



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 02:39 AM UTC

PDB ID : 8IVB / pdb_00008ivb
BMRB ID : 19045
Title : K113-Ubiquitinated BAK
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Deposited on : 2023-03-26

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

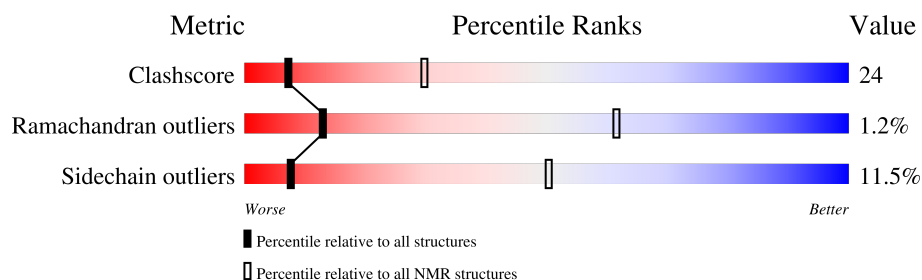
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 8%.

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	 63% 30% • 5%
2	B	169	 63% 33% •

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:72 (72)	0.17	11
2	B:18-B:186 (169)	0.26	12

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3851 atoms, of which 1912 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
			1235	379	631	105	118	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	CYS	GLY	conflict	UNP P62979

- Molecule 2 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms						Trace
2	B	169	Total	C	H	N	O	S	0
			2616	847	1281	233	249	6	

There is a discrepancy between the modelled and reference sequences:

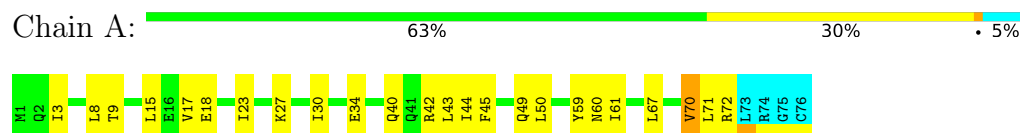
Chain	Residue	Modelled	Actual	Comment	Reference
B	113	CYS	LYS	engineered mutation	UNP Q16611

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ubiquitin



- Molecule 2: Bcl-2 homologous antagonist/killer

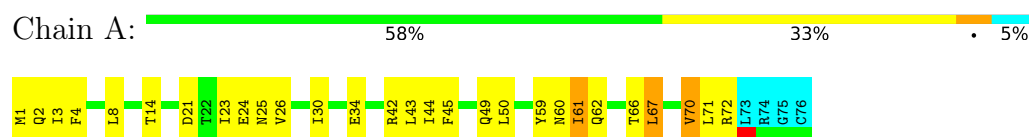


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

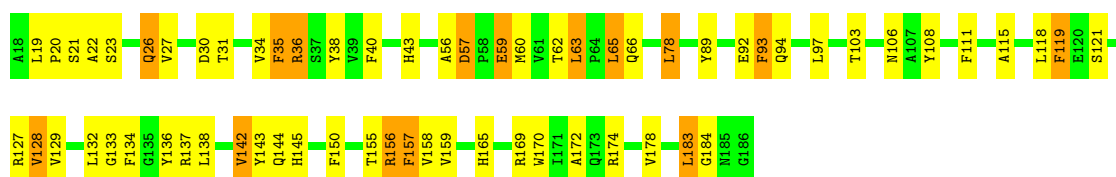
4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin



- Molecule 2: Bcl-2 homologous antagonist/killer



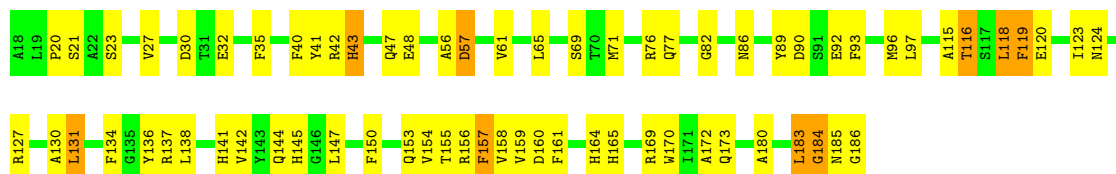


4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin

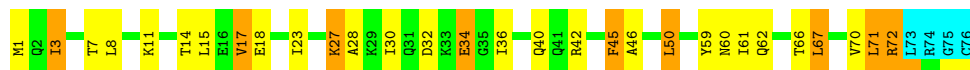


- Molecule 2: Bcl-2 homologous antagonist/killer

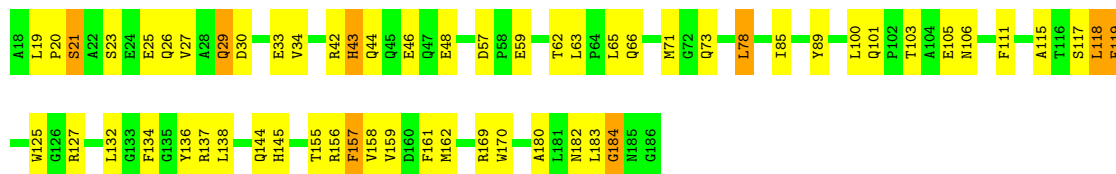


4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin



- Molecule 2: Bcl-2 homologous antagonist/killer



4.2.4 Score per residue for model 4

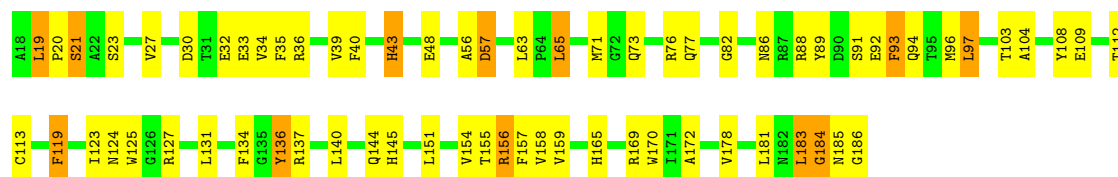
- Molecule 1: Ubiquitin

Chain A: 



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B: 



4.2.5 Score per residue for model 5

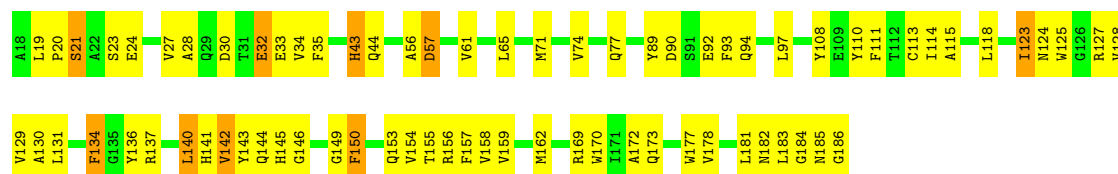
- Molecule 1: Ubiquitin

Chain A: 



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B: 



4.2.6 Score per residue for model 6

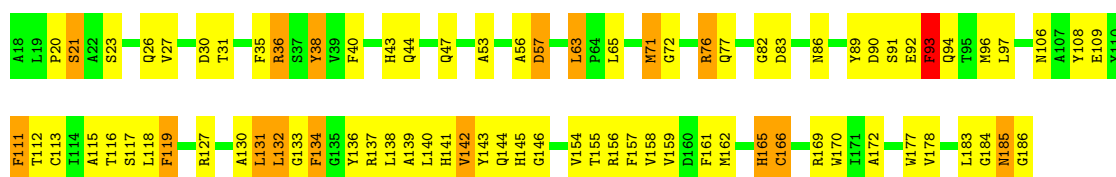
- Molecule 1: Ubiquitin

Chain A: 



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B: 



4.2.7 Score per residue for model 7

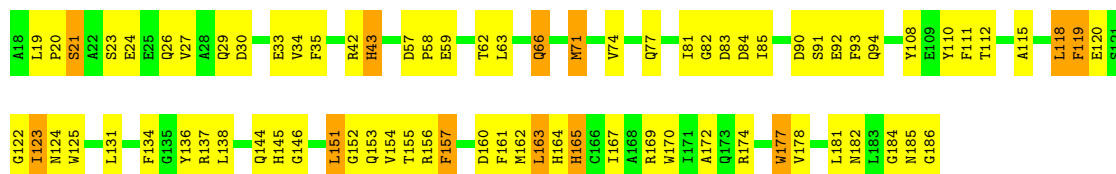
- Molecule 1: Ubiquitin

Chain A: 63% 24% 7% • 5%



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B: 54% 39% 7%



4.2.8 Score per residue for model 8

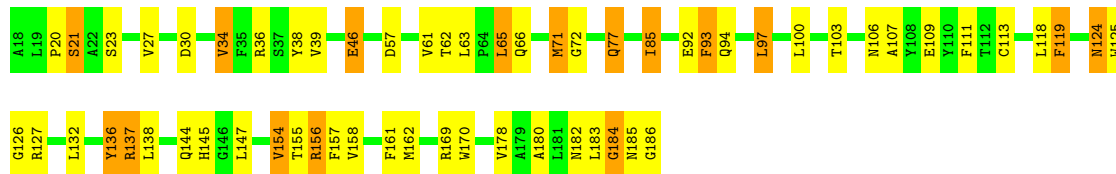
- Molecule 1: Ubiquitin

Chain A: 66% 22% 5% • 5%



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B: 64% 26% 9%



4.2.9 Score per residue for model 9

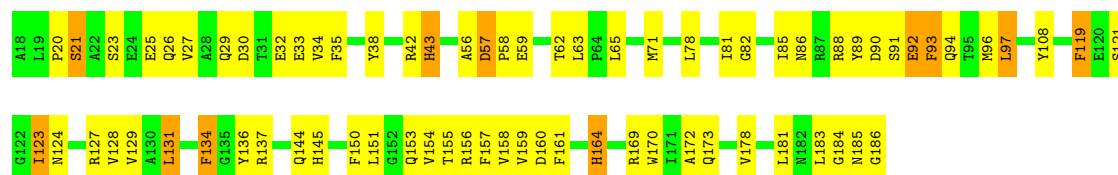
- Molecule 1: Ubiquitin

Chain A: 



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B: 



4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin

Chain A: 



- Molecule 2: Bcl-2 homologous antagonist/killer

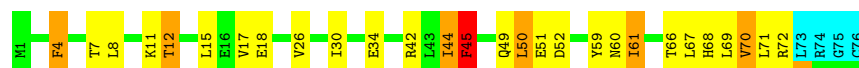
Chain B: 



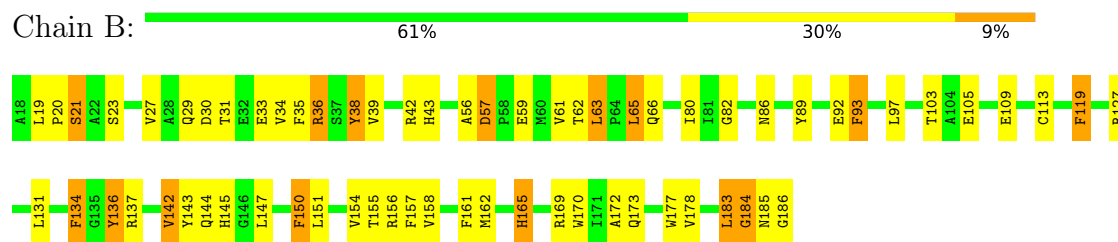
4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin

Chain A: 

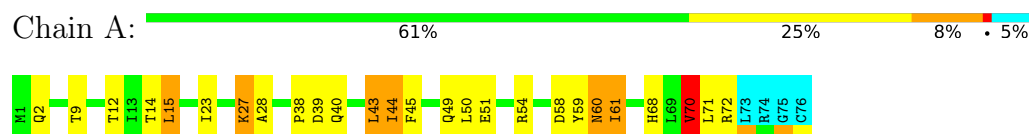


- Molecule 2: Bcl-2 homologous antagonist/killer

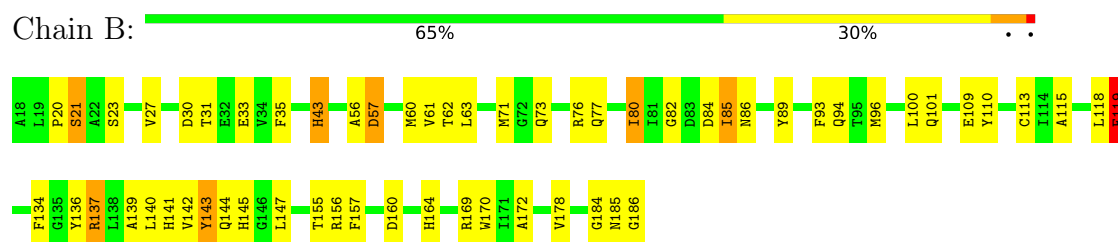


4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Ubiquitin

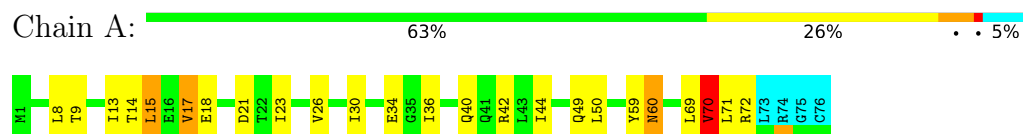


- Molecule 2: Bcl-2 homologous antagonist/killer

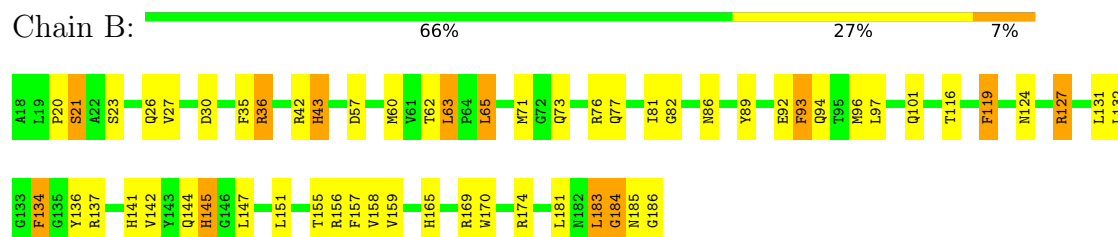


4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin



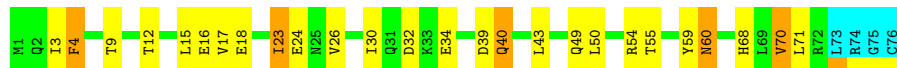
- Molecule 2: Bcl-2 homologous antagonist/killer



4.2.14 Score per residue for model 14

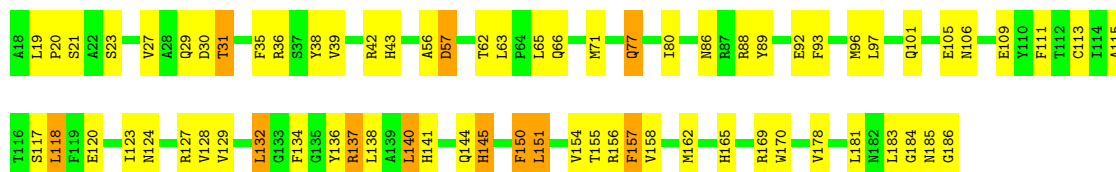
- Molecule 1: Ubiquitin

Chain A: 



