



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 05:23 AM UTC

PDB ID : 6UD0 / pdb_00006ud0
BMRB ID : 30675
Title : Solution-state NMR structural ensemble of human Tsg101 UEV in complex with K63-linked diubiquitin
Authors : Strickland, M.; Watanabe, S.; Bonn, S.M.; Camara, C.M.; Fushman, D.; Carter, C.A.; Tjandra, N.
Deposited on : 2019-09-18

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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

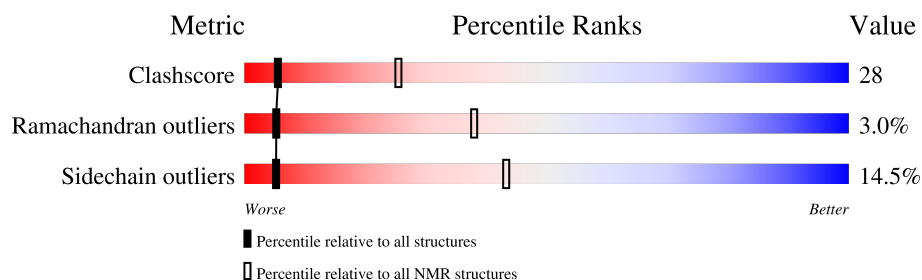
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 13%.

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	76	62% 33% . .
2	B	77	61% 32% . 5%
3	C	145	48% 41% 6% . .

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:73, C:3-C:143 (214)	0.06	4
2	B:1-B:73 (73)	0.08	6

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4766 atoms, of which 2415 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1232	378	629	107	117	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ARG	LYS	engineered mutation	UNP P0CG47

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
2	B	77	Total	C	H	N	O	S	0
			1241	382	631	106	121	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77	ASP	MET	engineered mutation	UNP P0CG47

- Molecule 3 is a protein called Tumor susceptibility gene 101 protein.

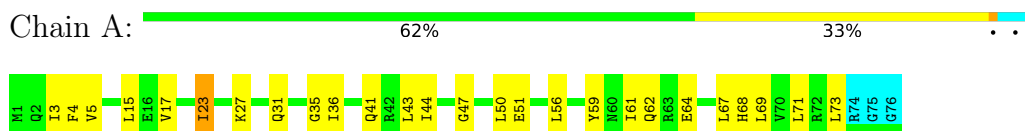
Mol	Chain	Residues	Atoms						Trace
3	C	141	Total	C	H	N	O	S	0
			2293	743	1155	182	207	6	

4 Residue-property plots [i](#)

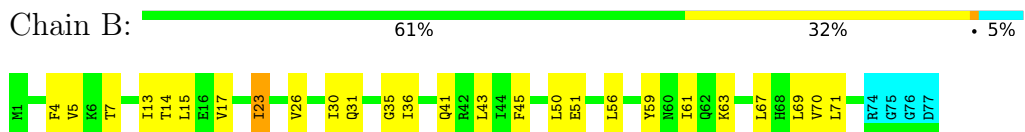
4.1 Average score per residue in the NMR ensemble

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

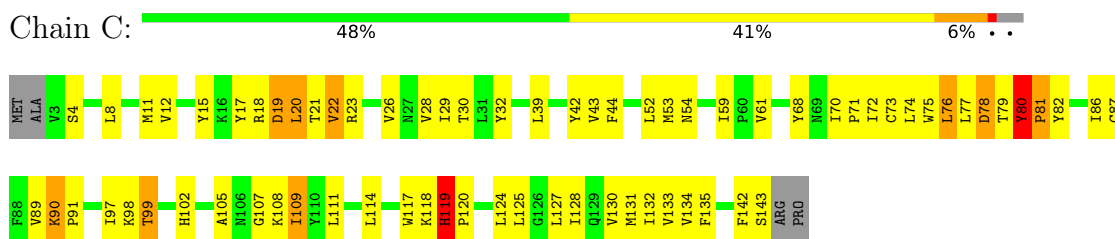
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin



- Molecule 3: Tumor susceptibility gene 101 protein



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

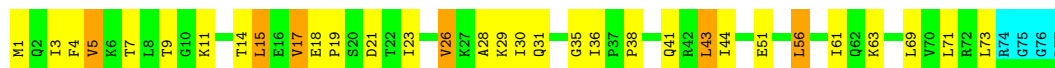
4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin

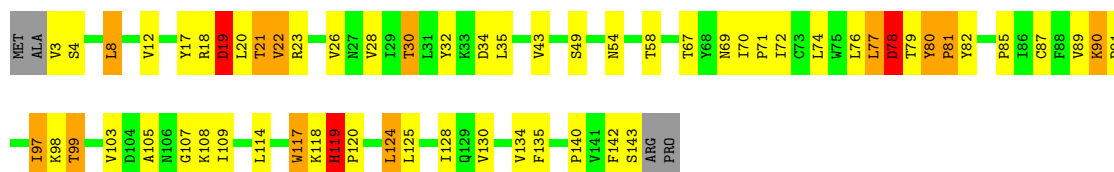




- Molecule 2: Ubiquitin



- Molecule 3: Tumor susceptibility gene 101 protein



4.2.2 Score per residue for model 2

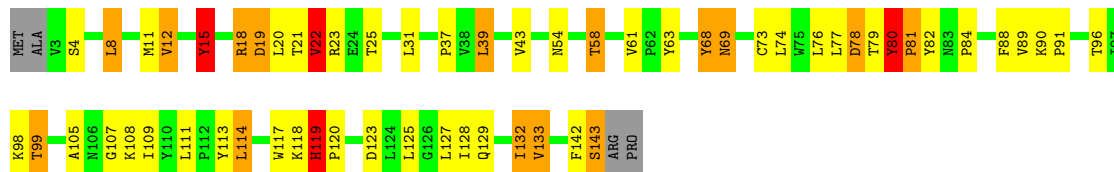
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin



- Molecule 3: Tumor susceptibility gene 101 protein



4.2.3 Score per residue for model 3

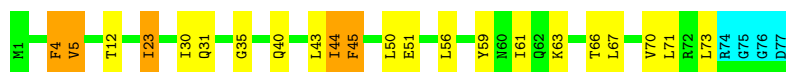
- Molecule 1: Ubiquitin

Chain A:  71% 17% 7% . .



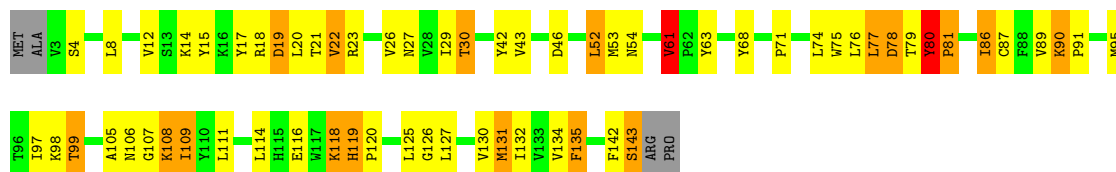
- Molecule 2: Ubiquitin

Chain B:  66% 22% 6% 5%



- Molecule 3: Tumor susceptibility gene 101 protein

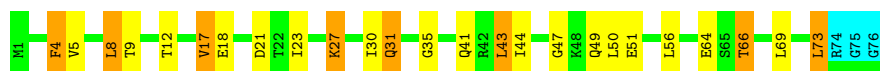
Chain C:  53% 31% 12% . .



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Ubiquitin

Chain A:  63% 22% 11% .

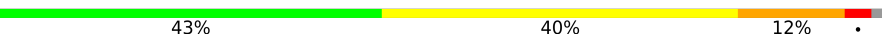


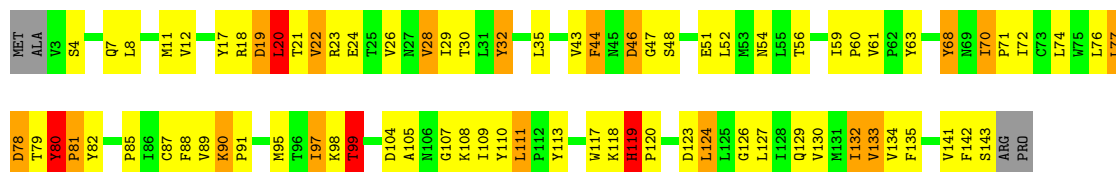
- Molecule 2: Ubiquitin

Chain B:  61% 23% 10% 5%



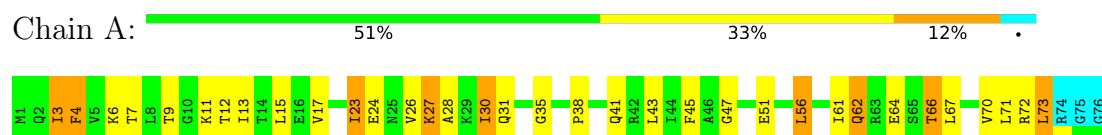
- Molecule 3: Tumor susceptibility gene 101 protein

Chain C:  43% 40% 12% . .

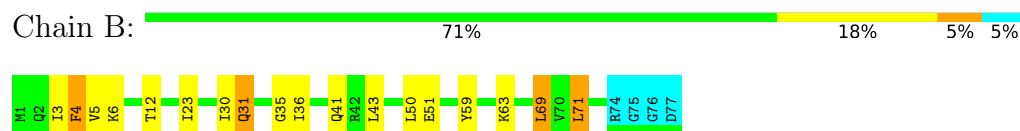


4.2.5 Score per residue for model 5

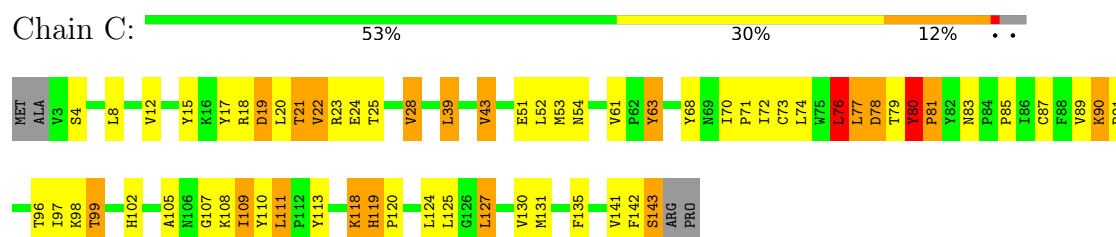
• Molecule 1: Ubiquitin



• Molecule 2: Ubiquitin

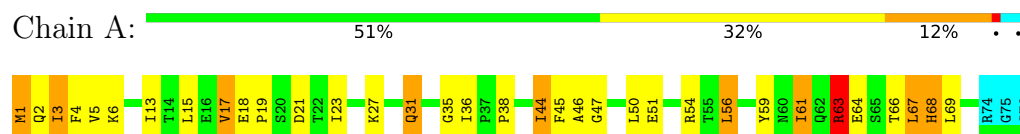


• Molecule 3: Tumor susceptibility gene 101 protein

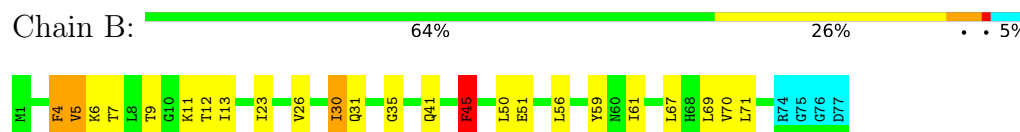


4.2.6 Score per residue for model 6

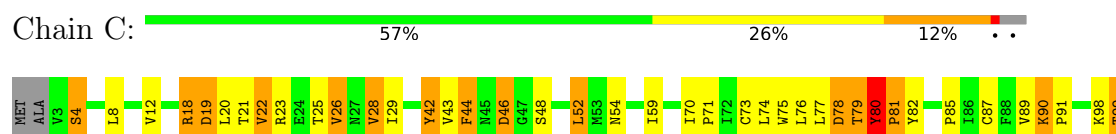
• Molecule 1: Ubiquitin

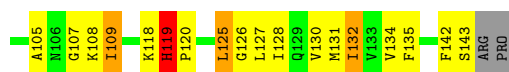


• Molecule 2: Ubiquitin



• Molecule 3: Tumor susceptibility gene 101 protein

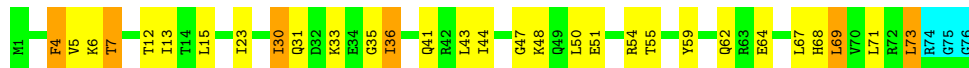




4.2.7 Score per residue for model 7

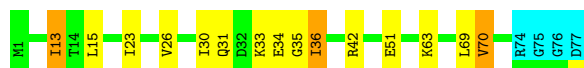
- Molecule 1: Ubiquitin

Chain A: 57% 32% 8% .



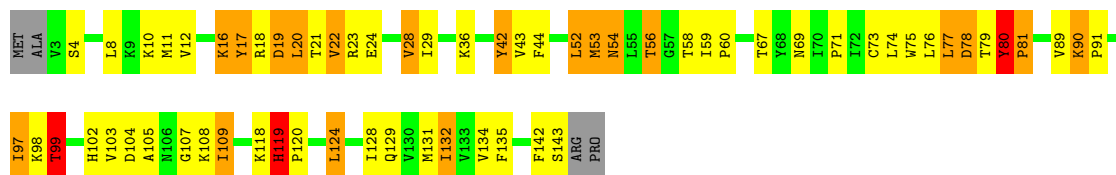
- Molecule 2: Ubiquitin

Chain B: 75% 16% . 5%



- Molecule 3: Tumor susceptibility gene 101 protein

Chain C: 53% 29% 13% . .



4.2.8 Score per residue for model 8

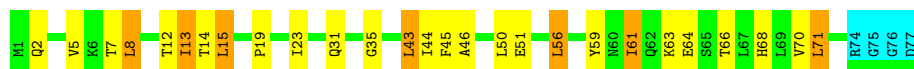
- Molecule 1: Ubiquitin

Chain A: 64% 29% . .



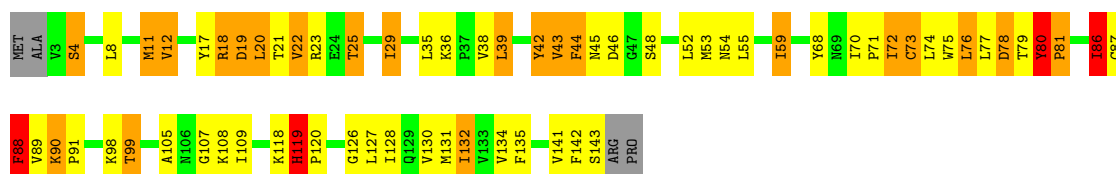
- Molecule 2: Ubiquitin

Chain B: 60% 26% 9% 5%



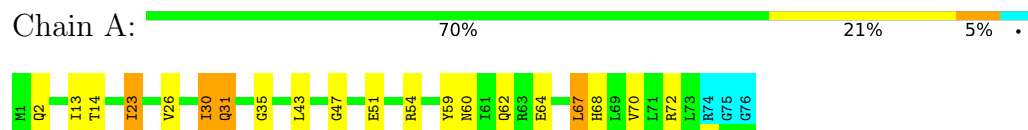
- Molecule 3: Tumor susceptibility gene 101 protein

Chain C: 51% 28% 15% . .

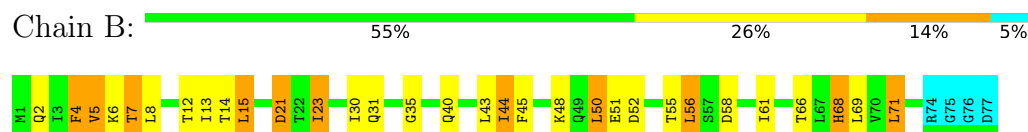


4.2.9 Score per residue for model 9

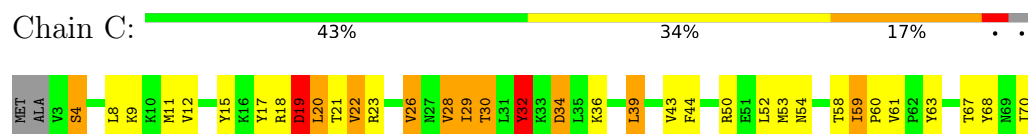
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin

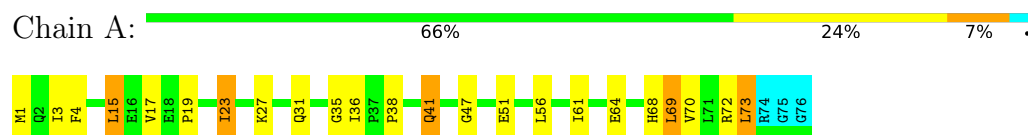


- Molecule 3: Tumor susceptibility gene 101 protein

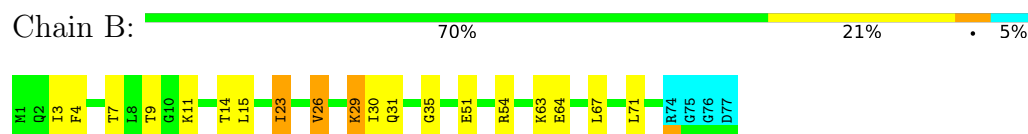


4.2.10 Score per residue for model 10

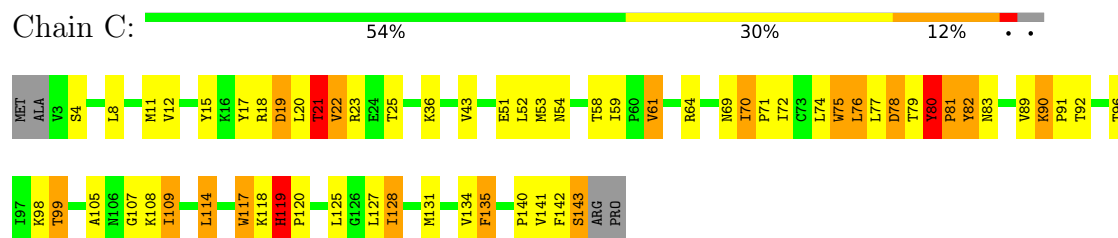
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin

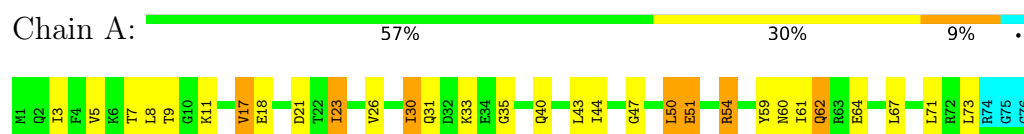


- Molecule 3: Tumor susceptibility gene 101 protein

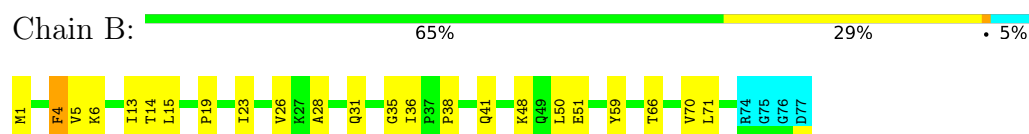


4.2.11 Score per residue for model 11

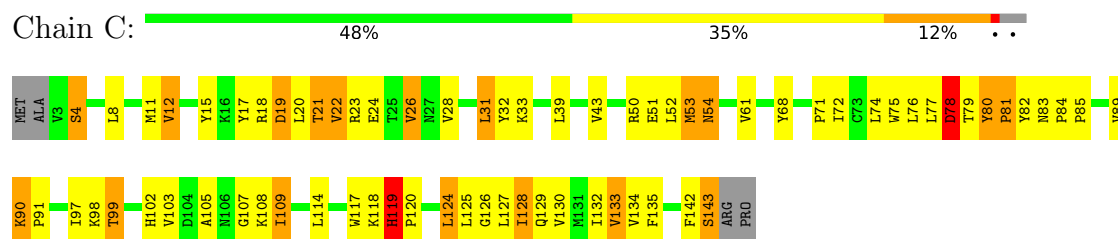
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin

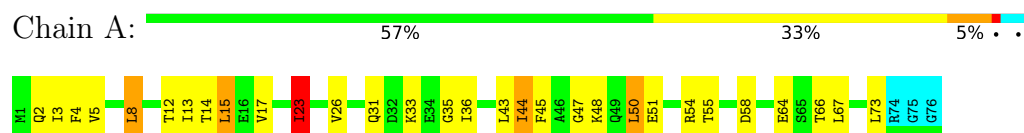


- Molecule 3: Tumor susceptibility gene 101 protein



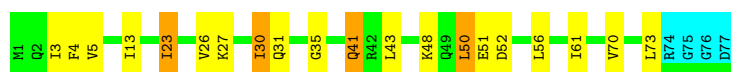
4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin



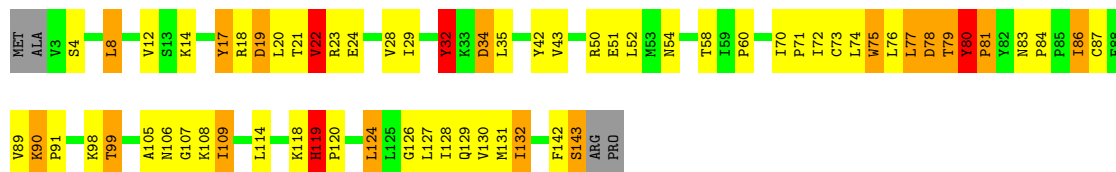
- Molecule 2: Ubiquitin





- Molecule 3: Tumor susceptibility gene 101 protein

Chain C: 



4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin

Chain A: 



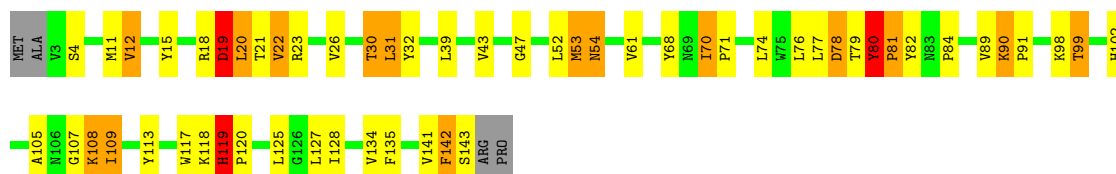
- Molecule 2: Ubiquitin

Chain B: 



- Molecule 3: Tumor susceptibility gene 101 protein

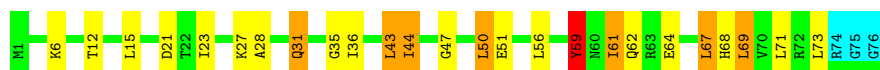
Chain C: 



4.2.14 Score per residue for model 14

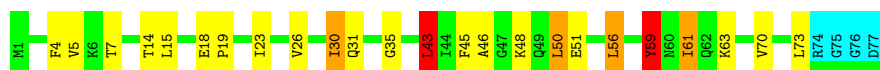
- Molecule 1: Ubiquitin

Chain A: 



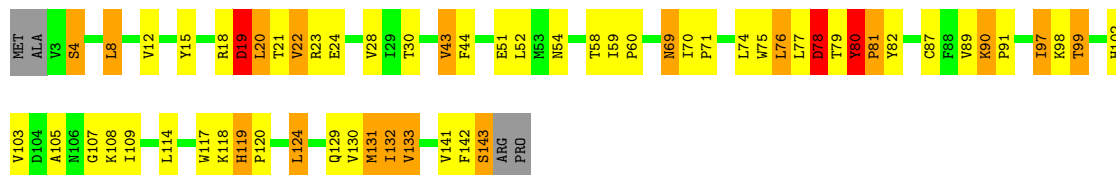
- Molecule 2: Ubiquitin

Chain B:  64% 23% 5% • 5%



- Molecule 3: Tumor susceptibility gene 101 protein

Chain C:  56% 28% 12% • •



4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin

Chain A:  64% 24% 8% •

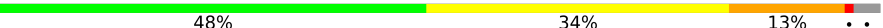


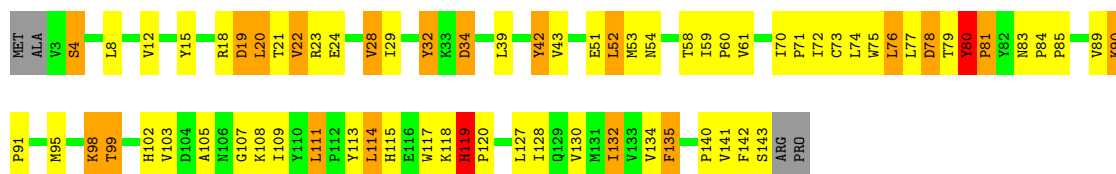
- Molecule 2: Ubiquitin

Chain B:  65% 23% 5% • 5%



- Molecule 3: Tumor susceptibility gene 101 protein

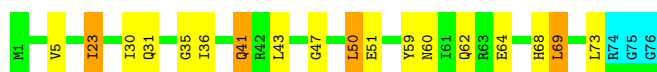
Chain C:  48% 34% 13% • •



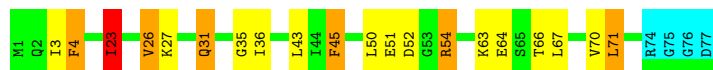
4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin

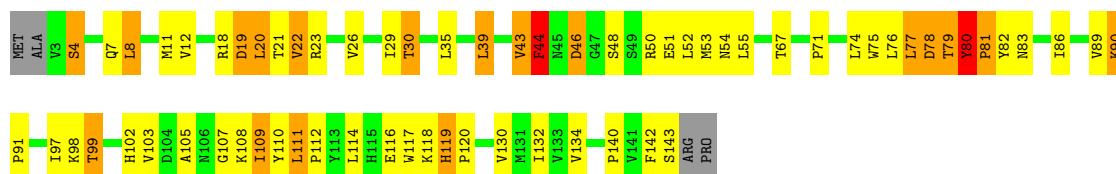
Chain A:  72% 18% 5% •



- Molecule 2: Ubiquitin



- Molecule 3: Tumor susceptibility gene 101 protein

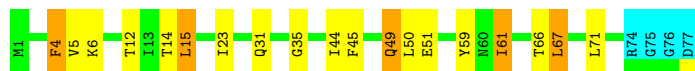


4.2.17 Score per residue for model 17

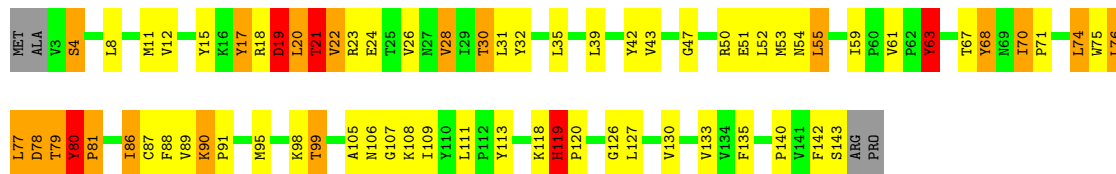
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin

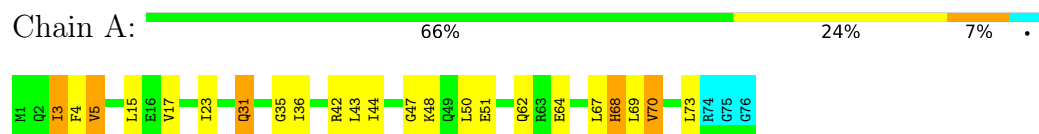


- Molecule 3: Tumor susceptibility gene 101 protein

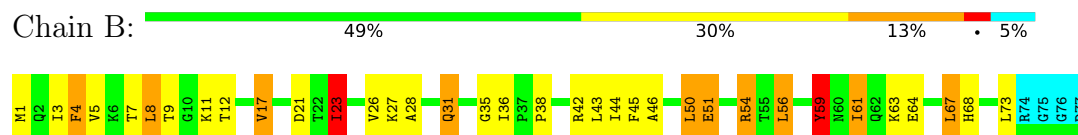


4.2.18 Score per residue for model 18

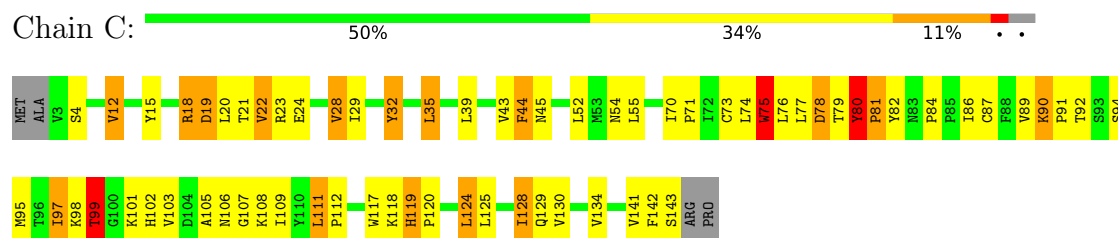
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin

