE1	1:B:29:GLU:HG3	0.53	2.38	17	3
1:A:44:LEU:CD1	1:A:47:PHE:CZ	0.53	2.92	9	3
1:B:49:ASN:O	1:B:79:VAL:HA	0.53	2.04	4	3
1:B:28:PHE:CE1	1:B:32:ILE:CD1	0.53	2.91	6	4
1:A:92:LEU:HD11	1:B:75:VAL:HG21	0.53	1.80	8	1
1:A:44:LEU:HB3	1:A:47:PHE:HE1	0.53	1.64	23	2
1:A:75:VAL:CB	1:B:92:LEU:HD21	0.53	2.34	19	2
1:B:7:ILE:HG21	1:B:25:LEU:CD2	0.53	2.30	18	1
1:A:35:THR:O	1:A:38:LYS:N	0.53	2.42	7	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:PHE:CE2	1:B:29:GLU:HG2	0.53	2.39	21	6
1:A:51:LYS:HG3	1:A:78:SER:CB	0.53	2.34	6	2
1:A:79:VAL:CG1	1:A:80:LYS:N	0.53	2.71	14	3
1:A:77:VAL:HG12	1:B:84:SER:CA	0.53	2.34	15	1
1:B:36:VAL:HG11	1:B:77:VAL:HB	0.53	1.78	18	1
1:A:20:SER:OG	1:A:23:LYS:CB	0.53	2.57	20	7
1:A:29:GLU:HG3	1:B:45:THR:HG21	0.53	1.80	20	6
1:A:14:THR:HG22	1:A:16:LEU:HD12	0.53	1.75	6	1
1:A:10:ILE:HG23	1:B:24:MET:HB3	0.53	1.80	16	3
1:A:35:THR:CG2	1:A:42:VAL:HG13	0.53	2.34	15	1
1:A:75:VAL:HB	1:B:92:LEU:HD21	0.53	1.81	17	2
1:A:86:LYS:HA	1:A:89:ALA:HB3	0.53	1.80	19	1
1:A:14:THR:HB	1:A:16:LEU:CD1	0.53	2.34	20	2
1:A:42:VAL:HG13	1:B:6:LEU:CD1	0.53	2.23	3	2
1:A:36:VAL:HB	1:B:85:LEU:HD21	0.53	1.78	5	2
1:A:19:VAL:CA	1:B:16:LEU:HD11	0.53	2.34	16	1
1:B:17:THR:HG22	1:B:19:VAL:N	0.52	2.19	4	17
1:B:45:THR:CG2	1:B:47:PHE:CE2	0.52	2.93	11	4
1:B:47:PHE:CD1	1:B:47:PHE:C	0.52	2.87	16	7
1:A:84:SER:O	1:B:77:VAL:HG11	0.52	2.03	4	2
1:B:43:GLN:C	1:B:44:LEU:HD23	0.52	2.29	4	2
1:A:45:THR:CG2	1:A:47:PHE:CD1	0.52	2.92	11	1
1:A:89:ALA:HB2	1:B:36:VAL:HG13	0.52	1.80	11	1
1:B:28:PHE:C	1:B:32:ILE:HD13	0.52	2.29	12	1
1:A:77:VAL:HG11	1:B:85:LEU:HD22	0.52	1.81	17	1
1:A:31:ILE:HA	1:A:34:GLU:HB2	0.52	1.80	23	2
1:A:50:ILE:CG2	1:A:79:VAL:HG12	0.52	2.33	23	1
1:B:7:ILE:HB	1:B:21:VAL:C	0.52	2.29	8	7
1:A:42:VAL:HG23	1:A:42:VAL:O	0.52	2.05	15	1
1:A:79:VAL:HG11	1:B:79:VAL:HB	0.52	1.80	15	1
1:B:3:LYS:CE	1:B:28:PHE:CD1	0.52	2.92	23	1
1:A:92:LEU:O	1:A:93:LYS:HG2	0.52	2.04	1	1
1:A:33:THR:HG23	1:B:88:ALA:HB2	0.52	1.79	17	5
1:B:26:ALA:O	1:B:30:LYS:HB2	0.52	2.04	9	2
1:A:48:LEU:CD2	1:B:50:ILE:HD11	0.52	2.35	7	2
1:B:25:LEU:HD12	1:B:25:LEU:O	0.52	2.03	19	3
1:B:2:ASN:O	1:B:6:LEU:N	0.52	2.34	23	1
1:A:28:PHE:O	1:A:32:ILE:HG13	0.52	2.04	8	4
1:A:33:THR:OG1	1:B:88:ALA:HB2	0.52	2.05	9	1
1:A:31:ILE:HA	1:A:34:GLU:HB3	0.52	1.81	15	1
1:A:84:SER:C	1:A:85:LEU:HG	0.52	2.30	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:50:ILE:N	1:B:80:LYS:CD	0.52	2.72	20	1
1:B:35:THR:O	1:B:36:VAL:C	0.52	2.52	4	14
1:B:44:LEU:CB	1:B:47:PHE:CE1	0.52	2.92	23	4
1:A:20:SER:O	1:A:24:MET:HG3	0.52	2.05	10	6
1:B:54:ALA:CA	1:B:75:VAL:N	0.52	2.71	10	2
1:A:9:ALA:HB1	1:B:31:ILE:CD1	0.52	2.33	9	1
1:A:50:ILE:CG1	1:A:79:VAL:HG12	0.52	2.35	17	1
1:B:94:TYR:CD1	1:B:95:GLU:N	0.52	2.78	11	4
1:B:7:ILE:CG2	1:B:8:LYS:N	0.52	2.72	9	6
1:B:95:GLU:O	1:B:96:ASP:C	0.52	2.52	5	1
1:B:23:LYS:HA	1:B:26:ALA:HB3	0.52	1.80	7	2
1:A:27:SER:O	1:A:31:ILE:CG2	0.52	2.56	9	1
1:A:44:LEU:HD12	1:A:47:PHE:CZ	0.52	2.39	9	1
1:A:16:LEU:CD1	1:B:20:SER:CB	0.52	2.87	2	4
1:A:32:ILE:CG2	1:B:47:PHE:CE2	0.52	2.93	23	7
1:B:45:THR:CG2	1:B:47:PHE:CD2	0.52	2.93	11	6
1:A:47:PHE:CD2	1:B:29:GLU:CG	0.52	2.91	7	3
1:A:85:LEU:HD13	1:B:33:THR:HA	0.52	1.81	9	2
1:B:48:LEU:HD12	1:B:49:ASN:N	0.52	2.20	23	1
1:A:89:ALA:HB3	1:B:75:VAL:CG1	0.52	2.30	3	1
1:A:20:SER:CB	1:B:14:THR:HG21	0.52	2.33	4	1
1:A:47:PHE:C	1:A:82:GLY:HA2	0.52	2.30	4	1
1:A:28:PHE:CE1	1:B:44:LEU:CD2	0.52	2.92	15	4
1:A:80:LYS:HB2	1:A:81:PRO:HD2	0.52	1.80	8	2
1:B:47:PHE:CE1	1:B:85:LEU:HD21	0.52	2.40	9	1
1:A:78:SER:C	1:A:79:VAL:HG23	0.52	2.29	16	1
1:A:1:MET:HB2	1:B:42:VAL:HG22	0.52	1.80	1	1
1:A:36:VAL:CG2	1:A:50:ILE:HG22	0.52	2.35	1	1
1:B:17:THR:O	1:B:17:THR:HG23	0.52	2.05	11	14
1:B:28:PHE:HA	1:B:31:ILE:HD11	0.52	1.81	5	7
1:B:28:PHE:CE2	1:B:29:GLU:HG3	0.52	2.40	21	8
1:B:14:THR:C	1:B:16:LEU:H	0.52	2.11	8	6
1:A:85:LEU:HD21	1:B:36:VAL:HB	0.52	1.79	7	3
1:A:10:ILE:CG2	1:B:24:MET:HG2	0.52	2.35	21	2
1:A:50:ILE:HG13	1:A:79:VAL:HG22	0.52	1.81	14	2
1:A:85:LEU:O	1:B:37:ALA:HB2	0.52	2.05	14	1
1:B:50:ILE:HG22	1:B:79:VAL:HG21	0.52	1.82	21	2
1:A:75:VAL:CA	1:B:94:TYR:CD1	0.52	2.93	23	2
1:A:92:LEU:HD12	1:A:93:LYS:N	0.52	2.20	3	3
1:B:42:VAL:HB	1:B:50:ILE:HB	0.52	1.81	11	2
1:A:25:LEU:CG	1:A:26:ALA:N	0.52	2.72	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:VAL:HA	1:B:16:LEU:HD11	0.52	1.82	16	1
1:B:47:PHE:CE2	1:B:48:LEU:HB3	0.52	2.39	23	1
1:B:50:ILE:CA	1:B:79:VAL:HG11	0.51	2.34	19	3
1:A:50:ILE:HG22	1:A:79:VAL:CB	0.51	2.34	6	2
1:A:52:PRO:HB2	1:A:75:VAL:CG1	0.51	2.34	15	2
1:A:8:LYS:CE	1:A:8:LYS:CA	0.51	2.88	9	1
1:A:16:LEU:CD1	1:A:16:LEU:H	0.51	2.17	17	3
1:B:50:ILE:HD12	1:B:79:VAL:HG22	0.51	1.82	13	1
1:B:44:LEU:C	1:B:45:THR:HG22	0.51	2.30	21	3
1:B:34:GLU:HG3	1:B:35:THR:N	0.51	2.19	23	1
1:B:31:ILE:O	1:B:35:THR:OG1	0.51	2.27	13	9
1:A:44:LEU:HB2	1:A:48:LEU:HB2	0.51	1.82	5	10
1:B:50:ILE:C	1:B:79:VAL:HG11	0.51	2.31	2	3
1:B:44:LEU:CB	1:B:47:PHE:HE1	0.51	2.19	3	1
1:A:77:VAL:HG12	1:B:86:LYS:HG3	0.51	1.81	7	3
1:A:33:THR:HA	1:B:85:LEU:CD2	0.51	2.36	10	1
1:A:75:VAL:HG21	1:B:94:TYR:HA	0.51	1.81	14	1
1:B:3:LYS:NZ	1:B:28:PHE:CD1	0.51	2.78	20	1
1:B:3:LYS:CB	1:B:25:LEU:HD13	0.51	2.34	23	1
1:B:48:LEU:CD1	1:B:80:LYS:HB3	0.51	2.34	9	2
1:B:31:ILE:HA	1:B:34:GLU:HB2	0.51	1.80	22	3
1:A:77:VAL:HG11	1:B:81:PRO:HB2	0.51	1.81	19	1
1:A:35:THR:CG2	1:A:40:ASP:CB	0.51	2.89	9	9
1:B:28:PHE:O	1:B:32:ILE:N	0.51	2.35	10	17
1:A:53:VAL:O	1:A:54:ALA:C	0.51	2.54	18	4
1:A:53:VAL:O	1:A:75:VAL:CG2	0.51	2.56	6	2
1:A:94:TYR:HE1	1:B:75:VAL:O	0.51	1.89	8	1
1:B:50:ILE:HD13	1:B:79:VAL:CB	0.51	2.32	8	1
1:A:6:LEU:HD11	1:B:42:VAL:HG11	0.51	1.81	9	2
1:B:52:PRO:O	1:B:53:VAL:HG13	0.51	2.05	10	1
1:A:36:VAL:CG1	1:A:77:VAL:HG23	0.51	2.14	13	1
1:A:44:LEU:C	1:A:45:THR:CG2	0.51	2.83	3	19
1:A:80:LYS:HB3	1:A:81:PRO:HD3	0.51	1.82	17	2
1:B:47:PHE:HD1	1:B:85:LEU:HD12	0.51	1.66	5	1
1:A:36:VAL:HG23	1:A:37:ALA:N	0.51	2.21	7	2
1:A:51:LYS:O	1:A:51:LYS:CG	0.51	2.58	9	1
1:A:81:PRO:HG3	1:B:79:VAL:HG12	0.51	1.83	9	1
1:A:94:TYR:HB2	1:B:75:VAL:HB	0.51	1.82	16	1
1:A:6:LEU:C	1:A:25:LEU:HD13	0.51	2.30	23	1
1:B:44:LEU:HB2	1:B:48:LEU:HB2	0.51	1.81	17	6
1:A:16:LEU:CD1	1:B:20:SER:HB3	0.51	2.36	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:SER:HB3	1:B:16:LEU:HD11	0.51	1.83	2	1
1:A:24:MET:HB3	1:B:14:THR:CG2	0.51	2.35	14	6
1:A:47:PHE:CE2	1:A:48:LEU:HG	0.51	2.41	11	3
1:B:24:MET:CE	1:B:25:LEU:HG	0.51	2.35	22	8
1:B:32:ILE:HD13	1:B:42:VAL:CG2	0.51	2.33	3	1
1:B:49:ASN:HB2	1:B:81:PRO:CG	0.51	2.36	6	1
1:A:37:ALA:O	1:B:92:LEU:HA	0.51	2.05	17	5
1:A:29:GLU:CG	1:B:47:PHE:CD1	0.51	2.94	10	2
1:A:37:ALA:HA	1:B:92:LEU:CB	0.51	2.35	17	2
1:A:22:SER:O	1:A:25:LEU:HG	0.51	2.05	13	1
1:A:36:VAL:N	1:A:40:ASP:HB2	0.51	2.20	20	1
1:A:32:ILE:CG2	1:B:47:PHE:CZ	0.51	2.93	2	7
1:B:5:GLU:HA	1:B:8:LYS:HE2	0.51	1.82	8	6
1:A:33:THR:HA	1:B:85:LEU:CD1	0.51	2.36	14	2
1:B:28:PHE:CE2	1:B:32:ILE:CD1	0.51	2.94	18	9
1:A:47:PHE:CE1	1:A:48:LEU:CB	0.51	2.94	7	1
1:A:16:LEU:CD2	1:B:20:SER:HB3	0.51	2.36	23	3
1:A:50:ILE:HG23	1:A:77:VAL:HG22	0.51	1.81	15	1
1:A:47:PHE:HA	1:A:82:GLY:CA	0.51	2.36	2	3
1:A:42:VAL:HG23	1:B:6:LEU:CD1	0.51	2.34	5	1
1:A:42:VAL:HG23	1:B:1:MET:HB3	0.51	1.80	8	1
1:A:92:LEU:HG	1:B:37:ALA:C	0.51	2.31	14	1
1:A:42:VAL:HG23	1:B:1:MET:HG3	0.51	1.81	16	2
1:A:1:MET:CE	1:A:6:LEU:HD23	0.51	2.35	16	5
1:A:28:PHE:CE1	1:A:29:GLU:HG3	0.51	2.41	8	2
1:A:24:MET:HE2	1:A:25:LEU:HG	0.51	1.82	4	2
1:A:37:ALA:CB	1:B:88:ALA:CB	0.51	2.88	18	4
1:A:51:LYS:HG3	1:A:51:LYS:O	0.51	2.06	6	2
1:A:29:GLU:O	1:A:33:THR:OG1	0.51	2.29	10	2
1:A:50:ILE:HD13	1:A:79:VAL:HG13	0.51	1.83	16	1
1:B:25:LEU:HD12	1:B:26:ALA:N	0.51	2.18	20	1
1:B:94:TYR:CE1	1:B:95:GLU:CG	0.51	2.94	20	1