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B: 



4.2.15 Score per residue for model 15

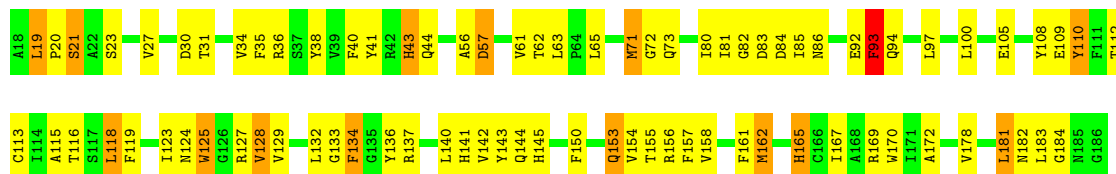
- Molecule 1: Ubiquitin

Chain A: 



- Molecule 2: Bcl-2 homologous antagonist/killer

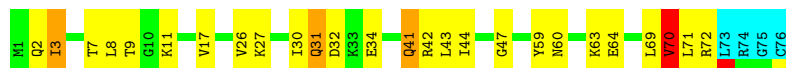
Chain B: 



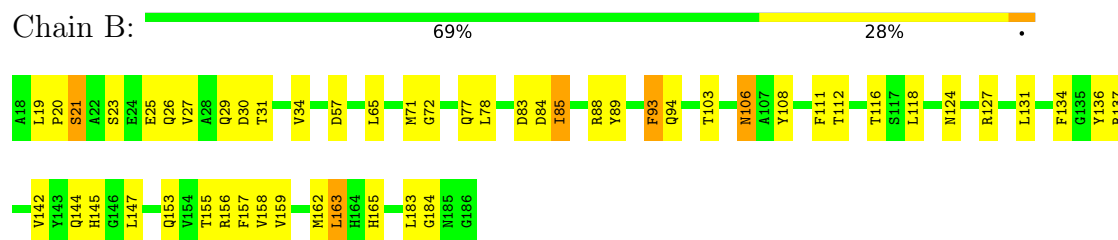
4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin

Chain A: 

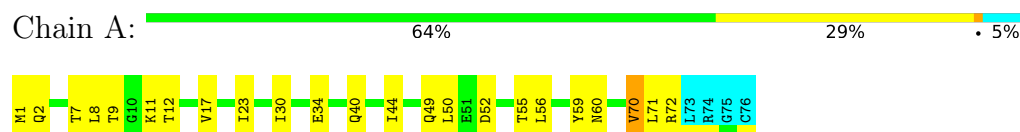


- Molecule 2: Bcl-2 homologous antagonist/killer

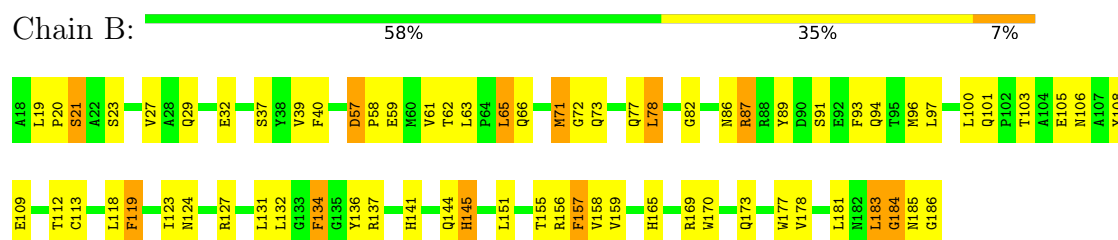


4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin

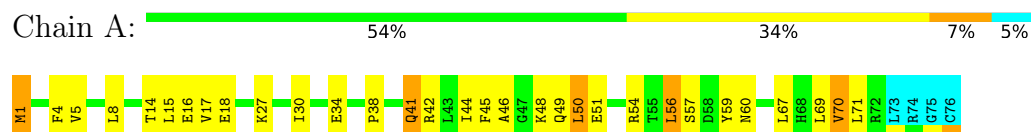


- Molecule 2: Bcl-2 homologous antagonist/killer

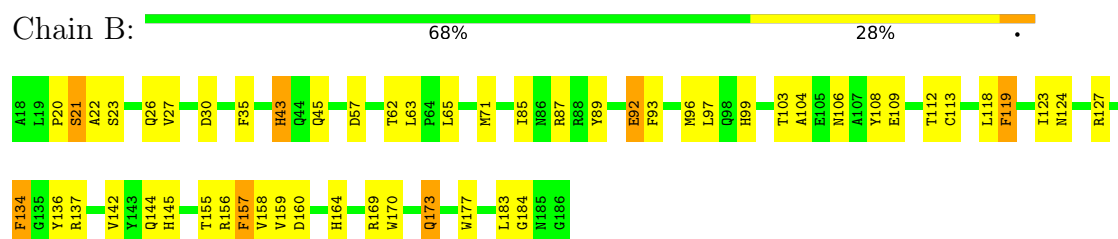


4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin



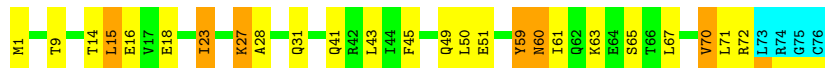
- Molecule 2: Bcl-2 homologous antagonist/killer



4.2.19 Score per residue for model 19

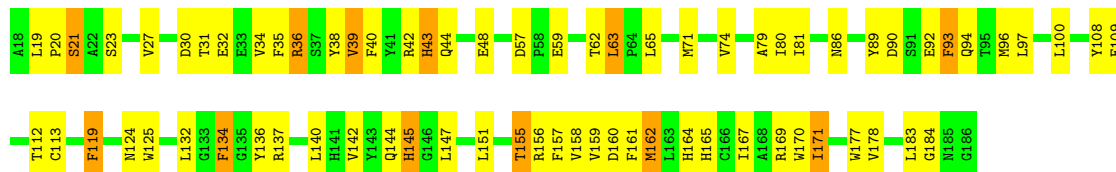
- Molecule 1: Ubiquitin

Chain A:  62% 25% 8% 5%



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B:  57% 36% 7%



4.2.20 Score per residue for model 20

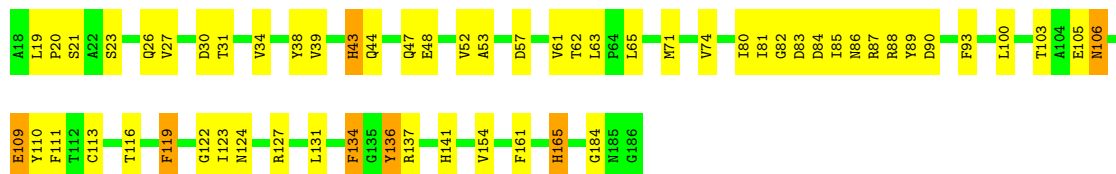
- Molecule 1: Ubiquitin

Chain A:  63% 28% 5%



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B:  65% 31%



5 Refinement protocol and experimental data overview

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

Of the 240 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	256
Number of shifts mapped to atoms	256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.51±0.05	0±1/581 (0.0± 0.1%)	1.26±0.02	0±1/784 (0.0± 0.1%)
2	B	1.48±0.03	0±0/1368 (0.0± 0.0%)	1.23±0.02	1±1/1858 (0.1± 0.1%)
All	All	1.49	4/38980 (0.0%)	1.24	31/52840 (0.1%)

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	36	ILE	N-CA	5.75	1.50	1.46	2	2
1	A	37	PRO	CA-C	5.09	1.56	1.52	9	1
1	A	70	VAL	N-CA	5.06	1.52	1.46	12	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
2	B	150	PHE	CA-CB-CG	-10.73	103.07	113.80	11	3
2	B	93	PHE	CA-CB-CG	-6.71	107.09	113.80	2	6
2	B	43	HIS	CA-CB-CG	-6.51	107.29	113.80	4	5
1	A	45	PHE	CA-CB-CG	-6.11	107.69	113.80	12	3
2	B	165	HIS	CA-CB-CG	-5.86	107.94	113.80	7	4
2	B	157	PHE	CA-CB-CG	-5.86	107.94	113.80	10	2
1	A	59	TYR	CA-CB-CG	-5.86	103.36	113.90	4	1
2	B	38	TYR	CB-CA-C	-5.50	101.55	110.79	11	1
2	B	119	PHE	CA-CB-CG	-5.50	108.30	113.80	12	1
1	A	68	HIS	CA-CB-CG	-5.38	108.42	113.80	12	2
2	B	164	HIS	CA-CB-CG	-5.16	108.64	113.80	9	1
2	B	161	PHE	CA-CB-CG	-5.05	108.75	113.80	3	1
2	B	111	PHE	CA-CB-CG	-5.01	108.79	113.80	6	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	574	600	599	25±7
2	B	1335	1281	1273	66±11
All	All	38180	37620	37440	1780