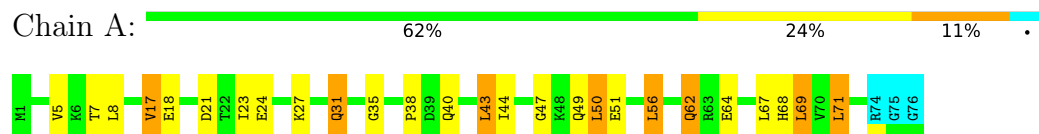


- Molecule 3: Tumor susceptibility gene 101 protein

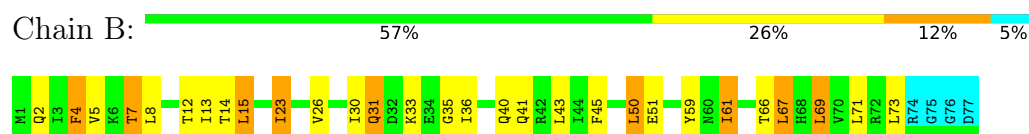


4.2.19 Score per residue for model 19

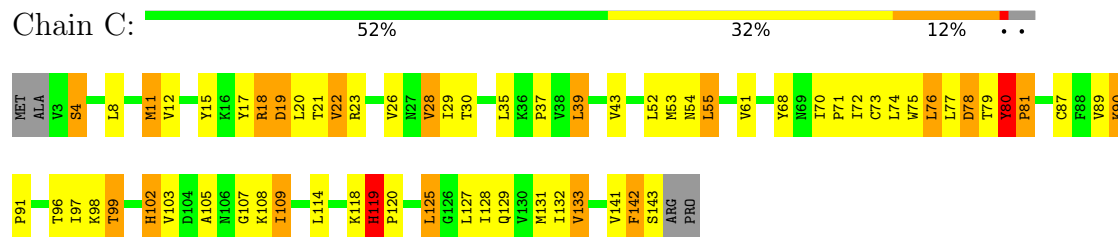
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin

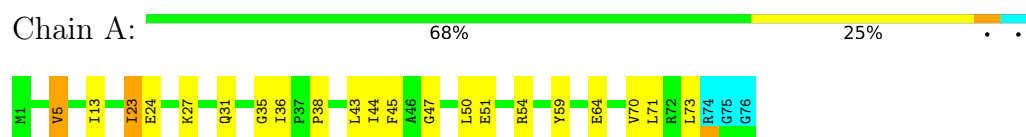


- Molecule 3: Tumor susceptibility gene 101 protein

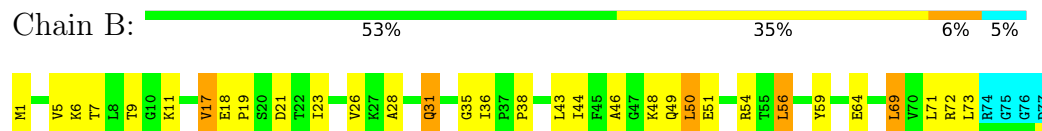


4.2.20 Score per residue for model 20

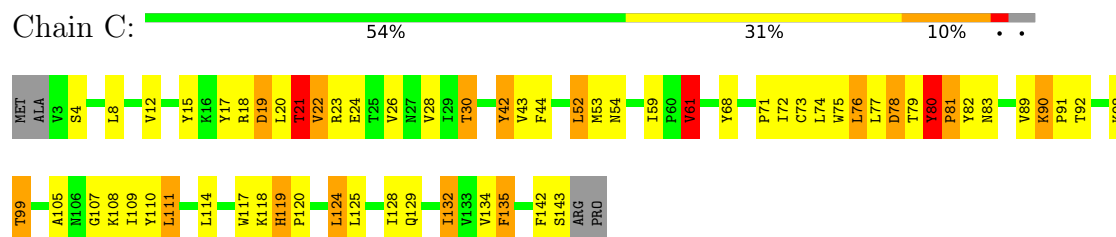
• Molecule 1: Ubiquitin



• Molecule 2: Ubiquitin



• Molecule 3: Tumor susceptibility gene 101 protein



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.51
X-PLOR NIH	structure calculation	2.51

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	542
Number of shifts mapped to atoms	541
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

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	0.61±0.04	0±1/591 (0.1± 0.1%)	1.09±0.04	1±1/798 (0.1± 0.1%)
2	B	0.61±0.03	0±0/589 (0.0± 0.1%)	1.10±0.04	1±1/795 (0.1± 0.1%)
3	C	0.67±0.03	0±1/1170 (0.0± 0.0%)	1.16±0.04	4±2/1596 (0.3± 0.1%)
All	All	0.64	18/47000 (0.0%)	1.13	106/63780 (0.2%)

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

Mol	Chain	Chirality	Planarity
3	C	0.0±0.0	0.2±0.4
All	All	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	63	ARG	CD-NE	8.77	1.58	1.46	6	1
2	B	41	GLN	CA-CB	-8.19	1.39	1.53	2	1
3	C	63	TYR	CB-CG	-6.87	1.36	1.51	17	1
3	C	61	VAL	CA-CB	6.50	1.62	1.54	20	1
2	B	23	ILE	CA-CB	-6.41	1.46	1.54	16	4
3	C	32	TYR	CB-CG	-6.19	1.38	1.51	12	3
1	A	23	ILE	CA-CB	-5.73	1.47	1.54	3	4
3	C	75	TRP	CA-CB	5.66	1.62	1.53	18	2
1	A	63	ARG	NE-CZ	5.56	1.39	1.33	6	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	61	ILE	N-CA-CB	12.89	126.34	111.39	14	1
3	C	12	VAL	CB-CA-C	10.48	128.47	111.29	2	1
3	C	81	PRO	CB-CA-C	-10.29	95.90	111.44	20	5
3	C	63	TYR	N-CA-CB	9.65	126.51	110.59	17	1
3	C	32	TYR	CA-CB-CG	-9.50	96.80	113.90	12	3
3	C	76	LEU	N-CA-CB	-8.98	96.47	110.57	5	6
3	C	63	TYR	CB-CA-C	-8.46	97.89	110.24	2	2
3	C	81	PRO	N-CA-CB	8.39	111.29	103.41	10	10
3	C	68	TYR	N-CA-CB	8.36	123.70	110.57	17	1
1	A	68	HIS	CA-CB-CG	-8.33	105.47	113.80	18	8
2	B	23	ILE	N-CA-CB	8.26	121.78	110.54	2	1
2	B	61	ILE	N-CA-CB	8.13	120.27	111.00	18	1
1	A	1	MET	N-CA-CB	-7.83	97.19	110.50	6	1
3	C	61	VAL	CB-CA-C	-7.70	97.35	111.36	20	2
2	B	59	TYR	N-CA-CB	7.47	121.55	110.49	14	2
1	A	61	ILE	CB-CA-C	-7.19	103.46	111.23	14	1
3	C	21	THR	N-CA-CB	7.17	121.90	109.72	20	3
3	C	80	TYR	N-CA-CB	6.99	122.81	110.37	15	1
2	B	56	LEU	N-CA-CB	6.81	120.35	110.20	15	2
3	C	80	TYR	CB-CA-C	-6.79	96.79	110.17	14	3
3	C	81	PRO	CA-N-CD	-6.76	102.53	112.00	11	20
3	C	20	LEU	N-CA-CB	6.62	121.68	110.49	4	1
1	A	59	TYR	N-CA-CB	6.46	120.05	110.49	14	1
3	C	88	PHE	N-CA-CB	6.45	121.48	110.77	8	1
2	B	45	PHE	CB-CA-C	-6.36	99.96	110.14	16	1
2	B	23	ILE	CB-CA-C	6.34	120.70	112.14	2	1
3	C	21	THR	CB-CA-C	-6.17	100.59	110.84	17	1
3	C	80	TYR	CA-CB-CG	-6.12	102.89	113.90	6	2
3	C	15	TYR	N-CA-CB	5.48	119.36	110.43	2	1
1	A	43	LEU	CB-CA-C	5.46	118.54	109.53	19	1
2	B	68	HIS	CA-CB-CG	-5.45	108.35	113.80	2	2
3	C	80	TYR	CB-CG-CD2	-5.43	112.65	120.80	14	1
2	B	45	PHE	CA-CB-CG	-5.38	108.42	113.80	14	2
3	C	86	ILE	N-CA-CB	5.38	117.48	111.89	8	1
3	C	117	TRP	CB-CA-C	-5.34	100.71	109.53	10	2
3	C	117	TRP	CB-CG-CD2	5.25	134.15	126.80	1	1
3	C	12	VAL	N-CA-CB	-5.18	102.68	111.23	8	1
3	C	102	HIS	CA-CB-CG	-5.17	108.63	113.80	19	1
2	B	43	LEU	CB-CA-C	5.14	118.02	109.53	14	1
3	C	119	HIS	CB-CA-C	-5.09	100.14	110.17	2	8
3	C	44	PHE	CB-CA-C	5.08	120.53	110.42	16	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
3	C	32	TYR	Sidechain	2
3	C	80	TYR	Sidechain	2

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	584	610	610	25±10
2	B	582	608	608	26±11
3	C	1138	1155	1155	83±16
All	All	46080	47460	47459	2588