1:A:11:ALA:HA	1:A:14:THR:OG1	0.51	2.06	1	4
1:A:84:SER:HB2	1:B:77:VAL:HG12	0.51	1.81	2	1
1:A:77:VAL:HG12	1:B:86:LYS:CD	0.51	2.36	13	2
1:B:7:ILE:HD13	1:B:21:VAL:HG23	0.51	1.82	8	3
1:A:36:VAL:CG1	1:B:85:LEU:HD23	0.51	2.30	18	1
1:A:5:GLU:HA	1:A:8:LYS:HE2	0.50	1.83	10	7
1:A:51:LYS:O	1:A:78:SER:N	0.50	2.44	19	7
1:B:24:MET:O	1:B:28:PHE:N	0.50	2.44	8	6
1:B:26:ALA:O	1:B:30:LYS:CB	0.50	2.59	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ASN:HB2	1:A:81:PRO:HG2	0.50	1.82	4	2
1:A:10:ILE:C	1:A:14:THR:OG1	0.50	2.53	18	10
1:A:45:THR:CG2	1:A:47:PHE:CD2	0.50	2.94	8	4
1:A:7:ILE:CG2	1:A:25:LEU:HD22	0.50	2.36	19	1
1:A:37:ALA:HA	1:B:89:ALA:CA	0.50	2.37	13	2
1:B:36:VAL:HG22	1:B:51:LYS:HA	0.50	1.82	2	1
1:B:44:LEU:HB3	1:B:47:PHE:HE1	0.50	1.66	3	3
1:A:94:TYR:CE1	1:B:75:VAL:CA	0.50	2.93	6	1
1:B:7:ILE:CA	1:B:25:LEU:HD12	0.50	2.35	21	3
1:A:29:GLU:O	1:A:33:THR:N	0.50	2.43	10	2
1:B:10:ILE:HG21	1:B:24:MET:HE2	0.50	1.83	10	1
1:A:84:SER:HA	1:B:77:VAL:CB	0.50	2.37	17	1
1:A:22:SER:O	1:A:26:ALA:CB	0.50	2.59	11	13
1:B:49:ASN:O	1:B:79:VAL:CB	0.50	2.59	1	1
1:A:85:LEU:N	1:A:85:LEU:CD2	0.50	2.60	17	3
1:A:82:GLY:O	1:A:84:SER:N	0.50	2.45	17	3
1:A:92:LEU:HG	1:B:37:ALA:HA	0.50	1.82	4	1
1:A:44:LEU:HB3	1:A:47:PHE:CE2	0.50	2.42	13	4
1:A:85:LEU:CD2	1:B:36:VAL:CG1	0.50	2.89	5	2
1:B:49:ASN:H	1:B:80:LYS:HA	0.50	1.66	20	3
1:B:35:THR:CG2	1:B:42:VAL:HG23	0.50	2.37	18	1
1:A:14:THR:CG2	1:A:16:LEU:HD13	0.50	2.32	21	1
1:A:1:MET:HA	1:A:5:GLU:CB	0.50	2.36	1	13
1:A:10:ILE:CA	1:A:14:THR:OG1	0.50	2.60	18	9
1:A:29:GLU:CG	1:B:47:PHE:CE1	0.50	2.95	3	4
1:A:20:SER:O	1:A:24:MET:N	0.50	2.39	15	6
1:B:94:TYR:CD1	1:B:96:ASP:OD1	0.50	2.64	5	1
1:A:94:TYR:CE1	1:B:75:VAL:HB	0.50	2.41	11	1
1:A:17:THR:HG23	1:A:17:THR:O	0.50	2.06	19	2
1:A:23:LYS:O	1:A:27:SER:CB	0.50	2.60	1	12
1:B:31:ILE:O	1:B:35:THR:HB	0.50	2.06	4	6
1:A:77:VAL:HG11	1:B:84:SER:HG	0.50	1.67	2	1
1:A:53:VAL:C	1:A:75:VAL:HG22	0.50	2.31	17	5
1:A:44:LEU:HD22	1:B:28:PHE:HE2	0.50	1.67	22	4
1:A:29:GLU:HG2	1:A:33:THR:OG1	0.50	2.06	10	2
1:A:85:LEU:C	1:A:85:LEU:HD23	0.50	2.31	15	1
1:A:50:ILE:HG12	1:A:79:VAL:HG12	0.50	1.83	17	1
1:B:47:PHE:CE1	1:B:48:LEU:HB2	0.50	2.42	11	3
1:A:85:LEU:HB2	1:B:77:VAL:CG2	0.50	2.37	4	1
1:A:94:TYR:CD1	1:A:94:TYR:C	0.50	2.88	5	3
1:B:48:LEU:CD2	1:B:82:GLY:HA2	0.50	2.37	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:LEU:CD1	1:B:36:VAL:HB	0.50	2.37	8	1
1:B:6:LEU:CB	1:B:25:LEU:HD11	0.50	2.36	12	1
1:A:36:VAL:HG22	1:A:52:PRO:CB	0.50	2.37	16	1
1:A:44:LEU:HD13	1:A:47:PHE:CZ	0.50	2.41	10	4
1:B:44:LEU:CD1	1:B:47:PHE:CZ	0.50	2.95	6	3
1:A:92:LEU:O	1:A:93:LYS:HB2	0.50	2.06	10	6
1:A:50:ILE:CB	1:A:79:VAL:HB	0.50	2.37	6	1
1:A:88:ALA:HB1	1:B:37:ALA:HB2	0.50	1.84	9	5
1:B:82:GLY:O	1:B:83:GLU:HB3	0.50	2.06	13	2
1:A:44:LEU:HD12	1:A:47:PHE:CE2	0.50	2.41	9	1
1:B:44:LEU:HB2	1:B:48:LEU:CB	0.50	2.36	19	4
1:B:79:VAL:HG12	1:B:80:LYS:N	0.50	2.20	13	1
1:A:79:VAL:HG22	1:A:80:LYS:H	0.50	1.66	20	2
1:B:50:ILE:CB	1:B:80:LYS:HD3	0.50	2.37	20	1
1:A:27:SER:HA	1:A:30:LYS:HB3	0.50	1.83	9	11
1:A:86:LYS:O	1:A:90:GLU:N	0.50	2.43	2	1
1:A:14:THR:HG23	1:B:20:SER:OG	0.50	2.07	4	2
1:A:3:LYS:HE3	1:A:29:GLU:CB	0.50	2.37	10	4
1:A:28:PHE:HA	1:A:31:ILE:HD11	0.50	1.83	6	7
1:A:37:ALA:CB	1:B:89:ALA:HA	0.50	2.35	7	1
1:B:85:LEU:HD23	1:B:85:LEU:C	0.50	2.30	7	1
1:A:77:VAL:HG13	1:B:81:PRO:HB2	0.50	1.84	12	2
1:A:7:ILE:CG2	1:A:8:LYS:N	0.50	2.74	17	1
1:A:53:VAL:HG23	1:A:76:GLY:O	0.50	2.07	22	1
1:A:28:PHE:CD1	1:A:32:ILE:HG13	0.50	2.41	23	6
1:A:47:PHE:CE2	1:B:32:ILE:CG2	0.50	2.95	4	6
1:B:44:LEU:CD1	1:B:47:PHE:CE1	0.50	2.95	23	4
1:A:36:VAL:HG11	1:A:77:VAL:HB	0.50	1.84	2	2
1:B:10:ILE:C	1:B:14:THR:OG1	0.50	2.55	6	5
1:A:44:LEU:N	1:A:48:LEU:O	0.50	2.45	23	4
1:A:94:TYR:CD1	1:B:75:VAL:CA	0.50	2.95	14	3
1:A:7:ILE:CG1	1:A:8:LYS:N	0.50	2.75	16	8
1:A:92:LEU:HA	1:B:37:ALA:O	0.50	2.06	13	3
1:A:35:THR:HA	1:A:38:LYS:HB2	0.50	1.82	21	2
1:B:79:VAL:CG1	1:B:80:LYS:N	0.50	2.75	13	1
1:B:7:ILE:HG22	1:B:25:LEU:HB2	0.50	1.84	14	1
1:A:3:LYS:O	1:A:7:ILE:HG23	0.50	2.06	19	1
1:B:50:ILE:HA	1:B:79:VAL:CB	0.49	2.36	1	1
1:A:37:ALA:O	1:B:92:LEU:CA	0.49	2.60	19	6
1:B:3:LYS:O	1:B:7:ILE:HG13	0.49	2.07	17	5
1:A:5:GLU:HA	1:A:8:LYS:HE3	0.49	1.84	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:THR:HG23	1:A:47:PHE:CD2	0.49	2.42	19	4
1:B:28:PHE:CD2	1:B:29:GLU:HG3	0.49	2.42	6	4
1:A:47:PHE:CD1	1:A:48:LEU:HB2	0.49	2.42	7	1
1:A:20:SER:HB3	1:B:16:LEU:CD2	0.49	2.37	13	1
1:B:35:THR:CG2	1:B:40:ASP:CB	0.49	2.90	22	16
1:B:47:PHE:HB2	1:B:85:LEU:CG	0.49	2.37	1	1
1:A:3:LYS:CE	1:A:29:GLU:CB	0.49	2.89	9	6
1:A:85:LEU:HD11	1:B:50:ILE:HG13	0.49	1.84	9	1
1:B:7:ILE:O	1:B:11:ALA:N	0.49	2.40	14	3
1:A:14:THR:CB	1:A:16:LEU:HD11	0.49	2.36	11	1
1:B:28:PHE:O	1:B:32:ILE:CD1	0.49	2.60	12	1
1:A:19:VAL:CG2	1:B:16:LEU:HD21	0.49	2.37	16	1
1:A:1:MET:CG	1:A:5:GLU:HB3	0.49	2.37	17	2
1:A:10:ILE:HA	1:A:14:THR:OG1	0.49	2.08	19	9
1:B:36:VAL:HG11	1:B:77:VAL:CG2	0.49	2.37	18	2
1:A:93:LYS:O	1:A:93:LYS:HG3	0.49	2.04	19	2
1:B:50:ILE:HG23	1:B:79:VAL:CG1	0.49	2.35	12	1
1:B:30:LYS:HA	1:B:34:GLU:CG	0.49	2.37	20	1
1:B:36:VAL:HG13	1:B:37:ALA:N	0.49	2.21	20	1
1:A:36:VAL:HG11	1:B:85:LEU:HB2	0.49	1.83	6	1
1:B:44:LEU:CD1	1:B:48:LEU:HB2	0.49	2.32	8	4
1:B:36:VAL:HG22	1:B:52:PRO:CG	0.49	2.38	11	2
1:A:83:GLU:O	1:A:83:GLU:HG3	0.49	2.08	17	1
1:A:35:THR:CG2	1:A:42:VAL:CG2	0.49	2.91	1	1
1:A:88:ALA:HB1	1:B:37:ALA:CB	0.49	2.37	19	5
1:B:8:LYS:O	1:B:12:GLN:N	0.49	2.45	22	12
1:B:22:SER:O	1:B:26:ALA:CB	0.49	2.60	15	11
1:B:85:LEU:N	1:B:85:LEU:HD23	0.49	2.22	2	1
1:A:25:LEU:O	1:A:28:PHE:HB3	0.49	2.07	15	2
1:A:19:VAL:HG13	1:A:20:SER:N	0.49	2.21	23	3
1:A:44:LEU:CD1	1:A:47:PHE:CE1	0.49	2.95	11	1
1:A:79:VAL:CG1	1:B:81:PRO:HD3	0.49	2.37	11	1
1:A:3:LYS:HG3	1:A:25:LEU:HB3	0.49	1.84	15	1
1:A:33:THR:HG22	1:B:85:LEU:HG	0.49	1.82	15	1
1:A:52:PRO:C	1:A:53:VAL:HG13	0.49	2.31	2	6
1:B:93:LYS:O	1:B:96:ASP:N	0.49	2.46	9	11
1:B:3:LYS:CD	1:B:25:LEU:HD11	0.49	2.34	6	2
1:A:54:ALA:HA	1:B:94:TYR:CE1	0.49	2.41	7	2
1:A:47:PHE:CZ	1:B:32:ILE:CG2	0.49	2.95	9	3
1:B:44:LEU:CB	1:B:47:PHE:CE2	0.49	2.96	9	1
1:B:14:THR:HG22	1:B:16:LEU:HD23	0.49	1.82	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:CG2	1:A:77:VAL:HG13	0.49	2.38	17	1
1:A:53:VAL:O	1:A:54:ALA:HB2	0.49	2.06	19	2
1:A:28:PHE:HE1	1:B:44:LEU:HD22	0.49	1.67	19	6
1:B:36:VAL:HG21	1:B:50:ILE:CG2	0.49	2.36	3	1
1:A:29:GLU:CG	1:B:45:THR:HG21	0.49	2.37	6	1
1:A:52:PRO:HB2	1:A:75:VAL:HG21	0.49	1.85	6	1
1:A:52:PRO:HB2	1:A:75:VAL:CG2	0.49	2.36	7	1
1:A:89:ALA:O	1:A:92:LEU:HG	0.49	2.06	8	2
1:B:45:THR:O	1:B:46:GLY:C	0.49	2.55	9	3
1:A:85:LEU:HB2	1:B:33:THR:OG1	0.49	2.08	15	1
1:B:1:MET:CB	1:B:5:GLU:CB	0.49	2.91	16	3
1:A:77:VAL:CG1	1:B:85:LEU:HB2	0.49	2.33	17	1
1:A:42:VAL:CG2	1:A:50:ILE:HB	0.49	2.37	20	2
1:B:49:ASN:C	1:B:79:VAL:CG2	0.49	2.85	1	1
1:A:19:VAL:CB	1:B:19:VAL:HB	0.49	2.38	20	2
1:B:28:PHE:O	1:B:32:ILE:HG13	0.49	2.08	20	7
1:A:14:THR:CG2	1:B:20:SER:CB	0.49	2.91	19	8
1:A:33:THR:O	1:A:36:VAL:CG2	0.49	2.60	23	2
1:A:45:THR:HG21	1:B:29:GLU:HB3	0.49	1.85	11	2
1:A:78:SER:O	1:A:79:VAL:HB	0.49	2.08	20	2
1:A:42:VAL:HG23	1:B:6:LEU:HD21	0.49	1.83	21	1
1:A:47:PHE:CD2	1:A:48:LEU:HG	0.49	2.43	1	1
1:B:21:VAL:HG23	1:B:22:SER:N	0.49	2.22	4	22
1:A:36:VAL:O	1:B:92:LEU:HD22	0.49	2.08	2	3
1:B:52:PRO:C	1:B:53:VAL:HG13	0.49	2.33	4	7
1:B:7:ILE:HG13	1:B:25:LEU:CD1	0.49	2.31	5	3
1:A:20:SER:HG	1:A:24:MET:N	0.49	2.06	6	1
1:B:35:THR:C	1:B:40:ASP:HB2	0.49	2.32	13	1
1:B:14:THR:CA	1:B:16:LEU:CD1	0.49	2.90	23	9
1:B:24:MET:O	1:B:28:PHE:CB	0.49	2.60	2	1
1:B:35:THR:CG2	1:B:42:VAL:HG13	0.49	2.34	23	2
1:A:50:ILE:HA	1:A:79:VAL:CG2	0.49	2.38	9	1
1:B:48:LEU:HD22	1:B:81:PRO:N	0.49	2.22	9	2