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:65:LEU:H	2:B:65:LEU:HD13	0.97	1.17	11	1
2:B:65:LEU:HD13	2:B:66:GLN:N	0.94	1.77	14	3
2:B:151:LEU:HD22	2:B:152:GLY:N	0.94	1.77	7	1
1:A:50:LEU:HD13	1:A:50:LEU:H	0.92	1.25	15	3
2:B:65:LEU:H	2:B:65:LEU:HD22	0.92	1.21	8	1
2:B:63:LEU:HD22	2:B:63:LEU:H	0.91	1.25	13	3
2:B:183:LEU:HD12	2:B:184:GLY:H	0.91	1.22	2	3
1:A:43:LEU:HD22	1:A:43:LEU:H	0.89	1.26	12	2
2:B:34:VAL:HG13	2:B:38:TYR:CE1	0.85	2.06	8	1
2:B:183:LEU:HD12	2:B:184:GLY:N	0.84	1.87	8	3
1:A:67:LEU:N	1:A:67:LEU:HD22	0.84	1.87	7	1
2:B:63:LEU:H	2:B:63:LEU:HD12	0.83	1.34	19	2
1:A:43:LEU:HD23	1:A:44:ILE:N	0.82	1.88	1	1
2:B:65:LEU:HD13	2:B:66:GLN:H	0.81	1.34	3	4
2:B:78:LEU:HD12	2:B:78:LEU:O	0.81	1.75	1	3
1:A:8:LEU:HD22	1:A:8:LEU:H	0.81	1.32	15	1
1:A:56:LEU:HD12	1:A:56:LEU:C	0.80	2.01	18	1
1:A:23:ILE:HD12	1:A:23:ILE:O	0.80	1.76	19	2
1:A:8:LEU:O	1:A:8:LEU:HD13	0.80	1.76	8	1
2:B:63:LEU:HD13	2:B:63:LEU:N	0.79	1.93	13	2
2:B:71:MET:O	2:B:74:VAL:HG22	0.78	1.78	7	4
2:B:136:TYR:CG	2:B:137:ARG:N	0.77	2.52	11	9
1:A:50:LEU:HD13	1:A:50:LEU:N	0.77	1.95	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:122:GLY:C	2:B:123:ILE:HD13	0.77	2.05	7	1
1:A:66:THR:C	1:A:67:LEU:HD23	0.76	2.06	1	2
2:B:63:LEU:HD22	2:B:63:LEU:N	0.75	1.96	1	7
2:B:38:TYR:CE2	2:B:132:LEU:HD22	0.75	2.17	1	1
1:A:66:THR:C	1:A:67:LEU:HD13	0.75	2.06	7	1
1:A:41:GLN:NE2	1:A:43:LEU:HD23	0.74	1.96	8	1
1:A:7:THR:HG22	1:A:11:LYS:O	0.74	1.82	11	5
2:B:123:ILE:HD13	2:B:123:ILE:H	0.73	1.44	5	1
1:A:67:LEU:HD22	1:A:67:LEU:H	0.73	1.41	7	1
2:B:147:LEU:HD22	2:B:147:LEU:N	0.73	1.99	19	1
2:B:63:LEU:HD12	2:B:63:LEU:N	0.72	1.99	7	6
2:B:132:LEU:HD23	2:B:133:GLY:N	0.72	2.00	6	1
1:A:70:VAL:HG23	1:A:71:LEU:H	0.72	1.43	8	3
2:B:43:HIS:NE2	2:B:136:TYR:CD1	0.71	2.58	10	3
2:B:158:VAL:CG1	2:B:162:MET:HE3	0.71	2.15	6	6
1:A:8:LEU:HD22	1:A:8:LEU:N	0.71	2.00	15	2
1:A:70:VAL:CG2	1:A:71:LEU:H	0.71	1.99	7	3
1:A:36:ILE:HG22	1:A:40:GLN:OE1	0.71	1.85	9	1
2:B:71:MET:O	2:B:74:VAL:HG12	0.71	1.86	10	1
1:A:50:LEU:H	1:A:50:LEU:CD1	0.70	1.99	3	3
1:A:50:LEU:O	1:A:50:LEU:HD12	0.70	1.84	8	1
2:B:35:PHE:O	2:B:132:LEU:HD11	0.70	1.86	1	1
1:A:59:TYR:CD1	1:A:59:TYR:O	0.70	2.45	19	2
1:A:44:ILE:HD12	2:B:92:GLU:OE1	0.70	1.86	10	1
2:B:181:LEU:H	2:B:181:LEU:HD22	0.69	1.46	7	2
2:B:65:LEU:HD13	2:B:65:LEU:N	0.69	2.00	11	1
2:B:97:LEU:HD13	2:B:97:LEU:O	0.69	1.86	5	9
2:B:89:TYR:O	2:B:89:TYR:CG	0.69	2.45	17	8
2:B:30:ASP:O	2:B:34:VAL:HG12	0.69	1.88	7	4
2:B:19:LEU:H	2:B:19:LEU:HD23	0.69	1.48	3	2
2:B:65:LEU:HD22	2:B:65:LEU:N	0.69	1.98	8	1
1:A:67:LEU:HD23	1:A:67:LEU:N	0.69	2.01	1	2
2:B:138:LEU:C	2:B:138:LEU:HD13	0.69	2.13	3	1
2:B:19:LEU:HD22	2:B:19:LEU:N	0.69	2.03	17	3
2:B:62:THR:HG22	2:B:63:LEU:H	0.68	1.49	14	5
1:A:68:HIS:CD2	2:B:88:ARG:NH2	0.68	2.61	4	1
2:B:23:SER:O	2:B:27:VAL:HG13	0.68	1.89	5	4
2:B:181:LEU:HD22	2:B:181:LEU:N	0.68	2.04	7	4
2:B:183:LEU:CD1	2:B:184:GLY:H	0.68	1.98	2	2
2:B:119:PHE:C	2:B:119:PHE:CD2	0.68	2.72	6	1
1:A:17:VAL:HG22	1:A:18:GLU:N	0.68	2.03	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:27:VAL:O	2:B:31:THR:HG23	0.68	1.89	10	4
2:B:93:PHE:CD2	2:B:93:PHE:C	0.67	2.73	9	7
1:A:68:HIS:CE1	2:B:88:ARG:NH2	0.67	2.62	4	1
1:A:17:VAL:HG22	1:A:18:GLU:H	0.67	1.50	6	3
2:B:65:LEU:H	2:B:65:LEU:CD1	0.67	2.01	11	2
2:B:62:THR:C	2:B:63:LEU:HD13	0.67	2.14	11	2
1:A:61:ILE:CD1	1:A:61:ILE:O	0.66	2.42	5	1
2:B:77:GLN:OE1	2:B:78:LEU:HD12	0.66	1.90	16	1
2:B:111:PHE:CE2	2:B:134:PHE:CZ	0.66	2.84	3	2
2:B:151:LEU:C	2:B:151:LEU:HD13	0.66	2.16	13	1
1:A:8:LEU:HD12	2:B:127:ARG:CZ	0.66	2.21	5	1
2:B:113:CYS:SG	2:B:114:ILE:N	0.65	2.69	5	1
1:A:46:ALA:HB3	1:A:59:TYR:OH	0.65	1.92	15	1
1:A:3:ILE:N	1:A:3:ILE:HD13	0.65	2.06	16	1
1:A:68:HIS:NE2	2:B:88:ARG:NH1	0.65	2.43	14	2
2:B:43:HIS:ND1	2:B:44:GLN:N	0.65	2.43	19	2
2:B:78:LEU:HD12	2:B:78:LEU:C	0.65	2.16	3	3
1:A:8:LEU:HD21	1:A:69:LEU:O	0.65	1.90	15	1
1:A:4:PHE:C	1:A:4:PHE:CD1	0.65	2.75	5	1
2:B:93:PHE:C	2:B:93:PHE:CD1	0.65	2.75	1	3
1:A:42:ARG:NH2	1:A:72:ARG:NH1	0.65	2.45	13	1
2:B:124:ASN:ND2	2:B:127:ARG:NH1	0.65	2.45	20	1
2:B:144:GLN:O	2:B:145:HIS:C	0.64	2.39	5	19
2:B:19:LEU:HD12	2:B:19:LEU:N	0.64	2.07	16	4
2:B:131:LEU:C	2:B:131:LEU:HD13	0.64	2.18	17	1
2:B:62:THR:HG22	2:B:63:LEU:N	0.64	2.07	7	5
2:B:136:TYR:CD2	2:B:137:ARG:N	0.64	2.66	8	4
2:B:185:ASN:ND2	2:B:185:ASN:N	0.64	2.45	6	1
1:A:44:ILE:C	1:A:44:ILE:HD12	0.64	2.18	11	1
1:A:8:LEU:O	2:B:127:ARG:NH1	0.64	2.30	6	3
2:B:119:PHE:C	2:B:119:PHE:CD1	0.64	2.76	4	1
2:B:134:PHE:CG	2:B:134:PHE:O	0.64	2.51	11	10
1:A:3:ILE:HD13	1:A:3:ILE:C	0.64	2.17	3	1
2:B:177:TRP:CD1	2:B:177:TRP:H	0.63	2.08	6	2
1:A:70:VAL:HG12	1:A:71:LEU:H	0.63	1.52	18	5
2:B:71:MET:SD	2:B:72:GLY:N	0.63	2.72	17	5
2:B:87:ARG:HH11	2:B:91:SER:N	0.63	1.91	17	1
2:B:43:HIS:ND1	2:B:43:HIS:C	0.63	2.57	5	6
1:A:61:ILE:O	1:A:61:ILE:HD12	0.63	1.93	5	1
1:A:50:LEU:HD22	1:A:50:LEU:O	0.63	1.92	15	2
2:B:63:LEU:H	2:B:63:LEU:CD1	0.63	2.07	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:93:PHE:CD1	2:B:94:GLN:N	0.63	2.67	15	2
2:B:150:PHE:CE2	2:B:153:GLN:NE2	0.63	2.67	15	1
1:A:17:VAL:HG12	1:A:18:GLU:N	0.62	2.09	18	1
2:B:42:ARG:NH2	2:B:86:ASN:HD22	0.62	1.91	13	1
2:B:151:LEU:N	2:B:151:LEU:HD23	0.62	2.09	9	1
2:B:132:LEU:HD23	2:B:132:LEU:C	0.62	2.19	1	1
2:B:23:SER:O	2:B:27:VAL:HG23	0.62	1.93	3	16
2:B:42:ARG:NH1	2:B:43:HIS:NE2	0.62	2.48	10	1
2:B:134:PHE:N	2:B:134:PHE:CD1	0.62	2.66	17	1
2:B:134:PHE:O	2:B:134:PHE:CD1	0.62	2.53	5	5
2:B:43:HIS:HD1	2:B:44:GLN:N	0.62	1.93	19	1
1:A:59:TYR:O	1:A:60:ASN:ND2	0.61	2.33	12	4
2:B:94:GLN:OE1	2:B:137:ARG:NH2	0.61	2.32	5	2
2:B:132:LEU:C	2:B:132:LEU:HD13	0.61	2.20	19	1
2:B:151:LEU:HD13	2:B:151:LEU:N	0.61	2.10	7	1
1:A:1:MET:SD	1:A:63:LYS:CB	0.61	2.88	9	1
2:B:89:TYR:CD1	2:B:89:TYR:O	0.61	2.53	5	4
1:A:1:MET:SD	1:A:2:GLN:N	0.61	2.74	9	1
2:B:63:LEU:N	2:B:63:LEU:CD1	0.61	2.63	13	8
2:B:115:ALA:HB1	2:B:119:PHE:CZ	0.61	2.31	3	1
2:B:30:ASP:O	2:B:34:VAL:HG22	0.61	1.96	15	4
2:B:41:TYR:CE2	2:B:45:GLN:NE2	0.60	2.69	10	1
2:B:103:THR:H	2:B:106:ASN:ND2	0.60	1.93	16	1
2:B:119:PHE:CG	2:B:119:PHE:O	0.60	2.54	13	5
1:A:45:PHE:CE1	1:A:59:TYR:CD1	0.60	2.89	19	1
2:B:136:TYR:CD1	2:B:137:ARG:N	0.60	2.69	4	4
1:A:50:LEU:N	1:A:50:LEU:CD1	0.60	2.65	18	1
2:B:92:GLU:H	2:B:92:GLU:CD	0.60	2.03	9	1
1:A:4:PHE:C	1:A:4:PHE:CD2	0.60	2.79	14	1
1:A:17:VAL:HG12	1:A:18:GLU:H	0.60	1.56	18	1
1:A:42:ARG:NH2	2:B:96:MET:SD	0.60	2.75	18	3
2:B:161:PHE:CZ	2:B:165:HIS:NE2	0.60	2.70	7	4
2:B:134:PHE:O	2:B:134:PHE:CG	0.60	2.55	20	4
2:B:141:HIS:CE1	2:B:145:HIS:NE2	0.59	2.70	12	2
2:B:31:THR:O	2:B:35:PHE:CG	0.59	2.56	12	1
2:B:119:PHE:CD1	2:B:119:PHE:N	0.59	2.67	12	3
1:A:2:GLN:C	1:A:3:ILE:HD13	0.59	2.22	16	1
2:B:119:PHE:CD2	2:B:119:PHE:O	0.59	2.55	19	2
1:A:56:LEU:C	1:A:56:LEU:CD1	0.59	2.75	18	1
1:A:70:VAL:O	1:A:71:LEU:HD23	0.59	1.98	12	2
2:B:19:LEU:H	2:B:19:LEU:CD2	0.59	2.10	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:59:GLU:H	2:B:62:THR:HG23	0.58	1.58	1	6
2:B:89:TYR:O	2:B:89:TYR:CD2	0.58	2.56	4	6
1:A:56:LEU:O	1:A:61:ILE:HG22	0.58	1.98	6	1
2:B:151:LEU:H	2:B:151:LEU:CD1	0.58	2.12	7	1
2:B:158:VAL:HG13	2:B:159:VAL:N	0.58	2.14	2	6
2:B:161:PHE:CE1	2:B:165:HIS:CD2	0.58	2.91	2	1
2:B:77:GLN:HE21	2:B:186:GLY:N	0.58	1.96	4	1
2:B:123:ILE:HD13	2:B:124:ASN:N	0.58	2.13	9	1
2:B:166:CYS:SG	2:B:166:CYS:O	0.58	2.62	6	1
1:A:59:TYR:CG	1:A:59:TYR:O	0.58	2.56	9	1
2:B:91:SER:O	2:B:95:THR:HG23	0.58	1.98	10	1
2:B:92:GLU:OE1	2:B:92:GLU:N	0.58	2.37	11	1
2:B:162:MET:SD	2:B:162:MET:N	0.58	2.77	15	1
2:B:89:TYR:O	2:B:93:PHE:CD1	0.58	2.56	20	1
2:B:92:GLU:CD	2:B:92:GLU:N	0.58	2.62	9	1
2:B:60:MET:SD	2:B:60:MET:N	0.58	2.76	10	2
2:B:119:PHE:CZ	2:B:165:HIS:NE2	0.58	2.72	4	1
1:A:67:LEU:N	1:A:67:LEU:CD2	0.58	2.61	7	3
2:B:134:PHE:CD2	2:B:134:PHE:O	0.58	2.57	7	3
1:A:68:HIS:CG	2:B:88:ARG:NH2	0.58	2.72	4	1
1:A:70:VAL:CG2	1:A:71:LEU:N	0.57	2.66	7	3
1:A:60:ASN:ND2	1:A:60:ASN:C	0.57	2.61	19	2
1:A:15:LEU:HD23	1:A:16:GLU:N	0.57	2.13	14	1
2:B:161:PHE:CZ	2:B:165:HIS:CE1	0.57	2.93	15	3
2:B:76:ARG:O	2:B:80:ILE:HG23	0.57	1.99	12	1
2:B:119:PHE:CD2	2:B:119:PHE:N	0.57	2.68	18	3
2:B:124:ASN:ND2	2:B:127:ARG:H	0.57	1.97	8	1
1:A:44:ILE:HD11	1:A:70:VAL:HG23	0.57	1.77	12	1
1:A:42:ARG:NH1	1:A:72:ARG:NH2	0.57	2.52	16	1
2:B:63:LEU:N	2:B:63:LEU:CD2	0.57	2.67	15	7
2:B:97:LEU:C	2:B:97:LEU:HD13	0.57	2.25	11	3
1:A:8:LEU:HD13	2:B:127:ARG:HH11	0.57	1.58	13	1
2:B:155:THR:C	2:B:157:PHE:H	0.57	2.07	6	19
2:B:158:VAL:HG23	2:B:159:VAL:N	0.57	2.14	4	4
2:B:63:LEU:H	2:B:63:LEU:CD2	0.57	2.06	11	2