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:132:ILE:HA	3:C:135:PHE:CE1	1.12	1.79	3	2
3:C:80:TYR:CE2	3:C:85:PRO:HA	1.08	1.84	6	3
1:A:59:TYR:CD1	1:A:59:TYR:O	1.06	2.09	13	1
3:C:32:TYR:CE2	3:C:58:THR:O	1.06	2.08	9	3
3:C:89:VAL:HG21	3:C:97:ILE:HD11	1.03	1.30	1	2
3:C:77:LEU:O	3:C:79:THR:N	1.03	1.89	1	20
3:C:15:TYR:CE2	3:C:17:TYR:O	1.01	2.13	17	1
1:A:2:GLN:H	1:A:63:ARG:HD2	0.98	1.18	6	1
3:C:32:TYR:HE2	3:C:58:THR:O	0.97	1.34	9	3
3:C:15:TYR:CD1	3:C:78:ASP:O	0.96	2.19	17	1
3:C:89:VAL:O	3:C:91:PRO:HD3	0.95	1.60	19	20
3:C:35:LEU:HD13	3:C:55:LEU:HD12	0.94	1.37	17	1
2:B:23:ILE:CD1	2:B:54:ARG:O	0.93	2.15	16	1
2:B:23:ILE:CD1	2:B:51:GLU:O	0.92	2.16	16	1
2:B:23:ILE:CG1	2:B:51:GLU:O	0.91	2.18	16	5
2:B:23:ILE:HD11	2:B:54:ARG:O	0.91	1.64	16	1
2:B:5:VAL:HG22	2:B:67:LEU:HD22	0.91	1.42	17	2
3:C:21:THR:OG1	3:C:80:TYR:CE1	0.90	2.24	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:27:LYS:NZ	2:B:36:ILE:O	0.90	2.04	2	1
1:A:63:ARG:HD3	1:A:64:GLU:H	0.89	1.26	6	1
3:C:111:LEU:HD21	3:C:134:VAL:HG21	0.88	1.44	16	2
3:C:17:TYR:CG	3:C:17:TYR:O	0.87	2.26	5	5
3:C:61:VAL:O	3:C:68:TYR:CE2	0.87	2.27	4	1
1:A:23:ILE:CG2	1:A:51:GLU:O	0.87	2.22	1	1
2:B:23:ILE:HD12	2:B:23:ILE:H	0.87	1.28	16	1
1:A:23:ILE:HD13	1:A:50:LEU:HB3	0.87	1.46	16	1
3:C:76:LEU:HA	3:C:80:TYR:CD2	0.86	2.04	6	3
3:C:77:LEU:O	3:C:80:TYR:CD2	0.86	2.28	17	3
3:C:16:LYS:CE	3:C:78:ASP:O	0.85	2.24	7	1
2:B:23:ILE:HG12	2:B:52:ASP:HA	0.84	1.48	12	1
2:B:23:ILE:CD1	2:B:23:ILE:H	0.84	1.83	16	1
3:C:114:LEU:O	3:C:117:TRP:HD1	0.84	1.56	1	5
2:B:23:ILE:HD13	2:B:51:GLU:O	0.84	1.73	16	1
3:C:68:TYR:CD1	3:C:70:ILE:HD13	0.84	2.08	13	2
3:C:15:TYR:CD1	3:C:80:TYR:OH	0.83	2.32	14	1
3:C:12:VAL:HB	3:C:15:TYR:CE2	0.82	2.09	2	1
3:C:61:VAL:HB	3:C:135:PHE:CE1	0.82	2.09	3	2
1:A:63:ARG:HD3	1:A:64:GLU:N	0.82	1.90	6	1
2:B:23:ILE:HG12	2:B:51:GLU:O	0.82	1.75	16	3
2:B:31:GLN:CD	2:B:36:ILE:O	0.81	2.23	16	1
2:B:23:ILE:HD12	2:B:23:ILE:N	0.81	1.87	16	1
1:A:15:LEU:HD23	1:A:17:VAL:HG13	0.80	1.53	10	1
3:C:80:TYR:N	3:C:81:PRO:CD	0.80	2.45	17	20
2:B:14:THR:C	2:B:15:LEU:HD22	0.80	2.02	10	1
3:C:80:TYR:HE2	3:C:85:PRO:HA	0.80	1.28	6	2
3:C:89:VAL:HG23	3:C:109:ILE:HD11	0.80	1.53	19	2
1:A:45:PHE:CD2	1:A:61:ILE:HD11	0.80	2.12	6	2
3:C:61:VAL:HG12	3:C:68:TYR:O	0.80	1.76	3	5
2:B:23:ILE:HD13	2:B:52:ASP:CA	0.79	2.07	16	1
2:B:45:PHE:CZ	2:B:67:LEU:HD12	0.79	2.13	19	2
3:C:16:LYS:HE2	3:C:78:ASP:O	0.79	1.76	7	1
1:A:4:PHE:CD1	1:A:12:THR:HG23	0.79	2.12	1	1
3:C:117:TRP:CE3	3:C:117:TRP:O	0.79	2.36	14	5
3:C:79:THR:C	3:C:81:PRO:HD2	0.78	2.03	10	20
1:A:63:ARG:CZ	1:A:63:ARG:HA	0.78	2.08	6	1
2:B:23:ILE:HD11	2:B:50:LEU:HD23	0.78	1.55	8	2
2:B:18:GLU:O	2:B:56:LEU:HD21	0.78	1.78	14	1
1:A:2:GLN:O	1:A:63:ARG:CD	0.78	2.32	6	1
1:A:2:GLN:N	1:A:63:ARG:HD2	0.78	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:41:GLN:CD	2:B:69:LEU:HD21	0.78	2.03	2	1
1:A:2:GLN:H	1:A:63:ARG:CD	0.78	1.91	6	1
1:A:23:ILE:HG21	1:A:51:GLU:O	0.78	1.78	1	1
3:C:15:TYR:CE1	3:C:18:ARG:HB3	0.78	2.13	2	1
2:B:14:THR:C	2:B:15:LEU:HD13	0.77	2.05	1	1
2:B:23:ILE:HG23	2:B:50:LEU:HD22	0.77	1.56	4	1
1:A:45:PHE:CZ	1:A:50:LEU:HD23	0.77	2.14	12	1
3:C:15:TYR:HD1	3:C:78:ASP:O	0.77	1.60	17	1
2:B:5:VAL:HG22	2:B:67:LEU:HD23	0.76	1.58	18	1
3:C:80:TYR:CD1	3:C:80:TYR:O	0.76	2.38	1	4
3:C:15:TYR:CZ	3:C:18:ARG:HA	0.76	2.15	2	1
1:A:23:ILE:HD12	1:A:51:GLU:O	0.76	1.80	16	1
2:B:45:PHE:CD1	2:B:50:LEU:HD13	0.76	2.16	3	3
3:C:61:VAL:O	3:C:63:TYR:CZ	0.76	2.39	17	1
2:B:27:LYS:O	2:B:27:LYS:HD3	0.75	1.81	2	1
3:C:15:TYR:CE1	3:C:18:ARG:CB	0.75	2.69	2	1
3:C:61:VAL:HG13	3:C:63:TYR:OH	0.75	1.80	17	1
3:C:15:TYR:CE2	3:C:18:ARG:HA	0.74	2.17	2	1
2:B:23:ILE:CG2	2:B:50:LEU:HD22	0.74	2.12	4	2
2:B:50:LEU:HD12	2:B:50:LEU:O	0.74	1.83	16	1
3:C:76:LEU:HD13	3:C:80:TYR:CE1	0.74	2.18	19	1
3:C:20:LEU:HD22	3:C:21:THR:H	0.74	1.40	4	1
2:B:23:ILE:HG21	2:B:50:LEU:HD13	0.74	1.59	16	1
1:A:31:GLN:HG3	1:A:36:ILE:O	0.74	1.83	14	2
3:C:132:ILE:CA	3:C:135:PHE:CE1	0.74	2.70	20	2
1:A:1:MET:CB	1:A:63:ARG:HE	0.74	1.96	6	1
3:C:55:LEU:HD21	3:C:76:LEU:HD11	0.74	1.57	19	1
3:C:17:TYR:CD1	3:C:81:PRO:HB3	0.73	2.17	5	5
3:C:61:VAL:HG21	3:C:135:PHE:CD2	0.73	2.18	15	2
3:C:55:LEU:O	3:C:55:LEU:HD23	0.73	1.83	17	1
3:C:77:LEU:C	3:C:79:THR:N	0.73	2.45	1	20
2:B:66:THR:HG21	3:C:46:ASP:CG	0.73	2.08	3	2
2:B:45:PHE:CD2	2:B:61:ILE:HD11	0.73	2.17	8	2
3:C:16:LYS:CE	3:C:17:TYR:H	0.73	1.95	7	1
3:C:77:LEU:HB2	3:C:80:TYR:CE1	0.73	2.19	6	2
3:C:76:LEU:HD12	3:C:80:TYR:HB3	0.73	1.59	8	1
2:B:43:LEU:CB	2:B:50:LEU:HD21	0.73	2.14	14	4
2:B:31:GLN:HG3	2:B:36:ILE:O	0.73	1.84	18	3
1:A:59:TYR:CZ	1:A:61:ILE:HD12	0.73	2.19	14	1
1:A:23:ILE:HG13	1:A:50:LEU:HD12	0.72	1.60	3	1
2:B:56:LEU:H	2:B:56:LEU:HD23	0.72	1.43	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:77:LEU:O	3:C:80:TYR:HD2	0.72	1.66	17	3
1:A:3:ILE:HG23	1:A:63:ARG:HH12	0.72	1.44	6	1
3:C:75:TRP:O	3:C:75:TRP:CD1	0.72	2.42	18	3
2:B:4:PHE:CE1	2:B:14:THR:HG22	0.72	2.18	14	1
3:C:74:LEU:HD13	3:C:124:LEU:HD21	0.72	1.61	4	1
1:A:56:LEU:O	1:A:59:TYR:CD1	0.72	2.42	14	1
1:A:23:ILE:CG1	1:A:50:LEU:HD22	0.72	2.15	12	1
3:C:12:VAL:HG12	3:C:53:MET:SD	0.72	2.23	13	1
1:A:63:ARG:HA	1:A:63:ARG:NE	0.72	1.99	6	1
3:C:77:LEU:O	3:C:80:TYR:CE2	0.72	2.42	14	3
3:C:12:VAL:HB	3:C:15:TYR:CD2	0.72	2.19	2	1
2:B:45:PHE:CE2	2:B:67:LEU:HD22	0.72	2.19	16	2
3:C:87:CYS:SG	3:C:109:ILE:HD13	0.71	2.25	3	2
1:A:43:LEU:HB2	1:A:50:LEU:HD11	0.71	1.60	12	2
3:C:82:TYR:O	3:C:117:TRP:CE3	0.71	2.42	20	5
1:A:61:ILE:HD11	1:A:67:LEU:HD21	0.71	1.60	14	1
3:C:76:LEU:HB3	3:C:80:TYR:CG	0.71	2.21	17	6
1:A:45:PHE:CE1	1:A:50:LEU:HD13	0.71	2.20	3	1
2:B:56:LEU:O	2:B:61:ILE:HG22	0.71	1.86	12	3
2:B:45:PHE:CE1	2:B:50:LEU:HD22	0.71	2.21	17	3
2:B:56:LEU:O	2:B:59:TYR:CD2	0.71	2.44	18	1
3:C:11:MET:HB3	3:C:39:LEU:HD12	0.71	1.60	8	4
3:C:89:VAL:CG2	3:C:97:ILE:HD11	0.71	2.14	14	2
2:B:67:LEU:C	2:B:67:LEU:HD23	0.71	2.10	17	2
3:C:15:TYR:CE2	3:C:21:THR:OG1	0.70	2.44	17	1
3:C:76:LEU:HB3	3:C:80:TYR:CD2	0.70	2.21	14	7
1:A:45:PHE:CE2	1:A:67:LEU:HD22	0.70	2.22	3	3
2:B:5:VAL:CG2	2:B:67:LEU:HD22	0.70	2.16	19	2
2:B:7:THR:HG23	2:B:9:THR:H	0.70	1.46	20	5
2:B:45:PHE:CD2	2:B:67:LEU:HD22	0.70	2.21	4	2
3:C:81:PRO:O	3:C:119:HIS:HB2	0.70	1.86	20	20
3:C:129:GLN:O	3:C:132:ILE:HG22	0.70	1.86	14	4
2:B:23:ILE:HD13	2:B:52:ASP:HA	0.70	1.61	16	1
2:B:50:LEU:HD23	2:B:59:TYR:CE1	0.70	2.21	15	1
1:A:43:LEU:HB2	1:A:50:LEU:HD21	0.70	1.64	11	2
3:C:76:LEU:HD12	3:C:80:TYR:CD1	0.69	2.22	20	2
3:C:114:LEU:HD13	3:C:115:HIS:N	0.69	2.01	15	1
3:C:21:THR:O	3:C:25:THR:HG23	0.69	1.86	6	3
1:A:50:LEU:HD22	1:A:54:ARG:NH2	0.69	2.02	7	1
3:C:102:HIS:CE1	3:C:134:VAL:HG11	0.69	2.23	9	1
3:C:63:TYR:CE1	3:C:68:TYR:HB2	0.69	2.22	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:32:TYR:CE1	3:C:60:PRO:HD3	0.69	2.23	15	3
3:C:17:TYR:HB3	3:C:20:LEU:HD21	0.69	1.65	4	1
3:C:32:TYR:CD1	3:C:128:ILE:HD12	0.68	2.23	13	2
1:A:2:GLN:O	1:A:3:ILE:HD13	0.68	1.88	17	3
3:C:114:LEU:O	3:C:117:TRP:CD1	0.68	2.45	1	5
1:A:43:LEU:CB	1:A:50:LEU:HD21	0.68	2.18	19	3
2:B:23:ILE:HD11	2:B:54:ARG:N	0.68	2.03	16	1
3:C:17:TYR:CB	3:C:20:LEU:HD21	0.68	2.18	4	1
1:A:45:PHE:CD2	1:A:67:LEU:HD22	0.68	2.22	12	3
1:A:2:GLN:N	1:A:63:ARG:CD	0.68	2.56	6	1
3:C:15:TYR:CE1	3:C:76:LEU:HD21	0.68	2.24	9	1
3:C:98:LYS:O	3:C:99:THR:C	0.68	2.37	1	20
3:C:53:MET:O	3:C:76:LEU:HD23	0.68	1.89	8	2
3:C:12:VAL:HG11	3:C:21:THR:HG21	0.68	1.66	11	1
3:C:28:VAL:HG23	3:C:125:LEU:HD13	0.67	1.64	6	2
3:C:32:TYR:CE1	3:C:35:LEU:HD22	0.67	2.24	18	1
3:C:15:TYR:CE1	3:C:78:ASP:O	0.67	2.48	17	1
3:C:113:TYR:CE2	3:C:127:LEU:HD12	0.67	2.23	4	1
1:A:4:PHE:CE2	1:A:14:THR:HG22	0.67	2.24	8	2
3:C:59:ILE:HD12	3:C:128:ILE:HG22	0.67	1.67	10	1
3:C:15:TYR:CG	3:C:80:TYR:OH	0.67	2.47	14	1
3:C:24:GLU:HB3	3:C:124:LEU:HD21	0.67	1.65	14	1
3:C:135:PHE:CE2	3:C:140:PRO:HD2	0.67	2.25	17	1
2:B:56:LEU:C	2:B:56:LEU:HD12	0.67	2.14	9	4
3:C:32:TYR:CE1	3:C:128:ILE:HD12	0.67	2.25	13	2
3:C:142:PHE:O	3:C:143:SER:C	0.67	2.37	1	20
3:C:89:VAL:HG23	3:C:109:ILE:CD1	0.67	2.20	20	2
3:C:61:VAL:HG22	3:C:61:VAL:O	0.67	1.88	20	1
3:C:61:VAL:HG13	3:C:61:VAL:O	0.67	1.90	3	2
3:C:16:LYS:HE2	3:C:79:THR:HA	0.67	1.64	7	1
3:C:39:LEU:HD22	3:C:39:LEU:O	0.67	1.90	5	1
3:C:28:VAL:HG21	3:C:124:LEU:HD22	0.67	1.66	11	2
3:C:61:VAL:CB	3:C:135:PHE:CE1	0.66	2.77	20	2
3:C:32:TYR:HB2	3:C:35:LEU:HD23	0.66	1.64	17	1
1:A:7:THR:HG23	1:A:9:THR:H	0.66	1.49	11	2
3:C:15:TYR:CD2	3:C:78:ASP:HA	0.66	2.25	5	3
2:B:50:LEU:O	2:B:50:LEU:HD13	0.66	1.90	4	2
3:C:77:LEU:C	3:C:79:THR:H	0.66	1.99	1	20
1:A:23:ILE:CG1	1:A:50:LEU:HD12	0.66	2.20	3	1
2:B:45:PHE:CE2	2:B:67:LEU:HB2	0.66	2.26	18	1
1:A:47:GLY:HA2	3:C:43:VAL:O	0.66	1.91	3	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:5:VAL:CG1	2:B:15:LEU:HD11	0.66	2.20	1	1
2:B:40:GLN:O	2:B:71:LEU:HD13	0.66	1.91	2	2
2:B:50:LEU:O	2:B:50:LEU:CD1	0.66	2.44	4	1
1:A:45:PHE:CD1	1:A:45:PHE:O	0.66	2.49	13	1
3:C:15:TYR:CE1	3:C:18:ARG:HA	0.66	2.26	2	1
3:C:109:ILE:HD11	3:C:135:PHE:CZ	0.66	2.26	7	2
1:A:45:PHE:CD1	1:A:59:TYR:CD1	0.66	2.84	13	1
3:C:35:LEU:HD13	3:C:55:LEU:CD1	0.65	2.20	17	1
3:C:80:TYR:CD2	3:C:85:PRO:HA	0.65	2.26	15	3
1:A:66:THR:C	1:A:67:LEU:HD23	0.65	2.15	3	2
3:C:76:LEU:HB3	3:C:80:TYR:CD1	0.65	2.27	17	3
3:C:61:VAL:HG11	3:C:135:PHE:CE2	0.65	2.25	15	1
3:C:76:LEU:O	3:C:76:LEU:HD23	0.65	1.91	9	1
3:C:129:GLN:O	3:C:133:VAL:HG13	0.65	1.91	11	5
1:A:45:PHE:CE1	1:A:50:LEU:HD12	0.65	2.26	6	1
2:B:43:LEU:HB2	2:B:50:LEU:HD21	0.65	1.67	14	3
1:A:50:LEU:CD1	1:A:50:LEU:O	0.65	2.45	12	1
1:A:23:ILE:HD11	1:A:59:TYR:CE1	0.65	2.27	16	1
2:B:15:LEU:H	2:B:15:LEU:HD22	0.65	1.50	1	1
3:C:132:ILE:HA	3:C:135:PHE:CD1	0.65	2.26	3	2
3:C:12:VAL:HG12	3:C:15:TYR:CG	0.65	2.25	11	1
3:C:20:LEU:HD22	3:C:21:THR:N	0.64	2.07	4	1
3:C:63:TYR:OH	3:C:68:TYR:HB3	0.64	1.90	17	1
3:C:124:LEU:O	3:C:128:ILE:HG23	0.64	1.91	18	1
2:B:59:TYR:O	2:B:59:TYR:CG	0.64	2.50	6	5
2:B:23:ILE:CD1	2:B:23:ILE:N	0.64	2.51	16	1
2:B:23:ILE:CG2	2:B:50:LEU:HD13	0.64	2.22	16	1
1:A:50:LEU:HD22	1:A:54:ARG:HH21	0.64	1.53	7	1
3:C:132:ILE:HA	3:C:135:PHE:CZ	0.64	2.26	20	1
3:C:17:TYR:O	3:C:17:TYR:CD2	0.64	2.50	10	4
3:C:77:LEU:O	3:C:78:ASP:C	0.64	2.39	1	20
3:C:17:TYR:CE2	3:C:81:PRO:HD3	0.64	2.28	11	5
3:C:15:TYR:CE1	3:C:18:ARG:CA	0.64	2.81	2	1
2:B:27:LYS:O	2:B:31:GLN:CD	0.64	2.39	16	2
3:C:61:VAL:HB	3:C:135:PHE:CZ	0.64	2.28	20	2
1:A:56:LEU:HD21	1:A:61:ILE:O	0.64	1.93	2	1
3:C:52:LEU:HD13	3:C:52:LEU:O	0.64	1.93	20	3
2:B:26:VAL:O	2:B:29:LYS:HD2	0.64	1.93	10	1
2:B:50:LEU:HD23	2:B:59:TYR:CD1	0.64	2.28	15	1
2:B:59:TYR:CD2	2:B:61:ILE:HD13	0.64	2.28	18	1
2:B:41:GLN:NE2	2:B:69:LEU:HD11	0.64	2.08	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:12:VAL:HG11	3:C:53:MET:HE3	0.64	1.67	5	2
3:C:29:ILE:HG23	3:C:35:LEU:O	0.63	1.94	16	1
2:B:56:LEU:O	2:B:59:TYR:HD2	0.63	1.73	18	1
3:C:42:TYR:O	3:C:42:TYR:CG	0.63	2.52	7	4
3:C:17:TYR:O	3:C:21:THR:HG22	0.63	1.94	10	2
3:C:135:PHE:CZ	3:C:140:PRO:HD2	0.63	2.29	17	2
3:C:11:MET:CB	3:C:39:LEU:HD12	0.63	2.23	2	3
1:A:2:GLN:N	1:A:63:ARG:NE	0.63	2.46	6	1
3:C:29:ILE:HD13	3:C:35:LEU:O	0.63	1.94	8	1
2:B:26:VAL:HG22	2:B:29:LYS:NZ	0.63	2.09	1	1
2:B:27:LYS:HE2	2:B:41:GLN:CB	0.63	2.24	2	1
2:B:8:LEU:HD13	2:B:8:LEU:O	0.63	1.93	8	1
3:C:118:LYS:O	3:C:119:HIS:CB	0.63	2.47	9	20
1:A:59:TYR:CE1	1:A:61:ILE:HB	0.63	2.29	14	1
3:C:17:TYR:HB3	3:C:20:LEU:HD11	0.62	1.71	4	1
1:A:69:LEU:HD22	1:A:70:VAL:N	0.62	2.09	10	1
3:C:12:VAL:O	3:C:12:VAL:HG23	0.62	1.93	13	2
1:A:23:ILE:CG1	1:A:50:LEU:HD13	0.62	2.24	20	1
1:A:59:TYR:HE1	1:A:61:ILE:HB	0.62	1.54	14	1
3:C:17:TYR:O	3:C:21:THR:HG23	0.62	1.94	3	2
2:B:43:LEU:HB3	2:B:50:LEU:HD21	0.62	1.71	16	1
3:C:12:VAL:HG12	3:C:15:TYR:CE1	0.62	2.29	9	3
3:C:70:ILE:HD11	3:C:141:VAL:CG2	0.62	2.24	13	1
2:B:23:ILE:HD13	2:B:52:ASP:C	0.62	2.19	16	1
2:B:7:THR:HG23	2:B:69:LEU:HD11	0.62	1.70	9	2
3:C:119:HIS:N	3:C:120:PRO:CD	0.62	2.62	13	20
1:A:5:VAL:HG13	1:A:69:LEU:HD23	0.62	1.71	4	1
3:C:24:GLU:O	3:C:28:VAL:HG23	0.62	1.95	17	5
2:B:18:GLU:O	2:B:56:LEU:HD11	0.62	1.94	15	1
3:C:8:LEU:HD13	3:C:8:LEU:O	0.62	1.95	20	1
2:B:23:ILE:HD11	2:B:54:ARG:H	0.61	1.54	16	1
1:A:68:HIS:HE2	1:A:70:VAL:HG23	0.61	1.54	18	1
2:B:59:TYR:CE2	2:B:61:ILE:HB	0.61	2.30	18	1
1:A:5:VAL:CG1	1:A:69:LEU:HD23	0.61	2.25	15	2
2:B:56:LEU:HG	2:B:61:ILE:HG21	0.61	1.72	12	1
3:C:16:LYS:HG3	3:C:78:ASP:O	0.61	1.94	7	1
3:C:75:TRP:HB2	3:C:86:ILE:CG2	0.61	2.26	8	1
2:B:23:ILE:HD12	2:B:50:LEU:HD22	0.61	1.72	12	1
3:C:20:LEU:H	3:C:20:LEU:HD13	0.61	1.54	4	1
3:C:80:TYR:CE1	3:C:124:LEU:HD23	0.61	2.30	12	1
1:A:59:TYR:CG	1:A:59:TYR:O	0.61	2.54	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:23:ILE:HB	2:B:51:GLU:O	0.61	1.95	3	16
3:C:59:ILE:HD11	3:C:72:ILE:HG12	0.61	1.71	9	1
1:A:68:HIS:NE2	1:A:70:VAL:HG23	0.61	2.10	18	1
1:A:69:LEU:O	1:A:69:LEU:HD23	0.61	1.96	19	1
3:C:61:VAL:O	3:C:61:VAL:HG13	0.61	1.96	20	1
3:C:89:VAL:O	3:C:91:PRO:CD	0.61	2.43	9	20
3:C:4:SER:O	3:C:8:LEU:HG	0.61	1.95	9	4
3:C:75:TRP:CE2	3:C:86:ILE:HD12	0.61	2.30	18	1
1:A:4:PHE:C	1:A:4:PHE:CD2	0.61	2.79	5	2
2:B:27:LYS:CE	2:B:41:GLN:HB2	0.61	2.26	2	1
2:B:19:PRO:C	2:B:56:LEU:HD21	0.60	2.21	14	1
2:B:19:PRO:CA	2:B:56:LEU:HD11	0.60	2.26	15	1
3:C:29:ILE:HD12	3:C:35:LEU:O	0.60	1.96	16	1
3:C:61:VAL:O	3:C:68:TYR:CD2	0.60	2.54	4	1
2:B:5:VAL:HG13	2:B:67:LEU:CD2	0.60	2.26	17	2
3:C:117:TRP:O	3:C:117:TRP:CD2	0.60	2.54	14	5
1:A:56:LEU:HG	1:A:61:ILE:HB	0.60	1.72	2	1
2:B:23:ILE:CG2	2:B:51:GLU:O	0.60	2.50	9	3
3:C:52:LEU:C	3:C:52:LEU:HD22	0.60	2.22	20	3
2:B:23:ILE:CD1	2:B:50:LEU:HD23	0.60	2.26	17	2
1:A:56:LEU:HD22	1:A:59:TYR:OH	0.60	1.97	14	1
2:B:27:LYS:CE	2:B:41:GLN:CB	0.60	2.80	2	1
3:C:15:TYR:OH	3:C:22:VAL:HG12	0.60	1.95	2	1
2:B:34:GLU:HB2	2:B:36:ILE:HD11	0.60	1.72	7	1
3:C:32:TYR:CZ	3:C:34:ASP:HB2	0.60	2.32	15	3
2:B:4:PHE:CZ	2:B:14:THR:HG22	0.60	2.31	14	1
2:B:45:PHE:CZ	2:B:50:LEU:HD22	0.60	2.32	3	3
2:B:30:ILE:HD13	2:B:69:LEU:HD21	0.60	1.72	5	1
1:A:5:VAL:HB	1:A:69:LEU:HD21	0.60	1.73	18	1
3:C:76:LEU:HD22	3:C:80:TYR:CD2	0.60	2.30	1	1
2:B:24:GLU:HA	2:B:27:LYS:HD3	0.60	1.74	13	1
2:B:50:LEU:N	2:B:50:LEU:HD22	0.60	2.12	14	1
1:A:23:ILE:HB	1:A:51:GLU:O	0.60	1.97	7	19
1:A:56:LEU:HD12	1:A:56:LEU:C	0.59	2.22	5	2
1:A:50:LEU:O	1:A:50:LEU:HD12	0.59	1.97	20	2
2:B:4:PHE:C	2:B:4:PHE:CD2	0.59	2.80	17	4
3:C:79:THR:C	3:C:81:PRO:CD	0.59	2.75	17	7
3:C:25:THR:O	3:C:29:ILE:HG22	0.59	1.97	8	1
3:C:15:TYR:HE2	3:C:21:THR:CB	0.59	2.10	17	1
3:C:39:LEU:HD13	3:C:39:LEU:N	0.59	2.12	8	5
3:C:32:TYR:CZ	3:C:35:LEU:HD22	0.59	2.31	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:36:ILE:HD12	2:B:41:GLN:OE1	0.59	1.97	19	1
2:B:43:LEU:O	2:B:44:ILE:HD13	0.59	1.97	8	2
3:C:63:TYR:OH	3:C:68:TYR:CB	0.59	2.50	17	1
3:C:11:MET:SD	3:C:53:MET:HE3	0.59	2.37	8	1
3:C:35:LEU:HD11	3:C:55:LEU:HB3	0.59	1.74	19	1
3:C:80:TYR:CE2	3:C:85:PRO:CA	0.59	2.76	6	2
3:C:11:MET:CG	3:C:39:LEU:HD12	0.59	2.27	16	1
3:C:35:LEU:C	3:C:35:LEU:HD13	0.59	2.23	19	1
1:A:3:ILE:HG23	1:A:63:ARG:NH1	0.59	2.12	6	1
2:B:15:LEU:HD22	2:B:15:LEU:N	0.58	2.13	1	1
3:C:119:HIS:N	3:C:120:PRO:HD2	0.58	2.13	16	18
1:A:23:ILE:O	1:A:27:LYS:HD2	0.58	1.98	4	1
1:A:40:GLN:O	1:A:71:LEU:HD13	0.58	1.97	11	1
3:C:24:GLU:O	3:C:28:VAL:HG13	0.58	1.98	5	2
2:B:50:LEU:CD1	2:B:50:LEU:O	0.58	2.51	12	1
1:A:67:LEU:HD13	1:A:68:HIS:N	0.58	2.13	9	1
3:C:111:LEU:HD11	3:C:134:VAL:HG21	0.58	1.75	15	1
3:C:18:ARG:O	3:C:19:ASP:C	0.58	2.45	3	20
3:C:82:TYR:O	3:C:117:TRP:CD1	0.58	2.56	18	6
3:C:15:TYR:CZ	3:C:18:ARG:CA	0.58	2.85	2	1
3:C:87:CYS:SG	3:C:109:ILE:HD12	0.58	2.38	5	1
1:A:15:LEU:C	1:A:15:LEU:HD22	0.58	2.24	10	1
1:A:50:LEU:HD22	1:A:50:LEU:N	0.58	2.11	11	3
3:C:35:LEU:HD21	3:C:55:LEU:HB3	0.58	1.74	19	1
2:B:7:THR:HG22	2:B:11:LYS:H	0.58	1.58	6	5
3:C:113:TYR:CD1	3:C:127:LEU:HG	0.58	2.34	2	1
1:A:8:LEU:CD2	1:A:9:THR:HG23	0.58	2.29	4	1
3:C:28:VAL:HG23	3:C:125:LEU:CD1	0.58	2.27	6	2
1:A:64:GLU:O	3:C:105:ALA:HB3	0.58	1.99	19	20
2:B:31:GLN:O	2:B:35:GLY:HA2	0.58	1.99	10	20
3:C:76:LEU:HD22	3:C:80:TYR:CG	0.58	2.33	1	1
2:B:23:ILE:HG13	2:B:52:ASP:HA	0.58	1.75	9	2
3:C:76:LEU:CB	3:C:80:TYR:CD2	0.58	2.87	2	2
2:B:43:LEU:HB2	2:B:50:LEU:HD11	0.58	1.76	12	3
3:C:71:PRO:HG2	3:C:90:LYS:O	0.58	1.99	4	19
3:C:61:VAL:O	3:C:61:VAL:HG22	0.58	1.98	3	1
1:A:31:GLN:O	1:A:35:GLY:HA2	0.58	1.99	3	20
3:C:44:PHE:CE1	3:C:46:ASP:CB	0.58	2.86	4	4
2:B:18:GLU:O	2:B:56:LEU:CD2	0.58	2.52	14	1
3:C:89:VAL:O	3:C:89:VAL:HG23	0.57	1.98	1	7
2:B:27:LYS:O	2:B:27:LYS:CD	0.57	2.50	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:68:TYR:CE2	3:C:95:MET:HE2	0.57	2.34	9	2
3:C:77:LEU:HD13	3:C:77:LEU:N	0.57	2.14	17	1
3:C:98:LYS:O	3:C:99:THR:O	0.57	2.22	1	20
1:A:44:ILE:HG23	1:A:68:HIS:CB	0.57	2.30	6	1
3:C:59:ILE:HG21	3:C:128:ILE:HD11	0.57	1.76	7	1
3:C:75:TRP:O	3:C:75:TRP:HD1	0.57	1.80	18	2
1:A:63:ARG:HA	1:A:63:ARG:NH1	0.57	2.14	6	1
1:A:24:GLU:HA	1:A:27:LYS:HD3	0.57	1.74	15	3
2:B:3:ILE:O	2:B:15:LEU:HD22	0.57	2.00	1	1
1:A:2:GLN:C	1:A:3:ILE:HD13	0.57	2.25	2	2
1:A:4:PHE:CE2	1:A:66:THR:HG23	0.57	2.34	5	2
3:C:24:GLU:HB3	3:C:124:LEU:HD22	0.57	1.75	7	1
3:C:42:TYR:HB3	3:C:52:LEU:HD12	0.57	1.76	15	3
3:C:8:LEU:O	3:C:12:VAL:HG23	0.57	2.00	11	1
3:C:77:LEU:N	3:C:80:TYR:HD2	0.57	1.97	2	2
3:C:76:LEU:HD22	3:C:80:TYR:CD1	0.57	2.34	13	3
3:C:28:VAL:HG23	3:C:124:LEU:HD13	0.57	1.77	20	1
3:C:123:ASP:O	3:C:127:LEU:HD13	0.57	1.98	2	1
3:C:16:LYS:HE3	3:C:17:TYR:H	0.57	1.57	7	1
3:C:75:TRP:CD1	3:C:75:TRP:C	0.57	2.83	9	4
2:B:23:ILE:CD1	2:B:50:LEU:HD22	0.57	2.28	12	1
1:A:43:LEU:CD2	1:A:50:LEU:HD22	0.57	2.30	4	2
2:B:71:LEU:HD22	2:B:71:LEU:O	0.57	2.00	4	2
2:B:50:LEU:HD21	2:B:59:TYR:CG	0.57	2.35	5	1
3:C:12:VAL:O	3:C:12:VAL:HG12	0.57	2.00	8	2
3:C:131:MET:HE3	3:C:132:ILE:HA	0.57	1.75	14	1
2:B:23:ILE:CG1	2:B:54:ARG:O	0.57	2.52	16	1
3:C:70:ILE:HD11	3:C:89:VAL:HG23	0.57	1.76	17	1
2:B:67:LEU:HD12	2:B:68:HIS:N	0.57	2.15	18	1
3:C:32:TYR:O	3:C:32:TYR:CD2	0.57	2.58	18	2
3:C:17:TYR:O	3:C:17:TYR:CD1	0.56	2.58	11	2
3:C:15:TYR:CD2	3:C:80:TYR:HE2	0.56	2.18	5	4
3:C:32:TYR:CE2	3:C:34:ASP:CB	0.56	2.88	15	3
3:C:51:GLU:C	3:C:52:LEU:HD22	0.56	2.24	12	3
2:B:31:GLN:CD	2:B:38:PRO:HD3	0.56	2.25	11	4
1:A:45:PHE:HE1	1:A:50:LEU:HD13	0.56	1.60	3	1
2:B:26:VAL:O	2:B:30:ILE:HG23	0.56	2.00	15	4
3:C:63:TYR:CB	3:C:68:TYR:CE2	0.56	2.88	4	1
1:A:61:ILE:HG22	1:A:61:ILE:O	0.56	2.01	6	1
1:A:7:THR:HG23	1:A:69:LEU:CD1	0.56	2.30	7	1
3:C:12:VAL:HB	3:C:15:TYR:CD1	0.56	2.35	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HD12	1:A:69:LEU:HD21	0.56	1.76	14	1
2:B:50:LEU:HD11	2:B:59:TYR:CE1	0.56	2.36	18	1
3:C:92:THR:HG23	3:C:94:SER:H	0.56	1.60	18	1
3:C:17:TYR:CD2	3:C:81:PRO:HD3	0.56	2.36	5	5
3:C:113:TYR:CD1	3:C:113:TYR:C	0.56	2.83	2	1
1:A:23:ILE:CD1	1:A:50:LEU:HD22	0.56	2.31	6	1
1:A:8:LEU:HD22	1:A:8:LEU:C	0.56	2.26	12	1
2:B:23:ILE:N	2:B:23:ILE:HD13	0.56	2.15	18	1
3:C:102:HIS:CE1	3:C:111:LEU:HD23	0.56	2.36	9	1
3:C:15:TYR:CE2	3:C:21:THR:CB	0.56	2.88	17	1
3:C:21:THR:OG1	3:C:80:TYR:CD1	0.56	2.58	17	1
3:C:8:LEU:O	3:C:12:VAL:HG22	0.56	2.00	15	14
2:B:23:ILE:HD11	2:B:50:LEU:CD2	0.56	2.28	8	2
1:A:72:ARG:O	1:A:73:LEU:CB	0.56	2.52	5	1
1:A:47:GLY:O	3:C:43:VAL:HG22	0.56	1.99	1	1
3:C:113:TYR:CD1	3:C:114:LEU:N	0.56	2.74	2	1
3:C:28:VAL:CG2	3:C:124:LEU:HD23	0.56	2.31	14	1
1:A:23:ILE:HG21	1:A:50:LEU:HG	0.56	1.76	1	1
3:C:87:CYS:HB3	3:C:109:ILE:HD12	0.56	1.77	8	5
2:B:23:ILE:HG21	2:B:50:LEU:HD22	0.56	1.78	16	1
3:C:111:LEU:HD23	3:C:112:PRO:HD2	0.56	1.78	16	2
3:C:15:TYR:OH	3:C:81:PRO:HD3	0.56	2.00	17	1
2:B:5:VAL:HG22	2:B:67:LEU:CD2	0.56	2.30	18	1
3:C:80:TYR:O	3:C:80:TYR:CG	0.56	2.58	11	10
3:C:87:CYS:HB3	3:C:109:ILE:HD13	0.56	1.76	1	2
1:A:45:PHE:CE2	1:A:67:LEU:HD13	0.56	2.36	3	2
2:B:45:PHE:CZ	2:B:50:LEU:HD23	0.56	2.36	16	2
2:B:71:LEU:HD22	2:B:71:LEU:C	0.56	2.26	4	1
3:C:79:THR:O	3:C:80:TYR:HD1	0.56	1.84	4	3
3:C:52:LEU:HD12	3:C:75:TRP:CZ3	0.56	2.36	9	2
3:C:17:TYR:CZ	3:C:21:THR:HB	0.56	2.35	10	2
3:C:75:TRP:C	3:C:76:LEU:HD22	0.56	2.25	20	2
2:B:56:LEU:HA	2:B:59:TYR:CE2	0.56	2.36	18	1