1:A:80:LYS:C	1:B:79:VAL:HG21	0.49	2.33	12	1
1:A:25:LEU:O	1:A:28:PHE:N	0.49	2.46	15	1
1:A:47:PHE:O	1:A:81:PRO:C	0.49	2.56	17	1
1:A:42:VAL:HG12	1:B:1:MET:HB3	0.49	1.83	20	1
1:A:35:THR:O	1:A:36:VAL:C	0.48	2.56	7	9
1:B:82:GLY:O	1:B:85:LEU:HD12	0.48	2.08	1	1
1:B:88:ALA:O	1:B:91:GLY:N	0.48	2.46	19	5
1:B:20:SER:HB3	1:B:23:LYS:HB2	0.48	1.85	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:LEU:CD1	1:B:33:THR:O	0.48	2.61	6	1
1:A:52:PRO:CB	1:A:75:VAL:HG11	0.48	2.38	8	2
1:A:9:ALA:HB1	1:B:31:ILE:HG21	0.48	1.83	12	1
1:B:79:VAL:HG23	1:B:80:LYS:N	0.48	2.23	17	1
1:A:33:THR:O	1:A:36:VAL:CG1	0.48	2.60	20	1
1:A:44:LEU:C	1:A:45:THR:HG22	0.48	2.32	22	2
1:A:92:LEU:O	1:A:93:LYS:CG	0.48	2.61	19	3
1:A:52:PRO:HA	1:A:77:VAL:HA	0.48	1.84	2	5
1:B:53:VAL:HG11	1:B:78:SER:OG	0.48	2.08	2	1
1:A:75:VAL:N	1:B:94:TYR:CD2	0.48	2.81	4	3
1:B:1:MET:O	1:B:2:ASN:HB3	0.48	2.09	19	2
1:A:17:THR:HB	1:B:17:THR:HG21	0.48	1.84	7	1
1:A:39:GLY:CA	1:B:97:PHE:CZ	0.48	2.95	7	1
1:B:28:PHE:CD2	1:B:32:ILE:CD1	0.48	2.95	12	1
1:A:82:GLY:O	1:A:85:LEU:HD13	0.48	2.07	17	1
1:B:7:ILE:N	1:B:25:LEU:CD1	0.48	2.76	1	3
1:B:20:SER:CB	1:B:23:LYS:CB	0.48	2.91	6	6
1:A:20:SER:CB	1:B:14:THR:CG2	0.48	2.91	16	7
1:A:49:ASN:C	1:A:79:VAL:CG2	0.48	2.87	19	3
1:A:47:PHE:CA	1:A:82:GLY:HA2	0.48	2.38	11	1
1:A:25:LEU:CD1	1:A:26:ALA:N	0.48	2.76	13	2
1:B:7:ILE:HD12	1:B:21:VAL:C	0.48	2.33	18	1
1:A:17:THR:O	1:A:17:THR:HG23	0.48	2.09	7	8
1:B:83:GLU:HA	1:B:86:LYS:HB2	0.48	1.86	3	1
1:A:50:ILE:CD1	1:A:79:VAL:CG2	0.48	2.91	12	3
1:A:44:LEU:CB	1:A:47:PHE:CZ	0.48	2.96	13	1
1:B:5:GLU:O	1:B:8:LYS:CG	0.48	2.61	13	1
1:B:77:VAL:O	1:B:79:VAL:HG12	0.48	2.08	17	1
1:B:42:VAL:HG13	1:B:50:ILE:HD11	0.48	1.83	21	1
1:A:4:THR:HG22	1:A:8:LYS:NZ	0.48	2.23	4	1
1:A:82:GLY:C	1:A:84:SER:N	0.48	2.69	17	3
1:A:83:GLU:O	1:A:86:LYS:N	0.48	2.44	4	2
1:B:14:THR:CG2	1:B:16:LEU:HD13	0.48	2.33	5	2
1:A:49:ASN:N	1:A:79:VAL:HG23	0.48	2.24	8	2
1:A:10:ILE:CG1	1:B:24:MET:HG2	0.48	2.38	21	2
1:A:75:VAL:HG23	1:B:94:TYR:HD1	0.48	1.69	22	2
1:A:47:PHE:CE2	1:B:32:ILE:HB	0.48	2.43	23	1
1:B:3:LYS:O	1:B:25:LEU:CD2	0.48	2.61	6	1
1:A:10:ILE:HD11	1:B:28:PHE:CA	0.48	2.38	7	1
1:A:44:LEU:CB	1:A:47:PHE:CE2	0.48	2.96	13	1
1:A:25:LEU:O	1:A:26:ALA:C	0.48	2.55	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:VAL:HG23	1:B:85:LEU:HD21	0.48	1.85	18	1
1:A:7:ILE:CA	1:A:25:LEU:HD12	0.48	2.38	18	6
1:A:16:LEU:HD12	1:A:16:LEU:H	0.48	1.69	20	2
1:A:50:ILE:HA	1:A:79:VAL:HA	0.48	1.84	23	3
1:B:10:ILE:HA	1:B:14:THR:OG1	0.48	2.08	16	2
1:A:85:LEU:CA	1:A:88:ALA:HB3	0.48	2.39	4	1
1:A:7:ILE:CG1	1:A:25:LEU:HD12	0.48	2.38	9	2
1:B:48:LEU:HD23	1:B:81:PRO:HA	0.48	1.86	17	1
1:A:30:LYS:HA	1:A:34:GLU:CG	0.48	2.39	20	1
1:B:44:LEU:CB	1:B:47:PHE:CZ	0.48	2.96	20	1
1:B:51:LYS:HG3	1:B:51:LYS:O	0.48	2.09	1	1
1:B:54:ALA:CB	1:B:75:VAL:N	0.48	2.76	8	3
1:A:85:LEU:HD12	1:B:33:THR:HG1	0.48	1.64	2	1
1:A:75:VAL:CB	1:B:94:TYR:HB2	0.48	2.38	20	4
1:A:28:PHE:CZ	1:A:32:ILE:CD1	0.48	2.97	7	2
1:A:31:ILE:HD12	1:A:32:ILE:HG12	0.48	1.85	21	3
1:A:89:ALA:HA	1:B:37:ALA:CB	0.48	2.39	12	1
1:B:35:THR:HG22	1:B:40:ASP:HA	0.48	1.84	13	1
1:A:75:VAL:CG2	1:B:94:TYR:HA	0.48	2.39	14	1
1:B:36:VAL:HG11	1:B:77:VAL:CB	0.48	2.38	18	1
1:B:44:LEU:CG	1:B:48:LEU:O	0.48	2.61	23	1
1:B:20:SER:O	1:B:24:MET:N	0.48	2.40	7	4
1:B:20:SER:HG	1:B:24:MET:H	0.48	1.52	4	1
1:A:50:ILE:HD11	1:A:79:VAL:CG2	0.48	2.38	15	1
1:A:5:GLU:HA	1:A:8:LYS:CE	0.48	2.38	12	4
1:B:93:LYS:O	1:B:93:LYS:HG3	0.48	2.09	5	1
1:A:88:ALA:HB2	1:B:33:THR:HG23	0.48	1.86	8	2
1:A:24:MET:CB	1:B:14:THR:HG21	0.48	2.33	11	1
1:A:47:PHE:HZ	1:B:32:ILE:HG21	0.48	1.68	11	1
1:A:21:VAL:O	1:A:25:LEU:HB3	0.48	2.09	19	3
1:B:36:VAL:CG2	1:B:50:ILE:CG2	0.48	2.91	18	1
1:A:53:VAL:CG2	1:A:76:GLY:O	0.48	2.62	22	1
1:A:10:ILE:HD11	1:B:24:MET:O	0.47	2.09	21	2
1:B:36:VAL:HG13	1:B:52:PRO:CD	0.47	2.39	2	2
1:A:88:ALA:HB1	1:B:34:GLU:OE2	0.47	2.08	3	1
1:B:44:LEU:CD1	1:B:48:LEU:CB	0.47	2.92	16	11
1:A:9:ALA:HB3	1:B:31:ILE:HD13	0.47	1.85	10	2
1:A:7:ILE:CG2	1:A:25:LEU:CD2	0.47	2.92	11	1
1:A:86:LYS:HG2	1:B:75:VAL:HG12	0.47	1.84	15	1
1:A:6:LEU:HD11	1:B:42:VAL:HG12	0.47	1.86	19	1
1:B:44:LEU:HB3	1:B:47:PHE:CZ	0.47	2.44	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:23:LYS:O	1:B:27:SER:HB2	0.47	2.09	2	1
1:A:92:LEU:N	1:B:37:ALA:CA	0.47	2.77	4	1
1:A:85:LEU:CB	1:B:77:VAL:HG11	0.47	2.39	20	2
1:A:92:LEU:HB3	1:B:37:ALA:C	0.47	2.35	7	5
1:B:44:LEU:CD1	1:B:47:PHE:CE2	0.47	2.96	9	1
1:A:16:LEU:HD12	1:A:16:LEU:N	0.47	2.24	17	2
1:A:84:SER:HA	1:B:77:VAL:HB	0.47	1.86	17	1
1:B:17:THR:HG23	1:B:19:VAL:N	0.47	2.24	19	1
1:A:14:THR:CG2	1:B:20:SER:HB3	0.47	2.39	15	4
1:A:47:PHE:CB	1:A:83:GLU:CB	0.47	2.92	4	1
1:A:14:THR:C	1:A:16:LEU:H	0.47	2.17	5	2
1:A:48:LEU:HD11	1:B:48:LEU:HD13	0.47	1.83	8	1
1:B:47:PHE:CD1	1:B:85:LEU:CD1	0.47	2.98	11	2
1:B:14:THR:HB	1:B:16:LEU:CD1	0.47	2.40	17	1
1:A:47:PHE:CD1	1:A:48:LEU:N	0.47	2.82	22	3
1:B:44:LEU:HD12	1:B:48:LEU:HG	0.47	1.85	23	1
1:A:88:ALA:CB	1:B:37:ALA:HB2	0.47	2.39	20	8
1:A:85:LEU:HB3	1:B:33:THR:O	0.47	2.09	17	2
1:B:82:GLY:C	1:B:84:SER:H	0.47	2.18	2	2
1:A:7:ILE:HD12	1:A:7:ILE:C	0.47	2.35	5	3
1:A:47:PHE:HB2	1:A:82:GLY:HA3	0.47	1.85	15	2
1:A:7:ILE:N	1:A:25:LEU:CD1	0.47	2.78	6	5
1:A:20:SER:CB	1:A:23:LYS:CB	0.47	2.92	3	10
1:A:89:ALA:CA	1:B:37:ALA:CB	0.47	2.92	6	3
1:B:10:ILE:CA	1:B:14:THR:OG1	0.47	2.63	16	4
1:A:11:ALA:CB	1:A:21:VAL:HG11	0.47	2.37	4	1
1:B:85:LEU:C	1:B:87:LYS:N	0.47	2.71	6	3
1:A:37:ALA:HB1	1:B:89:ALA:HA	0.47	1.86	7	1
1:A:47:PHE:CE1	1:A:48:LEU:HB2	0.47	2.45	7	2
1:B:47:PHE:CD2	1:B:48:LEU:HG	0.47	2.44	12	3
1:A:92:LEU:HG	1:B:38:LYS:CA	0.47	2.39	14	1
1:A:6:LEU:HD23	1:B:31:ILE:HD11	0.47	1.84	21	1
1:A:85:LEU:HG	1:B:33:THR:OG1	0.47	2.09	3	3
1:A:20:SER:C	1:A:24:MET:CG	0.47	2.86	22	8
1:A:3:LYS:NZ	1:A:25:LEU:O	0.47	2.48	7	2
1:A:20:SER:CB	1:B:16:LEU:CD1	0.47	2.92	17	4
1:A:28:PHE:CE2	1:A:32:ILE:HG13	0.47	2.45	11	1
1:A:31:ILE:HG23	1:B:13:ASP:OD2	0.47	2.09	13	1
1:B:36:VAL:HA	1:B:40:ASP:HB3	0.47	1.86	13	1
1:A:81:PRO:HB2	1:B:77:VAL:HG13	0.47	1.86	16	5
1:A:21:VAL:HG23	1:A:22:SER:N	0.47	2.25	3	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:CG1	1:A:37:ALA:N	0.47	2.78	1	1
1:B:20:SER:O	1:B:24:MET:HG3	0.47	2.09	1	2
1:B:11:ALA:CA	1:B:14:THR:OG1	0.47	2.63	23	9
1:A:24:MET:HE1	1:A:25:LEU:CD2	0.47	2.40	5	1
1:A:29:GLU:CG	1:B:47:PHE:CE2	0.47	2.97	5	5
1:B:47:PHE:CE1	1:B:48:LEU:CG	0.47	2.97	5	4
1:B:22:SER:HA	1:B:25:LEU:HD23	0.47	1.87	6	1
1:A:33:THR:HA	1:A:36:VAL:CG2	0.47	2.40	7	2
1:B:44:LEU:HB2	1:B:48:LEU:O	0.47	2.09	16	3
1:B:48:LEU:HB3	1:B:80:LYS:HD2	0.47	1.85	15	2
1:A:44:LEU:HD22	1:B:28:PHE:CE2	0.47	2.45	22	3
1:A:36:VAL:HG21	1:A:50:ILE:HG21	0.47	1.86	13	1
1:A:75:VAL:HB	1:B:89:ALA:CB	0.47	2.30	15	1
1:A:47:PHE:HB2	1:A:83:GLU:HG2	0.47	1.85	17	1
1:A:6:LEU:HD21	1:B:42:VAL:HG11	0.47	1.85	19	1
1:A:43:GLN:O	1:A:43:GLN:CG	0.47	2.62	19	2
1:A:1:MET:CB	1:A:5:GLU:CB	0.47	2.93	22	1
1:B:47:PHE:CA	1:B:82:GLY:HA3	0.47	2.39	23	1
1:A:19:VAL:HG13	1:A:24:MET:SD	0.47	2.50	1	4
1:A:33:THR:HG22	1:A:34:GLU:N	0.47	2.24	2	2
1:B:52:PRO:HA	1:B:77:VAL:HA	0.47	1.87	3	6
1:A:92:LEU:HD12	1:B:75:VAL:HG11	0.47	1.86	4	1
1:B:76:GLY:O	1:B:77:VAL:CG2	0.47	2.63	7	1
1:B:18:GLN:O	1:B:21:VAL:HG13	0.47	2.09	9	1
1:A:47:PHE:CA	1:A:82:GLY:CA	0.47	2.93	11	1
1:B:50:ILE:CD1	1:B:79:VAL:HG13	0.47	2.40	13	1
1:A:94:TYR:CD2	1:B:75:VAL:N	0.47	2.83	16	1
1:A:40:ASP:OD1	1:A:41:LYS:N	0.47	2.48	19	2
1:A:85:LEU:HD23	1:B:77:VAL:HG22	0.47	1.86	1	1
1:B:47:PHE:HB2	1:B:85:LEU:HD11	0.47	1.84	1	1
1:A:29:GLU:HB3	1:B:45:THR:HG21	0.47	1.87	2	4
1:A:3:LYS:CD	1:B:45:THR:HB	0.47	2.40	3	1
1:A:50:ILE:HD13	1:A:79:VAL:CG2	0.47	2.39	4	1
1:A:28:PHE:CD1	1:A:28:PHE:C	0.47	2.92	15	8
1:A:94:TYR:CD1	1:B:75:VAL:HB	0.47	2.44	23	3