1:A:61:ILE:HD12	1:A:62:GLN:O	0.57	1.98	1	2
2:B:125:TRP:CD2	2:B:125:TRP:N	0.57	2.71	15	1
2:B:147:LEU:N	2:B:147:LEU:CD2	0.57	2.68	19	1
2:B:162:MET:SD	2:B:163:LEU:N	0.57	2.77	16	1
2:B:43:HIS:NE2	2:B:136:TYR:CZ	0.57	2.72	20	1
1:A:42:ARG:NH2	1:A:72:ARG:HH12	0.57	1.97	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:HIS:NE2	2:B:89:TYR:OH	0.57	2.38	20	1
2:B:57:ASP:OD1	2:B:57:ASP:N	0.56	2.38	2	3
2:B:156:ARG:NH1	2:B:159:VAL:HG21	0.56	2.15	16	1
2:B:92:GLU:N	2:B:92:GLU:OE2	0.56	2.38	1	2
2:B:73:GLN:NE2	2:B:76:ARG:CZ	0.56	2.67	13	2
2:B:38:TYR:CD1	2:B:38:TYR:C	0.56	2.83	6	3
2:B:43:HIS:C	2:B:43:HIS:CD2	0.56	2.82	1	4
2:B:82:GLY:O	2:B:86:ASN:ND2	0.56	2.38	9	9
1:A:68:HIS:CG	2:B:88:ARG:HH22	0.56	2.17	4	1
2:B:73:GLN:NE2	2:B:76:ARG:NH1	0.56	2.53	4	2
2:B:57:ASP:OD2	2:B:57:ASP:N	0.56	2.38	5	5
1:A:49:GLN:H	1:A:49:GLN:CD	0.56	2.06	20	2
2:B:26:GLN:N	2:B:26:GLN:OE1	0.56	2.39	16	1
2:B:19:LEU:N	2:B:19:LEU:CD2	0.56	2.68	1	3
2:B:123:ILE:HD13	2:B:123:ILE:N	0.56	2.14	5	2
1:A:45:PHE:CD1	1:A:45:PHE:O	0.56	2.58	19	3
1:A:59:TYR:O	1:A:59:TYR:CD2	0.56	2.59	9	1
2:B:38:TYR:CD2	2:B:132:LEU:HD22	0.56	2.35	1	1
1:A:2:GLN:NE2	1:A:15:LEU:N	0.56	2.54	2	1
2:B:108:TYR:CE2	2:B:112:THR:OG1	0.56	2.59	16	3
1:A:60:ASN:CG	1:A:60:ASN:O	0.56	2.49	7	5
1:A:40:GLN:O	1:A:40:GLN:CG	0.56	2.53	4	4
2:B:19:LEU:HD23	2:B:19:LEU:N	0.56	2.16	3	2
2:B:151:LEU:N	2:B:151:LEU:CD1	0.56	2.69	7	3
1:A:42:ARG:NH1	1:A:72:ARG:NE	0.56	2.54	3	1
2:B:19:LEU:CD2	2:B:19:LEU:N	0.56	2.69	5	3
2:B:65:LEU:CD1	2:B:66:GLN:H	0.56	2.14	17	3
1:A:49:GLN:NE2	1:A:50:LEU:O	0.56	2.39	4	2
2:B:181:LEU:H	2:B:181:LEU:CD2	0.56	2.14	7	2
2:B:150:PHE:CG	2:B:151:LEU:N	0.56	2.74	11	2
2:B:137:ARG:NH2	2:B:144:GLN:OE1	0.56	2.39	17	1
2:B:124:ASN:ND2	2:B:127:ARG:CZ	0.56	2.69	20	1
1:A:42:ARG:NE	1:A:42:ARG:C	0.55	2.64	6	3
2:B:161:PHE:CE1	2:B:165:HIS:CE1	0.55	2.95	19	3
2:B:124:ASN:OD1	2:B:127:ARG:N	0.55	2.40	13	2
1:A:61:ILE:O	1:A:61:ILE:HG23	0.55	2.01	9	4
2:B:123:ILE:O	2:B:124:ASN:ND2	0.55	2.39	14	3
2:B:125:TRP:C	2:B:125:TRP:CD1	0.55	2.84	3	1
2:B:136:TYR:O	2:B:137:ARG:C	0.55	2.48	5	18
2:B:105:GLU:OE2	2:B:106:ASN:ND2	0.55	2.40	3	1
2:B:141:HIS:O	2:B:145:HIS:CD2	0.55	2.60	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ILE:HD11	1:A:70:VAL:CG2	0.55	2.31	13	2
2:B:73:GLN:HE21	2:B:76:ARG:NH1	0.55	1.99	13	1
2:B:161:PHE:CZ	2:B:165:HIS:CD2	0.55	2.94	19	4
2:B:109:GLU:O	2:B:113:CYS:SG	0.55	2.64	18	10
2:B:96:MET:SD	2:B:100:LEU:HD13	0.55	2.42	10	1
2:B:38:TYR:OH	2:B:86:ASN:ND2	0.55	2.39	20	1
2:B:185:ASN:ND2	2:B:185:ASN:H	0.55	1.98	6	1
2:B:111:PHE:CD1	2:B:138:LEU:HD21	0.55	2.37	8	1
1:A:59:TYR:O	1:A:60:ASN:CB	0.55	2.54	15	20
2:B:180:ALA:O	2:B:183:LEU:HD23	0.55	2.02	2	3
2:B:84:ASP:OD2	2:B:85:ILE:N	0.55	2.39	20	2
2:B:25:GLU:O	2:B:29:GLN:NE2	0.55	2.40	16	2
1:A:43:LEU:H	1:A:43:LEU:CD2	0.55	2.04	12	1
2:B:132:LEU:N	2:B:132:LEU:CD1	0.55	2.69	3	3
2:B:132:LEU:HD13	2:B:132:LEU:O	0.55	2.02	19	1
1:A:18:GLU:N	1:A:18:GLU:OE2	0.54	2.40	19	1
1:A:12:THR:C	1:A:13:ILE:HD12	0.54	2.28	20	1
2:B:65:LEU:CD1	2:B:66:GLN:N	0.54	2.64	14	3
2:B:165:HIS:O	2:B:165:HIS:CG	0.54	2.59	1	2
2:B:71:MET:N	2:B:71:MET:SD	0.54	2.80	13	5
1:A:60:ASN:ND2	1:A:60:ASN:O	0.54	2.41	7	2
1:A:68:HIS:CD2	2:B:89:TYR:OH	0.54	2.60	20	1
2:B:32:GLU:CD	2:B:33:GLU:N	0.54	2.66	4	1
2:B:24:GLU:OE1	2:B:169:ARG:CZ	0.54	2.56	7	1
2:B:26:GLN:NE2	2:B:29:GLN:OE1	0.54	2.40	10	1
2:B:150:PHE:CD2	2:B:153:GLN:NE2	0.54	2.75	15	1
1:A:2:GLN:HE21	1:A:15:LEU:N	0.54	2.00	2	1
1:A:45:PHE:O	1:A:45:PHE:CG	0.54	2.60	19	1
2:B:169:ARG:O	2:B:170:TRP:C	0.54	2.50	6	18
2:B:161:PHE:CE2	2:B:165:HIS:CD2	0.54	2.96	11	1
2:B:42:ARG:NH2	2:B:137:ARG:NH1	0.54	2.55	3	1
1:A:8:LEU:HD12	2:B:127:ARG:NH2	0.54	2.17	5	1
1:A:59:TYR:O	1:A:59:TYR:CG	0.54	2.60	12	2
2:B:30:ASP:O	2:B:34:VAL:HG13	0.54	2.03	11	4
2:B:34:VAL:O	2:B:34:VAL:HG22	0.54	2.03	7	2
2:B:29:GLN:NE2	2:B:30:ASP:OD1	0.54	2.41	3	1
2:B:137:ARG:O	2:B:141:HIS:CD2	0.54	2.61	20	2
2:B:185:ASN:N	2:B:185:ASN:HD22	0.54	2.01	6	1
1:A:8:LEU:H	1:A:8:LEU:CD2	0.54	2.11	15	1
1:A:42:ARG:O	1:A:42:ARG:HG3	0.53	2.02	18	5
1:A:41:GLN:HE22	1:A:43:LEU:HD23	0.53	1.63	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:36:ARG:HH11	2:B:151:LEU:HD11	0.53	1.62	11	1
2:B:124:ASN:OD1	2:B:125:TRP:CD2	0.53	2.61	19	2
1:A:40:GLN:CD	1:A:40:GLN:N	0.53	2.65	14	1
1:A:61:ILE:HD12	1:A:61:ILE:C	0.53	2.27	1	2
1:A:59:TYR:CD2	1:A:59:TYR:C	0.53	2.85	9	1
2:B:134:PHE:O	2:B:134:PHE:CD2	0.53	2.61	9	3
2:B:132:LEU:HD23	2:B:132:LEU:O	0.53	2.02	14	1
1:A:27:LYS:HD2	1:A:28:ALA:N	0.53	2.19	12	3
2:B:93:PHE:CG	2:B:94:GLN:N	0.53	2.76	8	8
2:B:109:GLU:N	2:B:109:GLU:OE1	0.53	2.42	8	3
2:B:83:ASP:N	2:B:83:ASP:OD1	0.53	2.42	6	3
2:B:23:SER:OG	2:B:26:GLN:NE2	0.53	2.41	7	1
1:A:49:GLN:N	2:B:92:GLU:OE1	0.53	2.42	18	1
1:A:14:THR:C	1:A:15:LEU:HD23	0.53	2.28	20	1
2:B:174:ARG:CZ	2:B:177:TRP:CZ3	0.53	2.91	7	1
2:B:38:TYR:OH	2:B:42:ARG:NH2	0.53	2.41	9	1
2:B:66:GLN:N	2:B:66:GLN:CD	0.53	2.66	11	1
2:B:84:ASP:OD1	2:B:85:ILE:N	0.53	2.42	12	2
2:B:108:TYR:CE1	2:B:109:GLU:OE2	0.53	2.62	19	1
1:A:8:LEU:CD2	1:A:8:LEU:N	0.53	2.72	3	1
1:A:68:HIS:NE2	2:B:88:ARG:NH2	0.53	2.57	4	1
2:B:183:LEU:CG	2:B:184:GLY:N	0.53	2.71	2	1
1:A:42:ARG:HH11	1:A:72:ARG:NH2	0.53	2.00	16	1
2:B:119:PHE:CD1	2:B:119:PHE:C	0.53	2.86	20	2
2:B:19:LEU:N	2:B:19:LEU:CD1	0.53	2.71	16	4
2:B:160:ASP:O	2:B:164:HIS:CD2	0.53	2.62	12	2
1:A:42:ARG:HH11	1:A:72:ARG:NE	0.53	2.01	3	1
2:B:52:VAL:CG1	2:B:137:ARG:HH22	0.53	2.16	10	1
2:B:153:GLN:N	2:B:153:GLN:OE1	0.52	2.42	7	2
2:B:38:TYR:CE1	2:B:132:LEU:HD21	0.52	2.39	6	1
1:A:18:GLU:N	1:A:18:GLU:OE1	0.52	2.41	10	1
1:A:1:MET:N	1:A:1:MET:SD	0.52	2.77	18	1
2:B:76:ARG:NH2	2:B:77:GLN:OE1	0.52	2.42	2	1
2:B:83:ASP:OD2	2:B:83:ASP:N	0.52	2.43	7	1
2:B:52:VAL:CG1	2:B:137:ARG:NH2	0.52	2.71	10	1
2:B:85:ILE:HD12	2:B:85:ILE:C	0.52	2.28	16	1
1:A:39:ASP:OD1	1:A:40:GLN:N	0.52	2.42	4	1
2:B:124:ASN:OD1	2:B:125:TRP:CE3	0.52	2.62	4	2
2:B:181:LEU:CD2	2:B:181:LEU:N	0.52	2.72	4	2
2:B:125:TRP:CD1	2:B:174:ARG:NH2	0.52	2.78	7	1
1:A:42:ARG:C	1:A:42:ARG:HE	0.52	2.13	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:132:LEU:HD12	2:B:132:LEU:N	0.52	2.19	13	3
2:B:65:LEU:HD12	2:B:65:LEU:H	0.52	1.64	13	1
2:B:165:HIS:O	2:B:165:HIS:ND1	0.52	2.42	14	4
2:B:181:LEU:N	2:B:181:LEU:HD22	0.52	2.20	4	2
2:B:125:TRP:N	2:B:125:TRP:CE3	0.52	2.78	15	1
2:B:137:ARG:HH12	2:B:144:GLN:HE22	0.52	1.47	17	1
1:A:31:GLN:O	1:A:35:GLY:N	0.52	2.43	20	1
2:B:73:GLN:HE22	2:B:76:ARG:CZ	0.52	2.17	4	1
2:B:71:MET:SD	2:B:71:MET:C	0.52	2.92	6	5
2:B:165:HIS:O	2:B:166:CYS:SG	0.52	2.68	6	1
2:B:160:ASP:O	2:B:164:HIS:ND1	0.52	2.43	7	2
1:A:4:PHE:CE2	1:A:14:THR:HG22	0.52	2.40	1	2
2:B:110:TYR:O	2:B:113:CYS:SG	0.52	2.68	5	1
2:B:124:ASN:OD1	2:B:125:TRP:N	0.52	2.43	7	1
2:B:103:THR:HG22	2:B:104:ALA:N	0.52	2.20	4	2
2:B:19:LEU:N	2:B:19:LEU:HD22	0.52	2.20	5	1
2:B:78:LEU:HD23	2:B:81:ILE:HD11	0.52	1.81	9	1
2:B:100:LEU:O	2:B:101:GLN:CG	0.52	2.58	12	2
2:B:39:VAL:O	2:B:43:HIS:ND1	0.52	2.43	4	2
2:B:181:LEU:N	2:B:181:LEU:CD2	0.52	2.73	9	4
1:A:42:ARG:NH1	1:A:72:ARG:CZ	0.51	2.73	3	1
1:A:53:GLY:O	1:A:54:ARG:NE	0.51	2.43	4	1
1:A:70:VAL:O	1:A:71:LEU:CD2	0.51	2.58	12	3
2:B:124:ASN:CG	2:B:126:GLY:H	0.51	2.13	8	1
1:A:60:ASN:O	1:A:60:ASN:CG	0.51	2.54	14	1
2:B:181:LEU:HD23	2:B:182:ASN:N	0.51	2.20	15	1
1:A:15:LEU:HD23	1:A:15:LEU:N	0.51	2.20	20	1
2:B:169:ARG:O	2:B:172:ALA:N	0.51	2.43	5	11
1:A:45:PHE:CZ	1:A:59:TYR:CD2	0.51	2.98	4	1
2:B:48:GLU:N	2:B:48:GLU:OE2	0.51	2.40	4	1
2:B:150:PHE:CE2	2:B:153:GLN:OE1	0.51	2.62	9	1
2:B:84:ASP:OD2	2:B:87:ARG:NH1	0.51	2.42	10	1
2:B:119:PHE:O	2:B:119:PHE:CG	0.51	2.63	4	1
2:B:90:ASP:OD1	2:B:91:SER:N	0.51	2.43	7	1
2:B:124:ASN:ND2	2:B:127:ARG:N	0.51	2.59	8	1
2:B:101:GLN:O	2:B:101:GLN:NE2	0.51	2.42	3	1
2:B:157:PHE:C	2:B:157:PHE:CD1	0.51	2.87	15	1
1:A:42:ARG:HH11	2:B:92:GLU:CG	0.51	2.19	18	1
1:A:8:LEU:HD12	1:A:8:LEU:N	0.51	2.21	1	4
2:B:150:PHE:CD1	2:B:153:GLN:NE2	0.51	2.78	2	1
2:B:39:VAL:HG13	2:B:43:HIS:CE1	0.51	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:127:ARG:O	2:B:131:LEU:HD23	0.51	2.05	4	1
2:B:35:PHE:CD2	2:B:35:PHE:C	0.51	2.87	5	1
2:B:124:ASN:O	2:B:128:VAL:HG13	0.51	2.06	5	4
1:A:2:GLN:NE2	1:A:15:LEU:C	0.51	2.68	2	1
1:A:18:GLU:N	1:A:18:GLU:CD	0.51	2.69	19	2
2:B:65:LEU:HD12	2:B:65:LEU:N	0.51	2.20	13	1
2:B:81:ILE:HD11	2:B:185:ASN:HD22	0.51	1.66	13	1
2:B:161:PHE:CE1	2:B:165:HIS:NE2	0.51	2.78	2	1
1:A:47:GLY:O	2:B:91:SER:OG	0.51	2.28	4	2
1:A:17:VAL:CG2	1:A:18:GLU:N	0.51	2.73	6	3
2:B:35:PHE:CD2	2:B:35:PHE:O	0.51	2.64	5	5