3:C:43:VAL:HG12	3:C:49:SER:OG	0.56	2.01	1	1
2:B:34:GLU:CB	2:B:36:ILE:HD11	0.56	2.31	7	1
1:A:2:GLN:O	1:A:63:ARG:NE	0.55	2.39	6	1
1:A:45:PHE:CE2	1:A:50:LEU:HG	0.55	2.36	13	1
1:A:23:ILE:HG23	1:A:51:GLU:O	0.55	1.98	1	1
2:B:23:ILE:CD1	2:B:50:LEU:HD12	0.55	2.32	20	1
3:C:74:LEU:HD13	3:C:124:LEU:CD2	0.55	2.31	4	1
2:B:71:LEU:H	2:B:71:LEU:HD13	0.55	1.60	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:17:VAL:HG22	2:B:21:ASP:CB	0.55	2.32	18	6
3:C:15:TYR:CD2	3:C:18:ARG:HA	0.55	2.36	2	1
3:C:61:VAL:HG22	3:C:68:TYR:O	0.55	2.01	19	3
2:B:44:ILE:HG23	2:B:68:HIS:CB	0.55	2.32	9	1
1:A:2:GLN:O	1:A:63:ARG:HD3	0.55	2.01	6	1
3:C:16:LYS:CE	3:C:79:THR:HA	0.55	2.31	7	1
3:C:52:LEU:HD23	3:C:75:TRP:CZ3	0.55	2.35	12	1
2:B:28:ALA:HA	2:B:31:GLN:CD	0.55	2.27	1	2
3:C:12:VAL:CG1	3:C:53:MET:HE3	0.55	2.32	5	2
1:A:69:LEU:HD12	1:A:70:VAL:N	0.55	2.17	17	1
3:C:63:TYR:HB3	3:C:68:TYR:CE2	0.55	2.37	4	1
2:B:19:PRO:HA	2:B:56:LEU:HD11	0.55	1.76	15	1
2:B:46:ALA:O	3:C:77:LEU:HD22	0.55	2.02	18	1
2:B:31:GLN:N	2:B:31:GLN:OE1	0.55	2.40	16	1
2:B:31:GLN:HG2	2:B:36:ILE:O	0.55	2.02	1	2
3:C:32:TYR:CZ	3:C:60:PRO:HD3	0.55	2.37	12	3
3:C:50:ARG:HG2	3:C:52:LEU:HD21	0.55	1.79	12	1
3:C:15:TYR:CE1	3:C:76:LEU:HD11	0.55	2.37	15	1
3:C:80:TYR:CD1	3:C:83:ASN:HB2	0.55	2.37	15	1
2:B:17:VAL:HG11	2:B:56:LEU:CD1	0.55	2.32	18	1
1:A:43:LEU:HD22	1:A:50:LEU:HD22	0.54	1.79	4	2
1:A:23:ILE:HG12	1:A:50:LEU:HD22	0.54	1.77	12	2
3:C:11:MET:O	3:C:53:MET:HE3	0.54	2.01	19	1
3:C:12:VAL:HA	3:C:15:TYR:CD1	0.54	2.37	5	4
1:A:1:MET:CB	1:A:63:ARG:NE	0.54	2.70	6	1
1:A:59:TYR:CD1	1:A:59:TYR:C	0.54	2.85	13	1
1:A:4:PHE:CD1	1:A:5:VAL:N	0.54	2.75	1	2
3:C:21:THR:CG2	3:C:22:VAL:N	0.54	2.71	5	3
2:B:41:GLN:HE21	2:B:69:LEU:HD11	0.54	1.61	2	1
3:C:102:HIS:O	3:C:109:ILE:HD13	0.54	2.03	11	2
1:A:43:LEU:N	1:A:43:LEU:HD13	0.54	2.17	13	2
2:B:71:LEU:O	3:C:117:TRP:CZ2	0.54	2.60	20	1
3:C:111:LEU:HD13	3:C:111:LEU:N	0.54	2.17	5	2
2:B:50:LEU:HD12	2:B:50:LEU:H	0.54	1.61	15	2
3:C:28:VAL:HG23	3:C:124:LEU:HD23	0.54	1.79	14	1
2:B:59:TYR:CG	2:B:61:ILE:HD13	0.54	2.37	18	1
2:B:50:LEU:CD1	2:B:59:TYR:CE1	0.54	2.90	18	1
3:C:16:LYS:HD2	3:C:17:TYR:N	0.54	2.18	7	1
3:C:16:LYS:CD	3:C:17:TYR:N	0.54	2.71	7	1
3:C:113:TYR:C	3:C:113:TYR:CD2	0.54	2.85	13	1
3:C:22:VAL:O	3:C:26:VAL:HG13	0.54	2.02	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:60:PRO:O	3:C:132:ILE:HD12	0.54	2.03	9	1
3:C:35:LEU:HD12	3:C:35:LEU:C	0.54	2.28	17	1
1:A:56:LEU:C	1:A:56:LEU:HD23	0.54	2.28	2	1
1:A:7:THR:HG22	1:A:11:LYS:H	0.54	1.61	5	2
2:B:59:TYR:O	2:B:59:TYR:CD2	0.54	2.61	11	2
3:C:52:LEU:HG	3:C:75:TRP:HE1	0.54	1.63	17	3
3:C:58:THR:OG1	3:C:69:ASN:O	0.54	2.25	2	1
3:C:95:MET:HB3	3:C:141:VAL:HG21	0.54	1.80	4	1
3:C:27:ASN:CB	3:C:125:LEU:HD11	0.54	2.33	3	1
3:C:15:TYR:OH	3:C:52:LEU:HA	0.54	2.02	19	4
3:C:113:TYR:CD2	3:C:127:LEU:HD13	0.54	2.38	13	1
1:A:23:ILE:HG12	1:A:50:LEU:HD13	0.54	1.79	20	1
3:C:128:ILE:O	3:C:132:ILE:HG23	0.53	2.02	8	5
2:B:66:THR:C	2:B:67:LEU:HD12	0.53	2.28	3	1
2:B:67:LEU:HD12	2:B:67:LEU:N	0.53	2.18	3	1
1:A:45:PHE:CD1	1:A:50:LEU:HD23	0.53	2.37	8	1
3:C:127:LEU:O	3:C:130:VAL:HG12	0.53	2.03	15	1
3:C:77:LEU:HD22	3:C:77:LEU:H	0.53	1.63	17	1
2:B:4:PHE:CD1	2:B:5:VAL:N	0.53	2.76	6	4
1:A:24:GLU:HA	1:A:27:LYS:HD2	0.53	1.78	5	1
3:C:87:CYS:CB	3:C:109:ILE:HD13	0.53	2.33	9	2
2:B:17:VAL:HG13	2:B:18:GLU:N	0.53	2.18	4	5
1:A:31:GLN:OE1	1:A:36:ILE:O	0.53	2.26	6	1
3:C:31:LEU:HD21	3:C:125:LEU:HD13	0.53	1.80	13	1
3:C:35:LEU:HD21	3:C:55:LEU:C	0.53	2.27	19	1
3:C:117:TRP:O	3:C:117:TRP:CG	0.53	2.62	18	5
3:C:52:LEU:HD11	3:C:77:LEU:HD23	0.53	1.79	8	2
2:B:56:LEU:HB3	2:B:61:ILE:CG2	0.53	2.33	6	2
3:C:75:TRP:CD1	3:C:86:ILE:HB	0.53	2.38	12	1
1:A:45:PHE:CD1	1:A:45:PHE:N	0.53	2.76	6	3
1:A:26:VAL:O	1:A:30:ILE:HG23	0.53	2.03	5	3
3:C:11:MET:HG3	3:C:12:VAL:HG13	0.53	1.80	9	2
1:A:3:ILE:HD11	1:A:61:ILE:HD11	0.53	1.80	13	1
1:A:56:LEU:HA	1:A:59:TYR:CE1	0.53	2.39	14	1
3:C:135:PHE:CE1	3:C:140:PRO:CG	0.53	2.92	17	2
3:C:39:LEU:HD13	3:C:39:LEU:H	0.53	1.64	16	5
3:C:70:ILE:HG23	3:C:70:ILE:O	0.53	2.04	17	6
3:C:135:PHE:C	3:C:135:PHE:CD2	0.53	2.87	10	1
2:B:14:THR:O	2:B:15:LEU:HD12	0.53	2.04	11	2
2:B:23:ILE:CD1	2:B:50:LEU:HD13	0.53	2.34	12	2
1:A:28:ALA:HA	1:A:31:GLN:OE1	0.53	2.03	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:114:LEU:HD22	3:C:114:LEU:O	0.53	2.02	15	1
3:C:111:LEU:HB2	3:C:113:TYR:CD1	0.53	2.39	9	1
1:A:64:GLU:O	3:C:105:ALA:CB	0.53	2.57	4	20
3:C:96:THR:HG22	3:C:142:PHE:O	0.53	2.03	19	4
1:A:41:GLN:CD	1:A:41:GLN:C	0.52	2.76	4	3
2:B:43:LEU:CB	2:B:50:LEU:HD11	0.52	2.33	2	3
3:C:18:ARG:O	3:C:22:VAL:HG13	0.52	2.04	12	2
1:A:23:ILE:HG13	1:A:52:ASP:HA	0.52	1.81	1	1
1:A:2:GLN:O	1:A:63:ARG:CZ	0.52	2.57	6	1
2:B:45:PHE:CD1	2:B:45:PHE:N	0.52	2.76	17	5
1:A:1:MET:HB3	1:A:63:ARG:HG2	0.52	1.81	6	1
2:B:56:LEU:HD13	2:B:61:ILE:HG22	0.52	1.81	8	1
3:C:102:HIS:CD2	3:C:102:HIS:O	0.52	2.62	9	1
1:A:59:TYR:CE1	1:A:61:ILE:HD12	0.52	2.39	14	1
3:C:17:TYR:CG	3:C:81:PRO:HG3	0.52	2.40	20	5
3:C:80:TYR:N	3:C:81:PRO:HD3	0.52	2.19	17	4
1:A:61:ILE:CG2	1:A:61:ILE:O	0.52	2.57	13	2
2:B:61:ILE:HG22	2:B:61:ILE:O	0.52	2.05	8	1
1:A:50:LEU:H	1:A:50:LEU:HD22	0.52	1.64	18	2
2:B:23:ILE:HG21	2:B:50:LEU:CD1	0.52	2.33	16	1
2:B:44:ILE:HD13	2:B:49:GLN:HA	0.52	1.82	20	2
3:C:12:VAL:HG23	3:C:15:TYR:CZ	0.52	2.40	2	1
3:C:28:VAL:CG2	3:C:124:LEU:HD13	0.52	2.35	20	1
2:B:26:VAL:HG22	2:B:29:LYS:HZ1	0.52	1.65	1	1
3:C:32:TYR:CE1	3:C:60:PRO:CD	0.52	2.92	12	3
3:C:63:TYR:HE2	3:C:135:PHE:CE2	0.52	2.23	17	1
3:C:89:VAL:HG22	3:C:107:GLY:CA	0.52	2.34	1	7
2:B:27:LYS:HE3	2:B:41:GLN:HB2	0.52	1.81	2	1
3:C:76:LEU:C	3:C:80:TYR:CD2	0.52	2.88	2	3
2:B:56:LEU:HD22	2:B:56:LEU:C	0.52	2.30	15	1
3:C:86:ILE:C	3:C:86:ILE:HD12	0.52	2.29	17	1
1:A:19:PRO:HA	1:A:56:LEU:HD22	0.52	1.82	2	1
3:C:44:PHE:CE1	3:C:46:ASP:HB2	0.52	2.40	8	4
3:C:76:LEU:HD22	3:C:76:LEU:N	0.52	2.19	20	2
3:C:31:LEU:CD2	3:C:125:LEU:HD13	0.52	2.35	13	1
3:C:113:TYR:CD1	3:C:130:VAL:HG21	0.52	2.40	15	1
3:C:61:VAL:HG23	3:C:135:PHE:CD1	0.52	2.40	20	2
3:C:27:ASN:O	3:C:125:LEU:HD21	0.52	2.05	3	1
2:B:27:LYS:HZ3	2:B:30:ILE:CG2	0.51	2.18	2	1
3:C:89:VAL:HG21	3:C:97:ILE:HD13	0.51	1.80	9	1
2:B:17:VAL:HG22	2:B:21:ASP:CG	0.51	2.30	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:15:TYR:CE2	3:C:21:THR:HB	0.51	2.40	2	2
3:C:135:PHE:CD2	3:C:135:PHE:O	0.51	2.63	15	3
1:A:15:LEU:N	1:A:15:LEU:HD13	0.51	2.20	2	1
3:C:61:VAL:CG2	3:C:135:PHE:CD1	0.51	2.93	20	2
1:A:17:VAL:HG22	1:A:21:ASP:CB	0.51	2.35	6	5
1:A:67:LEU:HD13	1:A:68:HIS:H	0.51	1.65	9	1
3:C:21:THR:HG1	3:C:80:TYR:HE1	0.51	1.46	2	1
3:C:61:VAL:O	3:C:61:VAL:CG1	0.51	2.55	3	2
1:A:7:THR:HG23	1:A:69:LEU:HD12	0.51	1.80	7	1
1:A:56:LEU:O	1:A:61:ILE:CG2	0.51	2.59	1	1
3:C:19:ASP:O	3:C:20:LEU:C	0.51	2.52	1	20
3:C:58:THR:OG1	3:C:69:ASN:C	0.51	2.53	1	4
3:C:76:LEU:C	3:C:80:TYR:CE2	0.51	2.89	14	1
3:C:113:TYR:OH	3:C:123:ASP:N	0.51	2.43	4	1
1:A:15:LEU:HD22	1:A:15:LEU:O	0.51	2.05	10	1
3:C:24:GLU:HB3	3:C:124:LEU:HD11	0.51	1.81	20	2
3:C:76:LEU:C	3:C:76:LEU:HD12	0.51	2.31	15	1
3:C:59:ILE:CD1	3:C:128:ILE:HG22	0.51	2.35	10	1
1:A:23:ILE:CD1	1:A:51:GLU:O	0.51	2.58	16	1
2:B:4:PHE:HD2	2:B:66:THR:HG22	0.51	1.65	3	1
3:C:51:GLU:C	3:C:52:LEU:HD12	0.51	2.31	4	3
2:B:36:ILE:HG21	2:B:41:GLN:NE2	0.51	2.21	5	1
1:A:59:TYR:O	1:A:60:ASN:CG	0.51	2.53	11	3
2:B:50:LEU:HD12	2:B:50:LEU:C	0.51	2.31	16	1
2:B:27:LYS:CD	2:B:27:LYS:C	0.51	2.84	2	1
3:C:12:VAL:CB	3:C:15:TYR:CE2	0.51	2.88	2	1
3:C:32:TYR:CZ	3:C:58:THR:O	0.51	2.61	9	3
1:A:69:LEU:C	1:A:69:LEU:HD13	0.51	2.31	10	1
3:C:89:VAL:HG21	3:C:97:ILE:CD1	0.51	2.27	14	1
2:B:67:LEU:C	2:B:67:LEU:CD2	0.51	2.82	17	2
1:A:5:VAL:CB	1:A:69:LEU:HD21	0.51	2.36	18	1
1:A:7:THR:HG22	1:A:69:LEU:HD22	0.51	1.83	19	1
2:B:23:ILE:HD11	2:B:50:LEU:HD13	0.51	1.83	6	1
2:B:28:ALA:HA	2:B:31:GLN:OE1	0.51	2.05	18	2
3:C:125:LEU:N	3:C:125:LEU:HD13	0.51	2.21	19	1
3:C:8:LEU:HD21	3:C:37:PRO:CG	0.50	2.35	2	1
1:A:2:GLN:O	1:A:63:ARG:NH1	0.50	2.44	6	1
1:A:59:TYR:O	1:A:59:TYR:CG	0.50	2.57	13	1
2:B:15:LEU:HG	2:B:29:LYS:HE2	0.50	1.83	1	1
3:C:54:ASN:HA	3:C:74:LEU:O	0.50	2.06	11	20
1:A:50:LEU:HD23	1:A:50:LEU:O	0.50	2.05	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:92:THR:HG22	3:C:95:MET:CG	0.50	2.36	18	1
3:C:17:TYR:OH	3:C:80:TYR:CD1	0.50	2.61	20	3
3:C:18:ARG:O	3:C:21:THR:CG2	0.50	2.59	10	2
1:A:43:LEU:HD22	1:A:43:LEU:H	0.50	1.67	13	2
3:C:77:LEU:C	3:C:80:TYR:CE2	0.50	2.89	14	1
3:C:18:ARG:O	3:C:21:THR:OG1	0.50	2.27	19	1
2:B:27:LYS:HD3	2:B:27:LYS:C	0.50	2.29	2	1
3:C:28:VAL:HG11	3:C:124:LEU:CB	0.50	2.37	5	1
1:A:2:GLN:NE2	1:A:14:THR:HG21	0.50	2.22	9	1
1:A:44:ILE:HD13	1:A:48:LYS:C	0.50	2.31	12	1
3:C:63:TYR:O	3:C:63:TYR:CG	0.50	2.64	9	2
2:B:71:LEU:HD12	2:B:71:LEU:O	0.50	2.07	5	2
3:C:75:TRP:C	3:C:75:TRP:CD1	0.50	2.89	16	2
1:A:8:LEU:H	1:A:8:LEU:HD13	0.50	1.66	4	1
2:B:50:LEU:HD12	2:B:50:LEU:N	0.50	2.22	12	3
3:C:76:LEU:HB3	3:C:80:TYR:CE1	0.50	2.42	5	1
3:C:75:TRP:C	3:C:76:LEU:HD12	0.50	2.30	11	3
2:B:14:THR:C	2:B:15:LEU:HD23	0.50	2.31	9	1
3:C:124:LEU:HD22	3:C:124:LEU:N	0.50	2.20	14	1
2:B:23:ILE:HD12	2:B:23:ILE:O	0.50	2.06	2	2
3:C:125:LEU:HD13	3:C:125:LEU:N	0.50	2.21	9	2
1:A:61:ILE:O	1:A:61:ILE:HG23	0.50	2.07	13	1
3:C:89:VAL:CG2	3:C:109:ILE:HD11	0.50	2.32	19	1
1:A:1:MET:HB3	1:A:63:ARG:NE	0.50	2.21	6	1
3:C:51:GLU:O	3:C:52:LEU:HD13	0.50	2.06	11	1
3:C:70:ILE:HD12	3:C:141:VAL:CG2	0.50	2.36	14	1
1:A:69:LEU:HD22	1:A:69:LEU:N	0.50	2.22	18	1
3:C:11:MET:HE2	3:C:37:PRO:HB2	0.50	1.83	19	1
1:A:23:ILE:CB	1:A:51:GLU:O	0.50	2.59	3	18
2:B:27:LYS:HD3	2:B:30:ILE:HG22	0.50	1.82	2	1
3:C:52:LEU:HD12	3:C:52:LEU:O	0.50	2.07	6	1
3:C:76:LEU:HD23	3:C:80:TYR:CD2	0.49	2.41	12	3
1:A:56:LEU:O	1:A:59:TYR:CE1	0.49	2.65	14	1
2:B:46:ALA:HB3	2:B:59:TYR:OH	0.49	2.07	20	1
2:B:23:ILE:CB	2:B:51:GLU:O	0.49	2.61	4	16
1:A:44:ILE:HD13	1:A:49:GLN:HA	0.49	1.83	2	3
3:C:20:LEU:HD13	3:C:20:LEU:N	0.49	2.22	4	1
3:C:73:CYS:O	3:C:88:PHE:HD1	0.49	1.90	8	1
2:B:71:LEU:HD22	2:B:71:LEU:N	0.49	2.22	9	2
1:A:27:LYS:HG2	1:A:38:PRO:HA	0.49	1.85	10	1
1:A:23:ILE:HG13	1:A:50:LEU:HD22	0.49	1.80	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:23:ILE:HB	2:B:50:LEU:HD22	0.49	1.82	12	1
3:C:84:PRO:HB2	3:C:114:LEU:HD23	0.49	1.84	15	1
3:C:15:TYR:CZ	3:C:17:TYR:O	0.49	2.63	17	1
2:B:5:VAL:HG23	2:B:69:LEU:HD13	0.49	1.82	1	1
2:B:15:LEU:HG	2:B:29:LYS:CE	0.49	2.37	1	1
3:C:44:PHE:CE1	3:C:48:SER:CB	0.49	2.94	6	4
3:C:70:ILE:HD11	3:C:141:VAL:CG1	0.49	2.37	4	1
3:C:125:LEU:HD22	3:C:125:LEU:H	0.49	1.67	6	3
3:C:102:HIS:O	3:C:103:VAL:HG23	0.49	2.08	19	4
3:C:124:LEU:HD23	3:C:128:ILE:HD13	0.49	1.84	11	1
2:B:56:LEU:HD23	2:B:56:LEU:N	0.49	2.15	14	2
2:B:70:VAL:HG11	3:C:117:TRP:CZ2	0.49	2.43	16	1
1:A:45:PHE:CG	1:A:59:TYR:CE2	0.49	3.00	1	1
1:A:73:LEU:N	1:A:73:LEU:HD13	0.49	2.22	2	1
1:A:27:LYS:CD	1:A:38:PRO:HB3	0.49	2.38	5	4
1:A:27:LYS:HG2	1:A:28:ALA:N	0.49	2.22	5	2
3:C:17:TYR:CE1	3:C:81:PRO:HB3	0.49	2.42	20	3
3:C:53:MET:SD	3:C:53:MET:N	0.49	2.84	11	1
1:A:41:GLN:OE1	1:A:69:LEU:HD11	0.49	2.06	16	1
2:B:61:ILE:CG2	2:B:61:ILE:O	0.49	2.60	17	2
1:A:50:LEU:HD12	1:A:50:LEU:C	0.49	2.32	20	1
2:B:66:THR:HG21	3:C:46:ASP:OD2	0.49	2.07	3	1
1:A:45:PHE:CZ	1:A:50:LEU:HD12	0.49	2.43	6	1
3:C:11:MET:CE	3:C:53:MET:HE3	0.49	2.37	8	1
3:C:75:TRP:CD1	3:C:76:LEU:N	0.49	2.81	11	3
3:C:81:PRO:O	3:C:119:HIS:CB	0.49	2.61	15	20
1:A:26:VAL:HG12	1:A:27:LYS:NZ	0.49	2.22	2	1
2:B:21:ASP:OD2	2:B:56:LEU:HD23	0.49	2.08	9	1
3:C:89:VAL:HG12	3:C:107:GLY:CA	0.49	2.37	17	1
3:C:107:GLY:O	3:C:109:ILE:HD13	0.49	2.07	20	1
1:A:43:LEU:C	1:A:50:LEU:HD11	0.49	2.33	11	1
1:A:50:LEU:HD13	1:A:50:LEU:H	0.49	1.67	19	2
3:C:82:TYR:O	3:C:117:TRP:CZ3	0.49	2.66	20	3
2:B:23:ILE:CD1	2:B:52:ASP:C	0.49	2.86	16	1
1:A:23:ILE:CG2	1:A:50:LEU:HD13	0.49	2.37	20	1
3:C:21:THR:HG22	3:C:22:VAL:N	0.49	2.20	17	2
2:B:43:LEU:HD22	2:B:43:LEU:N	0.49	2.22	19	2
2:B:56:LEU:O	2:B:59:TYR:CD1	0.49	2.65	14	1
3:C:89:VAL:HG13	3:C:109:ILE:HD11	0.48	1.85	1	1
3:C:77:LEU:N	3:C:80:TYR:CD2	0.48	2.81	14	3
1:A:3:ILE:HD11	1:A:17:VAL:CG1	0.48	2.38	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:127:LEU:C	3:C:127:LEU:HD13	0.48	2.33	17	1
3:C:21:THR:CG2	3:C:80:TYR:CE1	0.48	2.96	2	1
3:C:84:PRO:HD3	3:C:117:TRP:CD1	0.48	2.43	2	5
3:C:61:VAL:CG1	3:C:68:TYR:O	0.48	2.55	20	2
1:A:45:PHE:O	1:A:45:PHE:CG	0.48	2.66	13	1
3:C:55:LEU:O	3:C:55:LEU:CD2	0.48	2.59	17	1
3:C:130:VAL:O	3:C:133:VAL:HG22	0.48	2.08	17	1
1:A:50:LEU:O	1:A:50:LEU:CD2	0.48	2.62	11	2
2:B:43:LEU:HD22	2:B:67:LEU:HD11	0.48	1.85	18	1
2:B:43:LEU:HD22	2:B:69:LEU:HD21	0.48	1.83	20	1
2:B:43:LEU:HD22	2:B:43:LEU:H	0.48	1.68	1	2
3:C:117:TRP:C	3:C:117:TRP:CD1	0.48	2.91	4	1
2:B:5:VAL:CG1	2:B:69:LEU:HD13	0.48	2.38	5	1
3:C:109:ILE:HG22	3:C:111:LEU:CD1	0.48	2.38	5	2
3:C:124:LEU:HD22	3:C:124:LEU:H	0.48	1.69	14	1
3:C:89:VAL:O	3:C:89:VAL:HG13	0.48	2.08	17	1
2:B:17:VAL:HG11	2:B:56:LEU:HD11	0.48	1.84	18	1
2:B:23:ILE:HD11	2:B:50:LEU:HD12	0.48	1.84	20	1
2:B:71:LEU:O	3:C:117:TRP:CH2	0.48	2.67	20	1
1:A:17:VAL:HG13	1:A:18:GLU:N	0.48	2.24	19	5
3:C:80:TYR:N	3:C:80:TYR:CD2	0.48	2.79	5	2
3:C:135:PHE:O	3:C:135:PHE:HD2	0.48	1.91	15	2
3:C:21:THR:HB	3:C:80:TYR:CZ	0.48	2.43	19	1
3:C:28:VAL:CG1	3:C:29:ILE:N	0.48	2.77	7	4
3:C:75:TRP:N	3:C:75:TRP:CD1	0.48	2.81	20	3
1:A:45:PHE:HZ	1:A:50:LEU:HD23	0.48	1.67	12	1
1:A:50:LEU:CD1	1:A:50:LEU:C	0.48	2.86	12	1
2:B:27:LYS:O	2:B:31:GLN:NE2	0.48	2.46	16	1
2:B:45:PHE:CD2	2:B:59:TYR:CE1	0.48	3.01	18	1
1:A:54:ARG:HD3	1:A:55:THR:O	0.48	2.08	7	1
1:A:51:GLU:CG	1:A:54:ARG:HB2	0.48	2.39	11	1
3:C:74:LEU:HD11	3:C:87:CYS:SG	0.48	2.49	17	1
1:A:5:VAL:HG13	1:A:13:ILE:HB	0.48	1.86	20	1
1:A:3:ILE:HD11	1:A:67:LEU:HD13	0.48	1.85	11	1
1:A:50:LEU:HG	1:A:59:TYR:CD2	0.48	2.44	14	1
2:B:31:GLN:CG	2:B:36:ILE:O	0.48	2.62	16	1
2:B:36:ILE:HG21	2:B:41:GLN:OE1	0.48	2.09	2	1
3:C:22:VAL:CG2	3:C:23:ARG:N	0.48	2.76	2	2
2:B:43:LEU:CD2	2:B:69:LEU:HD11	0.48	2.39	5	1
3:C:12:VAL:HG12	3:C:15:TYR:HE1	0.48	1.69	14	2
1:A:50:LEU:HG	1:A:59:TYR:CE2	0.48	2.44	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:19:PRO:CA	2:B:56:LEU:HD21	0.48	2.38	14	1
2:B:70:VAL:HG13	3:C:117:TRP:CZ2	0.48	2.44	14	1
1:A:41:GLN:HG3	1:A:69:LEU:HD13	0.48	1.86	17	1
1:A:71:LEU:HD12	1:A:71:LEU:O	0.48	2.09	19	1
2:B:56:LEU:CG	2:B:61:ILE:HG21	0.47	2.37	12	1
3:C:124:LEU:HD23	3:C:124:LEU:N	0.47	2.25	7	1
3:C:75:TRP:HB2	3:C:86:ILE:HG23	0.47	1.85	8	1
2:B:4:PHE:CD2	2:B:66:THR:HG22	0.47	2.44	9	1
1:A:23:ILE:HD11	1:A:50:LEU:HD13	0.47	1.86	13	1
3:C:15:TYR:HE2	3:C:21:THR:OG1	0.47	1.87	17	1
3:C:89:VAL:O	3:C:89:VAL:HG12	0.47	2.09	20	2
3:C:15:TYR:CD1	3:C:18:ARG:HA	0.47	2.44	2	1
2:B:67:LEU:N	2:B:67:LEU:CD1	0.47	2.77	3	1
3:C:97:ILE:HD13	3:C:97:ILE:O	0.47	2.10	4	3
1:A:41:GLN:OE1	1:A:43:LEU:HD23	0.47	2.09	5	1
3:C:124:LEU:H	3:C:124:LEU:CD2	0.47	2.22	7	1
1:A:45:PHE:CD2	1:A:48:LYS:O	0.47	2.67	13	1
3:C:89:VAL:HG22	3:C:107:GLY:HA2	0.47	1.87	8	6
1:A:27:LYS:CG	1:A:38:PRO:HA	0.47	2.38	10	1
3:C:28:VAL:HG21	3:C:124:LEU:HB3	0.47	1.86	12	3
1:A:15:LEU:CD1	1:A:17:VAL:HG13	0.47	2.39	18	3
1:A:23:ILE:HD11	1:A:50:LEU:HD22	0.47	1.86	6	1
3:C:16:LYS:NZ	3:C:81:PRO:HD3	0.47	2.25	7	1
1:A:15:LEU:HD13	1:A:15:LEU:H	0.47	1.68	10	1
1:A:45:PHE:CE1	1:A:48:LYS:HB2	0.47	2.45	13	1
3:C:61:VAL:HB	3:C:68:TYR:CE1	0.47	2.44	13	1
2:B:50:LEU:H	2:B:50:LEU:HD13	0.47	1.70	14	1
3:C:124:LEU:H	3:C:124:LEU:HD13	0.47	1.69	14	1
2:B:23:ILE:CG1	2:B:50:LEU:HD23	0.47	2.40	19	1
2:B:43:LEU:HB3	2:B:50:LEU:HD11	0.47	1.86	2	2
2:B:8:LEU:HD22	2:B:8:LEU:H	0.47	1.70	4	2
3:C:77:LEU:CB	3:C:80:TYR:CE1	0.47	2.98	4	1
1:A:66:THR:C	1:A:67:LEU:HD12	0.47	2.35	5	1
3:C:43:VAL:O	3:C:43:VAL:CG2	0.47	2.63	5	4
3:C:16:LYS:HE3	3:C:78:ASP:O	0.47	2.08	7	1
3:C:52:LEU:CD1	3:C:77:LEU:HD23	0.47	2.40	8	2
2:B:54:ARG:HB2	2:B:59:TYR:OH	0.47	2.10	15	1
3:C:11:MET:HE2	3:C:53:MET:CG	0.47	2.39	17	1
2:B:23:ILE:CG1	2:B:50:LEU:HD13	0.47	2.40	18	1
1:A:62:GLN:NE2	3:C:105:ALA:O	0.47	2.47	19	1
1:A:59:TYR:O	1:A:59:TYR:CD2	0.47	2.68	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:118:LYS:CB	3:C:120:PRO:HD2	0.47	2.39	13	12
1:A:41:GLN:CD	1:A:41:GLN:O	0.47	2.58	2	1
2:B:23:ILE:HD12	2:B:23:ILE:C	0.47	2.34	2	2
3:C:12:VAL:HG23	3:C:15:TYR:OH	0.47	2.10	2	1
3:C:118:LYS:HB2	3:C:120:PRO:HD2	0.47	1.87	14	2
1:A:43:LEU:CD2	1:A:67:LEU:HD12	0.47	2.40	9	1
3:C:61:VAL:HG11	3:C:70:ILE:CD1	0.47	2.39	9	1
3:C:113:TYR:CE1	3:C:130:VAL:HB	0.47	2.45	9	1
2:B:5:VAL:HG13	2:B:67:LEU:HD22	0.47	1.85	17	2
1:A:67:LEU:N	1:A:67:LEU:HD22	0.47	2.24	19	1
2:B:5:VAL:HG12	2:B:15:LEU:HD21	0.47	1.87	1	1
3:C:17:TYR:CD1	3:C:20:LEU:HB2	0.47	2.44	10	2
3:C:52:LEU:HB2	3:C:75:TRP:NE1	0.47	2.25	3	1
1:A:36:ILE:HD12	1:A:71:LEU:HD22	0.47	1.86	7	1
1:A:23:ILE:CD1	1:A:50:LEU:HD23	0.47	2.40	4	2
3:C:76:LEU:HD12	3:C:76:LEU:N	0.47	2.25	11	1
3:C:80:TYR:CD2	3:C:80:TYR:N	0.47	2.81	17	1
2:B:30:ILE:HG22	2:B:36:ILE:CD1	0.46	2.40	7	1
2:B:7:THR:HG23	2:B:69:LEU:HD21	0.46	1.86	19	2
3:C:28:VAL:HG22	3:C:128:ILE:HD13	0.46	1.87	9	1
1:A:59:TYR:CE1	1:A:61:ILE:CB	0.46	2.99	14	1
2:B:43:LEU:C	2:B:50:LEU:HD11	0.46	2.35	14	1
3:C:75:TRP:CE3	3:C:86:ILE:HG21	0.46	2.44	17	1
2:B:23:ILE:HD13	2:B:54:ARG:O	0.46	2.11	20	1
1:A:60:ASN:O	1:A:60:ASN:OD1	0.46	2.33	9	3
3:C:12:VAL:HG13	3:C:53:MET:HG3	0.46	1.86	11	1
3:C:97:ILE:HD12	3:C:103:VAL:CG1	0.46	2.40	14	1
2:B:30:ILE:HG21	2:B:41:GLN:OE1	0.46	2.10	1	1
3:C:42:TYR:CG	3:C:75:TRP:NE1	0.46	2.83	3	1
3:C:127:LEU:O	3:C:130:VAL:HG22	0.46	2.10	17	8
3:C:111:LEU:O	3:C:111:LEU:HD12	0.46	2.10	9	1
1:A:6:LYS:HG2	1:A:12:THR:HG22	0.46	1.86	14	1
3:C:61:VAL:O	3:C:63:TYR:CE1	0.46	2.68	17	1
3:C:63:TYR:CE2	3:C:135:PHE:CE2	0.46	3.03	17	1
2:B:23:ILE:HG13	2:B:50:LEU:HD22	0.46	1.86	18	1
3:C:17:TYR:CD1	3:C:81:PRO:CB	0.46	2.97	5	4
3:C:26:VAL:O	3:C:30:THR:HG23	0.46	2.10	9	7
2:B:41:GLN:CD	2:B:41:GLN:C	0.46	2.84	12	1
1:A:43:LEU:HD12	1:A:69:LEU:CD2	0.46	2.40	14	1
2:B:31:GLN:NE2	2:B:36:ILE:O	0.46	2.47	20	2
3:C:17:TYR:HB3	3:C:20:LEU:CD2	0.46	2.38	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:86:ILE:O	3:C:86:ILE:HG22	0.46	2.10	12	1
2:B:5:VAL:HG13	2:B:69:LEU:HD23	0.46	1.86	20	1
3:C:76:LEU:CD1	3:C:80:TYR:CD1	0.46	2.98	20	1
3:C:54:ASN:CA	3:C:74:LEU:O	0.46	2.64	1	20
2:B:41:GLN:CD	2:B:41:GLN:O	0.46	2.59	12	1
3:C:12:VAL:O	3:C:12:VAL:CG2	0.46	2.64	13	1
2:B:23:ILE:HD12	2:B:50:LEU:HD13	0.46	1.87	18	1
1:A:23:ILE:HA	1:A:26:VAL:HG13	0.46	1.86	1	1
2:B:27:LYS:HE2	2:B:41:GLN:CG	0.46	2.40	2	1
3:C:75:TRP:CE3	3:C:86:ILE:HG23	0.46	2.46	3	1
3:C:110:TYR:O	3:C:111:LEU:HD12	0.46	2.10	4	1
3:C:113:TYR:HE2	3:C:127:LEU:HD12	0.46	1.66	4	1
3:C:54:ASN:HB2	3:C:74:LEU:O	0.46	2.10	11	2
3:C:97:ILE:HD12	3:C:140:PRO:O	0.46	2.11	9	1
1:A:43:LEU:O	1:A:44:ILE:HD13	0.46	2.11	18	2
1:A:43:LEU:HD13	1:A:68:HIS:O	0.46	2.10	19	1
2:B:56:LEU:C	2:B:56:LEU:CD1	0.46	2.86	9	3
1:A:38:PRO:O	1:A:41:GLN:HG3	0.46	2.11	2	1
3:C:86:ILE:O	3:C:88:PHE:CE1	0.46	2.69	8	1
3:C:135:PHE:CE1	3:C:140:PRO:HD2	0.46	2.45	10	2
3:C:61:VAL:O	3:C:63:TYR:CE2	0.46	2.68	17	1
3:C:72:ILE:CD1	3:C:131:MET:HE3	0.46	2.41	19	1
1:A:23:ILE:CD1	1:A:54:ARG:O	0.46	2.64	3	1
3:C:126:GLY:O	3:C:130:VAL:HG13	0.46	2.10	17	7
1:A:56:LEU:HB3	1:A:61:ILE:CG1	0.46	2.41	10	1
3:C:71:PRO:O	3:C:72:ILE:HD13	0.46	2.11	11	1
3:C:15:TYR:HB3	3:C:80:TYR:OH	0.45	2.10	2	1
1:A:44:ILE:HG23	1:A:68:HIS:HB2	0.45	1.87	6	2
1:A:43:LEU:HB2	1:A:50:LEU:CD1	0.45	2.41	20	2
2:B:30:ILE:CG2	2:B:36:ILE:HD11	0.45	2.42	19	1
2:B:15:LEU:HD13	2:B:15:LEU:N	0.45	2.25	1	1
3:C:80:TYR:CE1	3:C:85:PRO:HG3	0.45	2.47	11	2
2:B:43:LEU:HD21	2:B:69:LEU:HD11	0.45	1.87	4	1
3:C:26:VAL:O	3:C:30:THR:OG1	0.45	2.33	4	2
2:B:36:ILE:O	2:B:36:ILE:HG23	0.45	2.11	5	3
3:C:113:TYR:CD1	3:C:130:VAL:HG11	0.45	2.46	5	1
1:A:56:LEU:CD2	1:A:61:ILE:HG21	0.45	2.41	6	1
1:A:40:GLN:O	1:A:71:LEU:HD12	0.45	2.12	8	1
3:C:11:MET:CG	3:C:12:VAL:HG13	0.45	2.41	10	1
1:A:31:GLN:NE2	1:A:36:ILE:O	0.45	2.49	14	1
3:C:15:TYR:CD2	3:C:15:TYR:N	0.45	2.83	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:52:LEU:HD11	3:C:75:TRP:CE3	0.45	2.47	15	1