1:A:44:LEU:HB3	1:A:47:PHE:CZ	0.47	2.44	22	2
1:A:3:LYS:HE2	1:A:25:LEU:O	0.47	2.10	15	1
1:A:42:VAL:HA	1:B:1:MET:HB3	0.47	1.86	15	1
1:A:75:VAL:O	1:B:89:ALA:CB	0.47	2.62	15	1
1:B:85:LEU:HB2	1:B:88:ALA:HB3	0.47	1.86	18	1
1:B:42:VAL:HB	1:B:50:ILE:HG12	0.47	1.86	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:VAL:CG2	1:B:76:GLY:N	0.47	2.78	23	1
1:A:14:THR:CA	1:A:16:LEU:CD1	0.47	2.92	2	1
1:A:49:ASN:HB2	1:A:81:PRO:CG	0.47	2.40	4	2
1:B:14:THR:CG2	1:B:16:LEU:HD21	0.47	2.38	4	1
1:A:50:ILE:CG2	1:A:79:VAL:HG23	0.47	2.40	10	1
1:B:87:LYS:O	1:B:90:GLU:CG	0.47	2.63	13	3
1:A:50:ILE:CB	1:A:79:VAL:HG12	0.47	2.40	23	1
1:A:6:LEU:CD2	1:B:31:ILE:CD1	0.46	2.93	11	3
1:A:45:THR:CG2	1:B:3:LYS:HE3	0.46	2.41	15	2
1:A:85:LEU:N	1:A:85:LEU:CD1	0.46	2.77	17	2
1:A:36:VAL:CG1	1:B:85:LEU:HD22	0.46	2.39	5	1
1:A:7:ILE:O	1:A:11:ALA:N	0.46	2.44	19	6
1:A:85:LEU:CD2	1:B:77:VAL:HG11	0.46	2.40	6	1
1:A:1:MET:CB	1:B:42:VAL:HG12	0.46	2.40	8	1
1:B:45:THR:HG22	1:B:47:PHE:CD1	0.46	2.45	8	2
1:A:45:THR:HG22	1:A:47:PHE:CD1	0.46	2.45	11	1
1:A:5:GLU:O	1:A:8:LYS:CG	0.46	2.62	15	2
1:B:94:TYR:C	1:B:94:TYR:HD1	0.46	2.14	15	1
1:A:42:VAL:CG1	1:A:50:ILE:HB	0.46	2.40	16	1
1:A:78:SER:C	1:A:79:VAL:HG13	0.46	2.35	17	1
1:B:33:THR:O	1:B:36:VAL:CG2	0.46	2.62	22	2
1:A:44:LEU:HD12	1:A:48:LEU:CG	0.46	2.40	7	2
1:A:92:LEU:HD21	1:B:75:VAL:HG11	0.46	1.87	1	2
1:A:53:VAL:CG2	1:A:76:GLY:CA	0.46	2.93	6	1
1:A:1:MET:HG2	1:A:5:GLU:CB	0.46	2.41	15	3
1:B:36:VAL:HG11	1:B:77:VAL:HG22	0.46	1.88	9	1
1:B:20:SER:HB3	1:B:24:MET:N	0.46	2.26	12	2
1:B:28:PHE:CE2	1:B:32:ILE:HG13	0.46	2.44	14	1
1:A:31:ILE:CA	1:A:34:GLU:CG	0.46	2.91	15	1
1:B:7:ILE:CG1	1:B:8:LYS:N	0.46	2.76	18	9
1:B:54:ALA:HB2	1:B:75:VAL:N	0.46	2.26	1	1
1:A:36:VAL:HG23	1:A:42:VAL:HG12	0.46	1.87	5	1
1:A:11:ALA:HB2	1:A:21:VAL:CG1	0.46	2.40	7	1
1:B:36:VAL:HG12	1:B:37:ALA:N	0.46	2.24	12	3
1:B:42:VAL:HB	1:B:50:ILE:HD11	0.46	1.87	14	1
1:A:45:THR:N	1:B:29:GLU:OE1	0.46	2.48	19	1
1:A:33:THR:O	1:A:36:VAL:HG23	0.46	2.10	23	1
1:A:75:VAL:HA	1:B:94:TYR:CD1	0.46	2.46	23	1
1:B:28:PHE:HA	1:B:31:ILE:CD1	0.46	2.40	5	5
1:A:36:VAL:HG21	1:B:85:LEU:CG	0.46	2.41	7	1
1:A:49:ASN:O	1:A:79:VAL:CA	0.46	2.63	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LEU:HG	1:B:37:ALA:O	0.46	2.09	14	1
1:B:1:MET:HE2	1:B:6:LEU:HD21	0.46	1.85	21	1
1:B:36:VAL:HG22	1:B:52:PRO:CB	0.46	2.39	21	1
1:A:23:LYS:O	1:A:27:SER:HB3	0.46	2.10	20	5
1:B:45:THR:OG1	1:B:46:GLY:N	0.46	2.46	3	6
1:B:20:SER:C	1:B:22:SER:H	0.46	2.15	3	4
1:B:46:GLY:O	1:B:82:GLY:HA3	0.46	2.11	4	1
1:A:31:ILE:O	1:A:35:THR:HB	0.46	2.10	6	4
1:A:27:SER:HA	1:A:30:LYS:CB	0.46	2.40	10	2
1:B:54:ALA:CA	1:B:75:VAL:HA	0.46	2.35	11	1
1:A:50:ILE:CG1	1:A:79:VAL:HG23	0.46	2.41	15	1
1:A:44:LEU:CD2	1:B:28:PHE:CZ	0.46	2.98	18	1
1:A:77:VAL:CG1	1:B:84:SER:CB	0.46	2.92	18	1
1:A:78:SER:O	1:A:79:VAL:CG1	0.46	2.61	23	1
1:A:92:LEU:CG	1:A:93:LYS:N	0.46	2.79	1	6
1:B:93:LYS:O	1:B:97:PHE:CD2	0.46	2.68	1	2
1:B:92:LEU:HD11	1:B:94:TYR:HA	0.46	1.87	9	2
1:B:22:SER:O	1:B:26:ALA:HB2	0.46	2.11	4	7
1:A:47:PHE:CE1	1:A:48:LEU:CG	0.46	2.98	20	5
1:B:47:PHE:HD2	1:B:85:LEU:HD11	0.46	1.69	10	2
1:A:75:VAL:CB	1:B:94:TYR:CE2	0.46	2.99	14	1
1:A:44:LEU:CD1	1:A:48:LEU:CB	0.46	2.91	18	6
1:A:36:VAL:HG21	1:B:85:LEU:CD1	0.46	2.32	23	2
1:A:81:PRO:CB	1:B:77:VAL:HG11	0.46	2.41	2	1
1:A:7:ILE:HG22	1:A:25:LEU:HD12	0.46	1.86	5	2
1:B:21:VAL:CA	1:B:24:MET:HE2	0.46	2.38	20	3
1:B:48:LEU:HA	1:B:80:LYS:C	0.46	2.36	9	2
1:B:36:VAL:HA	1:B:52:PRO:HG3	0.46	1.86	12	2
1:A:89:ALA:HB1	1:B:75:VAL:CB	0.46	2.41	15	2
1:A:94:TYR:CG	1:A:95:GLU:N	0.46	2.84	16	2
1:A:75:VAL:CG1	1:A:76:GLY:N	0.46	2.79	19	1
1:A:13:ASP:HB3	1:B:27:SER:CB	0.46	2.41	20	1
1:A:94:TYR:CG	1:B:75:VAL:HG12	0.46	2.45	23	1
1:B:28:PHE:CZ	1:B:32:ILE:CD1	0.46	2.98	1	2
1:A:24:MET:CE	1:A:25:LEU:HG	0.46	2.41	22	6
1:A:85:LEU:HD12	1:B:77:VAL:CG2	0.46	2.40	4	1
1:A:18:GLN:O	1:A:19:VAL:O	0.46	2.34	10	4
1:B:48:LEU:HD22	1:B:82:GLY:HA2	0.46	1.87	6	1
1:A:2:ASN:N	1:A:5:GLU:HB2	0.46	2.25	17	2
1:A:47:PHE:CE2	1:B:29:GLU:CG	0.46	2.99	18	6
1:A:45:THR:CG2	1:B:29:GLU:HB3	0.46	2.41	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:VAL:HB	1:A:50:ILE:HG12	0.46	1.87	9	1
1:A:50:ILE:HD12	1:A:50:ILE:C	0.46	2.35	9	1
1:A:79:VAL:C	1:A:80:LYS:HG3	0.46	2.36	9	1
1:A:43:GLN:O	1:B:2:ASN:CB	0.46	2.64	18	1
1:A:3:LYS:CD	1:A:25:LEU:HD13	0.46	2.41	20	1
1:A:27:SER:OG	1:B:13:ASP:CB	0.46	2.64	20	1
1:A:77:VAL:HG11	1:B:84:SER:OG	0.46	2.11	2	1
1:A:37:ALA:C	1:B:92:LEU:CB	0.46	2.89	5	1
1:B:1:MET:CG	1:B:5:GLU:HB3	0.46	2.41	19	2
1:A:37:ALA:CA	1:B:88:ALA:O	0.46	2.63	9	3
1:B:14:THR:HA	1:B:16:LEU:CD1	0.46	2.40	10	3
1:B:2:ASN:O	1:B:6:LEU:HB2	0.46	2.10	12	2
1:B:51:LYS:HD3	1:B:53:VAL:HG13	0.46	1.88	18	1
1:A:20:SER:HG	1:B:14:THR:HG23	0.46	1.70	19	1
1:A:75:VAL:HG21	1:B:92:LEU:CD2	0.46	2.29	19	1
1:A:16:LEU:HD21	1:B:23:LYS:CE	0.46	2.41	20	1
1:A:28:PHE:CA	1:A:31:ILE:CG1	0.46	2.94	23	7
1:A:29:GLU:HG2	1:B:45:THR:CG2	0.46	2.40	3	1
1:A:48:LEU:CD2	1:A:82:GLY:HA2	0.46	2.39	4	1
1:A:91:GLY:C	1:A:93:LYS:H	0.46	2.18	6	4
1:A:92:LEU:HD21	1:B:36:VAL:O	0.46	2.11	4	1
1:B:24:MET:CE	1:B:25:LEU:CD2	0.46	2.94	17	6
1:B:79:VAL:O	1:B:80:LYS:CG	0.46	2.64	4	2
1:A:47:PHE:CB	1:B:33:THR:HG1	0.46	2.24	6	1
1:A:49:ASN:O	1:A:51:LYS:HG2	0.46	2.11	8	1
1:A:82:GLY:C	1:A:84:SER:H	0.46	2.18	19	2
1:B:44:LEU:HD12	1:B:47:PHE:CZ	0.46	2.45	9	1
1:B:52:PRO:O	1:B:53:VAL:CG1	0.46	2.64	10	1
1:A:20:SER:CB	1:A:23:LYS:HG3	0.46	2.41	11	1
1:A:85:LEU:CA	1:B:33:THR:OG1	0.46	2.64	11	2
1:B:54:ALA:N	1:B:75:VAL:HG22	0.46	2.25	13	1
1:A:50:ILE:HD11	1:B:48:LEU:HD21	0.46	1.87	22	1
1:A:7:ILE:HG13	1:A:8:LYS:H	0.45	1.71	4	3
1:B:50:ILE:CD1	1:B:79:VAL:CG1	0.45	2.94	6	1
1:A:37:ALA:CB	1:B:89:ALA:CA	0.45	2.94	7	1
1:B:3:LYS:O	1:B:7:ILE:HD12	0.45	2.11	16	1
1:B:19:VAL:HG22	1:B:24:MET:HG2	0.45	1.87	17	1
1:B:48:LEU:HB3	1:B:80:LYS:HG3	0.45	1.87	20	1
1:B:6:LEU:C	1:B:25:LEU:CD1	0.45	2.89	21	1
1:A:17:THR:CG2	1:A:19:VAL:N	0.45	2.80	13	10
1:B:53:VAL:HG23	1:B:53:VAL:O	0.45	2.11	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ILE:HG12	1:A:79:VAL:HG23	0.45	1.88	18	2
1:A:88:ALA:O	1:A:91:GLY:N	0.45	2.49	15	8
1:A:1:MET:HE1	1:B:31:ILE:HD13	0.45	1.87	6	1
1:A:42:VAL:O	1:A:50:ILE:CG1	0.45	2.64	6	1
1:A:92:LEU:CA	1:B:37:ALA:O	0.45	2.64	9	2
1:A:41:LYS:O	1:A:43:GLN:N	0.45	2.49	15	1
1:A:37:ALA:HB3	1:B:88:ALA:HB1	0.45	1.87	18	1
1:B:36:VAL:CG1	1:B:50:ILE:CG2	0.45	2.93	22	1
1:B:4:THR:HA	1:B:7:ILE:HG23	0.45	1.88	10	2
1:A:24:MET:O	1:A:28:PHE:CB	0.45	2.64	17	5
1:A:28:PHE:HA	1:A:31:ILE:CD1	0.45	2.41	6	5
1:A:75:VAL:CA	1:B:94:TYR:CE1	0.45	3.00	9	1
1:B:46:GLY:O	1:B:83:GLU:CB	0.45	2.65	9	1
1:A:19:VAL:CG2	1:A:20:SER:H	0.45	2.18	12	1
1:A:38:LYS:CA	1:B:92:LEU:HD12	0.45	2.41	13	1
1:A:11:ALA:CA	1:A:14:THR:OG1	0.45	2.64	1	4
1:A:16:LEU:CD1	1:B:20:SER:HB2	0.45	2.42	6	2
1:A:24:MET:HG2	1:B:10:ILE:CG2	0.45	2.42	5	1
1:B:93:LYS:CB	1:B:97:PHE:CZ	0.45	3.00	7	1
1:A:1:MET:CB	1:A:5:GLU:HB3	0.45	2.42	12	1
1:A:19:VAL:HB	1:B:19:VAL:CB	0.45	2.41	15	2
1:A:20:SER:CB	1:B:14:THR:HG23	0.45	2.41	19	1
1:A:3:LYS:HE3	1:A:29:GLU:HG3	0.45	1.89	20	1
1:A:77:VAL:CG1	1:B:84:SER:CA	0.45	2.95	20	1
1:A:6:LEU:HD11	1:B:42:VAL:HB	0.45	1.87	21	1
1:A:12:GLN:CG	1:A:13:ASP:N	0.45	2.80	18	6
1:A:37:ALA:O	1:B:92:LEU:HB3	0.45	2.10	23	5
1:A:54:ALA:HB2	1:A:75:VAL:CG2	0.45	2.34	3	1
1:A:33:THR:CA	1:B:85:LEU:HD13	0.45	2.39	4	1
1:A:52:PRO:HB2	1:A:75:VAL:HG11	0.45	1.87	8	3
1:B:20:SER:HG	1:B:24:MET:N	0.45	2.09	11	2
1:A:36:VAL:HG21	1:B:85:LEU:HD23	0.45	1.89	6	1
1:B:85:LEU:N	1:B:85:LEU:CD2	0.45	2.78	18	2
1:B:20:SER:C	1:B:24:MET:CG	0.45	2.90	14	2
1:B:50:ILE:HD13	1:B:79:VAL:HG23	0.45	1.87	10	1
1:A:7:ILE:O	1:A:11:ALA:CB	0.45	2.65	17	1