2:B:35:PHE:C	2:B:35:PHE:CD2	0.51	2.87	11	4
2:B:111:PHE:CD1	2:B:111:PHE:N	0.51	2.74	8	1
2:B:43:HIS:C	2:B:43:HIS:HD1	0.51	2.14	3	1
2:B:96:MET:C	2:B:96:MET:SD	0.51	2.94	4	7
1:A:60:ASN:OD1	1:A:60:ASN:C	0.51	2.54	13	3
2:B:111:PHE:N	2:B:111:PHE:CD2	0.51	2.78	1	1
2:B:123:ILE:N	2:B:123:ILE:CD1	0.51	2.74	5	1
2:B:34:VAL:O	2:B:38:TYR:CD1	0.51	2.64	8	2
1:A:44:ILE:HD12	1:A:45:PHE:N	0.51	2.20	11	1
1:A:23:ILE:HD12	1:A:23:ILE:C	0.51	2.30	19	1
1:A:8:LEU:N	1:A:8:LEU:CD2	0.50	2.74	5	2
2:B:66:GLN:O	2:B:66:GLN:NE2	0.50	2.43	7	1
2:B:151:LEU:HD23	2:B:151:LEU:H	0.50	1.64	9	1
2:B:150:PHE:CD2	2:B:150:PHE:N	0.50	2.77	11	2
2:B:20:PRO:O	2:B:21:SER:CB	0.50	2.59	20	20
1:A:42:ARG:NH1	2:B:92:GLU:OE1	0.50	2.45	2	1
2:B:151:LEU:HD12	2:B:151:LEU:N	0.50	2.21	17	2
2:B:153:GLN:N	2:B:153:GLN:CD	0.50	2.70	5	2
2:B:43:HIS:NE2	2:B:53:ALA:O	0.50	2.44	6	1
2:B:35:PHE:CD1	2:B:132:LEU:HD13	0.50	2.40	15	1
1:A:51:GLU:N	1:A:51:GLU:OE1	0.50	2.44	12	2
2:B:90:ASP:OD2	2:B:91:SER:N	0.50	2.44	9	1
1:A:59:TYR:CD1	1:A:59:TYR:C	0.50	2.88	8	2
1:A:8:LEU:HD13	2:B:127:ARG:NH1	0.50	2.22	13	1
1:A:61:ILE:HD11	1:A:65:SER:OG	0.50	2.05	19	1
2:B:35:PHE:C	2:B:35:PHE:CD1	0.50	2.87	2	3
2:B:183:LEU:CD1	2:B:184:GLY:N	0.50	2.72	3	3
2:B:150:PHE:CD1	2:B:150:PHE:C	0.50	2.89	11	2
1:A:51:GLU:OE1	1:A:54:ARG:NH1	0.50	2.45	18	1
2:B:157:PHE:CD2	2:B:157:PHE:C	0.50	2.89	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASN:O	1:A:60:ASN:OD1	0.50	2.30	12	3
2:B:182:ASN:C	2:B:182:ASN:OD1	0.50	2.54	10	1
1:A:39:ASP:O	1:A:72:ARG:CZ	0.50	2.60	12	2
1:A:54:ARG:NE	1:A:55:THR:O	0.50	2.43	14	1
2:B:87:ARG:O	2:B:87:ARG:NE	0.50	2.44	17	1
1:A:42:ARG:NH1	2:B:92:GLU:OE2	0.50	2.44	4	1
1:A:45:PHE:CE2	1:A:59:TYR:CG	0.50	3.00	4	1
2:B:122:GLY:C	2:B:127:ARG:NH1	0.50	2.70	20	1
2:B:124:ASN:ND2	2:B:127:ARG:NE	0.50	2.60	20	1
2:B:48:GLU:OE1	2:B:48:GLU:N	0.50	2.42	3	1
2:B:132:LEU:N	2:B:132:LEU:HD12	0.50	2.21	3	1
2:B:35:PHE:CD1	2:B:35:PHE:C	0.50	2.88	10	3
2:B:165:HIS:O	2:B:165:HIS:CD2	0.49	2.65	10	2
2:B:36:ARG:HH11	2:B:151:LEU:HD21	0.49	1.65	13	1
2:B:19:LEU:HD12	2:B:19:LEU:O	0.49	2.07	10	3
2:B:92:GLU:CD	2:B:93:PHE:N	0.49	2.70	11	2
2:B:92:GLU:CD	2:B:92:GLU:O	0.49	2.56	8	1
1:A:44:ILE:C	1:A:44:ILE:CD1	0.49	2.84	11	1
2:B:42:ARG:CZ	2:B:86:ASN:ND2	0.49	2.76	14	1
2:B:29:GLN:O	2:B:33:GLU:OE1	0.49	2.30	9	2
1:A:54:ARG:NE	1:A:58:ASP:OD1	0.49	2.45	12	1
1:A:43:LEU:HB3	1:A:50:LEU:HD11	0.49	1.85	4	1
2:B:108:TYR:O	2:B:112:THR:HG22	0.49	2.08	7	5
1:A:1:MET:SD	1:A:2:GLN:O	0.49	2.70	9	1
2:B:181:LEU:HD12	2:B:181:LEU:N	0.49	2.22	17	1
2:B:130:ALA:O	2:B:134:PHE:CD1	0.49	2.65	2	1
1:A:8:LEU:N	1:A:8:LEU:HD22	0.49	2.22	3	1
2:B:111:PHE:CZ	2:B:131:LEU:HD11	0.49	2.42	20	4
1:A:64:GLU:CD	1:A:64:GLU:O	0.49	2.56	9	1
2:B:151:LEU:H	2:B:151:LEU:CD2	0.49	2.21	9	1
2:B:23:SER:H	2:B:26:GLN:NE2	0.49	2.05	3	2
2:B:151:LEU:N	2:B:151:LEU:CD2	0.49	2.76	9	1
1:A:3:ILE:N	1:A:3:ILE:CD1	0.49	2.70	16	1
2:B:103:THR:H	2:B:106:ASN:HD21	0.49	1.50	16	1
1:A:50:LEU:HD13	1:A:51:GLU:H	0.49	1.66	11	1
2:B:32:GLU:OE1	2:B:36:ARG:NE	0.49	2.46	19	1
1:A:2:GLN:HE21	1:A:15:LEU:H	0.49	1.51	2	1
1:A:14:THR:HG22	1:A:15:LEU:N	0.49	2.23	4	4
2:B:25:GLU:N	2:B:25:GLU:OE2	0.49	2.45	3	1
2:B:119:PHE:CZ	2:B:165:HIS:CE1	0.49	3.01	4	1
1:A:54:ARG:HH11	1:A:55:THR:C	0.49	2.16	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LEU:N	1:A:8:LEU:CD1	0.48	2.76	10	4
2:B:30:ASP:OD2	2:B:31:THR:N	0.48	2.45	16	4
1:A:30:ILE:HG21	1:A:36:ILE:HD11	0.48	1.83	2	1
1:A:60:ASN:O	1:A:62:GLN:NE2	0.48	2.46	2	1
2:B:42:ARG:CZ	2:B:86:ASN:HD22	0.48	2.20	2	1
1:A:53:GLY:O	1:A:54:ARG:CZ	0.48	2.61	4	1
1:A:18:GLU:N	1:A:21:ASP:OD1	0.48	2.46	7	1
1:A:49:GLN:O	1:A:49:GLN:CD	0.48	2.56	8	4
1:A:70:VAL:O	1:A:71:LEU:HG	0.48	2.08	4	2
2:B:44:GLN:CD	2:B:44:GLN:C	0.48	2.81	15	3
1:A:59:TYR:O	1:A:60:ASN:OD1	0.48	2.32	13	3
1:A:56:LEU:HD12	1:A:57:SER:N	0.48	2.22	18	1
2:B:30:ASP:OD1	2:B:31:THR:N	0.48	2.45	19	1
2:B:35:PHE:CD1	2:B:35:PHE:O	0.48	2.66	10	3
1:A:64:GLU:O	1:A:64:GLU:CG	0.48	2.62	9	1
1:A:47:GLY:H	2:B:88:ARG:HH22	0.48	1.48	16	1
1:A:30:ILE:O	1:A:34:GLU:N	0.48	2.47	5	15
2:B:78:LEU:C	2:B:78:LEU:CD1	0.48	2.82	3	2
2:B:65:LEU:N	2:B:65:LEU:CD1	0.48	2.72	11	1
2:B:30:ASP:OD1	2:B:30:ASP:C	0.48	2.56	19	1
2:B:97:LEU:HD23	2:B:141:HIS:CE1	0.48	2.43	2	1
2:B:77:GLN:NE2	2:B:77:GLN:C	0.48	2.71	14	2
1:A:68:HIS:NE2	2:B:88:ARG:CZ	0.48	2.76	9	1
2:B:86:ASN:O	2:B:90:ASP:CG	0.48	2.57	20	2
2:B:128:VAL:CG2	2:B:129:VAL:N	0.48	2.76	1	5
2:B:40:PHE:CD2	2:B:65:LEU:HD21	0.48	2.43	4	1
1:A:59:TYR:C	1:A:60:ASN:CG	0.48	2.81	8	6
2:B:141:HIS:O	2:B:145:HIS:CG	0.48	2.67	6	2
1:A:46:ALA:HB2	1:A:59:TYR:OH	0.48	2.09	8	1
2:B:106:ASN:ND2	2:B:109:GLU:OE2	0.48	2.47	10	1
1:A:36:ILE:O	1:A:36:ILE:HG23	0.48	2.09	15	1
1:A:12:THR:O	1:A:12:THR:HG23	0.48	2.09	12	3
1:A:63:LYS:CG	1:A:64:GLU:N	0.48	2.76	7	2
2:B:136:TYR:CE1	2:B:140:LEU:HD23	0.48	2.44	14	1
2:B:27:VAL:O	2:B:30:ASP:OD2	0.48	2.32	12	4
2:B:35:PHE:O	2:B:132:LEU:CD1	0.48	2.61	1	1
1:A:3:ILE:C	1:A:3:ILE:CD1	0.48	2.84	3	1
1:A:27:LYS:CD	1:A:28:ALA:N	0.48	2.77	3	1
2:B:77:GLN:C	2:B:77:GLN:CD	0.48	2.82	14	2
1:A:1:MET:N	1:A:17:VAL:O	0.48	2.46	17	2
1:A:38:PRO:O	1:A:41:GLN:NE2	0.48	2.47	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:PHE:CD1	1:A:45:PHE:C	0.48	2.92	19	1
1:A:2:GLN:NE2	1:A:14:THR:OG1	0.48	2.46	2	1
1:A:61:ILE:O	1:A:61:ILE:CG2	0.48	2.62	3	4
2:B:30:ASP:OD1	2:B:177:TRP:CZ2	0.48	2.67	6	1
2:B:151:LEU:C	2:B:151:LEU:CD1	0.48	2.86	13	2
1:A:42:ARG:NE	1:A:42:ARG:CA	0.47	2.77	10	2
2:B:158:VAL:CG1	2:B:159:VAL:N	0.47	2.77	2	6
1:A:56:LEU:HB3	1:A:61:ILE:HG21	0.47	1.86	6	1
2:B:62:THR:CG2	2:B:63:LEU:N	0.47	2.77	7	5
2:B:161:PHE:CE2	2:B:165:HIS:CE1	0.47	3.02	15	1
2:B:77:GLN:NE2	2:B:185:ASN:CG	0.47	2.72	2	1
2:B:138:LEU:C	2:B:138:LEU:CD1	0.47	2.84	3	1
1:A:45:PHE:CZ	1:A:59:TYR:CG	0.47	3.03	4	1
2:B:30:ASP:OD2	2:B:30:ASP:O	0.47	2.32	8	1
2:B:31:THR:O	2:B:35:PHE:CD1	0.47	2.67	12	1
1:A:17:VAL:CG1	1:A:18:GLU:N	0.47	2.77	18	1
2:B:111:PHE:CE2	2:B:138:LEU:HD22	0.47	2.45	1	1
1:A:17:VAL:HG13	1:A:18:GLU:N	0.47	2.24	7	4
1:A:53:GLY:O	1:A:54:ARG:NH1	0.47	2.47	4	1
1:A:47:GLY:H	2:B:88:ARG:NH2	0.47	2.07	16	1
2:B:131:LEU:C	2:B:131:LEU:CD1	0.47	2.86	17	1
1:A:3:ILE:CG2	1:A:4:PHE:N	0.47	2.77	20	1
2:B:123:ILE:H	2:B:123:ILE:CD1	0.47	2.19	5	1
2:B:85:ILE:O	2:B:89:TYR:CE2	0.47	2.67	12	1
2:B:160:ASP:OD1	2:B:164:HIS:NE2	0.47	2.46	12	1
2:B:36:ARG:O	2:B:40:PHE:CD1	0.47	2.68	19	1
2:B:30:ASP:OD2	2:B:30:ASP:C	0.47	2.57	14	4
2:B:115:ALA:O	2:B:118:LEU:N	0.47	2.45	5	10
2:B:61:VAL:HG22	2:B:61:VAL:O	0.47	2.10	11	2
2:B:141:HIS:O	2:B:145:HIS:CE1	0.47	2.66	15	2
2:B:34:VAL:HG21	2:B:177:TRP:HE1	0.47	1.69	7	1
2:B:62:THR:C	2:B:63:LEU:HD12	0.47	2.33	18	4
2:B:97:LEU:HD23	2:B:137:ARG:HH21	0.47	1.70	13	1
1:A:27:LYS:HG2	1:A:28:ALA:N	0.47	2.25	2	1
2:B:142:VAL:HG12	2:B:147:LEU:HB2	0.47	1.85	2	2
1:A:49:GLN:OE1	1:A:49:GLN:O	0.47	2.33	18	2
2:B:119:PHE:O	2:B:119:PHE:CD1	0.47	2.67	11	2
2:B:42:ARG:NH2	2:B:86:ASN:ND2	0.47	2.62	13	1
2:B:132:LEU:C	2:B:132:LEU:CD2	0.47	2.87	1	1
1:A:30:ILE:CG2	1:A:36:ILE:HD11	0.47	2.40	2	1
2:B:140:LEU:N	2:B:140:LEU:CD2	0.47	2.77	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:162:MET:HA	2:B:167:ILE:HD12	0.47	1.86	7	2
1:A:27:LYS:NZ	1:A:38:PRO:CB	0.47	2.77	12	1
2:B:29:GLN:NE2	2:B:32:GLU:OE2	0.47	2.48	17	1
1:A:41:GLN:HE21	1:A:43:LEU:HD21	0.47	1.69	19	1
2:B:22:ALA:HB1	2:B:26:GLN:CD	0.47	2.34	1	1
1:A:69:LEU:C	1:A:69:LEU:HD23	0.47	2.35	13	5
2:B:151:LEU:HD22	2:B:152:GLY:H	0.47	1.65	7	1
1:A:50:LEU:N	1:A:50:LEU:HD13	0.47	2.25	18	1
2:B:34:VAL:HG23	2:B:74:VAL:HG23	0.47	1.86	5	1
2:B:179:ALA:O	2:B:182:ASN:OD1	0.47	2.32	10	1
2:B:137:ARG:NH2	2:B:141:HIS:ND1	0.47	2.63	13	1
2:B:38:TYR:CD2	2:B:38:TYR:C	0.47	2.92	20	3
2:B:29:GLN:O	2:B:33:GLU:OE2	0.47	2.33	7	2
2:B:28:ALA:O	2:B:32:GLU:CG	0.47	2.63	5	1
2:B:66:GLN:O	2:B:71:MET:HE1	0.47	2.10	8	2
2:B:141:HIS:NE2	2:B:145:HIS:NE2	0.47	2.63	10	1
2:B:27:VAL:O	2:B:30:ASP:OD1	0.47	2.33	19	1
2:B:40:PHE:O	2:B:43:HIS:ND1	0.47	2.46	19	1
2:B:169:ARG:O	2:B:173:GLN:OE1	0.46	2.33	9	2
1:A:66:THR:O	1:A:67:LEU:HD13	0.46	2.10	7	1
1:A:68:HIS:CD2	2:B:88:ARG:HH22	0.46	2.24	4	1
2:B:137:ARG:O	2:B:141:HIS:N	0.46	2.47	5	2
2:B:138:LEU:C	2:B:138:LEU:HD23	0.46	2.35	7	2
2:B:46:GLU:CD	2:B:46:GLU:C	0.46	2.83	8	2
2:B:103:THR:HG23	2:B:106:ASN:H	0.46	1.71	8	3
2:B:93:PHE:CD1	2:B:93:PHE:C	0.46	2.87	6	3
2:B:108:TYR:O	2:B:112:THR:HG23	0.46	2.11	6	1
2:B:38:TYR:CD2	2:B:78:LEU:HD21	0.46	2.45	1	1
1:A:56:LEU:C	1:A:61:ILE:HD11	0.46	2.35	5	1
1:A:61:ILE:HD12	1:A:61:ILE:N	0.46	2.26	5	1