3:C:12:VAL:HG13	3:C:12:VAL:O	0.45	2.11	6	1
3:C:16:LYS:CD	3:C:17:TYR:H	0.45	2.24	7	1
3:C:59:ILE:CD1	3:C:128:ILE:HG23	0.45	2.42	8	1
3:C:114:LEU:HD22	3:C:114:LEU:C	0.45	2.35	15	1
2:B:66:THR:C	2:B:67:LEU:HD23	0.45	2.37	16	1
1:A:23:ILE:HB	1:A:50:LEU:HD23	0.45	1.86	1	1
1:A:43:LEU:HD23	1:A:68:HIS:O	0.45	2.11	2	2
3:C:118:LYS:HB3	3:C:120:PRO:HD2	0.45	1.87	17	3
3:C:110:TYR:C	3:C:111:LEU:HD13	0.45	2.35	5	2
2:B:5:VAL:HG13	2:B:13:ILE:HB	0.45	1.88	9	1
2:B:23:ILE:HG23	2:B:51:GLU:O	0.45	2.10	9	1
3:C:39:LEU:C	3:C:39:LEU:HD13	0.45	2.36	15	2
3:C:22:VAL:O	3:C:23:ARG:C	0.45	2.58	3	20
1:A:23:ILE:HD13	1:A:54:ARG:O	0.45	2.12	3	3
1:A:27:LYS:O	1:A:31:GLN:CD	0.45	2.60	6	2
3:C:16:LYS:HD2	3:C:17:TYR:HB2	0.45	1.89	7	1
3:C:70:ILE:HD11	3:C:141:VAL:HG21	0.45	1.86	13	1
3:C:134:VAL:HG13	3:C:135:PHE:N	0.45	2.27	13	6
1:A:36:ILE:O	1:A:36:ILE:HG23	0.45	2.12	18	7
1:A:45:PHE:HE2	1:A:67:LEU:HD13	0.45	1.71	6	1
3:C:15:TYR:CZ	3:C:53:MET:SD	0.45	3.09	13	1
2:B:50:LEU:O	2:B:50:LEU:CD2	0.45	2.64	14	1
3:C:28:VAL:CG2	3:C:29:ILE:N	0.45	2.79	15	1
3:C:39:LEU:O	3:C:39:LEU:CD2	0.45	2.65	16	1
2:B:45:PHE:CE2	2:B:67:LEU:HD12	0.45	2.46	17	2
2:B:36:ILE:HB	2:B:41:GLN:NE2	0.45	2.26	19	1
2:B:1:MET:HE3	2:B:19:PRO:HG3	0.45	1.89	1	4
2:B:3:ILE:HG22	2:B:4:PHE:N	0.45	2.27	4	6
3:C:15:TYR:OH	3:C:22:VAL:CG1	0.45	2.65	2	1
3:C:15:TYR:OH	3:C:53:MET:N	0.45	2.49	15	2
3:C:7:GLN:HG3	3:C:11:MET:HE3	0.45	1.87	4	1
3:C:60:PRO:O	3:C:132:ILE:HG13	0.45	2.12	4	4
1:A:30:ILE:HG21	1:A:41:GLN:OE1	0.45	2.12	16	2
1:A:59:TYR:CE1	1:A:61:ILE:CG1	0.45	3.00	14	1
3:C:15:TYR:CE2	3:C:17:TYR:C	0.45	2.92	17	1
2:B:36:ILE:CG2	2:B:71:LEU:HD11	0.45	2.42	2	1
2:B:71:LEU:HD22	2:B:71:LEU:H	0.45	1.72	9	1
3:C:76:LEU:N	3:C:76:LEU:CD2	0.45	2.79	20	2
3:C:68:TYR:CD1	3:C:68:TYR:O	0.45	2.69	13	1
2:B:56:LEU:HA	2:B:59:TYR:CE1	0.45	2.47	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:27:LYS:O	2:B:30:ILE:HG13	0.45	2.12	15	1
3:C:86:ILE:HG22	3:C:86:ILE:O	0.45	2.11	16	1
2:B:45:PHE:CE1	2:B:50:LEU:HB2	0.45	2.47	19	2
3:C:44:PHE:CD2	3:C:44:PHE:N	0.45	2.84	18	1
3:C:21:THR:HG22	3:C:80:TYR:HD2	0.45	1.71	3	1
3:C:12:VAL:HA	3:C:15:TYR:CE1	0.45	2.47	14	3
3:C:135:PHE:CD1	3:C:140:PRO:CD	0.45	3.00	10	1
3:C:35:LEU:HD21	3:C:55:LEU:CB	0.45	2.41	19	1
2:B:4:PHE:CE2	2:B:14:THR:HG22	0.45	2.47	15	2
3:C:11:MET:HB2	3:C:39:LEU:HD12	0.45	1.89	2	1
1:A:66:THR:HG22	3:C:106:ASN:CG	0.45	2.37	3	2
3:C:102:HIS:O	3:C:103:VAL:HG13	0.45	2.12	7	1
3:C:114:LEU:HD13	3:C:114:LEU:C	0.45	2.36	15	1
3:C:11:MET:HG2	3:C:39:LEU:HD12	0.45	1.89	16	1
3:C:15:TYR:CD1	3:C:15:TYR:C	0.45	2.93	17	1
3:C:52:LEU:HD12	3:C:75:TRP:CE3	0.45	2.47	18	1
3:C:24:GLU:O	3:C:28:VAL:CG2	0.44	2.65	4	2
2:B:4:PHE:CE1	2:B:12:THR:HG22	0.44	2.47	5	2
2:B:12:THR:C	2:B:13:ILE:HD13	0.44	2.36	8	1
3:C:38:VAL:C	3:C:53:MET:HE1	0.44	2.36	8	1
3:C:42:TYR:CD1	3:C:42:TYR:C	0.44	2.94	8	1
2:B:50:LEU:H	2:B:50:LEU:HD22	0.44	1.72	9	1
3:C:20:LEU:HD21	3:C:119:HIS:CE1	0.44	2.46	9	2
3:C:61:VAL:HG11	3:C:70:ILE:HD12	0.44	1.89	9	1
1:A:15:LEU:HD12	1:A:17:VAL:HG13	0.44	1.87	1	2
2:B:61:ILE:O	2:B:61:ILE:HG23	0.44	2.12	6	2
3:C:12:VAL:HG12	3:C:53:MET:HG2	0.44	1.89	5	2
3:C:53:MET:O	3:C:76:LEU:HB2	0.44	2.12	5	1
3:C:73:CYS:O	3:C:75:TRP:CD1	0.44	2.71	7	3
3:C:12:VAL:O	3:C:12:VAL:CG1	0.44	2.65	8	2
1:A:45:PHE:CE1	1:A:50:LEU:HD23	0.44	2.46	12	1
3:C:103:VAL:HG11	3:C:140:PRO:HB3	0.44	1.89	16	1
2:B:30:ILE:HG21	2:B:36:ILE:HD11	0.44	1.90	19	1
1:A:22:THR:HG23	1:A:25:ASN:H	0.44	1.72	15	2
2:B:44:ILE:C	2:B:45:PHE:CD1	0.44	2.95	18	2
3:C:15:TYR:CE2	3:C:80:TYR:HE2	0.44	2.31	5	1
1:A:3:ILE:HD12	1:A:17:VAL:CG2	0.44	2.43	10	1
1:A:15:LEU:HD13	1:A:15:LEU:N	0.44	2.27	10	1
2:B:27:LYS:CD	2:B:38:PRO:HB3	0.44	2.42	13	1
3:C:15:TYR:OH	3:C:81:PRO:CD	0.44	2.65	17	1
3:C:134:VAL:HG23	3:C:135:PHE:N	0.44	2.28	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:32:TYR:CE1	3:C:35:LEU:HG	0.44	2.46	4	1
3:C:124:LEU:N	3:C:124:LEU:CD2	0.44	2.80	7	1
1:A:23:ILE:CD1	1:A:50:LEU:HB3	0.44	2.33	16	1
1:A:27:LYS:CD	1:A:41:GLN:CD	0.44	2.91	2	1
1:A:27:LYS:CG	1:A:41:GLN:CD	0.44	2.90	4	1
2:B:41:GLN:NE2	2:B:69:LEU:HD23	0.44	2.27	5	1
3:C:28:VAL:CG2	3:C:124:LEU:HB3	0.44	2.43	11	1
1:A:43:LEU:CD2	1:A:69:LEU:HD12	0.44	2.42	16	1
2:B:70:VAL:HG21	3:C:117:TRP:HZ2	0.44	1.73	16	1
1:A:43:LEU:HB3	1:A:50:LEU:HD21	0.44	1.89	20	1
2:B:43:LEU:N	2:B:43:LEU:HD13	0.44	2.27	1	1
3:C:97:ILE:HD13	3:C:140:PRO:O	0.44	2.13	1	1
3:C:51:GLU:O	3:C:52:LEU:HD12	0.44	2.12	14	3
3:C:125:LEU:C	3:C:125:LEU:HD23	0.44	2.37	11	1
3:C:11:MET:SD	3:C:39:LEU:HD12	0.44	2.52	16	1
2:B:5:VAL:CG1	2:B:69:LEU:HD23	0.44	2.42	20	1
2:B:13:ILE:HD12	2:B:33:LYS:HD3	0.44	1.90	7	1
3:C:75:TRP:HD1	3:C:86:ILE:H	0.44	1.55	18	2
3:C:74:LEU:HD23	3:C:87:CYS:SG	0.44	2.52	18	1
1:A:23:ILE:HD11	1:A:27:LYS:NZ	0.44	2.28	1	1
1:A:46:ALA:HB2	1:A:59:TYR:OH	0.44	2.13	1	2
3:C:71:PRO:CG	3:C:90:LYS:O	0.44	2.66	19	19
3:C:8:LEU:HD21	3:C:37:PRO:HG3	0.44	1.90	2	1
3:C:17:TYR:HB3	3:C:20:LEU:CD1	0.44	2.41	4	1
1:A:45:PHE:CE1	1:A:50:LEU:HB2	0.44	2.48	6	1
1:A:24:GLU:O	1:A:27:LYS:HG2	0.44	2.12	19	2
1:A:23:ILE:O	1:A:27:LYS:HG2	0.44	2.13	2	1
3:C:18:ARG:CG	3:C:19:ASP:H	0.44	2.26	2	1
2:B:8:LEU:HD22	2:B:8:LEU:N	0.44	2.28	18	2
1:A:17:VAL:HG11	1:A:56:LEU:HD13	0.44	1.89	6	1
1:A:4:PHE:CE1	1:A:12:THR:HG22	0.44	2.48	7	1
2:B:46:ALA:CB	2:B:59:TYR:OH	0.44	2.66	8	1
2:B:46:ALA:HB3	2:B:48:LYS:NZ	0.44	2.28	14	1
2:B:15:LEU:N	2:B:15:LEU:CD2	0.43	2.79	1	1
3:C:75:TRP:HE3	3:C:86:ILE:HG23	0.43	1.73	3	1
3:C:20:LEU:CD2	3:C:81:PRO:HB3	0.43	2.42	4	1
3:C:97:ILE:HD11	3:C:104:ASP:O	0.43	2.13	7	2
3:C:17:TYR:CD1	3:C:20:LEU:CB	0.43	3.00	10	3
3:C:59:ILE:CG2	3:C:132:ILE:HD11	0.43	2.43	9	1
1:A:27:LYS:CE	1:A:36:ILE:O	0.43	2.66	10	1
1:A:27:LYS:HD3	1:A:41:GLN:CG	0.43	2.42	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HB3	1:A:50:LEU:HD11	0.43	1.89	19	2
3:C:24:GLU:CB	3:C:124:LEU:HD21	0.43	2.40	14	1
1:A:17:VAL:HG21	1:A:56:LEU:CD1	0.43	2.43	15	1
3:C:135:PHE:CD2	3:C:135:PHE:C	0.43	2.96	15	1
3:C:111:LEU:HD21	3:C:134:VAL:CG2	0.43	2.32	16	1
3:C:114:LEU:HD11	3:C:127:LEU:HD11	0.43	1.90	19	1
1:A:56:LEU:O	1:A:61:ILE:HG22	0.43	2.13	1	1
3:C:21:THR:OG1	3:C:80:TYR:HE1	0.43	1.95	2	1
2:B:36:ILE:HG21	2:B:41:GLN:HE21	0.43	1.72	5	1
2:B:2:GLN:NE2	2:B:14:THR:OG1	0.43	2.52	9	2
2:B:21:ASP:OD1	2:B:21:ASP:C	0.43	2.61	9	1
3:C:83:ASN:CG	3:C:84:PRO:HD2	0.43	2.38	12	1
1:A:71:LEU:N	1:A:71:LEU:HD22	0.43	2.27	15	1
2:B:45:PHE:CE1	2:B:61:ILE:HD11	0.43	2.48	4	1
2:B:45:PHE:CD1	2:B:67:LEU:HD12	0.43	2.47	6	1
3:C:84:PRO:HB2	3:C:114:LEU:HD13	0.43	1.91	9	1
3:C:18:ARG:O	3:C:21:THR:HG23	0.43	2.12	10	1
3:C:42:TYR:CB	3:C:75:TRP:CZ3	0.43	3.02	12	1
3:C:61:VAL:O	3:C:61:VAL:CG2	0.43	2.53	20	1
3:C:54:ASN:CB	3:C:74:LEU:O	0.43	2.66	10	15
1:A:41:GLN:CG	1:A:69:LEU:HD13	0.43	2.44	17	1
2:B:71:LEU:HD12	2:B:71:LEU:H	0.43	1.74	17	1
3:C:63:TYR:CE1	3:C:68:TYR:CB	0.43	2.98	17	1
2:B:63:LYS:O	2:B:64:GLU:HB2	0.43	2.13	18	1
1:A:5:VAL:HG21	1:A:69:LEU:HD12	0.43	1.90	2	1
3:C:72:ILE:HG22	3:C:73:CYS:N	0.43	2.29	5	2
1:A:54:ARG:NH2	1:A:59:TYR:HB2	0.43	2.27	7	1
3:C:89:VAL:HG12	3:C:107:GLY:HA2	0.43	1.89	17	1
1:A:68:HIS:CE1	1:A:70:VAL:HG23	0.43	2.47	18	1
3:C:107:GLY:O	3:C:108:LYS:C	0.43	2.61	3	20
3:C:35:LEU:HD13	3:C:56:THR:C	0.43	2.39	4	1
2:B:14:THR:O	2:B:15:LEU:HD22	0.43	2.14	17	3
3:C:72:ILE:H	3:C:72:ILE:HD12	0.43	1.74	8	1
3:C:28:VAL:HG21	3:C:124:LEU:CD2	0.43	2.41	11	1
1:A:59:TYR:CD2	1:A:61:ILE:HB	0.43	2.48	13	1
2:B:19:PRO:C	2:B:56:LEU:HD11	0.43	2.37	15	1
2:B:45:PHE:CG	2:B:59:TYR:CE1	0.43	3.06	18	1
2:B:45:PHE:CE1	2:B:50:LEU:HD12	0.43	2.49	18	1
3:C:12:VAL:CG2	3:C:15:TYR:CE2	0.43	3.01	2	1
1:A:62:GLN:HB3	3:C:97:ILE:HD11	0.43	1.90	5	3
3:C:86:ILE:CG1	3:C:86:ILE:O	0.43	2.67	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:LEU:C	2:B:15:LEU:HD23	0.43	2.38	4	1
3:C:61:VAL:HB	3:C:135:PHE:CD2	0.43	2.49	10	1
2:B:36:ILE:HG23	2:B:41:GLN:NE2	0.43	2.29	11	1
3:C:17:TYR:CE2	3:C:20:LEU:HD23	0.43	2.49	12	1
1:A:49:GLN:O	2:B:46:ALA:HB1	0.43	2.14	13	1
3:C:15:TYR:CE1	3:C:80:TYR:OH	0.43	2.67	14	1
2:B:4:PHE:CD1	2:B:12:THR:HG23	0.43	2.48	17	1
1:A:43:LEU:HB2	1:A:50:LEU:CG	0.43	2.43	20	1
3:C:17:TYR:OH	3:C:80:TYR:CD2	0.43	2.71	1	2
3:C:39:LEU:N	3:C:39:LEU:CD1	0.43	2.82	8	1
3:C:73:CYS:O	3:C:88:PHE:CD1	0.43	2.71	8	1
2:B:23:ILE:CG1	2:B:52:ASP:HA	0.43	2.32	12	1
3:C:12:VAL:CB	3:C:15:TYR:CD1	0.43	3.01	14	1
3:C:63:TYR:CD1	3:C:63:TYR:N	0.43	2.83	17	1
3:C:70:ILE:CG1	3:C:135:PHE:HE1	0.43	2.27	17	1
2:B:23:ILE:HG12	2:B:54:ARG:O	0.43	2.13	18	1
1:A:67:LEU:HD23	1:A:67:LEU:N	0.43	2.29	3	1
3:C:68:TYR:CD2	3:C:68:TYR:N	0.43	2.87	4	1
1:A:43:LEU:HD12	1:A:43:LEU:H	0.43	1.74	7	1
1:A:54:ARG:CD	1:A:54:ARG:C	0.43	2.92	7	1
3:C:59:ILE:HB	3:C:132:ILE:HD11	0.43	1.91	9	1
3:C:127:LEU:HD23	3:C:131:MET:SD	0.43	2.54	10	1
2:B:56:LEU:C	2:B:61:ILE:HG22	0.43	2.39	12	1
3:C:59:ILE:CG2	3:C:131:MET:HE2	0.43	2.44	14	1
1:A:50:LEU:HD13	1:A:50:LEU:N	0.43	2.29	16	1
3:C:11:MET:HB2	3:C:53:MET:SD	0.43	2.53	19	1
3:C:117:TRP:CD1	3:C:117:TRP:C	0.43	2.95	18	6
1:A:43:LEU:C	1:A:50:LEU:HD22	0.43	2.39	3	1
2:B:5:VAL:HG13	2:B:69:LEU:HD13	0.43	1.90	5	1
3:C:114:LEU:HD22	3:C:114:LEU:N	0.43	2.29	12	1
1:A:23:ILE:HD12	1:A:23:ILE:O	0.42	2.13	1	1
1:A:23:ILE:HG12	1:A:51:GLU:O	0.42	2.15	1	1
3:C:28:VAL:CG1	3:C:32:TYR:CZ	0.42	3.01	4	1
3:C:43:VAL:HG13	3:C:47:GLY:O	0.42	2.14	13	3
1:A:62:GLN:HG3	3:C:97:ILE:HG22	0.42	1.91	9	1
2:B:8:LEU:HD23	2:B:71:LEU:HD23	0.42	1.91	9	1
2:B:44:ILE:HG23	2:B:68:HIS:HB2	0.42	1.91	9	1
2:B:15:LEU:HG	2:B:29:LYS:CD	0.42	2.44	10	1
2:B:23:ILE:HD12	2:B:50:LEU:CD2	0.42	2.43	12	1
2:B:23:ILE:HG13	2:B:50:LEU:HD13	0.42	1.90	18	1
3:C:28:VAL:HG12	3:C:32:TYR:CZ	0.42	2.49	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:127:LEU:C	3:C:127:LEU:HD23	0.42	2.39	4	1
1:A:27:LYS:HD3	1:A:38:PRO:HB3	0.42	1.90	5	1
3:C:109:ILE:HG22	3:C:111:LEU:HD12	0.42	1.91	5	1
1:A:44:ILE:C	1:A:45:PHE:CD1	0.42	2.97	6	1
1:A:56:LEU:HD23	1:A:61:ILE:HG21	0.42	1.91	6	1
2:B:71:LEU:O	2:B:71:LEU:CD2	0.42	2.67	8	1
1:A:3:ILE:HD12	1:A:4:PHE:O	0.42	2.14	18	1
2:B:46:ALA:HB3	2:B:59:TYR:HH	0.42	1.74	20	1
1:A:55:THR:HG22	1:A:58:ASP:CG	0.42	2.39	2	2
3:C:63:TYR:CB	3:C:68:TYR:HE2	0.42	2.24	4	1
3:C:113:TYR:CD2	3:C:113:TYR:C	0.42	2.97	4	1
3:C:25:THR:O	3:C:28:VAL:HG22	0.42	2.13	5	1
3:C:16:LYS:NZ	3:C:17:TYR:CB	0.42	2.82	7	1
2:B:23:ILE:HD13	2:B:43:LEU:HD12	0.42	1.90	9	1
3:C:15:TYR:OH	3:C:76:LEU:O	0.42	2.30	13	1
2:B:67:LEU:HD23	2:B:67:LEU:O	0.42	2.13	17	2
3:C:55:LEU:CD2	3:C:76:LEU:HD11	0.42	2.40	19	1
3:C:76:LEU:HB3	3:C:80:TYR:CZ	0.42	2.49	5	1
2:B:45:PHE:CE1	2:B:61:ILE:HD12	0.42	2.49	6	1
3:C:16:LYS:CD	3:C:79:THR:HA	0.42	2.44	7	1
3:C:109:ILE:HD13	3:C:131:MET:HE3	0.42	1.89	10	1
3:C:50:ARG:CG	3:C:52:LEU:HD21	0.42	2.45	11	1
2:B:24:GLU:O	2:B:27:LYS:HG2	0.42	2.15	13	1
1:A:44:ILE:CD1	3:C:44:PHE:O	0.42	2.67	14	1
2:B:43:LEU:HB3	2:B:50:LEU:CD2	0.42	2.42	16	1
3:C:50:ARG:HB3	3:C:52:LEU:HD21	0.42	1.92	17	2
3:C:42:TYR:CD2	3:C:75:TRP:CZ3	0.42	3.08	17	1
3:C:42:TYR:HB3	3:C:75:TRP:CZ3	0.42	2.50	12	1
2:B:40:GLN:O	2:B:41:GLN:NE2	0.42	2.53	19	1
1:A:1:MET:C	1:A:63:ARG:HE	0.42	2.22	6	1
3:C:54:ASN:CB	3:C:75:TRP:CD1	0.42	3.02	8	2
1:A:5:VAL:HG13	1:A:15:LEU:HD21	0.42	1.92	7	1
2:B:70:VAL:HG13	3:C:83:ASN:OD1	0.42	2.14	12	1
3:C:61:VAL:HG11	3:C:135:PHE:CD2	0.42	2.50	15	1
3:C:88:PHE:CE1	3:C:106:ASN:O	0.42	2.73	17	1
3:C:89:VAL:O	3:C:89:VAL:CG2	0.42	2.67	1	1
1:A:1:MET:HE2	1:A:19:PRO:HG3	0.42	1.90	10	2
3:C:96:THR:HG23	3:C:96:THR:O	0.42	2.14	2	3
1:A:56:LEU:HD23	1:A:61:ILE:HD13	0.42	1.90	6	1
1:A:3:ILE:HG22	1:A:4:PHE:N	0.42	2.30	10	1
3:C:70:ILE:HB	3:C:135:PHE:CE1	0.42	2.48	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:77:LEU:HD11	3:C:83:ASN:HD22	0.42	1.75	12	1
2:B:27:LYS:HG2	2:B:28:ALA:N	0.42	2.30	13	1
2:B:50:LEU:HD22	2:B:50:LEU:H	0.42	1.72	14	1
3:C:61:VAL:HG11	3:C:135:PHE:CZ	0.42	2.49	15	1
3:C:35:LEU:HD23	3:C:55:LEU:HB3	0.42	1.89	18	1
2:B:27:LYS:HE3	2:B:38:PRO:HA	0.42	1.91	2	1
2:B:30:ILE:HG21	2:B:41:GLN:HE21	0.42	1.75	2	1
2:B:45:PHE:CZ	2:B:67:LEU:HD23	0.42	2.49	3	1
1:A:4:PHE:O	1:A:67:LEU:HG	0.42	2.14	6	1
2:B:31:GLN:OE1	2:B:31:GLN:CA	0.42	2.67	16	1
2:B:45:PHE:CE2	2:B:67:LEU:HD13	0.42	2.50	16	1
3:C:68:TYR:HE2	3:C:95:MET:HE2	0.42	1.74	17	1
3:C:17:TYR:HD2	3:C:17:TYR:H	0.42	1.58	11	2
1:A:3:ILE:HB	1:A:15:LEU:HD21	0.42	1.90	2	1
3:C:21:THR:HG21	3:C:80:TYR:CE1	0.42	2.48	2	1
3:C:15:TYR:CE2	3:C:78:ASP:HA	0.42	2.50	5	2
3:C:63:TYR:CD1	3:C:68:TYR:CD1	0.42	3.08	5	1
1:A:27:LYS:CE	1:A:38:PRO:HA	0.42	2.44	10	1
3:C:11:MET:HB3	3:C:53:MET:HE2	0.42	1.90	11	1
1:A:45:PHE:HE2	1:A:67:LEU:HB3	0.42	1.75	12	1
3:C:55:LEU:HD22	3:C:74:LEU:HB2	0.42	1.92	17	1
1:A:8:LEU:HD13	1:A:8:LEU:N	0.42	2.30	4	1
3:C:28:VAL:O	3:C:32:TYR:CD2	0.42	2.73	4	1
2:B:7:THR:HG22	2:B:8:LEU:H	0.42	1.75	19	2
3:C:131:MET:HE3	3:C:132:ILE:CA	0.42	2.45	14	1
3:C:7:GLN:O	3:C:11:MET:HG3	0.42	2.14	16	1
3:C:52:LEU:HD22	3:C:53:MET:N	0.42	2.30	20	1
2:B:50:LEU:CD1	2:B:50:LEU:C	0.41	2.93	4	1
3:C:68:TYR:HD1	3:C:70:ILE:CD1	0.41	2.26	4	1
1:A:46:ALA:CB	1:A:59:TYR:OH	0.41	2.68	6	1
2:B:26:VAL:O	2:B:30:ILE:HG12	0.41	2.14	7	1
3:C:128:ILE:HA	3:C:131:MET:HE3	0.41	1.92	12	2
3:C:109:ILE:HD12	3:C:110:TYR:N	0.41	2.30	16	1
3:C:21:THR:HB	3:C:80:TYR:OH	0.41	2.15	19	1
2:B:23:ILE:HD12	2:B:43:LEU:HD12	0.41	1.90	3	1
3:C:75:TRP:CZ3	3:C:77:LEU:HB3	0.41	2.49	3	1
3:C:109:ILE:HD12	3:C:131:MET:CE	0.41	2.46	3	1
2:B:23:ILE:HG23	2:B:50:LEU:CD2	0.41	2.38	4	1
1:A:46:ALA:O	3:C:75:TRP:CH2	0.41	2.74	6	1
3:C:80:TYR:CD2	3:C:80:TYR:C	0.41	2.96	9	1
2:B:36:ILE:HG12	2:B:41:GLN:HG2	0.41	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:76:LEU:N	3:C:76:LEU:CD1	0.41	2.83	11	1
3:C:39:LEU:HD13	3:C:39:LEU:O	0.41	2.15	13	1
1:A:3:ILE:HD12	1:A:4:PHE:N	0.41	2.30	18	1
3:C:8:LEU:HD13	3:C:8:LEU:C	0.41	2.40	20	1
3:C:124:LEU:HD12	3:C:124:LEU:N	0.41	2.30	20	1
1:A:3:ILE:HG23	1:A:4:PHE:N	0.41	2.30	5	1
3:C:17:TYR:CZ	3:C:21:THR:OG1	0.41	2.73	5	1
3:C:131:MET:O	3:C:135:PHE:CG	0.41	2.73	6	2
2:B:42:ARG:HB3	2:B:70:VAL:HG22	0.41	1.91	7	1
3:C:54:ASN:HD21	3:C:56:THR:HG23	0.41	1.75	7	1
3:C:59:ILE:HG22	3:C:60:PRO:HD2	0.41	1.91	9	1
3:C:97:ILE:HD12	3:C:103:VAL:HG11	0.41	1.91	14	1
2:B:55:THR:O	2:B:59:TYR:CE1	0.41	2.73	15	1
2:B:23:ILE:HG13	2:B:54:ARG:O	0.41	2.15	16	1
2:B:5:VAL:O	2:B:5:VAL:HG22	0.41	2.15	1	1
3:C:12:VAL:CG2	3:C:15:TYR:CZ	0.41	3.03	2	1
3:C:31:LEU:HD12	3:C:32:TYR:CD2	0.41	2.49	11	1
3:C:102:HIS:CD2	3:C:103:VAL:HG12	0.41	2.51	18	1
3:C:17:TYR:CZ	3:C:81:PRO:HD3	0.41	2.51	11	2
1:A:4:PHE:O	1:A:67:LEU:HD12	0.41	2.15	2	1
1:A:5:VAL:O	1:A:5:VAL:HG13	0.41	2.16	6	2
3:C:113:TYR:HD1	3:C:130:VAL:HG11	0.41	1.74	5	1
3:C:28:VAL:HG12	3:C:29:ILE:N	0.41	2.31	7	1
2:B:8:LEU:HD23	2:B:71:LEU:CD2	0.41	2.46	9	1
3:C:97:ILE:HD11	3:C:103:VAL:CG2	0.41	2.46	9	1
1:A:12:THR:O	1:A:13:ILE:HD13	0.41	2.15	12	1
2:B:43:LEU:CA	2:B:50:LEU:HD21	0.41	2.45	14	1
3:C:124:LEU:N	3:C:124:LEU:HD13	0.41	2.30	14	1
3:C:61:VAL:CG1	3:C:135:PHE:CE2	0.41	3.01	15	1
3:C:70:ILE:CB	3:C:135:PHE:CE1	0.41	3.03	17	2
3:C:76:LEU:HA	3:C:80:TYR:HD2	0.41	1.66	15	1
3:C:128:ILE:CG1	3:C:129:GLN:N	0.41	2.83	18	1
2:B:73:LEU:HD12	2:B:73:LEU:N	0.41	2.31	20	1
3:C:52:LEU:C	3:C:52:LEU:CD2	0.41	2.91	20	1
3:C:67:THR:HG23	3:C:67:THR:O	0.41	2.14	17	5
2:B:41:GLN:NE2	2:B:69:LEU:HD21	0.41	2.29	2	1
1:A:43:LEU:CB	1:A:50:LEU:CD2	0.41	2.99	3	1
1:A:27:LYS:HG3	1:A:41:GLN:CD	0.41	2.40	4	1
1:A:30:ILE:HG23	1:A:36:ILE:HG23	0.41	1.92	7	1
3:C:72:ILE:O	3:C:72:ILE:HD12	0.41	2.15	9	1
3:C:61:VAL:HG21	3:C:135:PHE:CZ	0.41	2.49	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:48:LYS:HB3	2:B:59:TYR:CE1	0.41	2.51	11	1
2:B:45:PHE:CZ	2:B:50:LEU:CD2	0.41	3.03	16	1
3:C:21:THR:CG2	3:C:80:TYR:CZ	0.41	3.04	19	1
1:A:5:VAL:HG23	1:A:5:VAL:O	0.41	2.16	7	1
3:C:52:LEU:HB2	3:C:76:LEU:O	0.41	2.14	15	2
1:A:15:LEU:C	1:A:15:LEU:CD2	0.41	2.94	10	1
3:C:70:ILE:O	3:C:70:ILE:HG23	0.41	2.15	10	1
2:B:23:ILE:HD11	2:B:50:LEU:HD22	0.41	1.93	11	1
3:C:119:HIS:N	3:C:120:PRO:HD3	0.41	2.29	15	2
3:C:39:LEU:HB3	3:C:53:MET:HE1	0.41	1.93	19	1
3:C:97:ILE:HD13	3:C:141:VAL:HG12	0.41	1.92	19	1
3:C:12:VAL:CA	3:C:15:TYR:CD1	0.41	3.02	5	1
3:C:76:LEU:HB3	3:C:80:TYR:CE2	0.41	2.51	5	2
1:A:31:GLN:CD	1:A:38:PRO:HD3	0.41	2.40	6	1
1:A:6:LYS:O	1:A:69:LEU:CD2	0.41	2.69	7	1
3:C:15:TYR:N	3:C:15:TYR:CD2	0.41	2.88	9	2
2:B:70:VAL:HG13	3:C:117:TRP:HZ2	0.41	1.73	14	1
3:C:53:MET:HE2	3:C:76:LEU:HD12	0.41	1.91	16	1
3:C:35:LEU:C	3:C:35:LEU:CD1	0.41	2.92	17	1
3:C:35:LEU:HD22	3:C:55:LEU:HD11	0.41	1.92	17	1
3:C:107:GLY:O	3:C:109:ILE:HD12	0.41	2.15	19	1
1:A:23:ILE:HD11	1:A:27:LYS:HZ3	0.41	1.76	1	1
3:C:15:TYR:N	3:C:15:TYR:CD1	0.41	2.88	3	1
2:B:50:LEU:HD21	2:B:59:TYR:CD2	0.41	2.50	5	1
3:C:74:LEU:HD12	3:C:85:PRO:HB2	0.41	1.93	5	1
1:A:1:MET:HE3	1:A:19:PRO:CG	0.41	2.46	6	1
2:B:7:THR:OG1	2:B:69:LEU:HD11	0.41	2.16	6	1
3:C:130:VAL:O	3:C:134:VAL:HG22	0.41	2.16	6	1
3:C:11:MET:CB	3:C:53:MET:HE3	0.41	2.46	7	1
2:B:55:THR:HG22	2:B:58:ASP:CG	0.41	2.40	9	1
3:C:102:HIS:O	3:C:102:HIS:HD2	0.41	1.99	9	1
1:A:43:LEU:CA	1:A:50:LEU:HD21	0.41	2.46	11	1
1:A:50:LEU:HD22	1:A:50:LEU:H	0.41	1.73	11	1
2:B:27:LYS:HG2	2:B:41:GLN:CD	0.41	2.40	12	1
1:A:59:TYR:OH	1:A:61:ILE:HD12	0.41	2.15	14	1
2:B:18:GLU:O	2:B:56:LEU:CD1	0.41	2.69	15	1
2:B:19:PRO:HA	2:B:56:LEU:CD1	0.41	2.46	15	1
3:C:12:VAL:HG23	3:C:18:ARG:HG3	0.41	1.92	15	1
2:B:40:GLN:O	2:B:41:GLN:CD	0.41	2.64	19	1
3:C:42:TYR:CG	3:C:75:TRP:CD1	0.41	3.08	3	1
1:A:50:LEU:CD1	1:A:67:LEU:HD11	0.41	2.46	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:30:ILE:N	2:B:30:ILE:HD13	0.41	2.31	7	1
3:C:24:GLU:HB3	3:C:124:LEU:CD2	0.41	2.44	7	1
3:C:97:ILE:O	3:C:97:ILE:HG23	0.41	2.15	9	1
1:A:62:GLN:OE1	3:C:97:ILE:HB	0.41	2.16	11	1
1:A:50:LEU:N	1:A:50:LEU:CD1	0.41	2.84	14	1
2:B:59:TYR:CE1	2:B:61:ILE:HG13	0.41	2.50	14	1
3:C:24:GLU:O	3:C:28:VAL:CG1	0.41	2.69	15	1
3:C:61:VAL:CG2	3:C:135:PHE:CD2	0.41	3.01	15	1
3:C:70:ILE:HB	3:C:135:PHE:CZ	0.41	2.50	17	1
3:C:28:VAL:CG2	3:C:124:LEU:HD22	0.41	2.45	20	1
2:B:13:ILE:HD12	2:B:14:THR:N	0.40	2.31	4	1
2:B:71:LEU:CD1	2:B:71:LEU:H	0.40	2.29	4	1
2:B:19:PRO:HA	2:B:56:LEU:CG	0.40	2.46	8	2
3:C:76:LEU:HD12	3:C:80:TYR:CD2	0.40	2.50	9	1
1:A:69:LEU:HD22	1:A:69:LEU:C	0.40	2.41	10	1
3:C:70:ILE:HD12	3:C:70:ILE:HA	0.40	1.77	13	1
2:B:23:ILE:O	2:B:26:VAL:HG22	0.40	2.16	16	1
3:C:109:ILE:HD12	3:C:109:ILE:C	0.40	2.41	16	1
3:C:70:ILE:HG21	3:C:135:PHE:CE1	0.40	2.51	17	1
2:B:3:ILE:HB	2:B:15:LEU:HD23	0.40	1.94	1	1
3:C:20:LEU:O	3:C:21:THR:C	0.40	2.65	1	20
3:C:15:TYR:CD1	3:C:18:ARG:CA	0.40	3.05	2	1
3:C:12:VAL:CA	3:C:15:TYR:HD1	0.40	2.29	5	1
3:C:114:LEU:O	3:C:114:LEU:HD12	0.40	2.16	10	1
2:B:61:ILE:HG23	2:B:61:ILE:O	0.40	2.17	12	1
1:A:68:HIS:CE1	3:C:45:ASN:O	0.40	2.74	18	1
3:C:111:LEU:HB2	3:C:113:TYR:CE2	0.40	2.51	2	1
3:C:17:TYR:HB2	3:C:81:PRO:HG3	0.40	1.93	4	1
1:A:21:ASP:O	1:A:56:LEU:HG	0.40	2.16	14	1
2:B:15:LEU:HD11	2:B:30:ILE:HD12	0.40	1.92	14	1
2:B:50:LEU:HD11	2:B:59:TYR:CZ	0.40	2.51	18	1
3:C:12:VAL:HG12	3:C:15:TYR:HB2	0.40	1.92	18	1
1:A:59:TYR:CD2	1:A:59:TYR:O	0.40	2.75	2	1
1:A:45:PHE:CZ	1:A:50:LEU:HD13	0.40	2.50	3	1
3:C:109:ILE:HD13	3:C:131:MET:SD	0.40	2.57	7	1
3:C:31:LEU:HD11	3:C:128:ILE:HD11	0.40	1.92	13	1
3:C:70:ILE:HD12	3:C:141:VAL:HG21	0.40	1.93	14	1
3:C:75:TRP:CE3	3:C:86:ILE:HB	0.40	2.52	16	1
3:C:86:ILE:N	3:C:86:ILE:HD12	0.40	2.31	16	1
3:C:82:TYR:O	3:C:117:TRP:NE1	0.40	2.54	18	1
1:A:4:PHE:CE1	1:A:12:THR:HG23	0.40	2.50	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:13:ILE:HD11	2:B:30:ILE:HD12	0.40	1.93	7	1
1:A:45:PHE:CZ	1:A:50:LEU:CD2	0.40	2.98	12	1
1:A:45:PHE:CD1	1:A:59:TYR:CE1	0.40	3.10	13	1
3:C:75:TRP:CD1	3:C:86:ILE:H	0.40	2.35	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	72/76 (95%)	68±0 (95±1%)	3±0 (4±1%)	0±0 (1±1%)	20	70
2	B	72/77 (94%)	70±0 (97±1%)	2±0 (3±1%)	0±0 (0±0%)	100	100
3	C	139/145 (96%)	114±0 (82±0%)	18±0 (13±0%)	8±0 (6±0%)	2	20
All	All	5660/5960 (95%)	5028 (89%)	462 (8%)	170 (3%)	5	38