1:B:31:ILE:HD12	1:B:32:ILE:HG12	0.45	1.87	17	1
1:B:84:SER:HB3	1:B:86:LYS:HB2	0.45	1.89	18	1
1:B:3:LYS:HD3	1:B:25:LEU:HD13	0.45	1.87	20	1
1:A:33:THR:OG1	1:B:85:LEU:CB	0.45	2.64	23	1
1:A:38:LYS:HD3	1:B:92:LEU:HD13	0.45	1.88	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:ASN:N	1:B:79:VAL:HG23	0.45	2.27	1	1
1:A:33:THR:CA	1:B:85:LEU:HD22	0.45	2.42	4	1
1:B:76:GLY:C	1:B:77:VAL:CG2	0.45	2.89	7	1
1:A:29:GLU:HG2	1:B:44:LEU:HB3	0.45	1.88	9	1
1:B:27:SER:O	1:B:31:ILE:HG12	0.45	2.11	9	2
1:B:47:PHE:CD1	1:B:85:LEU:CD2	0.45	2.99	9	1
1:A:24:MET:O	1:B:10:ILE:CG1	0.45	2.65	11	1
1:A:43:GLN:C	1:A:44:LEU:HD23	0.45	2.36	11	1
1:A:50:ILE:HD13	1:A:79:VAL:HA	0.45	1.89	11	1
1:A:1:MET:HE2	1:A:6:LEU:HD21	0.45	1.84	12	1
1:A:3:LYS:HE2	1:A:28:PHE:HB3	0.45	1.88	15	1
1:B:44:LEU:HD12	1:B:48:LEU:HD12	0.45	1.89	17	3
1:A:92:LEU:HD21	1:B:75:VAL:CG1	0.45	2.41	1	1
1:B:87:LYS:O	1:B:90:GLU:HG3	0.45	2.11	1	1
1:A:7:ILE:HG22	1:A:21:VAL:O	0.45	2.12	4	3
1:B:7:ILE:HB	1:B:21:VAL:O	0.45	2.10	14	1
1:B:47:PHE:HB2	1:B:85:LEU:HD12	0.45	1.88	15	1
1:A:77:VAL:O	1:B:81:PRO:CB	0.45	2.65	16	1
1:B:1:MET:CB	1:B:5:GLU:HB3	0.45	2.42	18	3
1:B:94:TYR:CG	1:B:95:GLU:N	0.45	2.84	16	2
1:B:50:ILE:CD1	1:B:79:VAL:CG2	0.45	2.95	17	1
1:A:35:THR:CG2	1:A:40:ASP:HB2	0.45	2.39	19	1
1:B:34:GLU:CG	1:B:35:THR:N	0.45	2.79	23	1
1:A:14:THR:HG22	1:B:24:MET:HG2	0.45	1.89	2	1
1:A:83:GLU:O	1:A:83:GLU:CG	0.45	2.65	2	1
1:A:47:PHE:O	1:A:81:PRO:CA	0.45	2.65	13	1
1:B:7:ILE:HG13	1:B:8:LYS:H	0.45	1.71	21	3
1:B:47:PHE:HB2	1:B:85:LEU:HB3	0.45	1.89	14	1
1:B:6:LEU:O	1:B:7:ILE:C	0.45	2.60	18	2
1:B:50:ILE:HA	1:B:79:VAL:CG2	0.45	2.27	19	1
1:A:77:VAL:CG1	1:B:85:LEU:CD2	0.45	2.95	23	1
1:B:3:LYS:NZ	1:B:25:LEU:CD1	0.45	2.80	23	1
1:A:90:GLU:HA	1:A:94:TYR:HB2	0.45	1.88	1	1
1:A:45:THR:HG21	1:B:29:GLU:HG3	0.45	1.88	10	4
1:A:80:LYS:C	1:A:80:LYS:CD	0.45	2.90	9	2
1:B:18:GLN:O	1:B:19:VAL:O	0.45	2.35	19	5
1:B:9:ALA:O	1:B:13:ASP:OD2	0.45	2.34	9	1
1:A:7:ILE:HD12	1:A:25:LEU:CD2	0.45	2.41	17	1
1:A:47:PHE:O	1:A:82:GLY:HA2	0.45	2.12	17	1
1:B:27:SER:HA	1:B:30:LYS:CB	0.45	2.42	2	2
1:A:7:ILE:HG22	1:A:25:LEU:HB2	0.45	1.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:PHE:CD2	1:A:29:GLU:N	0.45	2.84	9	1
1:B:12:GLN:CG	1:B:13:ASP:N	0.44	2.80	1	5
1:A:8:LYS:O	1:A:12:GLN:N	0.44	2.49	11	5
1:A:49:ASN:CB	1:A:81:PRO:CD	0.44	2.95	4	1
1:B:1:MET:HA	1:B:5:GLU:HB2	0.44	1.89	6	4
1:A:36:VAL:HG13	1:A:52:PRO:CG	0.44	2.42	9	2
1:A:94:TYR:CD2	1:B:75:VAL:CB	0.44	3.00	10	1
1:A:28:PHE:CE1	1:B:44:LEU:HD21	0.44	2.48	15	1
1:B:50:ILE:HD12	1:B:50:ILE:O	0.44	2.12	19	1
1:B:3:LYS:HZ3	1:B:25:LEU:CD1	0.44	2.26	23	1
1:A:1:MET:HE1	1:B:31:ILE:CD1	0.44	2.42	6	1
1:B:80:LYS:N	1:B:80:LYS:CD	0.44	2.81	19	1
1:A:33:THR:CA	1:B:85:LEU:HD23	0.44	2.37	21	1
1:A:47:PHE:HB2	1:A:85:LEU:CG	0.44	2.42	21	1
1:A:6:LEU:C	1:A:25:LEU:CD1	0.44	2.91	23	1
1:A:47:PHE:CE2	1:A:85:LEU:HD21	0.44	2.47	23	1
1:B:2:ASN:OD1	1:B:3:LYS:N	0.44	2.51	23	1
1:A:35:THR:CG2	1:A:42:VAL:HG22	0.44	2.43	1	1
1:B:50:ILE:CA	1:B:79:VAL:HB	0.44	2.41	1	1
1:A:77:VAL:CG2	1:B:85:LEU:HB3	0.44	2.39	3	1
1:A:20:SER:OG	1:A:23:LYS:HG2	0.44	2.12	6	1
1:A:77:VAL:HG13	1:A:79:VAL:HG12	0.44	1.89	6	1
1:B:2:ASN:C	1:B:4:THR:H	0.44	2.21	6	5
1:B:1:MET:HG2	1:B:5:GLU:HB3	0.44	1.87	12	2
1:A:47:PHE:CB	1:A:82:GLY:HA3	0.44	2.43	15	1
1:A:36:VAL:CG1	1:B:88:ALA:HB1	0.44	2.41	20	1
1:A:47:PHE:HB2	1:A:83:GLU:HB3	0.44	1.90	4	1
1:A:54:ALA:N	1:A:75:VAL:HG22	0.44	2.27	4	1
1:A:85:LEU:CD1	1:B:77:VAL:HG11	0.44	2.42	5	1
1:A:29:GLU:CG	1:B:45:THR:HG22	0.44	2.42	11	3
1:B:7:ILE:HD12	1:B:25:LEU:CD2	0.44	2.42	9	1
1:B:11:ALA:CA	1:B:14:THR:HG1	0.44	2.25	23	3
1:A:3:LYS:CE	1:A:25:LEU:O	0.44	2.65	15	1
1:A:24:MET:HE1	1:A:25:LEU:HG	0.44	1.87	15	1
1:A:31:ILE:HD12	1:A:32:ILE:N	0.44	2.27	15	1
1:B:48:LEU:HD13	1:B:79:VAL:CG2	0.44	2.42	18	1
1:A:81:PRO:HA	1:A:85:LEU:HD13	0.44	1.89	20	1
1:A:14:THR:CG2	1:B:24:MET:HB3	0.44	2.42	2	2
1:A:35:THR:O	1:A:39:GLY:N	0.44	2.50	13	6
1:B:50:ILE:CD1	1:B:79:VAL:HG21	0.44	2.42	1	1
1:A:36:VAL:HG11	1:A:77:VAL:CB	0.44	2.42	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:SER:CB	1:B:23:LYS:CG	0.44	2.96	17	2
1:B:1:MET:CG	1:B:5:GLU:CB	0.44	2.96	6	2
1:B:28:PHE:CA	1:B:31:ILE:HG13	0.44	2.43	14	5
1:A:42:VAL:CG1	1:A:50:ILE:CG2	0.44	2.95	8	1
1:A:3:LYS:CE	1:A:26:ALA:O	0.44	2.66	9	1
1:B:36:VAL:N	1:B:40:ASP:HB2	0.44	2.27	13	1
1:A:20:SER:HB2	1:B:16:LEU:CD2	0.44	2.43	16	1
1:A:47:PHE:HD1	1:A:85:LEU:HD21	0.44	1.72	18	1
1:A:24:MET:CE	1:A:25:LEU:CD2	0.44	2.95	4	4
1:B:7:ILE:C	1:B:7:ILE:HD12	0.44	2.38	8	3
1:B:20:SER:O	1:B:20:SER:OG	0.44	2.34	2	1
1:A:22:SER:O	1:A:26:ALA:HB2	0.44	2.12	11	5
1:A:45:THR:HG21	1:B:29:GLU:CG	0.44	2.42	4	2
1:B:3:LYS:HE3	1:B:29:GLU:CB	0.44	2.43	17	2
1:A:17:THR:HG21	1:B:17:THR:HB	0.44	1.89	7	1
1:A:19:VAL:HG21	1:B:19:VAL:HG12	0.44	1.90	10	2
1:A:47:PHE:CG	1:A:48:LEU:N	0.44	2.86	17	1
1:B:47:PHE:O	1:B:81:PRO:CA	0.44	2.65	17	1
1:B:27:SER:O	1:B:31:ILE:CD1	0.44	2.65	18	1
1:A:94:TYR:HB2	1:B:75:VAL:CG1	0.44	2.43	23	1
1:B:42:VAL:HB	1:B:50:ILE:CG2	0.44	2.43	1	1
1:A:53:VAL:HG23	1:A:76:GLY:HA3	0.44	1.89	6	1
1:B:28:PHE:HA	1:B:31:ILE:HG13	0.44	1.89	6	3
1:B:35:THR:HA	1:B:38:LYS:CB	0.44	2.43	15	2
1:A:92:LEU:HG	1:A:93:LYS:H	0.44	1.73	8	1
1:A:54:ALA:HB2	1:B:97:PHE:CD2	0.44	2.48	9	1
1:B:44:LEU:CB	1:B:48:LEU:HB2	0.44	2.43	21	2
1:A:43:GLN:O	1:B:2:ASN:HA	0.44	2.13	21	2
1:A:85:LEU:HD11	1:B:36:VAL:HG21	0.44	1.90	15	1
1:A:31:ILE:HD11	1:B:6:LEU:CD2	0.44	2.43	18	1
1:B:47:PHE:HB2	1:B:85:LEU:CD1	0.44	2.42	18	2
1:B:75:VAL:HG13	1:B:76:GLY:N	0.44	2.28	17	4
1:A:47:PHE:CB	1:A:83:GLU:HB3	0.44	2.43	4	1
1:B:46:GLY:O	1:B:83:GLU:N	0.44	2.47	4	2
1:A:92:LEU:CG	1:B:37:ALA:O	0.44	2.65	6	1
1:B:85:LEU:O	1:B:86:LYS:C	0.44	2.61	6	1
1:A:81:PRO:CG	1:B:79:VAL:HG12	0.44	2.43	8	1
1:A:3:LYS:HG2	1:A:26:ALA:HA	0.44	1.89	9	1
1:A:7:ILE:CG2	1:A:8:LYS:HE3	0.44	2.40	9	1
1:B:28:PHE:CA	1:B:31:ILE:CG1	0.44	2.95	9	2
1:A:3:LYS:HD3	1:B:45:THR:CG2	0.44	2.42	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:GLY:N	1:A:85:LEU:HD11	0.44	2.27	21	1
1:A:47:PHE:CD2	1:A:85:LEU:CD2	0.44	3.00	23	1
1:A:35:THR:CG2	1:A:40:ASP:HB3	0.44	2.43	7	6
1:A:4:THR:O	1:A:5:GLU:C	0.44	2.61	4	8
1:A:90:GLU:HG3	1:A:91:GLY:N	0.44	2.28	5	2
1:B:20:SER:CB	1:B:23:LYS:HB3	0.44	2.42	10	1
1:A:49:ASN:H	1:A:80:LYS:HB2	0.44	1.73	11	1
1:A:51:LYS:HD2	1:A:53:VAL:HG13	0.44	1.88	11	1
1:B:36:VAL:CG1	1:B:37:ALA:N	0.44	2.81	20	2
1:B:42:VAL:CB	1:B:50:ILE:HD11	0.44	2.42	14	1
1:A:20:SER:OG	1:B:16:LEU:CD1	0.44	2.64	15	1
1:A:86:LYS:HD2	1:B:77:VAL:HG12	0.44	1.89	15	1
1:A:33:THR:O	1:A:36:VAL:HG12	0.44	2.13	20	1
1:A:50:ILE:O	1:A:50:ILE:HG22	0.44	2.13	20	1
1:A:77:VAL:HG12	1:B:84:SER:OG	0.44	2.13	20	1
1:B:50:ILE:C	1:B:50:ILE:HD12	0.44	2.38	21	1
1:A:36:VAL:CG1	1:A:50:ILE:CD1	0.44	2.96	23	1
1:A:10:ILE:HG13	1:B:24:MET:CB	0.43	2.43	1	2
1:A:79:VAL:CG1	1:B:81:PRO:HG3	0.43	2.43	2	1
1:B:75:VAL:HG22	1:B:76:GLY:N	0.43	2.28	3	1
1:A:85:LEU:CD2	1:B:77:VAL:CG1	0.43	2.96	6	1
1:A:36:VAL:O	1:A:52:PRO:CG	0.43	2.66	7	1
1:A:77:VAL:HG12	1:B:86:LYS:CG	0.43	2.42	7	1
1:B:20:SER:HB3	1:B:23:LYS:HB3	0.43	1.89	10	1
1:B:48:LEU:HA	1:B:80:LYS:O	0.43	2.12	14	2
1:A:42:VAL:HG12	1:B:1:MET:HG2	0.43	1.89	15	1
1:A:36:VAL:CG1	1:B:88:ALA:CB	0.43	2.96	20	1
1:B:24:MET:O	1:B:28:PHE:HB2	0.43	2.13	2	1
1:A:32:ILE:O	1:B:85:LEU:HD13	0.43	2.13	4	1
1:B:78:SER:O	1:B:79:VAL:HB	0.43	2.12	8	2
1:B:14:THR:CB	1:B:16:LEU:HD12	0.43	2.43	7	3
1:A:85:LEU:CD2	1:B:33:THR:HA	0.43	2.42	14	1
1:A:25:LEU:HA	1:A:28:PHE:CB	0.43	2.43	15	1
1:A:36:VAL:HG13	1:A:37:ALA:N	0.43	2.28	20	1
1:A:2:ASN:HA	1:B:43:GLN:O	0.43	2.14	3	2
1:A:28:PHE:C	1:A:28:PHE:CD1	0.43	2.96	21	3
1:B:50:ILE:CD1	1:B:79:VAL:HG23	0.43	2.43	4	1
1:A:51:LYS:O	1:A:78:SER:CB	0.43	2.66	6	1