2:B:89:TYR:OH	2:B:130:ALA:HB1	0.46	2.09	5	1
1:A:30:ILE:CG1	1:A:31:GLN:N	0.46	2.79	9	1
2:B:137:ARG:O	2:B:141:HIS:CG	0.46	2.68	20	1
1:A:71:LEU:CD2	2:B:120:GLU:OE1	0.46	2.64	2	1
1:A:45:PHE:O	1:A:46:ALA:HB3	0.46	2.11	4	7
1:A:2:GLN:N	1:A:2:GLN:CD	0.46	2.73	17	2
1:A:70:VAL:O	1:A:71:LEU:CG	0.46	2.63	4	2
2:B:62:THR:CG2	2:B:63:LEU:H	0.46	2.23	14	4
2:B:60:MET:C	2:B:60:MET:SD	0.46	2.98	13	1
1:A:43:LEU:HD23	1:A:44:ILE:H	0.46	1.67	1	1
1:A:1:MET:HE3	1:A:19:PRO:HD3	0.46	1.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:HIS:ND1	1:A:69:LEU:N	0.46	2.64	8	2
2:B:85:ILE:O	2:B:89:TYR:CZ	0.46	2.68	9	1
2:B:105:GLU:N	2:B:105:GLU:OE2	0.46	2.48	17	4
2:B:150:PHE:CZ	2:B:153:GLN:NE2	0.46	2.84	15	1
2:B:134:PHE:CD1	2:B:134:PHE:C	0.46	2.90	18	1
2:B:36:ARG:CD	2:B:36:ARG:N	0.46	2.78	1	1
2:B:36:ARG:CB	2:B:40:PHE:CZ	0.46	2.99	6	3
2:B:108:TYR:O	2:B:108:TYR:CG	0.46	2.69	1	3
2:B:155:THR:C	2:B:157:PHE:N	0.46	2.72	6	12
1:A:71:LEU:HD12	1:A:71:LEU:N	0.46	2.25	3	1
2:B:151:LEU:HD13	2:B:151:LEU:O	0.46	2.11	13	1
2:B:30:ASP:O	2:B:30:ASP:OD1	0.46	2.34	2	5
2:B:85:ILE:O	2:B:85:ILE:HD13	0.46	2.11	8	1
1:A:4:PHE:CE2	1:A:12:THR:OG1	0.46	2.64	11	1
2:B:73:GLN:O	2:B:77:GLN:OE1	0.46	2.35	12	2
2:B:103:THR:N	2:B:106:ASN:HD21	0.46	2.09	16	1
2:B:155:THR:O	2:B:157:PHE:N	0.45	2.50	6	10
1:A:3:ILE:HD13	1:A:3:ILE:O	0.45	2.11	3	1
1:A:16:GLU:N	1:A:16:GLU:OE2	0.45	2.49	8	1
2:B:161:PHE:N	2:B:161:PHE:CD2	0.45	2.82	9	1
2:B:124:ASN:HD22	2:B:127:ARG:NE	0.45	2.09	20	1
2:B:30:ASP:OD1	2:B:177:TRP:CE2	0.45	2.69	6	1
2:B:111:PHE:CE1	2:B:138:LEU:HD21	0.45	2.47	8	1
2:B:96:MET:SD	2:B:97:LEU:N	0.45	2.89	17	1
1:A:9:THR:O	1:A:9:THR:HG22	0.45	2.11	19	1
1:A:51:GLU:N	1:A:51:GLU:OE2	0.45	2.49	19	1
2:B:43:HIS:CE1	2:B:53:ALA:O	0.45	2.70	6	1
1:A:36:ILE:HG22	1:A:40:GLN:CD	0.45	2.36	9	1
2:B:128:VAL:CG1	2:B:129:VAL:N	0.45	2.79	15	1
2:B:178:VAL:O	2:B:181:LEU:HD22	0.45	2.11	15	1
2:B:39:VAL:HG13	2:B:40:PHE:CD2	0.45	2.46	17	1
2:B:119:PHE:CE2	2:B:165:HIS:NE2	0.45	2.84	4	1
2:B:93:PHE:CD1	2:B:93:PHE:O	0.45	2.70	5	1
2:B:94:GLN:CD	2:B:137:ARG:HH12	0.45	2.19	15	1
2:B:103:THR:OG1	2:B:106:ASN:OD1	0.45	2.34	16	2
2:B:185:ASN:O	2:B:186:GLY:OXT	0.45	2.35	6	4
2:B:124:ASN:ND2	2:B:126:GLY:N	0.45	2.64	8	1
2:B:136:TYR:CD2	2:B:136:TYR:C	0.45	2.93	8	1
2:B:185:ASN:O	2:B:186:GLY:O	0.45	2.34	12	7
2:B:80:ILE:CG2	2:B:81:ILE:N	0.45	2.80	20	3
2:B:158:VAL:CG1	2:B:162:MET:HE2	0.45	2.42	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:109:GLU:CD	2:B:109:GLU:C	0.45	2.85	20	1
1:A:17:VAL:CG2	1:A:18:GLU:H	0.45	2.20	6	2
2:B:124:ASN:HD21	2:B:126:GLY:CA	0.45	2.23	8	1
1:A:36:ILE:HG22	1:A:40:GLN:NE2	0.45	2.27	9	1
1:A:54:ARG:CZ	1:A:58:ASP:OD1	0.45	2.65	12	1
2:B:62:THR:C	2:B:63:LEU:HD22	0.45	2.36	14	3
2:B:115:ALA:HB1	2:B:119:PHE:CE2	0.45	2.46	12	1
1:A:42:ARG:CZ	2:B:96:MET:SD	0.45	3.05	2	1
2:B:163:LEU:O	2:B:163:LEU:HD13	0.45	2.11	7	1
2:B:82:GLY:O	2:B:86:ASN:CG	0.45	2.59	10	7
2:B:30:ASP:CG	2:B:71:MET:SD	0.45	2.99	5	2
2:B:77:GLN:HG3	2:B:186:GLY:OXT	0.45	2.11	5	1
2:B:34:VAL:HG11	2:B:177:TRP:NE1	0.45	2.27	7	1
2:B:107:ALA:O	2:B:111:PHE:CD2	0.45	2.69	8	1
1:A:12:THR:O	1:A:12:THR:CG2	0.45	2.65	12	1
1:A:17:VAL:CG2	1:A:21:ASP:OD1	0.45	2.65	15	1
2:B:83:ASP:OD1	2:B:84:ASP:N	0.45	2.48	16	2
1:A:17:VAL:CG1	1:A:18:GLU:H	0.45	2.25	18	1
2:B:133:GLY:O	2:B:136:TYR:CD1	0.45	2.70	6	2
1:A:42:ARG:NH2	2:B:96:MET:CE	0.45	2.80	2	1
2:B:48:GLU:C	2:B:48:GLU:CD	0.45	2.85	20	3
2:B:138:LEU:HD23	2:B:138:LEU:O	0.45	2.12	2	2
2:B:160:ASP:O	2:B:164:HIS:CG	0.45	2.70	2	2
1:A:50:LEU:O	1:A:50:LEU:HD22	0.45	2.12	4	2
2:B:43:HIS:NE2	2:B:136:TYR:CE1	0.45	2.85	4	1
2:B:77:GLN:OE1	2:B:81:ILE:CD1	0.45	2.65	7	1
1:A:39:ASP:O	1:A:72:ARG:NH1	0.45	2.49	12	1
1:A:42:ARG:CZ	1:A:49:GLN:NE2	0.45	2.79	15	1
2:B:57:ASP:OD2	2:B:58:PRO:N	0.45	2.50	17	1
2:B:151:LEU:O	2:B:155:THR:OG1	0.45	2.35	19	1
1:A:49:GLN:O	1:A:50:LEU:C	0.44	2.60	5	14
1:A:34:GLU:O	1:A:34:GLU:OE1	0.44	2.34	3	1
1:A:56:LEU:HD23	1:A:56:LEU:N	0.44	2.28	6	1
2:B:123:ILE:HD13	2:B:124:ASN:H	0.44	1.71	9	1
2:B:57:ASP:OD1	2:B:57:ASP:C	0.44	2.60	10	2
1:A:49:GLN:CD	1:A:49:GLN:N	0.44	2.75	20	1
2:B:142:VAL:HG21	2:B:150:PHE:CG	0.44	2.46	1	1
2:B:174:ARG:HH12	2:B:183:LEU:CD1	0.44	2.25	1	1
1:A:62:GLN:H	1:A:62:GLN:CD	0.44	2.19	2	1
1:A:34:GLU:OE1	1:A:36:ILE:CD1	0.44	2.65	3	1
1:A:39:ASP:OD1	1:A:39:ASP:C	0.44	2.59	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:89:TYR:OH	2:B:130:ALA:CB	0.44	2.65	5	2
2:B:36:ARG:NH1	2:B:151:LEU:HD21	0.44	2.28	11	1
2:B:94:GLN:CD	2:B:137:ARG:NH2	0.44	2.75	12	1
1:A:39:ASP:C	1:A:40:GLN:OE1	0.44	2.60	14	1
1:A:68:HIS:CD2	2:B:88:ARG:NH1	0.44	2.85	14	1
2:B:131:LEU:HD13	2:B:131:LEU:O	0.44	2.12	17	1
2:B:22:ALA:CB	2:B:26:GLN:NE2	0.44	2.81	18	1
2:B:92:GLU:CD	2:B:92:GLU:C	0.44	2.84	5	7
2:B:96:MET:SD	2:B:96:MET:O	0.44	2.75	4	2
1:A:2:GLN:N	1:A:2:GLN:OE1	0.44	2.49	12	1
2:B:94:GLN:CD	2:B:137:ARG:HH21	0.44	2.20	12	1
2:B:124:ASN:CG	2:B:127:ARG:HH11	0.44	2.19	15	1
1:A:41:GLN:CD	1:A:41:GLN:O	0.44	2.61	2	2
2:B:30:ASP:O	2:B:30:ASP:OD2	0.44	2.35	5	2
1:A:69:LEU:CD2	1:A:70:VAL:O	0.44	2.66	13	3
1:A:54:ARG:NH1	1:A:55:THR:O	0.44	2.50	14	1
2:B:56:ALA:O	2:B:57:ASP:OD1	0.44	2.35	15	1
1:A:21:ASP:OD1	1:A:25:ASN:ND2	0.44	2.51	1	1
2:B:158:VAL:CG2	2:B:159:VAL:N	0.44	2.80	4	2
2:B:29:GLN:CD	2:B:29:GLN:C	0.44	2.85	14	2
2:B:77:GLN:CD	2:B:77:GLN:C	0.44	2.86	6	2
2:B:144:GLN:O	2:B:146:GLY:N	0.44	2.51	5	4
2:B:94:GLN:CD	2:B:94:GLN:C	0.44	2.86	10	2
1:A:59:TYR:O	1:A:60:ASN:CG	0.44	2.61	8	4
2:B:34:VAL:O	2:B:34:VAL:HG12	0.44	2.13	9	3
2:B:90:ASP:OD1	2:B:90:ASP:O	0.44	2.35	5	1
2:B:42:ARG:NH1	2:B:136:TYR:CE1	0.44	2.86	11	1
2:B:76:ARG:HH11	2:B:77:GLN:HE21	0.44	1.54	13	1
2:B:84:ASP:OD1	2:B:84:ASP:N	0.44	2.47	15	1
2:B:173:GLN:CD	2:B:173:GLN:C	0.44	2.85	18	2
2:B:89:TYR:O	2:B:93:PHE:CG	0.44	2.71	20	1
2:B:100:LEU:CD2	2:B:110:TYR:CE2	0.44	3.01	20	1
2:B:97:LEU:HD13	2:B:97:LEU:C	0.44	2.38	5	2
2:B:85:ILE:N	2:B:85:ILE:HD12	0.44	2.26	18	2
2:B:182:ASN:O	2:B:182:ASN:OD1	0.44	2.36	7	4
1:A:72:ARG:HH22	2:B:96:MET:CE	0.44	2.26	4	1
2:B:140:LEU:N	2:B:140:LEU:HD22	0.44	2.26	6	5
2:B:178:VAL:HG12	2:B:178:VAL:O	0.44	2.12	17	3
1:A:55:THR:OG1	1:A:56:LEU:N	0.44	2.51	6	2
2:B:34:VAL:HG13	2:B:38:TYR:CZ	0.44	2.45	8	1
2:B:123:ILE:O	2:B:124:ASN:OD1	0.44	2.36	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:127:ARG:N	2:B:127:ARG:CD	0.44	2.81	10	1
1:A:42:ARG:NH2	1:A:72:ARG:CZ	0.44	2.81	13	1
2:B:153:GLN:CD	2:B:153:GLN:C	0.44	2.86	15	1
2:B:103:THR:OG1	2:B:106:ASN:ND2	0.44	2.51	20	1
2:B:44:GLN:O	2:B:48:GLU:OE1	0.44	2.36	3	1
2:B:124:ASN:ND2	2:B:125:TRP:CZ3	0.44	2.86	4	1
2:B:136:TYR:CE2	2:B:140:LEU:HD23	0.44	2.48	5	1
2:B:161:PHE:CD1	2:B:161:PHE:N	0.44	2.84	8	1
2:B:106:ASN:HD22	2:B:109:GLU:CD	0.44	2.21	10	1
2:B:42:ARG:NH1	2:B:86:ASN:ND2	0.44	2.66	14	1
1:A:3:ILE:HD11	1:A:17:VAL:HG22	0.44	1.89	16	1
2:B:45:GLN:CD	2:B:45:GLN:C	0.44	2.86	18	1
2:B:56:ALA:C	2:B:57:ASP:CG	0.43	2.84	5	8
2:B:142:VAL:O	2:B:143:TYR:C	0.43	2.60	12	7
2:B:100:LEU:CD2	2:B:100:LEU:C	0.43	2.91	3	2
1:A:39:ASP:O	1:A:39:ASP:OD2	0.43	2.36	7	1
2:B:36:ARG:NH1	2:B:154:VAL:CG1	0.43	2.80	8	1
2:B:153:GLN:CD	2:B:154:VAL:N	0.43	2.76	15	1
2:B:132:LEU:C	2:B:132:LEU:CD1	0.43	2.91	19	1
2:B:89:TYR:O	2:B:93:PHE:CE1	0.43	2.71	20	1
2:B:38:TYR:CE2	2:B:78:LEU:HD11	0.43	2.48	1	1
2:B:20:PRO:C	2:B:21:SER:OG	0.43	2.61	8	8
2:B:181:LEU:CD1	2:B:186:GLY:O	0.43	2.66	5	1
1:A:36:ILE:HD13	1:A:36:ILE:N	0.43	2.28	9	1
1:A:45:PHE:CD1	1:A:45:PHE:N	0.43	2.86	9	1
2:B:32:GLU:OE1	2:B:33:GLU:OE2	0.43	2.36	9	1
2:B:100:LEU:HD21	2:B:110:TYR:CG	0.43	2.48	12	1
2:B:60:MET:SD	2:B:60:MET:O	0.43	2.76	13	1
2:B:144:GLN:CG	2:B:145:HIS:N	0.43	2.81	17	1
2:B:167:ILE:O	2:B:171:ILE:HD12	0.43	2.12	19	1
1:A:1:MET:C	1:A:2:GLN:OE1	0.43	2.62	1	1
2:B:69:SER:OG	2:B:71:MET:CE	0.43	2.66	2	1
2:B:169:ARG:C	2:B:173:GLN:OE1	0.43	2.61	2	1
2:B:24:GLU:OE1	2:B:169:ARG:NE	0.43	2.51	7	1
2:B:65:LEU:N	2:B:65:LEU:CD2	0.43	2.70	8	1
1:A:8:LEU:O	2:B:127:ARG:NH2	0.43	2.52	15	1
1:A:32:ASP:O	1:A:32:ASP:OD1	0.43	2.36	14	2
2:B:36:ARG:O	2:B:40:PHE:CG	0.43	2.72	6	2
2:B:77:GLN:C	2:B:77:GLN:OE1	0.43	2.60	6	1
1:A:40:GLN:CD	1:A:71:LEU:HD22	0.43	2.37	12	1
2:B:42:ARG:CZ	2:B:86:ASN:HD21	0.43	2.27	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:42:ARG:NH1	2:B:79:ALA:O	0.43	2.51	19	1
2:B:103:THR:HG1	2:B:106:ASN:CG	0.43	2.21	1	1
1:A:27:LYS:O	1:A:30:ILE:HG13	0.43	2.14	4	1
2:B:103:THR:OG1	2:B:105:GLU:CD	0.43	2.62	11	1
2:B:181:LEU:N	2:B:181:LEU:CD1	0.43	2.81	17	1
2:B:30:ASP:OD1	2:B:71:MET:SD	0.43	2.77	18	1