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	4	SER	20
3	C	19	ASP	20
3	C	22	VAL	20
3	C	78	ASP	20
3	C	80	TYR	20
3	C	90	LYS	20
3	C	99	THR	20
3	C	119	HIS	20
1	A	73	LEU	10

6.3.2 Protein sidechains [i](#)

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	67/68 (99%)	57±3 (85±4%)	10±3 (15±4%)	5	43
2	B	67/69 (97%)	57±3 (85±4%)	10±3 (15±4%)	5	42
3	C	133/136 (98%)	114±3 (86±2%)	19±3 (14±2%)	5	44
All	All	5340/5460 (98%)	4564 (85%)	776 (15%)	5	43

All 180 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)
3	C	80	TYR	15
3	C	109	ILE	13
1	A	73	LEU	12
2	B	71	LEU	12
3	C	132	ILE	12
2	B	5	VAL	11
2	B	63	LYS	10
1	A	62	GLN	10
1	A	23	ILE	9
1	A	44	ILE	9
2	B	56	LEU	9
3	C	77	LEU	9
3	C	125	LEU	9
3	C	39	LEU	9
1	A	31	GLN	9
2	B	4	PHE	9
3	C	111	LEU	9
3	C	20	LEU	9
3	C	28	VAL	9
1	A	69	LEU	9
3	C	119	HIS	9
1	A	5	VAL	9
1	A	15	LEU	8
2	B	26	VAL	8
2	B	73	LEU	8
3	C	30	THR	8
3	C	124	LEU	8
2	B	50	LEU	8
2	B	30	ILE	8
2	B	13	ILE	8
3	C	44	PHE	8

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Mol	Chain	Res	Type	Models (Total)
2	B	15	LEU	7
3	C	8	LEU	7
3	C	70	ILE	7
3	C	72	ILE	7
1	A	13	ILE	7
1	A	71	LEU	7
2	B	6	LYS	7
2	B	23	ILE	7
2	B	70	VAL	7
3	C	143	SER	7
1	A	8	LEU	7
3	C	59	ILE	7
1	A	70	VAL	6
2	B	17	VAL	6
3	C	21	THR	6
3	C	114	LEU	6
1	A	67	LEU	6
3	C	29	ILE	6
2	B	31	GLN	6
3	C	75	TRP	6
1	A	50	LEU	6
1	A	72	ARG	5
2	B	61	ILE	5
3	C	19	ASP	5
3	C	97	ILE	5
1	A	3	ILE	5
1	A	33	LYS	5
2	B	12	THR	5
3	C	18	ARG	5
3	C	73	CYS	5
3	C	133	VAL	5
3	C	52	LEU	5
1	A	17	VAL	5
1	A	30	ILE	5
1	A	56	LEU	5
2	B	69	LEU	5
3	C	83	ASN	5
3	C	141	VAL	5
3	C	4	SER	5
3	C	42	TYR	5
3	C	17	TYR	5
2	B	67	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	4	PHE	4
1	A	26	VAL	4
2	B	43	LEU	4
2	B	44	ILE	4
3	C	34	ASP	4
3	C	130	VAL	4
2	B	41	GLN	4
2	B	54	ARG	4
3	C	31	LEU	4
3	C	86	ILE	4
3	C	135	PHE	4
1	A	43	LEU	4
3	C	43	VAL	4
3	C	76	LEU	4
3	C	79	THR	4
3	C	36	LYS	4
3	C	53	MET	4
2	B	7	THR	4
2	B	64	GLU	4
3	C	55	LEU	4
3	C	128	ILE	4
1	A	7	THR	3
1	A	40	GLN	3
1	A	61	ILE	3
3	C	35	LEU	3
3	C	78	ASP	3
1	A	27	LYS	3
3	C	68	TYR	3
3	C	88	PHE	3
1	A	41	GLN	3
3	C	61	VAL	3
3	C	118	LYS	3
3	C	131	MET	3
2	B	8	LEU	3
3	C	46	ASP	3
3	C	99	THR	3
3	C	26	VAL	3
3	C	54	ASN	3
1	A	54	ARG	3
2	B	48	LYS	3
2	B	66	THR	3
3	C	12	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	36	ILE	2
3	C	103	VAL	2
2	B	3	ILE	2
2	B	68	HIS	2
3	C	22	VAL	2
3	C	69	ASN	2
2	B	45	PHE	2
3	C	14	LYS	2
3	C	95	MET	2
3	C	108	LYS	2
3	C	116	GLU	2
1	A	12	THR	2
1	A	66	THR	2
3	C	32	TYR	2
1	A	6	LYS	2
3	C	102	HIS	2
1	A	63	ARG	2
3	C	82	TYR	2
1	A	48	LYS	2
3	C	11	MET	2
3	C	106	ASN	2
3	C	51	GLU	2
3	C	92	THR	2
1	A	51	GLU	2
1	A	59	TYR	2
3	C	142	PHE	2
2	B	59	TYR	2
1	A	42	ARG	2
1	A	65	SER	1
3	C	3	VAL	1
3	C	15	TYR	1
3	C	58	THR	1
3	C	127	LEU	1
1	A	68	HIS	1
2	B	36	ILE	1
3	C	10	LYS	1
3	C	16	LYS	1
3	C	56	THR	1
2	B	2	GLN	1
3	C	25	THR	1
3	C	45	ASN	1
2	B	21	ASP	1

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Mol	Chain	Res	Type	Models (Total)
2	B	40	GLN	1
3	C	9	LYS	1
3	C	50	ARG	1
2	B	29	LYS	1
3	C	64	ARG	1
3	C	33	LYS	1
2	B	27	LYS	1
1	A	24	GLU	1
3	C	98	LYS	1
1	A	9	THR	1
2	B	49	GLN	1
3	C	63	TYR	1
3	C	74	LEU	1
3	C	113	TYR	1
2	B	1	MET	1
2	B	42	ARG	1
2	B	51	GLU	1
3	C	101	LYS	1
2	B	33	LYS	1
3	C	87	CYS	1
1	A	45	PHE	1
2	B	72	ARG	1
3	C	129	GLN	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

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 13% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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

Total number of shifts	542
Number of shifts mapped to atoms	541
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	3	VAL	HT1	8.12385	.	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	271	0.02 ± 0.19	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 527 atoms were assigned a chemical shift out of a possible 4058. 0 out of 55 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	527/1414 (37%)	263/571 (46%)	0/574 (0%)	264/269 (98%)
Sidechain	0/2397 (0%)	0/1560 (0%)	0/754 (0%)	0/83 (0%)
Aromatic	0/247 (0%)	0/120 (0%)	0/120 (0%)	0/7 (0%)
Overall	527/4058 (13%)	263/2251 (12%)	0/1448 (0%)	264/359 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 13%, i.e. 541 atoms were assigned a chemical shift out of a possible 4137. 0 out of 55 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	541/1453 (37%)	270/589 (46%)	0/588 (0%)	271/276 (98%)
Sidechain	0/2437 (0%)	0/1584 (0%)	0/764 (0%)	0/89 (0%)
Aromatic	0/247 (0%)	0/120 (0%)	0/120 (0%)	0/7 (0%)
Overall	541/4137 (13%)	270/2293 (12%)	0/1472 (0%)	271/372 (73%)

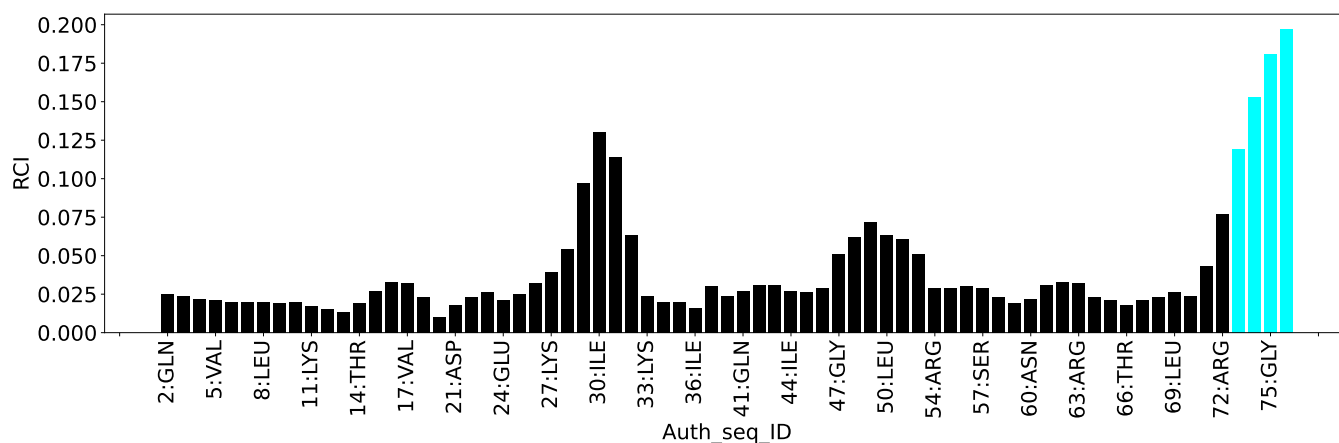
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

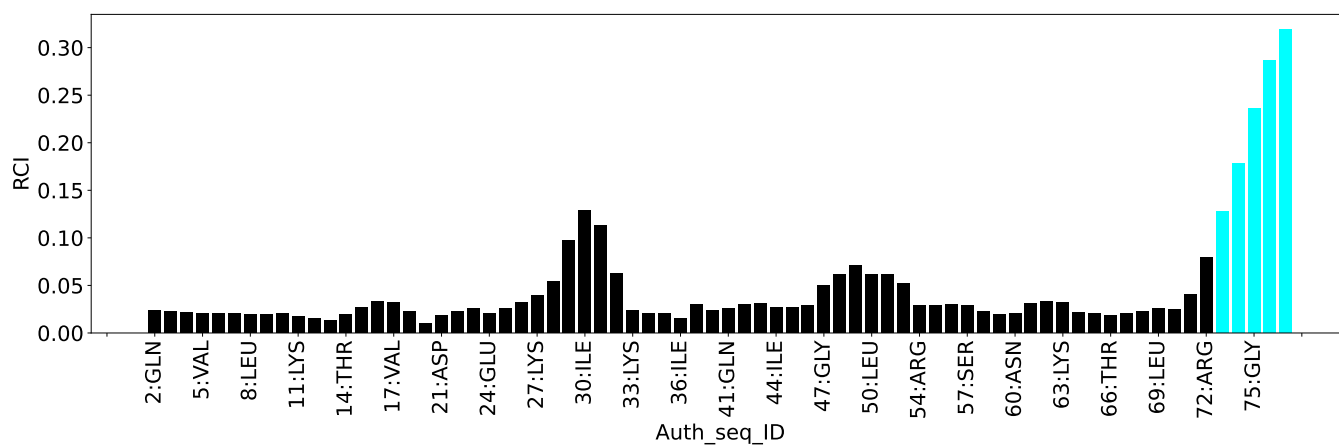
7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

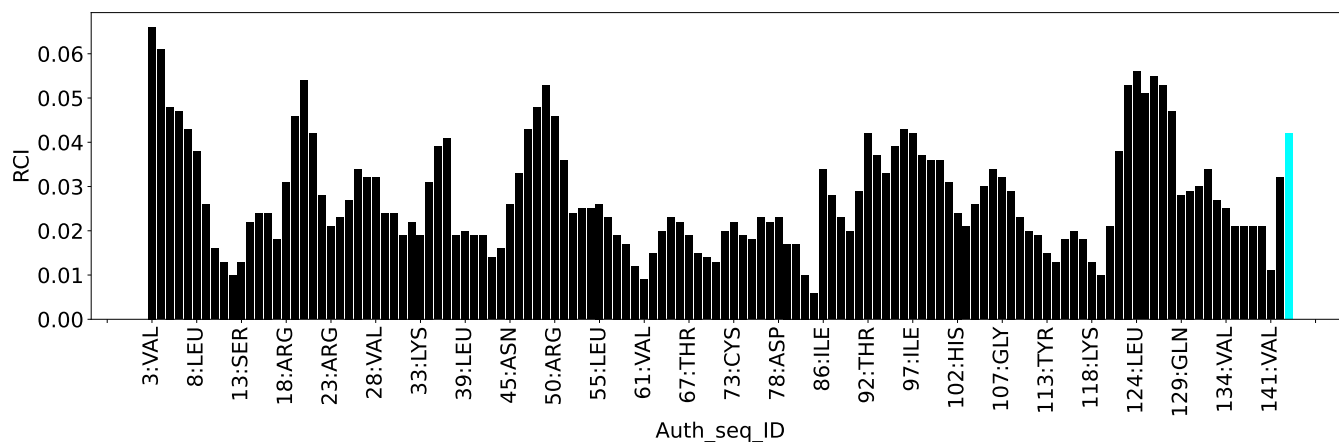
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	39
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	39
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.2	0.18
0.2-0.5 (Medium)	1.2	0.48
>0.5 (Large)	22.0	23.28

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

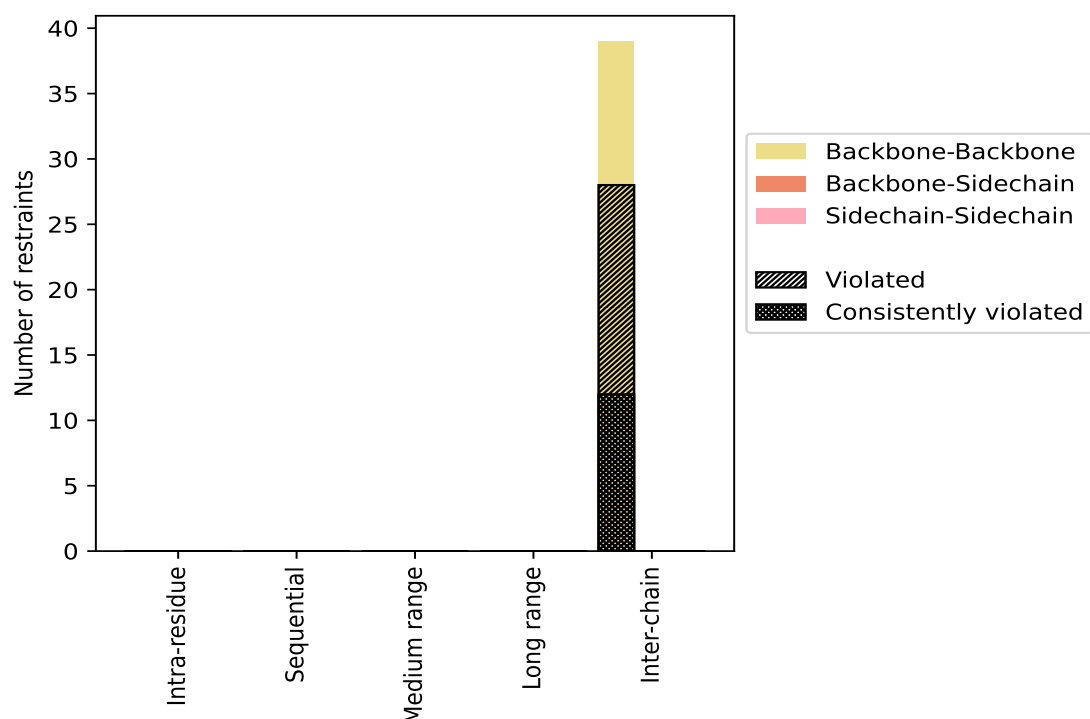
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	39	100.0	28	71.8	71.8	12	30.8	30.8
Backbone-Backbone	39	100.0	28	71.8	71.8	12	30.8	30.8
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	39	100.0	28	71.8	71.8	12	30.8	30.8
Backbone-Backbone	39	100.0	28	71.8	71.8	12	30.8	30.8
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	25	25	5.7	22.65	6.49	3.85
2	0	0	0	0	23	23	6.28	21.77	5.61	4.72
3	0	0	0	0	23	23	4.8	15.39	3.62	4.85
4	0	0	0	0	26	26	5.54	22.83	6.03	4.04
5	0	0	0	0	22	22	6.19	16.82	3.88	6.04
6	0	0	0	0	22	22	6.62	22.89	6.35	4.61
7	0	0	0	0	21	21	5.16	16.33	3.55	5.15
8	0	0	0	0	21	21	4.53	13.02	3.1	4.02
9	0	0	0	0	22	22	5.95	22.16	6.26	3.8
10	0	0	0	0	24	24	5.36	18.43	4.09	5.64

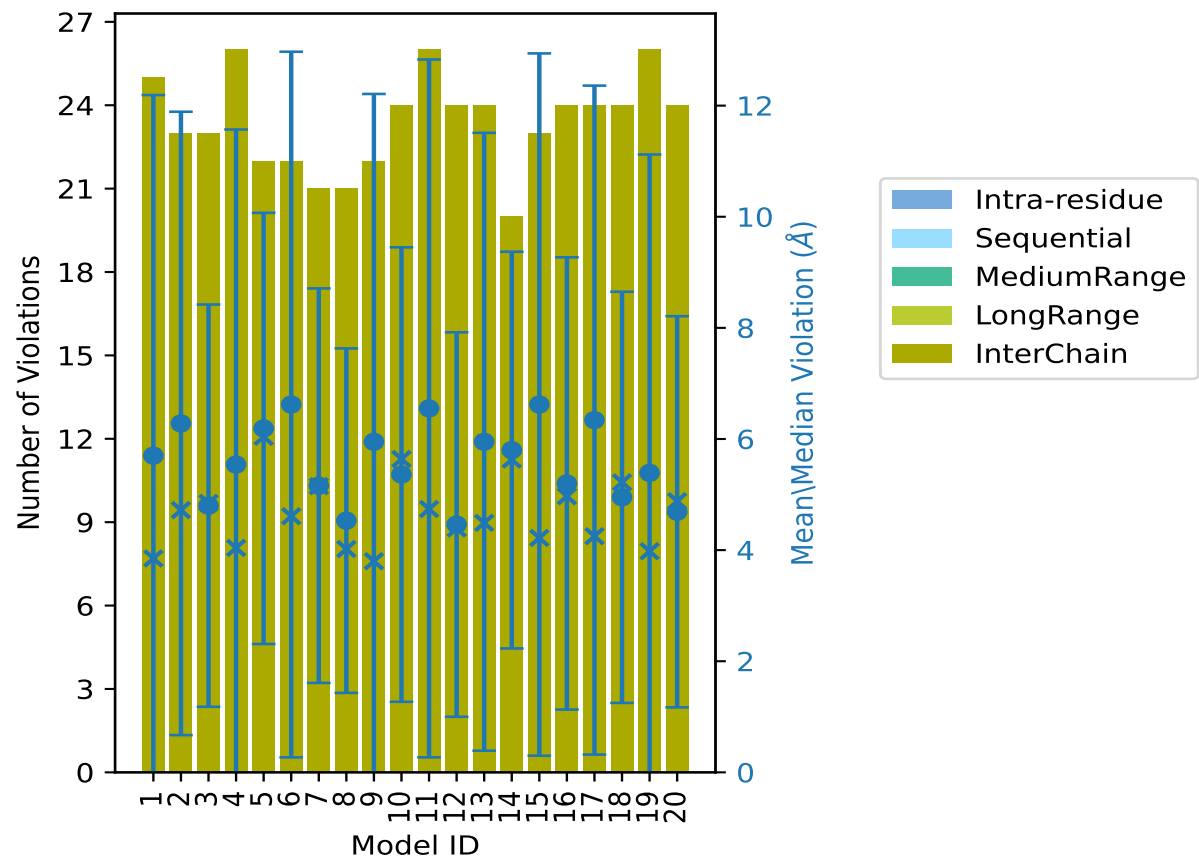
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	26	26	6.55	23.21	6.28	4.74
12	0	0	0	0	24	24	4.46	13.76	3.46	4.39
13	0	0	0	0	24	24	5.95	21.69	5.56	4.49
14	0	0	0	0	20	20	5.8	15.51	3.57	5.63
15	0	0	0	0	23	23	6.62	23.28	6.32	4.22
16	0	0	0	0	24	24	5.2	17.76	4.07	4.97
17	0	0	0	0	24	24	6.34	22.74	6.02	4.25
18	0	0	0	0	24	24	4.95	17.88	3.7	5.22
19	0	0	0	0	26	26	5.39	21.14	5.73	3.98
20	0	0	0	0	24	24	4.69	14.47	3.52	4.88

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

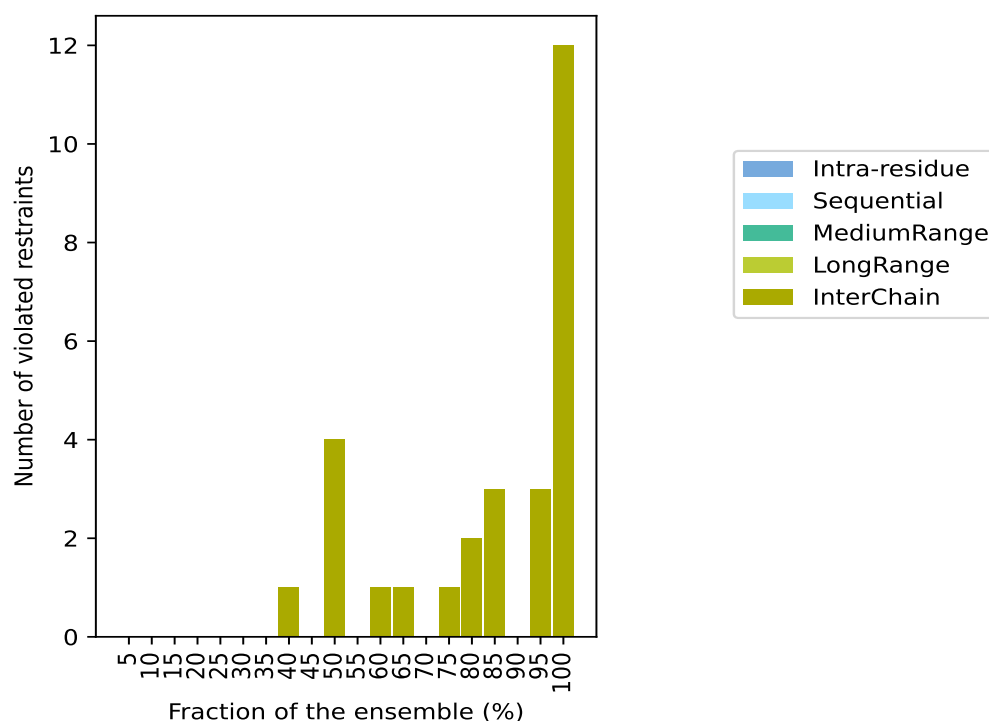
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 11(IR:0, SQ:0, MR:0, LR:0, IC:11) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	1	1	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	4	4	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	1	1	12	60.0
0	0	0	0	1	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	1	1	15	75.0
0	0	0	0	2	2	16	80.0
0	0	0	0	3	3	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	3	3	19	95.0
0	0	0	0	12	12	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