1:A:85:LEU:CD1	1:B:36:VAL:CB	0.43	2.97	8	1
1:B:14:THR:C	1:B:16:LEU:N	0.43	2.76	22	4
1:B:30:LYS:HA	1:B:34:GLU:HG3	0.43	1.90	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:HB2	1:B:42:VAL:CG2	0.43	2.44	1	1
1:A:24:MET:HE3	1:A:25:LEU:CD2	0.43	2.42	9	2
1:B:4:THR:HA	1:B:7:ILE:CG2	0.43	2.43	10	2
1:A:33:THR:CG2	1:A:34:GLU:N	0.43	2.82	2	1
1:A:1:MET:CE	1:A:6:LEU:CD2	0.43	2.96	17	3
1:A:32:ILE:HG22	1:B:47:PHE:CE2	0.43	2.48	8	3
1:B:42:VAL:HG13	1:B:42:VAL:O	0.43	2.14	3	1
1:A:91:GLY:C	1:B:37:ALA:HB1	0.43	2.38	4	1
1:A:92:LEU:CA	1:B:37:ALA:HA	0.43	2.43	4	1
1:A:44:LEU:HD12	1:A:48:LEU:HG	0.43	1.90	7	1
1:A:44:LEU:HB2	1:A:47:PHE:CD1	0.43	2.48	11	1
1:B:32:ILE:HG22	1:B:33:THR:N	0.43	2.28	12	1
1:B:42:VAL:HG23	1:B:50:ILE:HD11	0.43	1.88	19	2
1:A:3:LYS:NZ	1:A:29:GLU:HB2	0.43	2.28	15	1
1:B:3:LYS:CE	1:B:26:ALA:HA	0.43	2.43	15	1
1:B:20:SER:OG	1:B:23:LYS:HB3	0.43	2.14	15	2
1:B:30:LYS:C	1:B:34:GLU:CG	0.43	2.91	20	1
1:A:42:VAL:O	1:A:42:VAL:HG12	0.43	2.13	23	1
1:B:44:LEU:HD12	1:B:48:LEU:CG	0.43	2.43	23	1
1:B:47:PHE:CB	1:B:85:LEU:HD21	0.43	2.44	4	1
1:A:20:SER:C	1:A:22:SER:H	0.43	2.15	13	3
1:A:29:GLU:HG3	1:B:45:THR:CG2	0.43	2.44	6	1
1:A:85:LEU:HD13	1:B:77:VAL:HG13	0.43	1.85	7	1
1:A:20:SER:CB	1:A:23:LYS:CG	0.43	2.97	11	1
1:A:24:MET:CA	1:B:10:ILE:HG13	0.43	2.43	18	1
1:B:42:VAL:O	1:B:50:ILE:HG13	0.43	2.14	19	1
1:B:50:ILE:CG1	1:B:50:ILE:O	0.43	2.66	19	1
1:B:47:PHE:HB2	1:B:85:LEU:HG	0.43	1.89	20	1
1:B:8:LYS:O	1:B:12:GLN:CG	0.43	2.66	22	1
1:B:24:MET:HE3	1:B:24:MET:HB3	0.43	1.60	23	1
1:A:53:VAL:C	1:A:76:GLY:H	0.43	2.21	2	1
1:A:79:VAL:O	1:A:80:LYS:CG	0.43	2.66	2	2
1:B:44:LEU:CG	1:B:48:LEU:HB2	0.43	2.44	4	1
1:A:42:VAL:N	1:A:50:ILE:HG13	0.43	2.28	6	1
1:B:80:LYS:CB	1:B:81:PRO:CD	0.43	2.96	23	2
1:A:1:MET:HA	1:A:5:GLU:HB2	0.43	1.91	8	2
1:B:51:LYS:O	1:B:51:LYS:HD3	0.43	2.13	9	1
1:B:3:LYS:O	1:B:7:ILE:CD1	0.43	2.67	11	2
1:B:20:SER:OG	1:B:23:LYS:HE3	0.43	2.14	14	1
1:B:52:PRO:HB2	1:B:75:VAL:CG2	0.43	2.43	15	1
1:B:19:VAL:HG13	1:B:24:MET:SD	0.43	2.53	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:PHE:HB3	1:B:84:SER:HB3	0.43	1.91	19	1
1:A:82:GLY:H	1:A:85:LEU:HD11	0.43	1.74	21	1
1:A:36:VAL:CG2	1:B:85:LEU:CD1	0.43	2.88	23	1
1:A:75:VAL:HG13	1:B:86:LYS:HG2	0.43	1.91	1	1
1:B:77:VAL:HG12	1:B:79:VAL:CG1	0.43	2.43	1	1
1:A:33:THR:OG1	1:B:47:PHE:CD2	0.43	2.71	3	1
1:B:50:ILE:HG12	1:B:79:VAL:HG23	0.43	1.90	7	2
1:B:8:LYS:O	1:B:12:GLN:HB3	0.43	2.13	16	4
1:B:17:THR:CG2	1:B:19:VAL:N	0.43	2.82	16	6
1:B:94:TYR:C	1:B:94:TYR:CD1	0.43	2.97	5	1
1:B:79:VAL:HG22	1:B:80:LYS:H	0.43	1.71	8	1
1:A:20:SER:HB3	1:A:23:LYS:HG3	0.43	1.89	11	1
1:B:5:GLU:HA	1:B:8:LYS:CE	0.43	2.42	12	1
1:B:34:GLU:O	1:B:37:ALA:C	0.43	2.59	14	1
1:A:22:SER:HA	1:A:25:LEU:HD23	0.43	1.89	16	1
1:B:42:VAL:CG1	1:B:50:ILE:CG2	0.43	2.96	20	1
1:B:48:LEU:CD1	1:B:80:LYS:CG	0.43	2.88	20	1
1:A:28:PHE:CA	1:A:31:ILE:HG13	0.43	2.44	3	8
1:A:85:LEU:N	1:B:33:THR:OG1	0.43	2.52	1	3
1:A:32:ILE:O	1:A:36:VAL:CG2	0.43	2.67	7	1
1:A:37:ALA:HB1	1:B:92:LEU:HG	0.43	1.90	7	1
1:B:97:PHE:CD1	1:B:97:PHE:N	0.43	2.83	7	1
1:B:35:THR:O	1:B:39:GLY:N	0.43	2.52	20	2
1:B:34:GLU:HA	1:B:37:ALA:HB3	0.43	1.90	9	1
1:A:13:ASP:OD2	1:B:31:ILE:HG23	0.43	2.14	10	1
1:A:52:PRO:CB	1:A:75:VAL:CG1	0.43	2.97	11	2
1:A:28:PHE:CD2	1:A:32:ILE:HG13	0.43	2.49	13	1
1:A:36:VAL:HG13	1:B:88:ALA:CB	0.43	2.42	20	1
1:A:47:PHE:HA	1:A:82:GLY:HA3	0.43	1.90	20	1
1:B:4:THR:CA	1:B:7:ILE:HG23	0.43	2.44	1	2
1:A:81:PRO:CB	1:B:77:VAL:O	0.43	2.67	18	3
1:B:89:ALA:O	1:B:92:LEU:HD23	0.43	2.13	5	1
1:B:27:SER:O	1:B:30:LYS:HB3	0.43	2.14	18	2
1:A:14:THR:CG2	1:B:20:SER:HG	0.43	2.27	13	1
1:A:47:PHE:O	1:A:48:LEU:HD23	0.43	2.13	13	1
1:B:3:LYS:CE	1:B:28:PHE:HD1	0.43	2.26	23	1
1:B:48:LEU:HD11	1:B:79:VAL:HG22	0.43	1.90	23	1
1:A:36:VAL:HG11	1:B:85:LEU:HB3	0.43	1.91	1	1
1:A:44:LEU:HB2	1:A:48:LEU:CB	0.43	2.44	12	4
1:B:52:PRO:HB2	1:B:75:VAL:CG1	0.43	2.44	2	1
1:A:2:ASN:O	1:A:4:THR:N	0.43	2.52	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:VAL:O	1:A:80:LYS:HB3	0.43	2.14	6	3
1:A:1:MET:O	1:B:43:GLN:CG	0.43	2.67	7	1
1:A:31:ILE:CD1	1:B:9:ALA:HB1	0.43	2.35	9	1
1:B:36:VAL:HG21	1:B:50:ILE:HD12	0.43	1.91	9	1
1:A:89:ALA:N	1:B:37:ALA:HB2	0.43	2.29	21	3
1:A:79:VAL:HG21	1:B:48:LEU:HD21	0.43	1.91	16	1
1:A:3:LYS:HD3	1:A:25:LEU:HD11	0.43	1.91	17	1
1:B:53:VAL:O	1:B:75:VAL:HG23	0.43	2.14	23	1
1:A:28:PHE:HA	1:A:31:ILE:HG13	0.42	1.90	4	1
1:A:85:LEU:C	1:A:88:ALA:HB3	0.42	2.39	4	1
1:A:36:VAL:CG2	1:B:85:LEU:CD2	0.42	2.97	11	2
1:A:45:THR:HG22	1:A:47:PHE:CE2	0.42	2.49	8	1
1:A:86:LYS:O	1:B:75:VAL:HG11	0.42	2.13	11	1
1:A:24:MET:O	1:A:28:PHE:HB3	0.42	2.14	19	1
1:B:20:SER:OG	1:B:23:LYS:HG2	0.42	2.14	2	1
1:B:35:THR:CG2	1:B:40:ASP:HB3	0.42	2.43	4	4
1:B:47:PHE:HB2	1:B:85:LEU:CD2	0.42	2.43	2	1
1:A:1:MET:HG2	1:A:5:GLU:HB3	0.42	1.91	4	2
1:B:7:ILE:CD1	1:B:25:LEU:CD2	0.42	2.95	9	1
1:A:20:SER:HB3	1:A:23:LYS:CG	0.42	2.45	11	1
1:B:42:VAL:O	1:B:50:ILE:N	0.42	2.52	20	2
1:B:53:VAL:HG11	1:B:78:SER:HB2	0.42	1.90	11	1
1:A:20:SER:OG	1:B:14:THR:HG23	0.42	2.14	19	1
1:A:47:PHE:HB3	1:A:84:SER:CB	0.42	2.43	20	1
1:B:19:VAL:HG13	1:B:20:SER:N	0.42	2.24	1	1
1:A:6:LEU:CB	1:A:25:LEU:CD1	0.42	2.97	5	1
1:A:44:LEU:CD1	1:A:48:LEU:CD1	0.42	2.97	5	1
1:B:25:LEU:HG	1:B:26:ALA:H	0.42	1.69	6	1
1:A:36:VAL:C	1:A:52:PRO:HG3	0.42	2.39	7	1
1:A:77:VAL:CG2	1:B:84:SER:O	0.42	2.66	10	1
1:B:4:THR:O	1:B:5:GLU:C	0.42	2.61	19	2
1:A:36:VAL:CB	1:B:85:LEU:CD2	0.42	2.98	11	1
1:A:20:SER:HB2	1:B:16:LEU:CD1	0.42	2.44	17	1
1:B:94:TYR:CE1	1:B:95:GLU:HG2	0.42	2.49	20	1
1:B:77:VAL:O	1:B:77:VAL:HG13	0.42	2.14	22	1
1:B:49:ASN:O	1:B:80:LYS:N	0.42	2.52	23	1
1:A:10:ILE:O	1:A:14:THR:HG23	0.42	2.14	1	2
1:A:10:ILE:CG1	1:B:24:MET:CB	0.42	2.98	20	3
1:A:90:GLU:HA	1:A:94:TYR:CB	0.42	2.44	1	1
1:A:2:ASN:C	1:A:4:THR:N	0.42	2.77	4	13
1:A:24:MET:C	1:A:27:SER:HG	0.42	2.22	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:SER:O	1:B:22:SER:C	0.42	2.61	7	2
1:A:24:MET:HG2	1:B:14:THR:CG2	0.42	2.45	14	3
1:A:29:GLU:OE1	1:B:45:THR:N	0.42	2.53	9	1
1:B:3:LYS:HE3	1:B:29:GLU:CD	0.42	2.39	9	1
1:B:23:LYS:O	1:B:27:SER:HB3	0.42	2.14	9	1
1:A:78:SER:C	1:A:79:VAL:CG1	0.42	2.93	13	1
1:B:89:ALA:C	1:B:91:GLY:N	0.42	2.74	13	1
1:A:36:VAL:O	1:B:92:LEU:CB	0.42	2.67	14	1
1:B:43:GLN:O	1:B:43:GLN:CG	0.42	2.67	16	1
1:A:35:THR:O	1:A:40:ASP:N	0.42	2.52	19	1
1:A:89:ALA:C	1:A:91:GLY:N	0.42	2.76	20	1
1:A:92:LEU:CD1	1:A:93:LYS:N	0.42	2.83	1	1
1:A:10:ILE:HG21	1:A:24:MET:HE1	0.42	1.91	2	1
1:B:47:PHE:HB3	1:B:84:SER:CB	0.42	2.45	12	3
1:A:42:VAL:CG1	1:A:42:VAL:O	0.42	2.67	6	1
1:B:3:LYS:O	1:B:25:LEU:HD21	0.42	2.14	6	1
1:A:86:LYS:HG3	1:B:77:VAL:HG21	0.42	1.92	7	1
1:B:84:SER:HB2	1:B:86:LYS:HD2	0.42	1.92	10	1
1:A:23:LYS:HG3	1:B:14:THR:HG23	0.42	1.90	11	1
1:A:28:PHE:CZ	1:B:44:LEU:CD2	0.42	3.03	16	2
1:B:78:SER:C	1:B:79:VAL:HG23	0.42	2.34	13	1
1:A:19:VAL:HG23	1:B:16:LEU:CG	0.42	2.45	16	1
1:A:33:THR:OG1	1:B:85:LEU:HG	0.42	2.13	16	1
1:A:84:SER:O	1:A:84:SER:OG	0.42	2.32	17	1
1:B:33:THR:O	1:B:37:ALA:HB2	0.42	2.14	17	1
1:B:94:TYR:CD1	1:B:94:TYR:O	0.42	2.73	19	2
1:A:20:SER:OG	1:A:23:LYS:HB3	0.42	2.14	20	1
1:A:10:ILE:CG1	1:B:24:MET:O	0.42	2.68	21	1
1:A:75:VAL:HG22	1:A:76:GLY:N	0.42	2.30	1	1
1:B:47:PHE:HA	1:B:83:GLU:H	0.42	1.74	2	1
1:B:92:LEU:O	1:B:93:LYS:HB2	0.42	2.15	22	6
1:A:1:MET:CA	1:A:5:GLU:HB3	0.42	2.45	4	3
1:B:2:ASN:C	1:B:4:THR:N	0.42	2.77	8	10
1:A:36:VAL:HG11	1:B:85:LEU:HG	0.42	1.89	8	1
1:B:94:TYR:CE1	1:B:95:GLU:HG3	0.42	2.50	20	2
1:B:53:VAL:N	1:B:76:GLY:O	0.42	2.52	10	1
1:A:10:ILE:HG23	1:B:24:MET:CB	0.42	2.45	19	1
1:A:2:ASN:O	1:A:3:LYS:C	0.42	2.62	20	1
1:A:81:PRO:CB	1:B:77:VAL:HG13	0.42	2.45	23	1
1:A:3:LYS:HE2	1:A:26:ALA:HA	0.42	1.90	6	3