2:B:97:LEU:HD12	2:B:100:LEU:HD12	0.43	1.91	19	1
2:B:87:ARG:O	2:B:88:ARG:C	0.43	2.62	20	1
1:A:42:ARG:NH1	1:A:43:LEU:O	0.43	2.47	6	2
2:B:90:ASP:O	2:B:90:ASP:OD2	0.43	2.36	6	2
1:A:43:LEU:HD11	1:A:67:LEU:CB	0.43	2.43	6	1
2:B:185:ASN:HD22	2:B:186:GLY:N	0.43	2.12	6	1
1:A:71:LEU:HD22	2:B:117:SER:O	0.43	2.13	3	1
1:A:42:ARG:NE	1:A:43:LEU:O	0.43	2.51	6	1
1:A:36:ILE:HG22	1:A:40:GLN:HE22	0.43	1.73	9	1
2:B:80:ILE:O	2:B:83:ASP:CG	0.43	2.62	20	1
2:B:35:PHE:CZ	2:B:36:ARG:NH2	0.43	2.87	4	1
2:B:173:GLN:O	2:B:173:GLN:NE2	0.43	2.52	5	1
2:B:178:VAL:O	2:B:178:VAL:HG22	0.43	2.14	6	5
2:B:161:PHE:CE2	2:B:165:HIS:NE2	0.43	2.86	11	1
2:B:101:GLN:OE1	2:B:101:GLN:O	0.43	2.36	13	2
2:B:94:GLN:CD	2:B:94:GLN:O	0.43	2.62	17	1
2:B:99:HIS:CD2	2:B:99:HIS:O	0.43	2.71	18	1
1:A:32:ASP:O	1:A:32:ASP:OD2	0.43	2.37	8	4
1:A:34:GLU:OE1	1:A:34:GLU:C	0.43	2.61	3	2
1:A:6:LYS:NZ	1:A:66:THR:HG21	0.43	2.29	6	1
2:B:56:ALA:O	2:B:57:ASP:OD2	0.43	2.36	6	1
2:B:57:ASP:OD2	2:B:57:ASP:C	0.43	2.60	6	2
2:B:185:ASN:C	2:B:186:GLY:O	0.43	2.62	12	2
1:A:45:PHE:CD1	1:A:59:TYR:CE1	0.43	3.07	19	1
2:B:40:PHE:CD2	2:B:41:TYR:N	0.43	2.87	2	2
2:B:127:ARG:O	2:B:131:LEU:HD13	0.43	2.14	13	4
2:B:73:GLN:CD	2:B:73:GLN:N	0.43	2.77	3	1
1:A:13:ILE:HD13	1:A:34:GLU:CD	0.42	2.39	4	2
2:B:108:TYR:O	2:B:112:THR:CG2	0.42	2.67	7	2
2:B:139:ALA:O	2:B:142:VAL:HG23	0.42	2.14	6	1
1:A:61:ILE:HD12	1:A:61:ILE:O	0.42	2.14	7	1
1:A:16:GLU:N	1:A:16:GLU:OE1	0.42	2.52	19	3
2:B:65:LEU:C	2:B:66:GLN:OE1	0.42	2.62	11	1
2:B:108:TYR:CZ	2:B:109:GLU:OE2	0.42	2.72	19	1
2:B:158:VAL:HG22	2:B:162:MET:SD	0.42	2.54	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:83:ASP:OD1	2:B:83:ASP:N	0.42	2.45	20	1
2:B:183:LEU:CD2	2:B:184:GLY:H	0.42	2.26	4	3
1:A:42:ARG:NH2	1:A:72:ARG:NH2	0.42	2.67	13	1
1:A:42:ARG:CZ	1:A:49:GLN:HE21	0.42	2.28	15	1
2:B:57:ASP:OD1	2:B:59:GLU:CD	0.42	2.62	10	1
1:A:43:LEU:HD22	1:A:43:LEU:N	0.42	2.10	12	1
1:A:17:VAL:CG2	1:A:21:ASP:OD2	0.42	2.67	13	1
2:B:26:GLN:CD	2:B:26:GLN:C	0.42	2.87	13	1
1:A:34:GLU:C	1:A:34:GLU:OE2	0.42	2.63	16	1
1:A:47:GLY:N	2:B:88:ARG:NH2	0.42	2.67	16	1
2:B:35:PHE:O	2:B:39:VAL:HG22	0.42	2.14	19	1
2:B:124:ASN:OD1	2:B:125:TRP:CZ3	0.42	2.72	4	1
2:B:30:ASP:OD2	2:B:71:MET:SD	0.42	2.77	5	1
1:A:42:ARG:NH1	2:B:92:GLU:O	0.42	2.53	9	1
1:A:23:ILE:C	1:A:23:ILE:CD1	0.42	2.92	19	1
2:B:29:GLN:C	2:B:29:GLN:OE1	0.42	2.63	3	1
2:B:43:HIS:ND1	2:B:43:HIS:N	0.42	2.66	4	1
2:B:149:GLY:O	2:B:153:GLN:OE1	0.42	2.37	5	1
2:B:58:PRO:O	2:B:59:GLU:CD	0.42	2.62	7	2
1:A:18:GLU:O	1:A:21:ASP:OD1	0.42	2.38	9	1
1:A:50:LEU:HD13	1:A:51:GLU:N	0.42	2.28	11	1
1:A:40:GLN:O	1:A:40:GLN:HG2	0.42	2.13	3	1
2:B:100:LEU:C	2:B:100:LEU:HD23	0.42	2.39	3	2
1:A:72:ARG:HH22	2:B:96:MET:HE2	0.42	1.74	4	1
2:B:34:VAL:O	2:B:34:VAL:CG1	0.42	2.67	9	2
1:A:68:HIS:HD1	1:A:69:LEU:N	0.42	2.13	8	1
1:A:8:LEU:CD1	1:A:68:HIS:NE2	0.42	2.83	15	1
1:A:3:ILE:HD11	1:A:17:VAL:CG2	0.42	2.45	16	1
2:B:38:TYR:CE2	2:B:132:LEU:HD12	0.42	2.49	19	1
2:B:47:GLN:CD	2:B:47:GLN:C	0.42	2.87	6	3
2:B:166:CYS:SG	2:B:170:TRP:CZ3	0.42	3.02	6	1
1:A:61:ILE:O	1:A:61:ILE:CG1	0.42	2.68	7	1
2:B:144:GLN:CD	2:B:144:GLN:C	0.42	2.87	8	1
1:A:14:THR:O	1:A:15:LEU:HD22	0.42	2.15	13	1
2:B:108:TYR:CZ	2:B:112:THR:OG1	0.42	2.72	16	1
2:B:86:ASN:O	2:B:90:ASP:OD1	0.42	2.38	20	1
1:A:24:GLU:CD	1:A:24:GLU:C	0.42	2.88	1	2
2:B:182:ASN:O	2:B:182:ASN:CG	0.42	2.63	8	2
2:B:173:GLN:O	2:B:173:GLN:CD	0.42	2.63	5	2
1:A:31:GLN:CD	1:A:31:GLN:C	0.42	2.88	16	2
2:B:52:VAL:O	2:B:53:ALA:C	0.42	2.61	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:106:ASN:OD1	2:B:106:ASN:C	0.42	2.62	18	3
1:A:42:ARG:NH1	1:A:72:ARG:HH11	0.42	2.12	8	1
2:B:80:ILE:O	2:B:83:ASP:OD1	0.42	2.38	20	1
1:A:6:LYS:NZ	1:A:66:THR:CG2	0.42	2.83	6	1
2:B:111:PHE:CD1	2:B:111:PHE:C	0.42	2.97	6	1
2:B:107:ALA:O	2:B:111:PHE:CG	0.42	2.73	8	1
1:A:54:ARG:NH1	1:A:58:ASP:OD1	0.42	2.53	9	2
1:A:60:ASN:OD1	1:A:60:ASN:O	0.42	2.37	13	1
2:B:36:ARG:NH1	2:B:155:THR:OG1	0.42	2.53	13	1
2:B:153:GLN:O	2:B:157:PHE:CD1	0.42	2.72	16	1
2:B:158:VAL:O	2:B:159:VAL:C	0.41	2.61	5	4
1:A:71:LEU:CD2	2:B:117:SER:O	0.41	2.68	3	1
2:B:46:GLU:O	2:B:46:GLU:CD	0.41	2.63	3	1
1:A:1:MET:SD	1:A:63:LYS:HB3	0.41	2.54	9	1
2:B:25:GLU:CD	2:B:25:GLU:C	0.41	2.87	10	1
2:B:65:LEU:HD13	2:B:66:GLN:C	0.41	2.40	1	1
2:B:109:GLU:N	2:B:109:GLU:CD	0.41	2.78	4	1
2:B:76:ARG:HG3	2:B:77:GLN:N	0.41	2.29	6	1
1:A:3:ILE:CG2	1:A:67:LEU:HD21	0.41	2.45	7	1
1:A:49:GLN:O	1:A:49:GLN:OE1	0.41	2.38	8	1
1:A:4:PHE:CD1	1:A:4:PHE:O	0.41	2.73	11	1
2:B:33:GLU:OE2	2:B:71:MET:SD	0.41	2.78	12	1
1:A:62:GLN:OE1	1:A:62:GLN:N	0.41	2.52	3	1
1:A:61:ILE:HG22	1:A:61:ILE:O	0.41	2.15	11	1
2:B:150:PHE:CD1	2:B:151:LEU:N	0.41	2.88	11	1
2:B:34:VAL:O	2:B:34:VAL:CG2	0.41	2.68	7	1
2:B:89:TYR:C	2:B:92:GLU:OE1	0.41	2.63	11	1
2:B:124:ASN:HD21	2:B:127:ARG:CG	0.41	2.29	13	1
2:B:32:GLU:CD	2:B:32:GLU:C	0.41	2.88	9	2
2:B:101:GLN:O	2:B:101:GLN:CD	0.41	2.64	3	1
2:B:66:GLN:NE2	2:B:71:MET:SD	0.41	2.94	7	1
2:B:73:GLN:CD	2:B:73:GLN:O	0.41	2.63	15	1
1:A:41:GLN:NE2	1:A:43:LEU:H	0.41	2.13	16	1
2:B:59:GLU:CD	2:B:60:MET:H	0.41	2.24	1	1
1:A:27:LYS:CG	1:A:28:ALA:N	0.41	2.83	2	1
1:A:31:GLN:HA	1:A:35:GLY:H	0.41	1.76	5	1
2:B:26:GLN:CD	2:B:26:GLN:N	0.41	2.79	20	2
1:A:52:ASP:C	1:A:52:ASP:OD2	0.41	2.62	17	2
1:A:42:ARG:CD	1:A:49:GLN:NE2	0.41	2.84	11	1
2:B:160:ASP:CG	2:B:164:HIS:CD2	0.41	2.98	12	1
2:B:132:LEU:CD2	2:B:132:LEU:C	0.41	2.94	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:134:PHE:CZ	2:B:138:LEU:HD11	0.41	2.50	1	1
1:A:21:ASP:O	1:A:56:LEU:HG	0.41	2.16	5	1
2:B:139:ALA:O	2:B:142:VAL:CG2	0.41	2.68	6	1
2:B:66:GLN:O	2:B:66:GLN:CD	0.41	2.63	7	1
1:A:42:ARG:NE	1:A:49:GLN:NE2	0.41	2.69	11	1
2:B:105:GLU:OE2	2:B:105:GLU:N	0.41	2.53	11	1
1:A:7:THR:HG23	1:A:9:THR:H	0.41	1.75	17	2
2:B:103:THR:OG1	2:B:106:ASN:CG	0.41	2.64	20	1
1:A:41:GLN:CD	1:A:41:GLN:C	0.41	2.88	2	1
1:A:43:LEU:HD12	1:A:43:LEU:N	0.41	2.30	5	1
1:A:67:LEU:N	1:A:67:LEU:HD13	0.41	2.30	7	1
2:B:42:ARG:NH2	2:B:82:GLY:O	0.41	2.52	7	1
2:B:120:GLU:O	2:B:120:GLU:CD	0.41	2.63	7	1
1:A:43:LEU:CB	1:A:50:LEU:HD21	0.41	2.45	8	1
2:B:120:GLU:C	2:B:120:GLU:CD	0.41	2.89	10	1
1:A:1:MET:SD	1:A:63:LYS:HA	0.41	2.55	19	1
2:B:115:ALA:O	2:B:116:THR:C	0.41	2.62	6	2
2:B:136:TYR:O	2:B:138:LEU:N	0.41	2.54	6	2
1:A:4:PHE:CE1	1:A:14:THR:HG22	0.41	2.50	10	1
1:A:52:ASP:OD2	1:A:52:ASP:C	0.41	2.63	11	1
2:B:139:ALA:O	2:B:143:TYR:CD2	0.41	2.74	12	1
2:B:119:PHE:N	2:B:119:PHE:CD2	0.41	2.88	15	1
2:B:118:LEU:CD2	2:B:127:ARG:NH1	0.41	2.84	16	1
2:B:89:TYR:C	2:B:92:GLU:OE2	0.41	2.64	1	1
2:B:101:GLN:CD	2:B:101:GLN:C	0.41	2.89	3	1
2:B:33:GLU:OE1	2:B:71:MET:SD	0.41	2.79	5	1
2:B:61:VAL:O	2:B:61:VAL:HG12	0.41	2.16	5	2
1:A:70:VAL:HG12	1:A:71:LEU:N	0.41	2.31	6	1
2:B:131:LEU:HD12	2:B:134:PHE:CE1	0.41	2.51	7	1
2:B:96:MET:SD	2:B:96:MET:C	0.41	3.03	10	1
2:B:100:LEU:CD2	2:B:110:TYR:CE1	0.41	3.04	15	1
2:B:140:LEU:HD12	2:B:143:TYR:CD1	0.40	2.50	12	1
2:B:100:LEU:HD21	2:B:110:TYR:CE1	0.40	2.51	15	1
1:A:34:GLU:OE2	1:A:34:GLU:O	0.40	2.39	16	1
1:A:48:LYS:C	2:B:92:GLU:OE1	0.40	2.64	18	1
2:B:77:GLN:NE2	2:B:186:GLY:CA	0.40	2.85	4	1
2:B:181:LEU:HD12	2:B:186:GLY:O	0.40	2.15	5	1
2:B:106:ASN:CG	2:B:109:GLU:OE1	0.40	2.63	6	1
1:A:70:VAL:O	1:A:71:LEU:HD12	0.40	2.15	10	1
1:A:5:VAL:HG22	1:A:13:ILE:O	0.40	2.17	15	1
2:B:133:GLY:O	2:B:136:TYR:CD2	0.40	2.74	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:32:GLU:OE1	2:B:36:ARG:CD	0.40	2.69	19	1
2:B:151:LEU:CD2	2:B:152:GLY:N	0.40	2.67	7	1
1:A:66:THR:O	1:A:66:THR:HG23	0.40	2.17	11	1
2:B:123:ILE:O	2:B:123:ILE:HG23	0.40	2.16	20	1
2:B:178:VAL:O	2:B:178:VAL:HG12	0.40	2.16	1	1
1:A:8:LEU:N	1:A:8:LEU:HD12	0.40	2.31	2	1
1:A:31:GLN:NE2	1:A:38:PRO:CG	0.40	2.85	4	1
2:B:24:GLU:OE2	2:B:24:GLU:N	0.40	2.50	5	1
2:B:125:TRP:O	2:B:128:VAL:HG22	0.40	2.16	5	1
2:B:142:VAL:HG11	2:B:150:PHE:CG	0.40	2.52	5	1
2:B:185:ASN:O	2:B:186:GLY:C	0.40	2.63	5	2
1:A:22:THR:OG1	1:A:25:ASN:OD1	0.40	2.37	9	1
2:B:93:PHE:CE1	2:B:134:PHE:CD1	0.40	3.09	11	1
2:B:162:MET:SD	2:B:162:MET:C	0.40	3.04	16	1
2:B:39:VAL:HG11	2:B:136:TYR:CD1	0.40	2.52	19	1
1:A:2:GLN:C	1:A:3:ILE:HD12	0.40	2.41	20	1
2:B:83:ASP:OD2	2:B:84:ASP:N	0.40	2.52	7	1
2:B:77:GLN:CG	2:B:186:GLY:O	0.40	2.69	12	1
2:B:113:CYS:O	2:B:117:SER:OG	0.40	2.37	14	1
2:B:112:THR:O	2:B:116:THR:HG23	0.40	2.17	15	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/76 (93%)	63±1 (89±1%)	6±1 (9±1%)	1±0 (1±0%)	11	57
2	B	167/169 (99%)	145±3 (87±2%)	20±2 (12±1%)	2±0 (1±0%)	14	63
All	All	4760/4900 (97%)	4173 (88%)	528 (11%)	59 (1%)	13	61