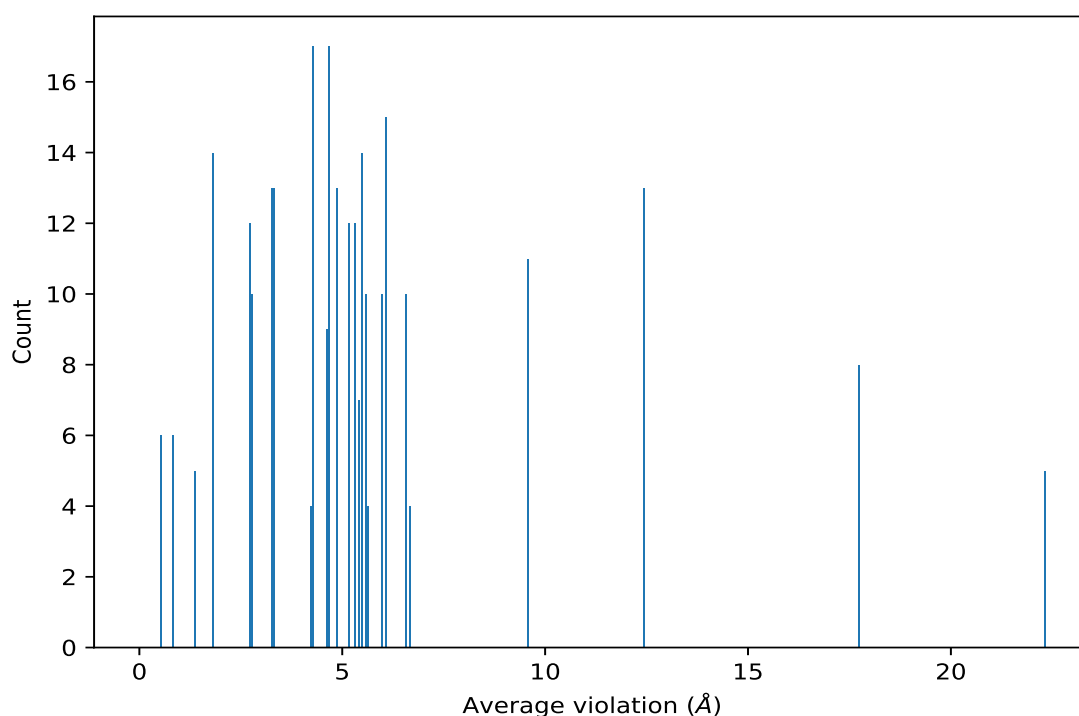
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,5)	2:66:B:THR:HG21	3:113:C:TYR:O	20	12.44	8.58	10.66
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HH	20	12.44	8.58	10.66
(3,5)	2:71:B:LEU:O	3:113:C:TYR:O	20	12.44	8.58	10.66
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HE2	20	12.44	8.58	10.66
(3,5)	2:44:B:ILE:HD13	3:113:C:TYR:O	20	12.44	8.58	10.66
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HD2	20	12.44	8.58	10.66
(3,5)	2:71:B:LEU:HD12	3:113:C:TYR:O	20	12.44	8.58	10.66
(3,5)	2:71:B:LEU:HD22	3:113:C:TYR:O	20	12.44	8.58	10.66
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HB2	20	12.44	8.58	10.66
(3,5)	2:71:B:LEU:HD13	3:113:C:TYR:O	20	12.44	8.58	10.66
(3,5)	2:71:B:LEU:HD11	3:113:C:TYR:O	20	12.44	8.58	10.66
(3,5)	2:66:B:THR:HG22	3:113:C:TYR:O	20	12.44	8.58	10.66
(3,5)	2:44:B:ILE:HD12	3:113:C:TYR:O	20	12.44	8.58	10.66
(2,11)	2:71:B:LEU:HD12	3:39:C:LEU:HD22	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:H	3:39:C:LEU:HD23	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	20	9.56	6.51	8.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,11)	2:71:B:LEU:HD11	3:39:C:LEU:HD22	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:HD13	3:39:C:LEU:HD12	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:HD11	3:43:C:VAL:O	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:H	3:39:C:LEU:HD21	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:HD12	3:39:C:LEU:HD23	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:H	3:39:C:LEU:HD11	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:HD23	3:39:C:LEU:HD13	20	9.56	6.51	8.7
(2,11)	2:71:B:LEU:H	3:39:C:LEU:HD22	20	9.56	6.51	8.7
(3,9)	2:48:B:LYS:H	3:44:C:PHE:N	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HE1	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:HZ3	3:44:C:PHE:HE1	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:HZ3	3:44:C:PHE:N	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HE2	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HZ	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:HZ1	3:44:C:PHE:O	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:HB2	3:44:C:PHE:HZ	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:HG2	3:44:C:PHE:N	20	6.6	3.93	5.79
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HD1	20	6.6	3.93	5.79
(2,7)	2:48:B:LYS:H	3:39:C:LEU:O	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:HZ1	3:43:C:VAL:HA	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HG21	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:HZ3	3:43:C:VAL:HA	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HA	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HG22	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:HZ1	3:39:C:LEU:HD13	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:HZ3	3:39:C:LEU:HD11	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:HZ2	3:43:C:VAL:HA	20	5.96	1.84	5.61
(2,7)	2:48:B:LYS:HE2	3:43:C:VAL:HA	20	5.96	1.84	5.61
(3,10)	2:62:B:GLN:HE22	3:44:C:PHE:O	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:O	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:HD1	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:HG2	3:44:C:PHE:HB2	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:HB3	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:H	3:44:C:PHE:HZ	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:OE1	3:44:C:PHE:O	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:OE1	3:44:C:PHE:HB2	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:H	3:44:C:PHE:HD1	20	5.58	1.69	5.58
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:HZ	20	5.58	1.69	5.58
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG13	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG23	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG11	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HA	20	5.47	3.62	4.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HG12	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:H	3:43:C:VAL:HA	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:OE1	3:43:C:VAL:HG11	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:OE1	3:43:C:VAL:HG13	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:HB2	3:43:C:VAL:HG11	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HB	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HA	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HG11	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HG13	20	5.47	3.62	4.22
(2,8)	2:62:B:GLN:H	3:43:C:VAL:HG12	20	5.47	3.62	4.22
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HB	20	5.41	0.28	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG12	20	5.41	0.28	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG11	20	5.41	0.28	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG23	20	5.41	0.28	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG21	20	5.41	0.28	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG13	20	5.41	0.28	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG22	20	5.41	0.28	5.27
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG13	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:OE1	3:43:C:VAL:HG13	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG11	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG12	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG23	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:OE1	3:43:C:VAL:HG12	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:OE2	3:43:C:VAL:HG21	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:OE1	3:43:C:VAL:HG11	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG21	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:OE2	3:43:C:VAL:HG22	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:OE1	3:43:C:VAL:HG21	20	5.31	2.51	5.46
(2,9)	2:64:B:GLU:OE2	3:43:C:VAL:HG13	20	5.31	2.51	5.46
(3,11)	2:64:B:GLU:O	3:44:C:PHE:H	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:OE1	3:44:C:PHE:H	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HD1	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:HG2	3:44:C:PHE:HE1	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HB3	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:OE1	3:44:C:PHE:HE1	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HZ	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HB2	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:OE2	3:44:C:PHE:HD1	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:OE2	3:44:C:PHE:HE1	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:HG3	3:44:C:PHE:HE1	20	5.18	1.04	5.26
(3,11)	2:64:B:GLU:OE2	3:44:C:PHE:HB3	20	5.18	1.04	5.26
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	20	4.64	3.96	4.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HE1	20	4.64	3.96	4.41
(3,8)	2:47:B:GLY:HA3	3:44:C:PHE:HZ	20	4.64	3.96	4.41
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HE2	20	4.64	3.96	4.41
(3,8)	2:47:B:GLY:N	3:44:C:PHE:HZ	20	4.64	3.96	4.41
(3,8)	2:47:B:GLY:HA2	3:44:C:PHE:HZ	20	4.64	3.96	4.41
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HB3	20	4.64	3.96	4.41
(3,8)	2:47:B:GLY:N	3:44:C:PHE:N	20	4.64	3.96	4.41
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HD1	20	4.64	3.96	4.41
(2,6)	2:47:B:GLY:HA2	3:39:C:LEU:O	20	4.26	2.25	3.9
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HA	20	4.26	2.25	3.9
(2,6)	2:47:B:GLY:N	3:43:C:VAL:HA	20	4.26	2.25	3.9
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HG22	20	4.26	2.25	3.9
(2,6)	2:47:B:GLY:HA3	3:39:C:LEU:HD11	20	4.26	2.25	3.9
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HG21	20	4.26	2.25	3.9
(2,6)	2:47:B:GLY:HA3	3:43:C:VAL:HA	20	4.26	2.25	3.9
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HG23	20	4.26	2.25	3.9
(2,6)	2:47:B:GLY:N	3:43:C:VAL:O	20	4.26	2.25	3.9
(3,4)	2:62:B:GLN:HE22	3:47:C:GLY:O	20	1.82	0.96	1.74
(3,4)	2:64:B:GLU:OE1	3:47:C:GLY:O	20	1.82	0.96	1.74
(3,4)	2:66:B:THR:HG23	3:47:C:GLY:N	20	1.82	0.96	1.74
(3,4)	2:62:B:GLN:HE22	3:47:C:GLY:HA3	20	1.82	0.96	1.74
(3,4)	2:66:B:THR:HG21	3:47:C:GLY:H	20	1.82	0.96	1.74
(3,4)	2:62:B:GLN:OE1	3:47:C:GLY:HA3	20	1.82	0.96	1.74
(3,4)	2:66:B:THR:HG22	3:47:C:GLY:H	20	1.82	0.96	1.74
(3,4)	2:64:B:GLU:HB3	3:47:C:GLY:O	20	1.82	0.96	1.74
(3,4)	2:66:B:THR:HG1	3:47:C:GLY:N	20	1.82	0.96	1.74
(3,4)	2:66:B:THR:HG23	3:47:C:GLY:H	20	1.82	0.96	1.74
(3,4)	2:66:B:THR:HG1	3:47:C:GLY:O	20	1.82	0.96	1.74
(3,4)	2:66:B:THR:HG1	3:47:C:GLY:H	20	1.82	0.96	1.74
(3,4)	2:66:B:THR:HG21	3:47:C:GLY:O	20	1.82	0.96	1.74
(3,4)	2:62:B:GLN:HE22	3:47:C:GLY:HA2	20	1.82	0.96	1.74
(3,7)	2:44:B:ILE:O	3:44:C:PHE:H	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HD13	3:44:C:PHE:HE1	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HD12	3:44:C:PHE:HZ	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HG22	3:44:C:PHE:H	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HD13	3:115:C:HIS:HD2	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:O	3:44:C:PHE:HE1	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HD13	3:44:C:PHE:H	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HD12	3:115:C:HIS:O	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HG22	3:44:C:PHE:HZ	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HG23	3:44:C:PHE:N	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HG23	3:44:C:PHE:HE1	19	6.09	4.23	8.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,7)	2:44:B:ILE:HG22	3:44:C:PHE:HE2	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HG21	3:44:C:PHE:H	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HG13	3:115:C:HIS:HA	19	6.09	4.23	8.23
(3,7)	2:44:B:ILE:HG21	3:44:C:PHE:HE1	19	6.09	4.23	8.23
(2,5)	2:44:B:ILE:HD11	3:39:C:LEU:HD12	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HD12	3:43:C:VAL:HA	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HD11	3:39:C:LEU:HD11	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HG22	3:43:C:VAL:HA	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HD13	3:39:C:LEU:HD23	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HG21	3:43:C:VAL:HA	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HD12	3:39:C:LEU:O	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HG22	3:43:C:VAL:O	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HG23	3:43:C:VAL:HA	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HD13	3:39:C:LEU:O	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HG22	3:39:C:LEU:O	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HG23	3:43:C:VAL:O	19	4.89	3.63	5.87
(2,5)	2:44:B:ILE:HD12	3:39:C:LEU:HD23	19	4.89	3.63	5.87
(2,1)	2:44:B:ILE:HD11	3:39:C:LEU:HD12	19	4.66	3.59	4.22
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HA	19	4.66	3.59	4.22
(2,1)	2:44:B:ILE:HD11	3:39:C:LEU:HD11	19	4.66	3.59	4.22
(2,1)	2:48:B:LYS:HZ2	3:39:C:LEU:HA	19	4.66	3.59	4.22
(2,1)	2:44:B:ILE:HD13	3:39:C:LEU:HD23	19	4.66	3.59	4.22
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HG	19	4.66	3.59	4.22
(2,1)	2:48:B:LYS:HZ2	3:39:C:LEU:HB2	19	4.66	3.59	4.22
(2,1)	2:44:B:ILE:HD12	3:39:C:LEU:O	19	4.66	3.59	4.22
(2,1)	2:48:B:LYS:HZ1	3:39:C:LEU:HD13	19	4.66	3.59	4.22
(2,1)	2:66:B:THR:HG1	3:39:C:LEU:HD13	19	4.66	3.59	4.22
(2,1)	2:48:B:LYS:HZ3	3:39:C:LEU:HD11	19	4.66	3.59	4.22
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HD13	19	4.66	3.59	4.22
(2,1)	2:44:B:ILE:HD13	3:39:C:LEU:O	19	4.66	3.59	4.22
(2,1)	2:66:B:THR:HG1	3:39:C:LEU:HD23	19	4.66	3.59	4.22
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HD21	19	4.66	3.59	4.22
(2,1)	2:44:B:ILE:HD12	3:39:C:LEU:HD23	19	4.66	3.59	4.22
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HD11	19	4.66	3.59	4.22
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:H	17	2.8	1.66	3.42
(3,12)	2:66:B:THR:HG22	3:44:C:PHE:H	17	2.8	1.66	3.42
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:HD1	17	2.8	1.66	3.42
(3,12)	2:66:B:THR:OG1	3:44:C:PHE:HB3	17	2.8	1.66	3.42
(3,12)	2:66:B:THR:HG23	3:44:C:PHE:H	17	2.8	1.66	3.42
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:HD2	17	2.8	1.66	3.42
(3,12)	2:66:B:THR:HG22	3:44:C:PHE:HB2	17	2.8	1.66	3.42
(3,12)	2:66:B:THR:HB	3:44:C:PHE:H	17	2.8	1.66	3.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:HE2	17	2.8	1.66	3.42
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:HB3	17	2.8	1.66	3.42
(3,1)	2:62:B:GLN:HE22	3:44:C:PHE:O	17	2.7	1.77	3.42
(3,1)	2:66:B:THR:HG22	3:44:C:PHE:H	17	2.7	1.77	3.42
(3,1)	2:66:B:THR:HG1	3:44:C:PHE:HD1	17	2.7	1.77	3.42
(3,1)	2:47:B:GLY:HA3	3:44:C:PHE:HZ	17	2.7	1.77	3.42
(3,1)	2:66:B:THR:HG23	3:44:C:PHE:H	17	2.7	1.77	3.42
(3,1)	2:66:B:THR:HG1	3:44:C:PHE:H	17	2.7	1.77	3.42
(3,1)	2:66:B:THR:HG1	3:44:C:PHE:HD2	17	2.7	1.77	3.42
(3,1)	2:47:B:GLY:HA2	3:44:C:PHE:HZ	17	2.7	1.77	3.42
(3,1)	2:66:B:THR:HB	3:44:C:PHE:H	17	2.7	1.77	3.42
(3,1)	2:47:B:GLY:H	3:44:C:PHE:HE2	17	2.7	1.77	3.42
(3,1)	2:66:B:THR:OG1	3:44:C:PHE:HB3	17	2.7	1.77	3.42
(3,1)	2:44:B:ILE:HG21	3:44:C:PHE:HE1	17	2.7	1.77	3.42
(1,7)	1:62:A:GLN:HG3	3:98:C:LYS:N	17	0.85	0.25	0.9
(1,7)	1:62:A:GLN:HG2	3:98:C:LYS:N	17	0.85	0.25	0.9
(1,7)	1:62:A:GLN:HE22	3:98:C:LYS:HA	17	0.85	0.25	0.9
(1,7)	1:62:A:GLN:OE1	3:98:C:LYS:N	17	0.85	0.25	0.9
(1,7)	1:62:A:GLN:HE21	3:98:C:LYS:HA	17	0.85	0.25	0.9
(1,7)	1:62:A:GLN:HE21	3:98:C:LYS:N	17	0.85	0.25	0.9
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:HG12	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG22	3:43:C:VAL:HG22	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:HG11	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG22	3:43:C:VAL:O	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG21	3:43:C:VAL:O	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:HA	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:OG1	3:43:C:VAL:O	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:HG23	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HB	3:43:C:VAL:HG22	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:HA	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:O	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:O	16	3.34	2.21	4.24
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:HG13	16	3.34	2.21	4.24
(2,4)	2:66:B:THR:HG1	3:43:C:VAL:HG12	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:HG22	3:43:C:VAL:HG22	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:HG11	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:HG22	3:43:C:VAL:O	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:HG21	3:43:C:VAL:O	16	3.3	2.18	4.04
(2,4)	2:47:B:GLY:H	3:43:C:VAL:HA	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:OG1	3:43:C:VAL:O	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:HG23	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:HB	3:43:C:VAL:HG22	16	3.3	2.18	4.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:HA	16	3.3	2.18	4.04
(2,4)	2:47:B:GLY:HA3	3:43:C:VAL:HA	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:O	16	3.3	2.18	4.04
(2,4)	2:66:B:THR:HG1	3:43:C:VAL:HG13	16	3.3	2.18	4.04
(3,2)	2:62:B:GLN:HE22	3:45:C:ASN:O	15	4.27	2.46	5.19
(3,2)	2:62:B:GLN:HE21	3:45:C:ASN:O	15	4.27	2.46	5.19
(3,2)	2:66:B:THR:HG23	3:45:C:ASN:O	15	4.27	2.46	5.19
(3,2)	2:62:B:GLN:OE1	3:45:C:ASN:O	15	4.27	2.46	5.19
(3,2)	2:66:B:THR:HG22	3:45:C:ASN:HB2	15	4.27	2.46	5.19
(3,2)	2:66:B:THR:HG22	3:45:C:ASN:OD1	15	4.27	2.46	5.19
(3,2)	2:66:B:THR:HG1	3:45:C:ASN:HB2	15	4.27	2.46	5.19
(3,2)	2:66:B:THR:HG23	3:45:C:ASN:HB2	15	4.27	2.46	5.19
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	13	5.64	2.93	6.82
(2,2)	2:48:B:LYS:HZ2	3:40:C:ASP:O	13	5.64	2.93	6.82
(2,2)	2:66:B:THR:HG1	3:40:C:ASP:HA	13	5.64	2.93	6.82
(2,2)	2:47:B:GLY:HA2	3:40:C:ASP:OD2	13	5.64	2.93	6.82
(1,6)	1:62:A:GLN:OE1	3:92:C:THR:O	12	1.36	0.8	1.47
(1,6)	1:62:A:GLN:HE22	3:92:C:THR:O	12	1.36	0.8	1.47
(1,6)	1:62:A:GLN:HB3	3:92:C:THR:O	12	1.36	0.8	1.47
(1,6)	1:62:A:GLN:HG3	3:92:C:THR:O	12	1.36	0.8	1.47
(1,6)	1:62:A:GLN:HG2	3:92:C:THR:O	12	1.36	0.8	1.47
(3,6)	2:66:B:THR:HG1	3:115:C:HIS:HA	10	22.3	0.62	22.24
(3,6)	2:47:B:GLY:HA3	3:115:C:HIS:N	10	22.3	0.62	22.24
(3,6)	2:66:B:THR:HG23	3:115:C:HIS:HA	10	22.3	0.62	22.24
(3,6)	2:66:B:THR:HG21	3:115:C:HIS:HA	10	22.3	0.62	22.24
(3,6)	2:66:B:THR:HG22	3:115:C:HIS:HA	10	22.3	0.62	22.24
(3,13)	2:71:B:LEU:HD12	3:44:C:PHE:H	10	17.74	0.61	17.87
(3,13)	2:71:B:LEU:H	3:44:C:PHE:HE1	10	17.74	0.61	17.87
(3,13)	2:71:B:LEU:H	3:44:C:PHE:H	10	17.74	0.61	17.87
(3,13)	2:71:B:LEU:HD13	3:44:C:PHE:H	10	17.74	0.61	17.87
(3,13)	2:71:B:LEU:HD22	3:44:C:PHE:H	10	17.74	0.61	17.87
(3,13)	2:71:B:LEU:HD12	3:44:C:PHE:HE2	10	17.74	0.61	17.87
(3,13)	2:71:B:LEU:HD23	3:44:C:PHE:H	10	17.74	0.61	17.87
(3,13)	2:71:B:LEU:HD12	3:44:C:PHE:HE1	10	17.74	0.61	17.87
(2,3)	2:47:B:GLY:HA3	3:41:C:SER:HA	10	6.68	1.54	7.12
(2,3)	2:48:B:LYS:HZ2	3:41:C:SER:HA	10	6.68	1.54	7.12
(2,3)	2:48:B:LYS:HE2	3:41:C:SER:HA	10	6.68	1.54	7.12
(2,3)	2:66:B:THR:HG23	3:41:C:SER:HG	10	6.68	1.54	7.12
(3,3)	2:62:B:GLN:HE22	3:46:C:ASP:O	10	4.24	1.31	4.18
(3,3)	2:64:B:GLU:OE1	3:46:C:ASP:O	10	4.24	1.31	4.18
(3,3)	2:64:B:GLU:OE2	3:46:C:ASP:O	10	4.24	1.31	4.18
(3,3)	2:64:B:GLU:HG2	3:46:C:ASP:O	10	4.24	1.31	4.18

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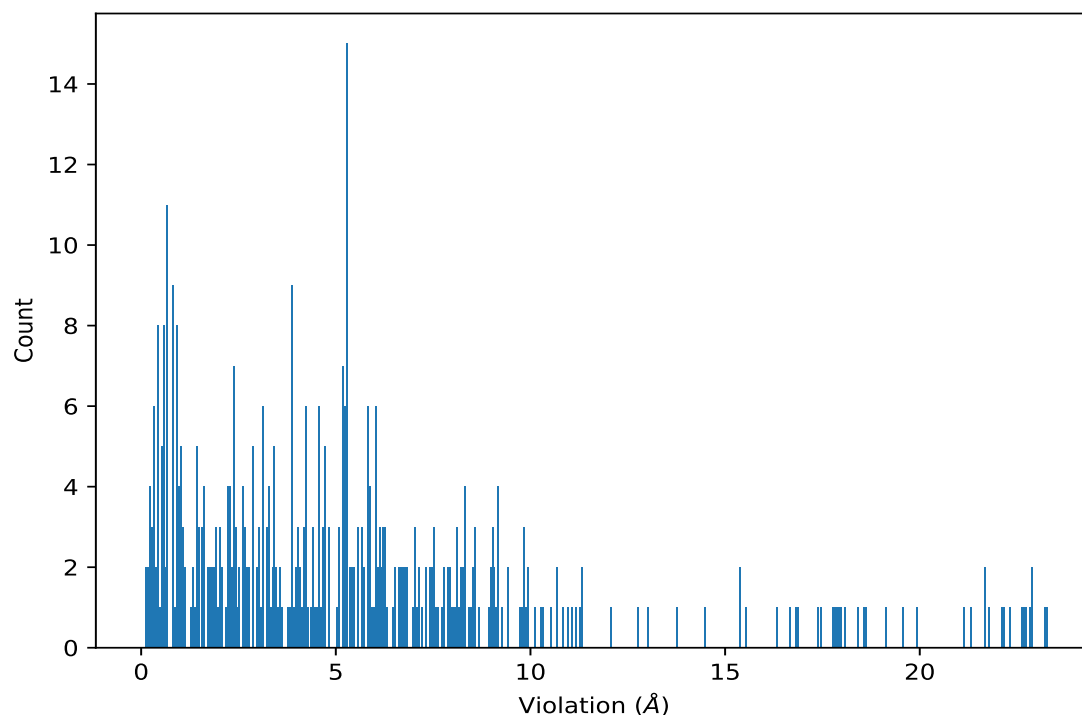
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:44:A:ILE:HD13	3:46:C:ASP:N	8	0.5	0.13	0.54
(1,4)	1:44:A:ILE:HG23	3:46:C:ASP:N	8	0.5	0.13	0.54
(1,4)	1:44:A:ILE:HG22	3:46:C:ASP:N	8	0.5	0.13	0.54
(1,4)	1:44:A:ILE:HD12	3:46:C:ASP:N	8	0.5	0.13	0.54
(1,4)	1:44:A:ILE:HG21	3:46:C:ASP:N	8	0.5	0.13	0.54
(1,4)	1:44:A:ILE:HG13	3:46:C:ASP:N	8	0.5	0.13	0.54