1:A:7:ILE:CG2	1:A:21:VAL:O	0.42	2.67	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:GLY:C	1:A:93:LYS:N	0.42	2.78	4	1
1:A:51:LYS:HG2	1:A:78:SER:CB	0.42	2.44	6	1
1:A:31:ILE:CG2	1:B:13:ASP:OD2	0.42	2.68	7	1
1:B:94:TYR:CE1	1:B:95:GLU:CD	0.42	2.98	8	1
1:B:52:PRO:HB2	1:B:75:VAL:HG21	0.42	1.91	15	2
1:A:14:THR:CG2	1:B:19:VAL:CG2	0.42	2.97	10	1
1:A:37:ALA:HA	1:B:88:ALA:O	0.42	2.14	10	1
1:B:35:THR:CG2	1:B:40:ASP:O	0.42	2.68	11	1
1:B:51:LYS:O	1:B:51:LYS:CG	0.42	2.68	11	1
1:A:44:LEU:CD2	1:B:28:PHE:CE1	0.42	3.03	12	2
1:B:33:THR:O	1:B:37:ALA:HB3	0.42	2.15	14	1
1:B:7:ILE:CG1	1:B:25:LEU:HD12	0.42	2.44	22	1
1:A:14:THR:CB	1:A:16:LEU:CD1	0.42	2.98	1	1
1:A:77:VAL:O	1:A:77:VAL:HG13	0.42	2.14	2	2
1:A:42:VAL:HB	1:A:50:ILE:HD11	0.42	1.90	10	2
1:B:21:VAL:CG2	1:B:22:SER:N	0.42	2.83	6	2
1:B:82:GLY:O	1:B:84:SER:N	0.42	2.49	7	1
1:B:28:PHE:CE1	1:B:32:ILE:CG1	0.42	3.02	8	1
1:A:25:LEU:CD1	1:A:29:GLU:OE2	0.42	2.68	11	1
1:A:8:LYS:O	1:A:12:GLN:CG	0.42	2.67	17	2
1:B:5:GLU:O	1:B:9:ALA:N	0.42	2.50	18	1
1:A:24:MET:HE3	1:A:24:MET:HB2	0.42	1.74	19	1
1:B:25:LEU:CD1	1:B:26:ALA:N	0.42	2.80	20	1
1:A:85:LEU:HA	1:B:33:THR:OG1	0.42	2.15	22	1
1:A:1:MET:HB2	1:B:42:VAL:HG12	0.42	1.92	23	1
1:A:90:GLU:OE1	1:A:94:TYR:CD2	0.42	2.73	17	2
1:A:20:SER:HB3	1:B:16:LEU:HD13	0.42	1.90	2	1
1:A:45:THR:OG1	1:A:46:GLY:N	0.42	2.51	14	7
1:B:51:LYS:O	1:B:51:LYS:HG3	0.42	2.14	2	1
1:A:36:VAL:CG1	1:B:85:LEU:CD2	0.42	2.97	5	1
1:B:1:MET:HG2	1:B:5:GLU:CB	0.42	2.45	6	1
1:B:1:MET:HA	1:B:5:GLU:HB3	0.42	1.91	8	1
1:B:50:ILE:HG12	1:B:80:LYS:CG	0.42	2.45	9	2
1:B:28:PHE:CG	1:B:32:ILE:HD13	0.42	2.50	12	1
1:B:87:LYS:O	1:B:90:GLU:HB2	0.42	2.15	14	1
1:A:42:VAL:CG2	1:A:50:ILE:CG2	0.42	2.98	15	1
1:B:14:THR:O	1:B:16:LEU:N	0.42	2.53	16	1
1:A:6:LEU:CD1	1:B:42:VAL:CG2	0.42	2.94	20	1
1:A:85:LEU:O	1:A:89:ALA:HB2	0.42	2.15	21	1
1:B:47:PHE:CZ	1:B:48:LEU:HB3	0.42	2.49	23	1
1:A:42:VAL:O	1:A:50:ILE:N	0.42	2.53	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD13	1:B:28:PHE:CE1	0.42	2.50	1	2
1:A:85:LEU:CD2	1:B:77:VAL:CG2	0.42	2.98	1	1
1:A:28:PHE:O	1:A:32:ILE:CB	0.42	2.68	4	1
1:A:85:LEU:O	1:A:88:ALA:CB	0.42	2.65	4	1
1:A:42:VAL:H	1:A:50:ILE:HD11	0.42	1.75	6	1
1:B:83:GLU:O	1:B:85:LEU:CA	0.42	2.67	6	1
1:A:23:LYS:O	1:A:27:SER:HB2	0.42	2.15	7	1
1:B:47:PHE:CZ	1:B:48:LEU:HD12	0.42	2.50	8	1
1:B:4:THR:O	1:B:7:ILE:CB	0.42	2.68	9	1
1:A:11:ALA:O	1:A:15:GLY:CA	0.42	2.68	10	1
1:A:37:ALA:HB2	1:B:88:ALA:HA	0.42	1.92	10	1
1:A:47:PHE:CA	1:A:82:GLY:HA3	0.42	2.45	15	1
1:B:43:GLN:HA	1:B:48:LEU:O	0.42	2.15	18	1
1:B:25:LEU:CD1	1:B:29:GLU:OE2	0.42	2.68	19	1
1:B:49:ASN:C	1:B:50:ILE:HG23	0.42	2.39	19	1
1:B:41:LYS:CG	1:B:51:LYS:CB	0.42	2.98	20	1
1:B:42:VAL:CG2	1:B:50:ILE:CG2	0.42	2.97	23	1
1:A:81:PRO:CG	1:B:77:VAL:O	0.41	2.69	3	1
1:A:8:LYS:HE3	1:A:8:LYS:N	0.41	2.29	9	1
1:B:47:PHE:CG	1:B:48:LEU:N	0.41	2.88	9	1
1:A:2:ASN:CB	1:B:43:GLN:O	0.41	2.68	12	2
1:A:31:ILE:O	1:A:32:ILE:C	0.41	2.61	15	1
1:A:21:VAL:C	1:A:24:MET:HE2	0.41	2.39	17	1
1:A:20:SER:HB2	1:A:23:LYS:CB	0.41	2.45	19	1
1:A:75:VAL:N	1:B:94:TYR:CG	0.41	2.88	19	1
1:A:44:LEU:CB	1:A:48:LEU:HB2	0.41	2.46	2	1
1:A:1:MET:HA	1:A:5:GLU:HB3	0.41	1.93	23	2
1:A:88:ALA:HB2	1:B:33:THR:HA	0.41	1.92	4	1
1:A:47:PHE:HD1	1:A:85:LEU:HD12	0.41	1.74	7	1
1:A:1:MET:CG	1:A:5:GLU:CB	0.41	2.98	19	2
1:B:53:VAL:O	1:B:76:GLY:CA	0.41	2.68	15	1
1:A:20:SER:HG	1:A:23:LYS:HB3	0.41	1.75	18	1
1:A:7:ILE:HA	1:A:25:LEU:CD1	0.41	2.45	1	1
1:A:22:SER:O	1:A:26:ALA:HB3	0.41	2.15	1	1
1:A:4:THR:HG22	1:A:8:LYS:HZ1	0.41	1.73	4	1
1:A:36:VAL:HA	1:A:52:PRO:HG3	0.41	1.92	6	1
1:A:7:ILE:HG12	1:A:25:LEU:CG	0.41	2.45	9	1
1:B:23:LYS:O	1:B:27:SER:N	0.41	2.46	23	2
1:B:80:LYS:C	1:B:80:LYS:CD	0.41	2.93	11	1
1:A:94:TYR:CE1	1:B:75:VAL:HA	0.41	2.50	14	1
1:B:36:VAL:HA	1:B:40:ASP:O	0.41	2.14	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:51:LYS:HD3	1:B:51:LYS:O	0.41	2.15	18	2
1:A:20:SER:CB	1:B:16:LEU:HD21	0.41	2.32	19	1
1:B:3:LYS:HD3	1:B:25:LEU:CD1	0.41	2.45	20	1
1:A:28:PHE:CE1	1:A:32:ILE:CG1	0.41	3.03	1	1
1:A:85:LEU:CD2	1:B:77:VAL:HG13	0.41	2.45	1	1
1:B:48:LEU:HD22	1:B:48:LEU:HA	0.41	1.69	11	2
1:B:36:VAL:CG2	1:B:50:ILE:C	0.41	2.94	2	1
1:A:24:MET:HB3	1:B:10:ILE:CG2	0.41	2.43	4	2
1:A:2:ASN:O	1:A:6:LEU:HB2	0.41	2.15	6	1
1:A:20:SER:OG	1:A:23:LYS:CE	0.41	2.68	7	1
1:A:48:LEU:HD22	1:B:50:ILE:HD11	0.41	1.92	7	1
1:A:76:GLY:C	1:A:77:VAL:CG2	0.41	2.93	8	1
1:A:6:LEU:CD2	1:B:31:ILE:HD12	0.41	2.46	9	1
1:A:24:MET:CB	1:B:10:ILE:HG13	0.41	2.45	9	1
1:B:44:LEU:HD12	1:B:47:PHE:CE2	0.41	2.51	9	1
1:A:4:THR:O	1:A:7:ILE:N	0.41	2.54	22	2
1:A:37:ALA:HB2	1:B:88:ALA:HB3	0.41	1.91	13	1
1:B:77:VAL:O	1:B:77:VAL:HG22	0.41	2.15	13	1
1:A:75:VAL:HG11	1:B:92:LEU:HD21	0.41	1.91	15	1
1:B:16:LEU:HD12	1:B:17:THR:HB	0.41	1.91	16	1
1:B:91:GLY:C	1:B:93:LYS:H	0.41	2.23	19	1
1:B:50:ILE:HB	1:B:80:LYS:CD	0.41	2.46	20	1
1:A:29:GLU:CG	1:B:47:PHE:HE2	0.41	2.29	2	1
1:A:52:PRO:C	1:A:53:VAL:CG1	0.41	2.94	18	2
1:A:2:ASN:CA	1:A:6:LEU:HD12	0.41	2.45	4	2
1:B:47:PHE:CD2	1:B:85:LEU:HD11	0.41	2.51	6	1
1:A:33:THR:HA	1:A:36:VAL:HG21	0.41	1.92	7	1
1:B:45:THR:HG23	1:B:47:PHE:HD1	0.41	1.74	7	1
1:A:32:ILE:HG21	1:B:47:PHE:HZ	0.41	1.71	9	1
1:B:7:ILE:HG22	1:B:21:VAL:O	0.41	2.15	12	1
1:B:50:ILE:HA	1:B:79:VAL:O	0.41	2.15	15	1
1:A:35:THR:CG2	1:A:40:ASP:O	0.41	2.69	16	1
1:A:30:LYS:HA	1:A:34:GLU:HG3	0.41	1.93	20	1
1:B:90:GLU:HG2	1:B:91:GLY:N	0.41	2.31	20	1
1:A:11:ALA:O	1:A:15:GLY:HA2	0.41	2.15	23	1
1:A:77:VAL:CG2	1:B:85:LEU:HG	0.41	2.45	23	1
1:A:94:TYR:CB	1:B:75:VAL:CG1	0.41	2.98	23	1
1:A:10:ILE:O	1:A:14:THR:CG2	0.41	2.69	7	2
1:A:48:LEU:HD23	1:A:48:LEU:HA	0.41	1.63	2	3
1:B:85:LEU:O	1:B:88:ALA:CB	0.41	2.68	4	1
1:B:44:LEU:HB2	1:B:47:PHE:CE1	0.41	2.50	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:THR:CG2	1:B:17:THR:CG2	0.41	2.98	7	1
1:B:85:LEU:CD2	1:B:85:LEU:C	0.41	2.93	7	1
1:A:27:SER:HB3	1:B:13:ASP:CG	0.41	2.41	9	1
1:A:3:LYS:HD2	1:B:45:THR:HB	0.41	1.92	11	1
1:A:94:TYR:HE1	1:B:75:VAL:CB	0.41	2.28	11	1
1:A:9:ALA:O	1:A:13:ASP:HB2	0.41	2.16	16	4
1:B:1:MET:CA	1:B:5:GLU:HB2	0.41	2.45	14	1
1:B:3:LYS:O	1:B:7:ILE:CG1	0.41	2.69	17	1
1:B:28:PHE:C	1:B:28:PHE:CD1	0.41	2.97	17	1
1:B:80:LYS:N	1:B:81:PRO:CD	0.41	2.83	20	1
1:A:43:GLN:N	1:B:1:MET:O	0.41	2.52	22	1
1:A:88:ALA:HB3	1:B:37:ALA:CB	0.41	2.45	3	2
1:A:49:ASN:HB3	1:A:81:PRO:CD	0.41	2.46	4	1
1:B:93:LYS:O	1:B:97:PHE:CE2	0.41	2.73	7	1
1:A:2:ASN:C	1:A:4:THR:H	0.41	2.24	8	1
1:A:45:THR:HG22	1:A:47:PHE:CE1	0.41	2.51	9	1
1:B:85:LEU:HB3	1:B:88:ALA:CB	0.41	2.42	10	1
1:B:79:VAL:O	1:B:80:LYS:HB3	0.41	2.16	13	1
1:B:45:THR:O	1:B:45:THR:OG1	0.41	2.37	14	1
1:A:7:ILE:HG13	1:A:25:LEU:CG	0.41	2.45	15	1
1:A:25:LEU:HG	1:A:26:ALA:H	0.41	1.74	16	1
1:A:90:GLU:HA	1:A:94:TYR:HB3	0.41	1.91	20	1
1:B:2:ASN:N	1:B:5:GLU:HB2	0.41	2.30	20	1
1:B:36:VAL:HG23	1:B:52:PRO:CG	0.41	2.46	20	1
1:B:4:THR:O	1:B:7:ILE:N	0.41	2.53	21	1
1:A:81:PRO:O	1:A:83:GLU:N	0.41	2.54	1	1
1:A:7:ILE:CG2	1:A:25:LEU:HD12	0.41	2.45	5	1
1:B:49:ASN:HB3	1:B:81:PRO:CD	0.41	2.44	6	1
1:A:81:PRO:HG3	1:B:77:VAL:O	0.41	2.16	7	1
1:A:16:LEU:CB	1:B:19:VAL:HG23	0.41	2.42	14	1
1:B:52:PRO:C	1:B:53:VAL:CG1	0.41	2.93	14	1
1:A:14:THR:HG21	1:B:24:MET:CB	0.41	2.46	18	2
1:A:83:GLU:HA	1:A:86:LYS:HB2	0.41	1.93	21	1
1:A:44:LEU:CG	1:A:48:LEU:HB2	0.41	2.45	22	1
1:B:45:THR:O	1:B:84:SER:CB	0.41	2.68	23	1
1:B:1:MET:CE	1:B:6:LEU:CD2	0.41	2.99	10	2
1:A:1:MET:SD	1:B:42:VAL:HG22	0.41	2.55	2	1
1:A:34:GLU:O	1:A:37:ALA:N	0.41	2.54	3	1
1:B:3:LYS:CG	1:B:29:GLU:CD	0.41	2.94	22	3
1:B:85:LEU:O	1:B:89:ALA:HB2	0.41	2.16	3	1
1:B:92:LEU:O	1:B:93:LYS:HG2	0.41	2.16	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:VAL:H	1:A:50:ILE:CD1	0.41	2.29	6	1
1:A:47:PHE:CD2	1:B:33:THR:OG1	0.41	2.73	6	1
1:A:89:ALA:HA	1:B:37:ALA:HB1	0.41	1.91	6	1
1:A:13:ASP:CB	1:B:27:SER:OG	0.41	2.69	22	2
1:A:42:VAL:CG1	1:B:6:LEU:CD1	0.41	2.95	9	1
1:A:51:LYS:CE	1:A:78:SER:CB	0.41	2.99	9	1
1:B:89:ALA:HA	1:B:92:LEU:CD2	0.41	2.45	9	1
1:B:34:GLU:O	1:B:37:ALA:HB3	0.41	2.15	11	1
1:B:48:LEU:HD23	1:B:48:LEU:HA	0.41	1.73	12	1
1:B:3:LYS:CE	1:B:29:GLU:HB3	0.41	2.45	13	1
1:B:47:PHE:CB	1:B:84:SER:CB	0.41	2.99	19	2
1:B:52:PRO:HB2	1:B:75:VAL:HG11	0.41	1.93	13	1
1:A:45:THR:HG22	1:B:29:GLU:CG	0.41	2.46	14	1
1:A:75:VAL:HB	1:B:94:TYR:CD1	0.41	2.50	14	1
1:A:94:TYR:CD1	1:B:75:VAL:HA	0.41	2.51	14	1
1:A:94:TYR:CD2	1:A:95:GLU:N	0.41	2.88	15	1
1:A:4:THR:O	1:A:7:ILE:HG22	0.41	2.16	17	1
1:A:35:THR:HA	1:A:38:LYS:CB	0.41	2.46	18	1
1:A:3:LYS:HD3	1:A:25:LEU:CD1	0.41	2.46	19	1
1:A:36:VAL:HB	1:B:85:LEU:CD2	0.41	2.46	22	1
1:A:51:LYS:O	1:A:51:LYS:HD3	0.41	2.16	22	1
1:A:85:LEU:CD2	1:B:32:ILE:HG22	0.41	2.46	22	1
1:B:51:LYS:HG3	1:B:78:SER:HB3	0.41	1.93	1	1
1:B:20:SER:OG	1:B:23:LYS:C	0.41	2.63	2	1
1:A:24:MET:HA	1:A:27:SER:OG	0.41	2.15	4	1
1:B:47:PHE:CD2	1:B:85:LEU:HB2	0.41	2.51	8	1
1:A:42:VAL:HB	1:A:50:ILE:CD1	0.41	2.45	10	1
1:A:35:THR:HG21	1:A:42:VAL:HB	0.41	1.92	13	1
1:A:80:LYS:HG2	1:A:81:PRO:N	0.41	2.30	17	1
1:B:75:VAL:CG1	1:B:76:GLY:N	0.41	2.84	18	1
1:B:7:ILE:CG2	1:B:22:SER:HA	0.41	2.46	19	1
1:B:7:ILE:CD1	1:B:22:SER:HA	0.41	2.46	22	1
1:A:36:VAL:HG11	1:B:85:LEU:CB	0.40	2.46	1	1
1:A:42:VAL:CB	1:A:50:ILE:CG1	0.40	2.99	9	1
1:A:27:SER:OG	1:B:13:ASP:HB3	0.40	2.17	10	1
1:A:19:VAL:HG23	1:B:16:LEU:CB	0.40	2.42	11	1
1:B:46:GLY:C	1:B:84:SER:HB2	0.40	2.41	11	1
1:A:47:PHE:CD1	1:A:85:LEU:HD11	0.40	2.42	13	1
1:A:43:GLN:HG3	1:B:1:MET:O	0.40	2.16	14	1
1:A:19:VAL:C	1:B:16:LEU:HD13	0.40	2.41	17	1
1:A:84:SER:OG	1:B:77:VAL:HG23	0.40	2.16	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:GLN:HA	1:A:48:LEU:O	0.40	2.15	21	1
1:A:50:ILE:HG22	1:A:79:VAL:HG21	0.40	1.90	3	1
1:A:85:LEU:O	1:A:88:ALA:CA	0.40	2.69	4	1
1:A:91:GLY:O	1:A:93:LYS:N	0.40	2.55	4	1
1:A:24:MET:CB	1:B:10:ILE:CG1	0.40	2.98	6	1
1:A:53:VAL:N	1:A:75:VAL:CG2	0.40	2.84	6	1
1:A:44:LEU:CD1	1:A:48:LEU:HB3	0.40	2.46	7	1
1:A:6:LEU:CD1	1:B:44:LEU:HD21	0.40	2.46	9	1
1:B:92:LEU:O	1:B:92:LEU:CG	0.40	2.69	10	1
1:A:24:MET:CE	1:A:25:LEU:HB3	0.40	2.45	11	1
1:A:79:VAL:CB	1:B:81:PRO:HD3	0.40	2.46	11	1
1:B:40:ASP:CG	1:B:41:LYS:N	0.40	2.79	13	1
1:A:24:MET:SD	1:A:25:LEU:HD23	0.40	2.56	15	1
1:B:11:ALA:O	1:B:15:GLY:N	0.40	2.54	15	1
1:A:49:ASN:HB3	1:A:81:PRO:CG	0.40	2.45	17	1
1:A:3:LYS:CG	1:A:29:GLU:CD	0.40	2.94	18	1
1:A:36:VAL:HA	1:A:40:ASP:CB	0.40	2.46	20	1
1:A:47:PHE:HB2	1:A:85:LEU:CD1	0.40	2.46	22	1
1:A:47:PHE:CD2	1:B:29:GLU:HG2	0.40	2.51	23	1
1:A:37:ALA:CA	1:B:89:ALA:HA	0.40	2.46	1	1
1:B:27:SER:O	1:B:30:LYS:N	0.40	2.54	2	1
1:B:33:THR:HG22	1:B:34:GLU:N	0.40	2.31	3	2
1:A:20:SER:HB3	1:A:23:LYS:HB3	0.40	1.92	4	1
1:B:7:ILE:O	1:B:11:ALA:HB2	0.40	2.17	7	1
1:A:27:SER:O	1:A:30:LYS:N	0.40	2.54	10	1
1:A:1:MET:O	1:A:2:ASN:HB3	0.40	2.17	13	1
1:A:54:ALA:CB	1:A:75:VAL:HA	0.40	2.47	14	1
1:A:27:SER:CB	1:B:13:ASP:HB3	0.40	2.46	15	1
1:B:30:LYS:O	1:B:34:GLU:HG2	0.40	2.14	22	1
1:A:77:VAL:CG1	1:B:85:LEU:HD21	0.40	2.45	23	1
1:B:2:ASN:O	1:B:3:LYS:C	0.40	2.62	23	1
1:B:3:LYS:HZ3	1:B:25:LEU:HD12	0.40	1.76	23	1
1:B:25:LEU:O	1:B:28:PHE:HB3	0.40	2.16	1	1
1:A:92:LEU:CD2	1:B:37:ALA:C	0.40	2.94	2	1
1:B:3:LYS:HG2	1:B:29:GLU:OE1	0.40	2.15	3	1
1:B:81:PRO:C	1:B:83:GLU:H	0.40	2.24	8	1
1:A:94:TYR:HE1	1:B:54:ALA:HA	0.40	1.76	9	1
1:B:54:ALA:CA	1:B:75:VAL:CA	0.40	2.95	10	1
1:A:8:LYS:O	1:A:12:GLN:HB3	0.40	2.17	15	1
1:A:50:ILE:CG2	1:A:77:VAL:CG2	0.40	2.99	15	1
1:B:50:ILE:HG12	1:B:80:LYS:HG2	0.40	1.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ASP:OD1	1:A:50:ILE:CG2	0.40	2.68	19	1
1:B:48:LEU:HD13	1:B:49:ASN:H	0.40	1.75	19	1
1:B:89:ALA:O	1:B:90:GLU:C	0.40	2.65	22	1
1:A:25:LEU:O	1:A:29:GLU:OE1	0.40	2.39	3	1
1:A:39:GLY:HA3	1:B:97:PHE:CE1	0.40	2.51	7	1
1:B:50:ILE:CB	1:B:80:LYS:HG2	0.40	2.47	9	1
1:A:3:LYS:CD	1:A:29:GLU:OE1	0.40	2.70	11	1
1:B:48:LEU:CD2	1:B:80:LYS:O	0.40	2.70	14	1
1:A:5:GLU:O	1:A:8:LYS:HG3	0.40	2.17	15	1
1:A:77:VAL:HG12	1:A:79:VAL:HG13	0.40	1.89	19	1
1:A:84:SER:HA	1:B:77:VAL:HG21	0.40	1.92	19	1
1:A:83:GLU:O	1:A:87:LYS:N	0.40	2.40	20	1
1:B:52:PRO:CB	1:B:75:VAL:CG1	0.40	2.99	20	1
1:B:33:THR:HA	1:B:36:VAL:HG21	0.40	1.94	23	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	74/99 (75%)	54±2 (72±3%)	12±2 (17±3%)	8±2 (11±3%)	1	8
1	B	76/99 (77%)	55±3 (72±3%)	13±2 (18±3%)	8±2 (10±2%)	1	9
All	All	3450/4554 (76%)	2494 (72%)	591 (17%)	365 (11%)	1	8

All 52 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	19	VAL	23
1	A	21	VAL	23
1	B	19	VAL	23
1	B	21	VAL	23
1	B	45	THR	23
1	A	79	VAL	22
1	A	45	THR	21

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Mol	Chain	Res	Type	Models (Total)
1	B	79	VAL	20
1	B	77	VAL	20
1	A	77	VAL	19
1	B	75	VAL	16
1	A	75	VAL	15
1	B	84	SER	9
1	B	85	LEU	9
1	A	93	LYS	7
1	A	84	SER	6
1	A	85	LEU	6
1	A	95	GLU	6
1	B	2	ASN	6
1	A	81	PRO	5
1	A	53	VAL	5
1	B	78	SER	4
1	A	78	SER	3
1	A	82	GLY	3
1	B	39	GLY	3
1	A	3	LYS	3
1	B	3	LYS	3
1	B	82	GLY	3
1	A	17	THR	3
1	A	54	ALA	3
1	B	16	LEU	2
1	A	80	LYS	2
1	B	81	PRO	2
1	B	94	TYR	2
1	B	80	LYS	2
1	A	94	TYR	2
1	A	2	ASN	2
1	A	41	LYS	2
1	A	92	LEU	1
1	B	95	GLU	1
1	B	96	ASP	1
1	B	97	PHE	1
1	A	46	GLY	1
1	B	47	PHE	1
1	B	41	LYS	1
1	B	93	LYS	1
1	A	42	VAL	1
1	A	83	GLU	1
1	B	92	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	40	ASP	1
1	B	44	LEU	1
1	B	54	ALA	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	62/81 (77%)	34±2 (55±4%)	28±2 (45±4%)	0	3
1	B	64/81 (79%)	36±3 (56±4%)	28±3 (44±4%)	0	3
All	All	2898/3726 (78%)	1612 (56%)	1286 (44%)	0	3

All 113 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	17	THR	23
1	B	17	THR	23
1	B	33	THR	23
1	A	7	ILE	22
1	B	7	ILE	22
1	B	40	ASP	22
1	A	24	MET	21
1	A	40	ASP	21
1	B	92	LEU	21
1	A	23	LYS	20
1	A	33	THR	20
1	B	3	LYS	20
1	B	19	VAL	20
1	A	19	VAL	19
1	A	38	LYS	19
1	B	31	ILE	19
1	A	14	THR	19
1	A	20	SER	18
1	A	45	THR	18
1	A	92	LEU	18
1	B	24	MET	18

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Mol	Chain	Res	Type	Models (Total)
1	B	32	ILE	18
1	B	38	LYS	18
1	B	45	THR	18
1	B	80	LYS	18
1	A	78	SER	17
1	B	10	ILE	17
1	B	23	LYS	17
1	A	75	VAL	17
1	A	85	LEU	17
1	B	25	LEU	17
1	A	3	LYS	16
1	A	80	LYS	16
1	B	20	SER	16
1	B	85	LEU	16
1	A	31	ILE	16
1	A	32	ILE	16
1	A	93	LYS	15
1	B	29	GLU	15
1	B	78	SER	15
1	A	28	PHE	15
1	B	5	GLU	14
1	B	8	LYS	14
1	B	14	THR	14
1	B	84	SER	14
1	A	29	GLU	14
1	A	90	GLU	14
1	B	96	ASP	14
1	A	84	SER	14
1	A	5	GLU	13
1	A	8	LYS	13
1	A	10	ILE	13
1	A	25	LEU	13
1	B	36	VAL	13
1	B	48	LEU	13
1	B	51	LYS	13
1	B	75	VAL	13
1	B	28	PHE	13
1	A	36	VAL	12
1	A	50	ILE	12
1	B	97	PHE	12
1	B	49	ASN	11
1	B	93	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	B	87	LYS	10
1	B	94	TYR	10
1	A	48	LEU	10
1	A	86	LYS	10
1	A	1	MET	9
1	A	41	LYS	9
1	A	49	ASN	9
1	A	87	LYS	9
1	B	41	LYS	9
1	A	16	LEU	9
1	A	94	TYR	8
1	B	50	ILE	8
1	B	86	LYS	8
1	A	51	LYS	7
1	B	43	GLN	7
1	B	90	GLU	7
1	A	79	VAL	7
1	B	16	LEU	7
1	B	1	MET	7
1	B	83	GLU	6
1	A	12	GLN	6
1	A	43	GLN	6
1	B	79	VAL	5
1	A	22	SER	5
1	A	83	GLU	5
1	A	35	THR	4
1	B	22	SER	4
1	A	42	VAL	4
1	A	6	LEU	4
1	B	6	LEU	3
1	B	12	GLN	3
1	B	2	ASN	3
1	B	47	PHE	2
1	A	30	LYS	2
1	A	77	VAL	2
1	A	34	GLU	2
1	B	35	THR	2
1	A	2	ASN	2
1	A	4	THR	2
1	A	53	VAL	2
1	A	95	GLU	1
1	B	27	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	B	30	LYS	1
1	B	77	VAL	1
1	B	42	VAL	1
1	B	21	VAL	1
1	B	95	GLU	1
1	A	13	ASP	1
1	A	47	PHE	1
1	B	34	GLU	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 oligosaccharides 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

No chemical shift data were provided