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,5)	2:66:B:THR:HG21	3:113:C:TYR:O	15	23.28
(3,6)	2:66:B:THR:HG23	3:115:C:HIS:HA	11	23.21
(3,6)	2:66:B:THR:HG23	3:115:C:HIS:HA	6	22.89
(3,6)	2:66:B:THR:HG21	3:115:C:HIS:HA	15	22.87
(3,6)	2:47:B:GLY:HA3	3:115:C:HIS:N	4	22.83
(3,5)	2:66:B:THR:HG22	3:113:C:TYR:O	17	22.74
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HD2	11	22.67
(3,5)	2:66:B:THR:HG21	3:113:C:TYR:O	1	22.65
(3,6)	2:66:B:THR:HG1	3:115:C:HIS:HA	1	22.31
(3,6)	2:47:B:GLY:HA3	3:115:C:HIS:N	9	22.16
(3,6)	2:66:B:THR:HG22	3:115:C:HIS:HA	17	22.12
(3,6)	2:47:B:GLY:HA3	3:115:C:HIS:N	2	21.77
(3,6)	2:47:B:GLY:HA3	3:115:C:HIS:N	13	21.69
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HD2	6	21.67
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HB2	9	21.3
(3,6)	2:47:B:GLY:HA3	3:115:C:HIS:N	19	21.14
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HE2	4	19.92
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HD2	19	19.58
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HE2	13	19.1
(3,13)	2:71:B:LEU:HD12	3:44:C:PHE:H	1	18.63
(3,13)	2:71:B:LEU:H	3:44:C:PHE:H	4	18.56
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	10	18.43
(3,13)	2:71:B:LEU:HD12	3:44:C:PHE:HE2	11	18.09
(3,13)	2:71:B:LEU:HD13	3:44:C:PHE:H	6	17.98
(3,13)	2:71:B:LEU:HD22	3:44:C:PHE:H	9	17.92
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	18	17.88
(3,13)	2:71:B:LEU:HD12	3:44:C:PHE:HE1	19	17.81
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	16	17.76
(3,13)	2:71:B:LEU:H	3:44:C:PHE:HE1	13	17.49
(3,13)	2:71:B:LEU:H	3:44:C:PHE:HE1	2	17.39
(3,13)	2:71:B:LEU:HD23	3:44:C:PHE:H	15	16.88
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	5	16.82
(3,13)	2:71:B:LEU:HD12	3:44:C:PHE:HE2	17	16.68
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	7	16.33
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	14	15.51
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	3	15.39
(3,5)	2:47:B:GLY:HA3	3:113:C:TYR:HH	2	15.36
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	20	14.47
(2,11)	2:71:B:LEU:H	3:43:C:VAL:O	12	13.76
(2,11)	2:71:B:LEU:HD11	3:43:C:VAL:O	8	13.02
(3,9)	2:48:B:LYS:H	3:44:C:PHE:N	11	12.75
(3,7)	2:44:B:ILE:O	3:44:C:PHE:H	11	12.1
(3,9)	2:48:B:LYS:H	3:44:C:PHE:N	15	11.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	2:62:B:GLN:HB2	3:43:C:VAL:HG11	12	11.31
(2,8)	2:62:B:GLN:H	3:43:C:VAL:HG12	20	11.29
(3,9)	2:48:B:LYS:H	3:44:C:PHE:N	2	11.17
(3,9)	2:48:B:LYS:H	3:44:C:PHE:N	1	11.1
(3,9)	2:48:B:LYS:HZ3	3:44:C:PHE:N	6	10.96
(2,8)	2:62:B:GLN:H	3:43:C:VAL:HA	8	10.83
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	11	10.67
(3,7)	2:44:B:ILE:O	3:44:C:PHE:H	6	10.66
(3,7)	2:44:B:ILE:O	3:44:C:PHE:H	1	10.52
(3,9)	2:48:B:LYS:H	3:44:C:PHE:N	17	10.34
(3,7)	2:44:B:ILE:O	3:44:C:PHE:H	15	10.28
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HA	16	10.12
(3,7)	2:44:B:ILE:HD13	3:44:C:PHE:HE1	2	9.95
(2,5)	2:44:B:ILE:HG22	3:43:C:VAL:O	10	9.92
(3,7)	2:44:B:ILE:HG21	3:44:C:PHE:H	17	9.86
(2,1)	2:48:B:LYS:HZ2	3:39:C:LEU:HA	5	9.84
(3,7)	2:44:B:ILE:HG22	3:44:C:PHE:H	4	9.83
(3,9)	2:48:B:LYS:H	3:44:C:PHE:N	4	9.8
(2,5)	2:44:B:ILE:HG22	3:43:C:VAL:HA	5	9.79
(3,7)	2:44:B:ILE:HG22	3:44:C:PHE:H	19	9.74
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HA	5	9.45
(2,7)	2:48:B:LYS:HZ2	3:43:C:VAL:HA	14	9.45
(3,9)	2:48:B:LYS:H	3:44:C:PHE:N	9	9.29
(3,10)	2:62:B:GLN:H	3:44:C:PHE:HD1	12	9.16
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	1	9.16
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG23	5	9.16
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	15	9.15
(3,9)	2:48:B:LYS:HG2	3:44:C:PHE:N	19	9.14
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	2	9.07
(2,5)	2:44:B:ILE:HG22	3:43:C:VAL:HA	16	9.07
(3,10)	2:62:B:GLN:H	3:44:C:PHE:HD1	20	9.03
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	6	9.03
(3,7)	2:44:B:ILE:HG23	3:44:C:PHE:N	13	9.01
(2,9)	2:64:B:GLU:OE2	3:43:C:VAL:HG22	16	8.99
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	14	8.99
(2,5)	2:44:B:ILE:HG23	3:43:C:VAL:HA	14	8.91
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HA	16	8.69
(2,7)	2:48:B:LYS:HZ3	3:43:C:VAL:HA	5	8.59
(2,2)	2:48:B:LYS:HZ2	3:40:C:ASP:O	5	8.57
(2,3)	2:48:B:LYS:HZ2	3:41:C:SER:HA	5	8.56
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HD13	14	8.54
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HA	3	8.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	2:48:B:LYS:HE2	3:41:C:SER:HA	10	8.47
(2,5)	2:44:B:ILE:HG23	3:43:C:VAL:O	18	8.41
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HD21	18	8.34
(3,2)	2:62:B:GLN:HE21	3:45:C:ASN:O	2	8.33
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	10	8.31
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	17	8.3
(3,9)	2:48:B:LYS:HZ1	3:44:C:PHE:O	13	8.28
(2,5)	2:44:B:ILE:HG22	3:43:C:VAL:HA	7	8.27
(3,7)	2:44:B:ILE:HD13	3:44:C:PHE:H	9	8.23
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HA	7	8.22
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HB	14	8.2
(2,7)	2:48:B:LYS:HZ1	3:39:C:LEU:HD13	10	8.13
(2,1)	2:48:B:LYS:HZ1	3:39:C:LEU:HD13	10	8.13
(2,8)	2:62:B:GLN:OE1	3:43:C:VAL:HG13	10	8.1
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG12	12	8.07
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG11	3	8.04
(2,7)	2:48:B:LYS:HZ1	3:43:C:VAL:HA	3	7.95
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HG	7	7.94
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	16	7.9
(2,6)	2:47:B:GLY:N	3:43:C:VAL:HA	10	7.89
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	4	7.86
(2,6)	2:47:B:GLY:N	3:43:C:VAL:HA	5	7.79
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG11	3	7.77
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HA	18	7.71
(2,3)	2:47:B:GLY:HA3	3:41:C:SER:HA	18	7.63
(2,9)	2:64:B:GLU:OE2	3:43:C:VAL:HG21	8	7.6
(3,8)	2:47:B:GLY:N	3:44:C:PHE:N	19	7.54
(2,3)	2:66:B:THR:HG23	3:41:C:SER:HG	14	7.53
(2,3)	2:47:B:GLY:HA3	3:41:C:SER:HA	16	7.53
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	18	7.49
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	9	7.46
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HA	14	7.4
(2,5)	2:44:B:ILE:HD12	3:43:C:VAL:HA	3	7.4
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG13	7	7.31
(2,9)	2:64:B:GLU:OE2	3:43:C:VAL:HG13	20	7.31
(2,5)	2:44:B:ILE:HG21	3:43:C:VAL:HA	12	7.2
(3,10)	2:62:B:GLN:HG2	3:44:C:PHE:HB2	5	7.14
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG23	14	7.14
(2,7)	2:48:B:LYS:HE2	3:43:C:VAL:HA	16	7.08
(2,9)	2:64:B:GLU:OE1	3:43:C:VAL:HG11	10	7.05
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG11	18	7.02
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:O	2	7.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	2:47:B:GLY:H	3:44:C:PHE:N	13	6.97
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	3	6.82
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	7	6.82
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HG12	7	6.79
(2,5)	2:44:B:ILE:HG21	3:43:C:VAL:HA	20	6.78
(2,3)	2:47:B:GLY:HA3	3:41:C:SER:HA	3	6.72
(3,2)	2:62:B:GLN:HE22	3:45:C:ASN:O	11	6.7
(3,11)	2:64:B:GLU:O	3:44:C:PHE:H	11	6.69
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HA	3	6.65
(3,2)	2:62:B:GLN:HE21	3:45:C:ASN:O	15	6.64
(3,11)	2:64:B:GLU:OE1	3:44:C:PHE:H	2	6.61
(2,3)	2:47:B:GLY:HA3	3:41:C:SER:HA	7	6.53
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:O	16	6.52
(3,2)	2:62:B:GLN:HE22	3:45:C:ASN:O	17	6.49
(2,1)	2:48:B:LYS:HZ2	3:39:C:LEU:HB2	8	6.31
(2,7)	2:48:B:LYS:HZ3	3:39:C:LEU:HD11	20	6.3
(2,1)	2:47:B:GLY:HA3	3:39:C:LEU:HD11	20	6.29
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HB	1	6.27
(2,6)	2:47:B:GLY:HA3	3:43:C:VAL:HA	16	6.24
(2,4)	2:47:B:GLY:HA3	3:43:C:VAL:HA	16	6.24
(3,3)	2:64:B:GLU:OE1	3:46:C:ASP:O	2	6.23
(3,11)	2:64:B:GLU:OE2	3:44:C:PHE:HD1	13	6.19
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	20	6.16
(3,11)	2:64:B:GLU:HG2	3:44:C:PHE:HE1	4	6.14
(3,3)	2:64:B:GLU:OE2	3:46:C:ASP:O	11	6.13
(2,6)	2:47:B:GLY:N	3:43:C:VAL:HA	7	6.13
(3,11)	2:64:B:GLU:OE1	3:44:C:PHE:H	19	6.09
(3,10)	2:62:B:GLN:HE22	3:44:C:PHE:O	17	6.09
(3,10)	2:62:B:GLN:HE22	3:44:C:PHE:O	11	6.05
(2,10)	2:66:B:THR:HG22	3:43:C:VAL:O	5	6.04
(2,4)	2:66:B:THR:HG22	3:43:C:VAL:O	5	6.04
(2,7)	2:48:B:LYS:H	3:39:C:LEU:O	11	6.03
(3,10)	2:62:B:GLN:OE1	3:44:C:PHE:HB2	10	6.02
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HB2	12	6.0
(3,5)	2:44:B:ILE:HD13	3:113:C:TYR:O	5	5.96
(3,2)	2:62:B:GLN:HE22	3:45:C:ASN:O	6	5.92
(3,11)	2:64:B:GLU:OE2	3:44:C:PHE:HB3	20	5.89
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:O	15	5.88
(2,6)	2:47:B:GLY:N	3:43:C:VAL:O	18	5.88
(2,5)	2:44:B:ILE:HG21	3:43:C:VAL:HA	8	5.87
(3,11)	2:64:B:GLU:HG3	3:44:C:PHE:HE1	17	5.83
(2,10)	2:66:B:THR:OG1	3:43:C:VAL:O	10	5.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	2:66:B:THR:OG1	3:43:C:VAL:O	10	5.82
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG22	16	5.82
(2,7)	2:48:B:LYS:HZ3	3:43:C:VAL:HA	8	5.81
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG23	5	5.81
(3,11)	2:64:B:GLU:O	3:44:C:PHE:H	15	5.74
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG21	8	5.73
(3,10)	2:62:B:GLN:HE22	3:44:C:PHE:O	13	5.69
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG23	14	5.68
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HG13	18	5.67
(3,5)	2:44:B:ILE:HD12	3:113:C:TYR:O	18	5.59
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:HD1	14	5.58
(3,10)	2:62:B:GLN:HE22	3:44:C:PHE:O	6	5.57
(3,2)	2:62:B:GLN:HE22	3:45:C:ASN:O	19	5.47
(3,5)	2:71:B:LEU:O	3:113:C:TYR:O	10	5.45
(3,3)	2:64:B:GLU:HG2	3:46:C:ASP:O	17	5.44
(2,7)	2:48:B:LYS:H	3:39:C:LEU:O	15	5.41
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	12	5.39
(2,3)	2:47:B:GLY:HA3	3:41:C:SER:HA	20	5.37
(3,2)	2:62:B:GLN:HE22	3:45:C:ASN:O	13	5.28
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG12	2	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG12	3	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG11	7	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG12	10	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG13	12	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG12	18	5.27
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG11	20	5.27
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HB3	5	5.26
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG11	15	5.26
(3,11)	2:64:B:GLU:O	3:44:C:PHE:H	9	5.25
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG11	4	5.25
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG11	6	5.25
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG11	9	5.25
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG12	11	5.25
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG11	17	5.24
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:O	18	5.22
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:O	18	5.22
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG13	13	5.22
(1,15)	1:71:A:LEU:N	3:43:C:VAL:HG13	19	5.22
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HG22	17	5.2
(3,2)	2:62:B:GLN:HE22	3:45:C:ASN:O	4	5.19
(2,6)	2:47:B:GLY:HA3	3:39:C:LEU:HD11	12	5.19
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:HD1	3	5.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	2:48:B:LYS:H	3:39:C:LEU:O	1	5.17
(3,10)	2:62:B:GLN:HE22	3:44:C:PHE:O	4	5.16
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:HB3	7	5.15
(3,10)	2:62:B:GLN:H	3:44:C:PHE:HZ	8	5.15
(2,6)	2:47:B:GLY:HA3	3:43:C:VAL:HA	20	5.1
(3,11)	2:64:B:GLU:O	3:44:C:PHE:H	1	5.08
(3,10)	2:62:B:GLN:HE22	3:44:C:PHE:O	19	5.07
(3,11)	2:64:B:GLU:OE1	3:44:C:PHE:HE1	6	5.01
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:HG11	3	4.85
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:HG11	3	4.85
(2,3)	2:47:B:GLY:HA3	3:41:C:SER:HA	12	4.83
(3,12)	2:66:B:THR:HG23	3:44:C:PHE:H	11	4.74
(3,1)	2:66:B:THR:HG23	3:44:C:PHE:H	11	4.74
(3,12)	2:66:B:THR:HG22	3:44:C:PHE:H	2	4.72
(3,1)	2:66:B:THR:HG22	3:44:C:PHE:H	2	4.72
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HD1	3	4.7
(2,7)	2:48:B:LYS:H	3:39:C:LEU:O	6	4.69
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:HG13	20	4.67
(2,4)	2:66:B:THR:HG1	3:43:C:VAL:HG13	20	4.67
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HG21	4	4.64
(3,12)	2:66:B:THR:HB	3:44:C:PHE:H	13	4.59
(3,1)	2:66:B:THR:HB	3:44:C:PHE:H	13	4.59
(2,2)	2:47:B:GLY:HA3	3:40:C:ASP:O	8	4.58
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:HG12	12	4.56
(2,4)	2:66:B:THR:HG1	3:43:C:VAL:HG12	12	4.56
(3,3)	2:62:B:GLN:HE22	3:46:C:ASP:O	19	4.55
(3,3)	2:64:B:GLU:OE1	3:46:C:ASP:O	6	4.52
(3,2)	2:62:B:GLN:HE22	3:45:C:ASN:O	1	4.46
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:HA	8	4.42
(3,12)	2:66:B:THR:HG22	3:44:C:PHE:H	19	4.41
(3,1)	2:66:B:THR:HG22	3:44:C:PHE:H	19	4.41
(2,11)	2:71:B:LEU:H	3:39:C:LEU:HD11	13	4.39
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HB3	7	4.28
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HG22	9	4.24
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:H	15	4.22
(3,1)	2:66:B:THR:HG1	3:44:C:PHE:H	15	4.22
(2,7)	2:48:B:LYS:HZ3	3:39:C:LEU:HD11	12	4.22
(2,1)	2:48:B:LYS:HZ3	3:39:C:LEU:HD11	12	4.22
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HB2	18	4.21
(3,12)	2:66:B:THR:HG22	3:44:C:PHE:H	4	4.18
(3,2)	2:62:B:GLN:OE1	3:45:C:ASN:O	9	4.18
(3,1)	2:66:B:THR:HG22	3:44:C:PHE:H	4	4.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	2:64:B:GLU:OE2	3:44:C:PHE:HE1	16	4.12
(2,10)	2:66:B:THR:HG21	3:43:C:VAL:O	7	4.06
(2,4)	2:66:B:THR:HG21	3:43:C:VAL:O	7	4.06
(3,10)	2:62:B:GLN:OE1	3:44:C:PHE:O	9	4.03
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HA	8	4.02
(2,4)	2:47:B:GLY:H	3:43:C:VAL:HA	8	4.02
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HB3	10	3.98
(3,5)	2:71:B:LEU:HD11	3:113:C:TYR:O	16	3.98
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HB2	14	3.91
(2,7)	2:48:B:LYS:H	3:43:C:VAL:HG21	13	3.9
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG12	4	3.89
(3,12)	2:66:B:THR:HG23	3:44:C:PHE:H	6	3.87
(3,5)	2:71:B:LEU:HD22	3:113:C:TYR:O	8	3.87
(3,4)	2:66:B:THR:HG1	3:47:C:GLY:H	16	3.87
(3,1)	2:66:B:THR:HG23	3:44:C:PHE:H	6	3.87
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:H	1	3.85
(3,10)	2:62:B:GLN:HE22	3:44:C:PHE:O	1	3.85
(3,1)	2:62:B:GLN:HE22	3:44:C:PHE:O	1	3.85
(3,3)	2:64:B:GLU:HG2	3:46:C:ASP:O	15	3.83
(2,6)	2:47:B:GLY:HA2	3:39:C:LEU:O	11	3.78
(2,3)	2:47:B:GLY:HA3	3:41:C:SER:HA	8	3.61
(3,3)	2:62:B:GLN:HE22	3:46:C:ASP:O	13	3.58
(2,11)	2:71:B:LEU:H	3:39:C:LEU:HD21	9	3.58
(2,7)	2:48:B:LYS:H	3:39:C:LEU:O	19	3.55
(2,11)	2:71:B:LEU:HD11	3:39:C:LEU:HD22	4	3.48
(2,11)	2:71:B:LEU:HD23	3:39:C:LEU:HD13	15	3.45
(3,4)	2:64:B:GLU:HB3	3:47:C:GLY:O	11	3.43
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:HA	14	3.43
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:HA	14	3.43
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:H	9	3.42
(3,1)	2:66:B:THR:HG1	3:44:C:PHE:H	9	3.42
(3,5)	2:71:B:LEU:HD11	3:113:C:TYR:O	14	3.37
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG11	13	3.37
(3,3)	2:62:B:GLN:HE22	3:46:C:ASP:O	4	3.31
(3,12)	2:66:B:THR:HG22	3:44:C:PHE:H	17	3.3
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HD1	20	3.3
(3,1)	2:66:B:THR:HG22	3:44:C:PHE:H	17	3.3
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HE1	14	3.28
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HG23	17	3.24
(2,9)	2:64:B:GLU:OE1	3:43:C:VAL:HG21	19	3.21
(2,11)	2:71:B:LEU:HD12	3:39:C:LEU:HD22	17	3.2
(3,5)	2:71:B:LEU:HD13	3:113:C:TYR:O	20	3.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HZ	12	3.13
(3,5)	2:71:B:LEU:HD12	3:113:C:TYR:O	7	3.12
(3,5)	2:71:B:LEU:HD13	3:113:C:TYR:O	12	3.12
(2,9)	2:64:B:GLU:OE1	3:43:C:VAL:HG13	2	3.12
(2,11)	2:71:B:LEU:HD12	3:39:C:LEU:HD23	11	3.1
(3,4)	2:66:B:THR:HG22	3:47:C:GLY:H	10	3.06
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG21	17	3.04
(3,10)	2:62:B:GLN:H	3:44:C:PHE:HD1	18	3.02
(2,5)	2:44:B:ILE:HG22	3:39:C:LEU:O	17	3.02
(2,6)	2:47:B:GLY:HA2	3:39:C:LEU:O	15	2.97
(2,11)	2:71:B:LEU:H	3:39:C:LEU:HD22	19	2.96
(3,4)	2:64:B:GLU:OE1	3:47:C:GLY:O	2	2.89
(2,6)	2:47:B:GLY:HA2	3:39:C:LEU:O	1	2.89
(2,7)	2:48:B:LYS:H	3:39:C:LEU:O	2	2.88
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HZ	10	2.86
(3,5)	2:71:B:LEU:O	3:113:C:TYR:O	3	2.86
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HE1	7	2.8
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HG11	17	2.77
(2,11)	2:71:B:LEU:HD13	3:39:C:LEU:HD12	6	2.71
(2,8)	2:62:B:GLN:OE1	3:43:C:VAL:HG13	13	2.7
(3,9)	2:48:B:LYS:HZ3	3:44:C:PHE:HE1	5	2.69
(2,11)	2:71:B:LEU:HD12	3:39:C:LEU:HD22	1	2.69
(3,3)	2:62:B:GLN:HE22	3:46:C:ASP:O	1	2.66
(3,11)	2:64:B:GLU:O	3:44:C:PHE:HZ	8	2.65
(3,9)	2:48:B:LYS:HB2	3:44:C:PHE:HZ	18	2.64
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG12	9	2.62
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HE2	8	2.61
(3,7)	2:44:B:ILE:HG22	3:44:C:PHE:HE2	16	2.53
(1,6)	1:62:A:GLN:HB3	3:92:C:THR:O	7	2.52
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HG12	11	2.47
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HE1	3	2.44
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG21	11	2.44
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HG22	9	2.44
(3,7)	2:44:B:ILE:HG23	3:44:C:PHE:HE1	14	2.4
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG23	2	2.4
(2,9)	2:64:B:GLU:OE1	3:43:C:VAL:HG12	6	2.39
(2,5)	2:44:B:ILE:HD11	3:39:C:LEU:HD11	11	2.38
(3,7)	2:44:B:ILE:HD12	3:115:C:HIS:O	10	2.37
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG13	1	2.36
(1,6)	1:62:A:GLN:HB3	3:92:C:THR:O	13	2.35
(2,9)	2:64:B:GLU:O	3:43:C:VAL:HG12	15	2.33
(1,6)	1:62:A:GLN:HB3	3:92:C:THR:O	11	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	2:71:B:LEU:H	3:39:C:LEU:HD23	2	2.28
(3,4)	2:62:B:GLN:HE22	3:47:C:GLY:HA2	19	2.26
(3,4)	2:66:B:THR:HG23	3:47:C:GLY:N	5	2.25
(2,1)	2:66:B:THR:HG1	3:39:C:LEU:HD13	11	2.25
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG11	15	2.23
(3,7)	2:44:B:ILE:HD13	3:115:C:HIS:HD2	5	2.22
(3,3)	2:62:B:GLN:HE22	3:46:C:ASP:O	9	2.2
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG11	6	2.2
(2,1)	2:66:B:THR:HG1	3:39:C:LEU:HD23	17	2.19
(3,4)	2:66:B:THR:HG21	3:47:C:GLY:O	17	2.08
(2,6)	2:47:B:GLY:HA2	3:39:C:LEU:O	6	2.07
(3,4)	2:66:B:THR:HG23	3:47:C:GLY:H	18	2.04
(2,6)	2:47:B:GLY:HA2	3:39:C:LEU:O	4	2.02
(3,9)	2:48:B:LYS:H	3:44:C:PHE:HE2	16	2.0
(3,7)	2:44:B:ILE:HG13	3:115:C:HIS:HA	18	1.97
(3,4)	2:62:B:GLN:HE22	3:47:C:GLY:HA3	13	1.93
(2,6)	2:47:B:GLY:H	3:43:C:VAL:HG21	13	1.92
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG11	4	1.91
(1,6)	1:62:A:GLN:HG3	3:92:C:THR:O	8	1.86
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HB3	18	1.85
(3,4)	2:66:B:THR:HG1	3:47:C:GLY:O	15	1.84
(1,6)	1:62:A:GLN:HG3	3:92:C:THR:O	14	1.83
(3,10)	2:62:B:GLN:HE21	3:44:C:PHE:HZ	16	1.77
(2,8)	2:62:B:GLN:HE22	3:43:C:VAL:HG13	19	1.77
(2,5)	2:44:B:ILE:HD12	3:39:C:LEU:O	13	1.71
(2,1)	2:44:B:ILE:HD12	3:39:C:LEU:O	13	1.71
(3,4)	2:66:B:THR:HG1	3:47:C:GLY:N	20	1.64
(3,4)	2:66:B:THR:HG23	3:47:C:GLY:N	3	1.63
(3,4)	2:64:B:GLU:OE1	3:47:C:GLY:O	6	1.63
(3,2)	2:66:B:THR:HG23	3:45:C:ASN:HB2	20	1.6
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:HE2	16	1.55
(2,5)	2:44:B:ILE:HD13	3:39:C:LEU:O	15	1.55
(2,1)	2:44:B:ILE:HD13	3:39:C:LEU:O	15	1.55
(1,6)	1:62:A:GLN:HG3	3:92:C:THR:O	19	1.49
(3,4)	2:62:B:GLN:HE22	3:47:C:GLY:HA3	4	1.48
(2,2)	2:66:B:THR:HG1	3:40:C:ASP:HA	11	1.46
(2,8)	2:62:B:GLN:OE1	3:43:C:VAL:HG11	9	1.45
(1,6)	1:62:A:GLN:HG2	3:92:C:THR:O	18	1.45
(3,2)	2:66:B:THR:HG23	3:45:C:ASN:O	8	1.43
(3,12)	2:66:B:THR:OG1	3:44:C:PHE:HB3	18	1.41
(3,1)	2:66:B:THR:OG1	3:44:C:PHE:HB3	18	1.41
(3,7)	2:44:B:ILE:HD12	3:44:C:PHE:HZ	3	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,12)	2:66:B:THR:OG1	3:44:C:PHE:HB3	5	1.33
(3,4)	2:66:B:THR:HG1	3:47:C:GLY:N	12	1.33
(3,7)	2:44:B:ILE:HG22	3:44:C:PHE:HZ	12	1.29
(3,4)	2:66:B:THR:HG21	3:47:C:GLY:H	7	1.15
(2,8)	2:62:B:GLN:HE21	3:43:C:VAL:HG13	1	1.15
(1,7)	1:62:A:GLN:HG3	3:98:C:LYS:N	9	1.09
(3,2)	2:66:B:THR:HG1	3:45:C:ASN:HB2	16	1.08
(1,7)	1:62:A:GLN:HG3	3:98:C:LYS:N	1	1.05
(1,7)	1:62:A:GLN:HG3	3:98:C:LYS:N	6	1.04
(1,7)	1:62:A:GLN:HG3	3:98:C:LYS:N	10	1.04
(1,7)	1:62:A:GLN:HG3	3:98:C:LYS:N	12	1.04
(2,6)	2:47:B:GLY:HA2	3:39:C:LEU:O	19	1.03
(1,7)	1:62:A:GLN:HG3	3:98:C:LYS:N	20	1.02
(1,7)	1:62:A:GLN:HG2	3:98:C:LYS:N	15	0.99
(3,8)	2:47:B:GLY:HA3	3:44:C:PHE:HZ	5	0.98
(3,2)	2:66:B:THR:HG22	3:45:C:ASN:OD1	12	0.98
(3,1)	2:47:B:GLY:HA3	3:44:C:PHE:HZ	5	0.98
(3,7)	2:44:B:ILE:O	3:44:C:PHE:HE1	7	0.95
(1,6)	1:62:A:GLN:OE1	3:92:C:THR:O	20	0.94
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:HG23	19	0.93
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:HG23	19	0.93
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HE1	14	0.92
(1,7)	1:62:A:GLN:HE21	3:98:C:LYS:N	19	0.92
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HD1	20	0.9
(1,7)	1:62:A:GLN:HE21	3:98:C:LYS:HA	18	0.9
(1,7)	1:62:A:GLN:HG2	3:98:C:LYS:N	4	0.86
(1,7)	1:62:A:GLN:HG2	3:98:C:LYS:N	16	0.83
(2,5)	2:44:B:ILE:HD11	3:39:C:LEU:HD11	4	0.82
(2,5)	2:44:B:ILE:HD13	3:39:C:LEU:HD23	6	0.82
(2,1)	2:44:B:ILE:HD11	3:39:C:LEU:HD11	4	0.82
(2,1)	2:44:B:ILE:HD13	3:39:C:LEU:HD23	6	0.82
(1,7)	1:62:A:GLN:HG2	3:98:C:LYS:N	3	0.82
(1,7)	1:62:A:GLN:HG2	3:98:C:LYS:N	5	0.82
(1,7)	1:62:A:GLN:HG2	3:98:C:LYS:N	2	0.81
(1,7)	1:62:A:GLN:HG2	3:98:C:LYS:N	17	0.81
(3,12)	2:66:B:THR:HG22	3:44:C:PHE:HB2	12	0.7
(3,4)	2:66:B:THR:HG23	3:47:C:GLY:N	8	0.7
(3,8)	2:47:B:GLY:N	3:44:C:PHE:HZ	10	0.69
(3,8)	2:47:B:GLY:HA2	3:44:C:PHE:HZ	12	0.68
(3,1)	2:47:B:GLY:HA2	3:44:C:PHE:HZ	12	0.68
(2,10)	2:66:B:THR:HG1	3:43:C:VAL:HG12	1	0.68
(2,10)	2:66:B:THR:HG22	3:43:C:VAL:HG22	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	2:66:B:THR:HG1	3:43:C:VAL:HG12	1	0.68
(2,4)	2:66:B:THR:HG22	3:43:C:VAL:HG22	2	0.68
(1,4)	1:44:A:ILE:HG23	3:46:C:ASP:N	2	0.65
(1,4)	1:44:A:ILE:HG22	3:46:C:ASP:N	4	0.65
(2,10)	2:66:B:THR:HB	3:43:C:VAL:HG22	13	0.62
(2,4)	2:66:B:THR:HB	3:43:C:VAL:HG22	13	0.62
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:HB3	20	0.6
(1,6)	1:62:A:GLN:OE1	3:92:C:THR:O	3	0.6
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:HD2	10	0.58
(3,1)	2:66:B:THR:HG1	3:44:C:PHE:HD2	10	0.58
(1,4)	1:44:A:ILE:HD12	3:46:C:ASP:N	8	0.57
(1,4)	1:44:A:ILE:HG13	3:46:C:ASP:N	19	0.57
(2,10)	2:66:B:THR:HG22	3:43:C:VAL:HG22	4	0.56
(2,4)	2:66:B:THR:HG22	3:43:C:VAL:HG22	4	0.56
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HE2	8	0.54
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HE1	7	0.53
(3,4)	2:62:B:GLN:OE1	3:47:C:GLY:HA3	9	0.52
(1,4)	1:44:A:ILE:HG13	3:46:C:ASP:N	18	0.52
(2,2)	2:47:B:GLY:HA2	3:40:C:ASP:OD2	17	0.51
(2,6)	2:47:B:GLY:HA2	3:39:C:LEU:O	2	0.48
(3,7)	2:44:B:ILE:HG21	3:44:C:PHE:HE1	20	0.44
(3,1)	2:44:B:ILE:HG21	3:44:C:PHE:HE1	20	0.44
(2,5)	2:44:B:ILE:HD12	3:39:C:LEU:O	9	0.43
(2,1)	2:44:B:ILE:HD12	3:39:C:LEU:O	9	0.43
(1,4)	1:44:A:ILE:HD13	3:46:C:ASP:N	1	0.42
(3,4)	2:66:B:THR:HG23	3:47:C:GLY:H	14	0.4
(2,5)	2:44:B:ILE:HD11	3:39:C:LEU:HD12	1	0.4
(2,1)	2:44:B:ILE:HD11	3:39:C:LEU:HD12	1	0.4
(1,6)	1:62:A:GLN:HE22	3:92:C:THR:O	16	0.37
(1,6)	1:62:A:GLN:OE1	3:92:C:THR:O	10	0.36
(2,10)	2:66:B:THR:HG23	3:43:C:VAL:HG23	11	0.35
(2,4)	2:66:B:THR:HG23	3:43:C:VAL:HG23	11	0.35
(1,4)	1:44:A:ILE:HD13	3:46:C:ASP:N	17	0.35
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HE2	16	0.34
(3,1)	2:47:B:GLY:H	3:44:C:PHE:HE2	16	0.34
(2,2)	2:47:B:GLY:HA2	3:40:C:ASP:OD2	15	0.34
(3,2)	2:66:B:THR:HG22	3:45:C:ASN:HB2	10	0.29
(1,4)	1:44:A:ILE:HG21	3:46:C:ASP:N	12	0.29
(1,6)	1:62:A:GLN:HE22	3:92:C:THR:O	4	0.27
(3,8)	2:47:B:GLY:H	3:44:C:PHE:HE1	3	0.24
(3,4)	2:62:B:GLN:HE22	3:47:C:GLY:O	1	0.23
(1,7)	1:62:A:GLN:HE22	3:98:C:LYS:HA	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:62:A:GLN:OE1	3:98:C:LYS:N	11	0.22
(3,12)	2:66:B:THR:HG1	3:44:C:PHE:HD1	3	0.18
(3,1)	2:66:B:THR:HG1	3:44:C:PHE:HD1	3	0.18
(2,5)	2:44:B:ILE:HD12	3:39:C:LEU:HD23	19	0.12
(2,1)	2:44:B:ILE:HD12	3:39:C:LEU:HD23	19	0.12

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found