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	70	VAL	20

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Mol	Chain	Res	Type	Models (Total)
2	B	184	GLY	20
2	B	156	ARG	18
1	A	60	ASN	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/69 (96%)	58±3 (88±4%)	8±3 (12±4%)	7	48
2	B	137/137 (100%)	122±4 (89±3%)	15±4 (11±3%)	8	51
All	All	4060/4120 (99%)	3593 (88%)	467 (12%)	8	50

All 111 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)
2	B	57	ASP	20
1	A	71	LEU	16
2	B	65	LEU	16
2	B	119	PHE	15
2	B	183	LEU	15
2	B	21	SER	15
1	A	70	VAL	14
2	B	93	PHE	11
2	B	154	VAL	11
2	B	134	PHE	11
1	A	23	ILE	10
2	B	43	HIS	10
1	A	15	LEU	10
1	A	26	VAL	9
1	A	9	THR	9
2	B	118	LEU	9
2	B	63	LEU	8
2	B	142	VAL	8
1	A	44	ILE	8
1	A	3	ILE	7
1	A	67	LEU	7

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Mol	Chain	Res	Type	Models (Total)
2	B	36	ARG	7
2	B	157	PHE	7
2	B	71	MET	7
2	B	127	ARG	6
1	A	27	LYS	6
1	A	50	LEU	6
2	B	97	LEU	6
1	A	60	ASN	6
1	A	61	ILE	5
2	B	177	TRP	5
2	B	39	VAL	5
2	B	116	THR	4
2	B	131	LEU	4
1	A	17	VAL	4
1	A	45	PHE	4
1	A	43	LEU	4
2	B	123	ILE	4
2	B	136	TYR	4
2	B	178	VAL	4
1	A	8	LEU	4
2	B	61	VAL	4
2	B	147	LEU	4
1	A	40	GLN	4
2	B	145	HIS	4
2	B	78	LEU	3
2	B	156	ARG	3
1	A	1	MET	3
2	B	162	MET	3
2	B	19	LEU	3
1	A	4	PHE	3
2	B	132	LEU	3
2	B	151	LEU	3
2	B	163	LEU	3
1	A	41	GLN	3
2	B	85	ILE	3
2	B	137	ARG	3
2	B	80	ILE	3
2	B	31	THR	3
2	B	35	PHE	2
2	B	121	SER	2
2	B	128	VAL	2
1	A	49	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	63	LYS	2
1	A	72	ARG	2
1	A	5	VAL	2
2	B	140	LEU	2
1	A	56	LEU	2
2	B	110	TYR	2
2	B	77	GLN	2
1	A	36	ILE	2
2	B	92	GLU	2
1	A	12	THR	2
2	B	106	ASN	2
2	B	87	ARG	2
2	B	26	GLN	1
2	B	59	GLU	1
1	A	34	GLU	1
2	B	29	GLN	1
1	A	66	THR	1
2	B	32	GLU	1
1	A	11	LYS	1
2	B	38	TYR	1
2	B	76	ARG	1
2	B	166	CYS	1
2	B	185	ASN	1
2	B	66	GLN	1
2	B	34	VAL	1
2	B	46	GLU	1
2	B	113	CYS	1
2	B	124	ASN	1
1	A	30	ILE	1
1	A	64	GLU	1
2	B	30	ASP	1
2	B	167	ILE	1
2	B	143	TYR	1
2	B	174	ARG	1
2	B	138	LEU	1
2	B	125	TRP	1
2	B	153	GLN	1
2	B	181	LEU	1
1	A	31	GLN	1
2	B	37	SER	1
2	B	89	TYR	1
2	B	173	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	59	TYR	1
2	B	155	THR	1
2	B	171	ILE	1
1	A	7	THR	1
2	B	109	GLU	1
2	B	165	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no 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 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *wk11_CS*

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	256
Number of shifts mapped to atoms	256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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	128	1.15 ± 0.16	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 254 atoms were assigned a chemical shift out of a possible 3317. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	254/1206 (21%)	127/492 (26%)	0/482 (0%)	127/232 (55%)
Sidechain	0/1837 (0%)	0/1196 (0%)	0/568 (0%)	0/73 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/274 (0%)	0/133 (0%)	0/124 (0%)	0/17 (0%)
Overall	254/3317 (8%)	127/1821 (7%)	0/1174 (0%)	127/322 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 256 atoms were assigned a chemical shift out of a possible 3372. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	256/1227 (21%)	128/501 (26%)	0/490 (0%)	128/236 (54%)
Sidechain	0/1871 (0%)	0/1218 (0%)	0/577 (0%)	0/76 (0%)
Aromatic	0/274 (0%)	0/133 (0%)	0/124 (0%)	0/17 (0%)
Overall	256/3372 (8%)	128/1852 (7%)	0/1191 (0%)	128/329 (39%)

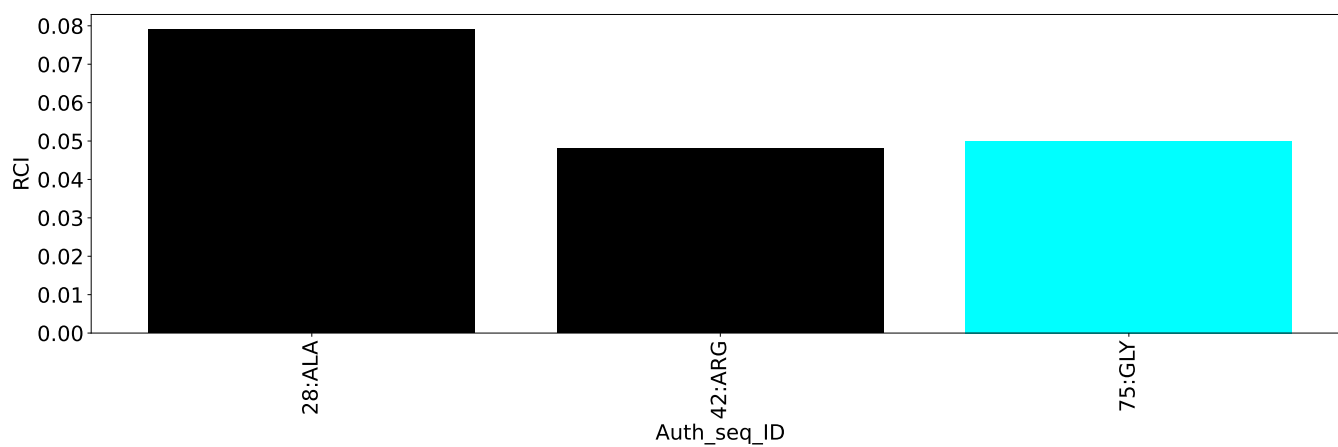
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

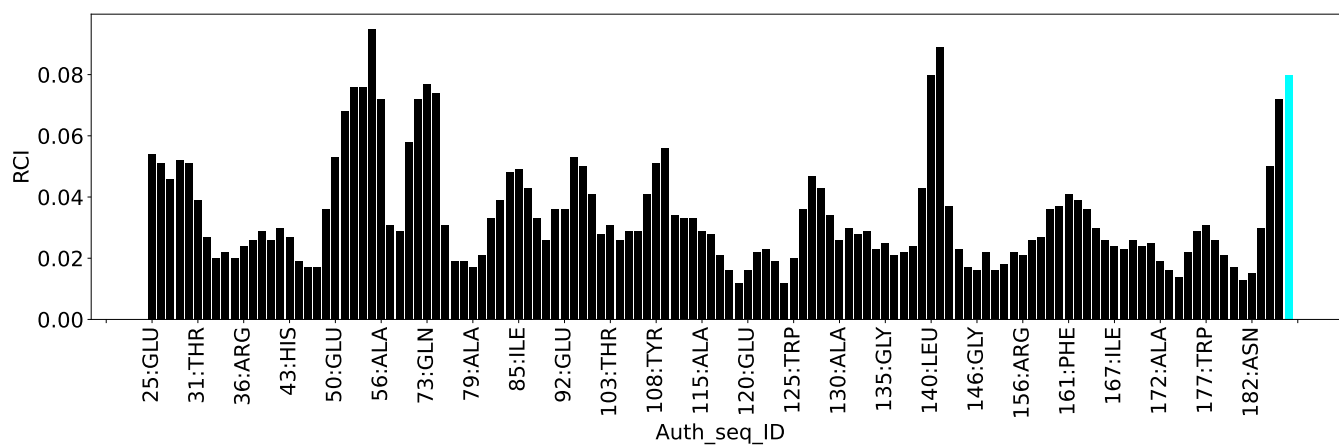
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



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	14
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	14
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)	1.4	0.2
0.2-0.5 (Medium)	3.6	0.5
>0.5 (Large)	4.2	1.68

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 ⓘ

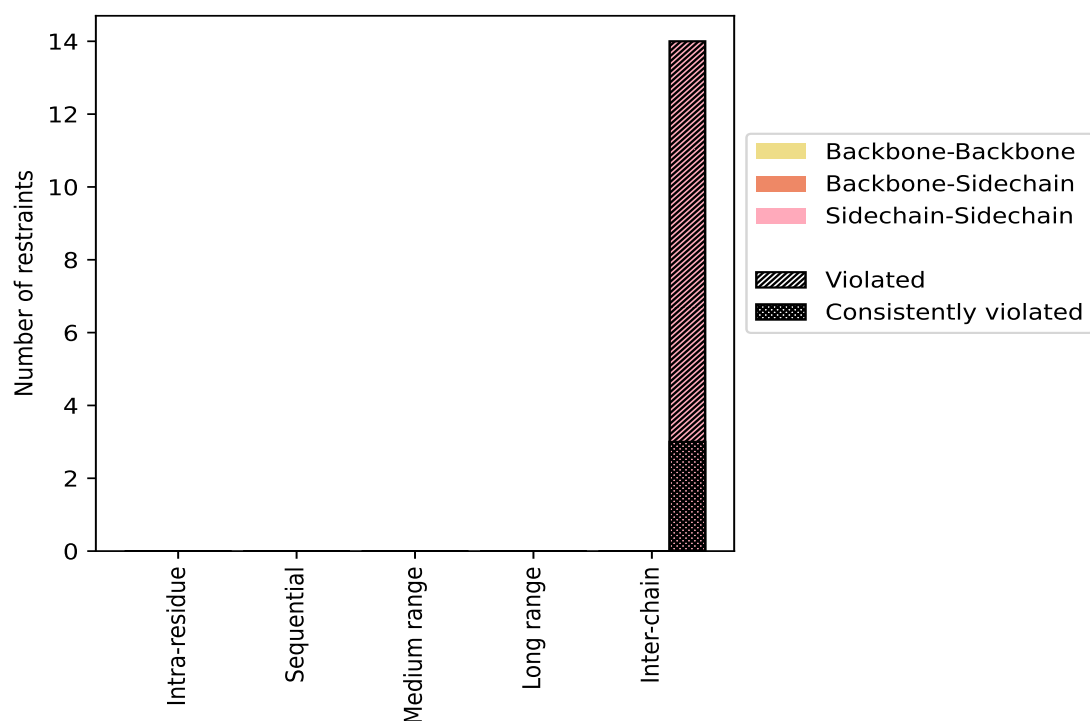
9.1 Summary of distance violations ⓘ

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	14	100.0	14	100.0	100.0	3	21.4	21.4
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	14	100.0	14	100.0	100.0	3	21.4	21.4
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	14	100.0	14	100.0	100.0	3	21.4	21.4
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	14	100.0	14	100.0	100.0	3	21.4	21.4

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	8	8	0.56	1.15	0.33	0.43
2	0	0	0	0	10	10	0.48	1.12	0.31	0.4
3	0	0	0	0	7	7	0.58	1.1	0.36	0.5
4	0	0	0	0	10	10	0.6	1.19	0.37	0.5
5	0	0	0	0	10	10	0.58	1.68	0.5	0.4
6	0	0	0	0	8	8	0.65	1.15	0.32	0.57
7	0	0	0	0	12	12	0.59	1.55	0.44	0.48
8	0	0	0	0	8	8	0.68	1.29	0.42	0.74
9	0	0	0	0	10	10	0.56	1.02	0.28	0.44
10	0	0	0	0	9	9	0.58	1.27	0.33	0.47

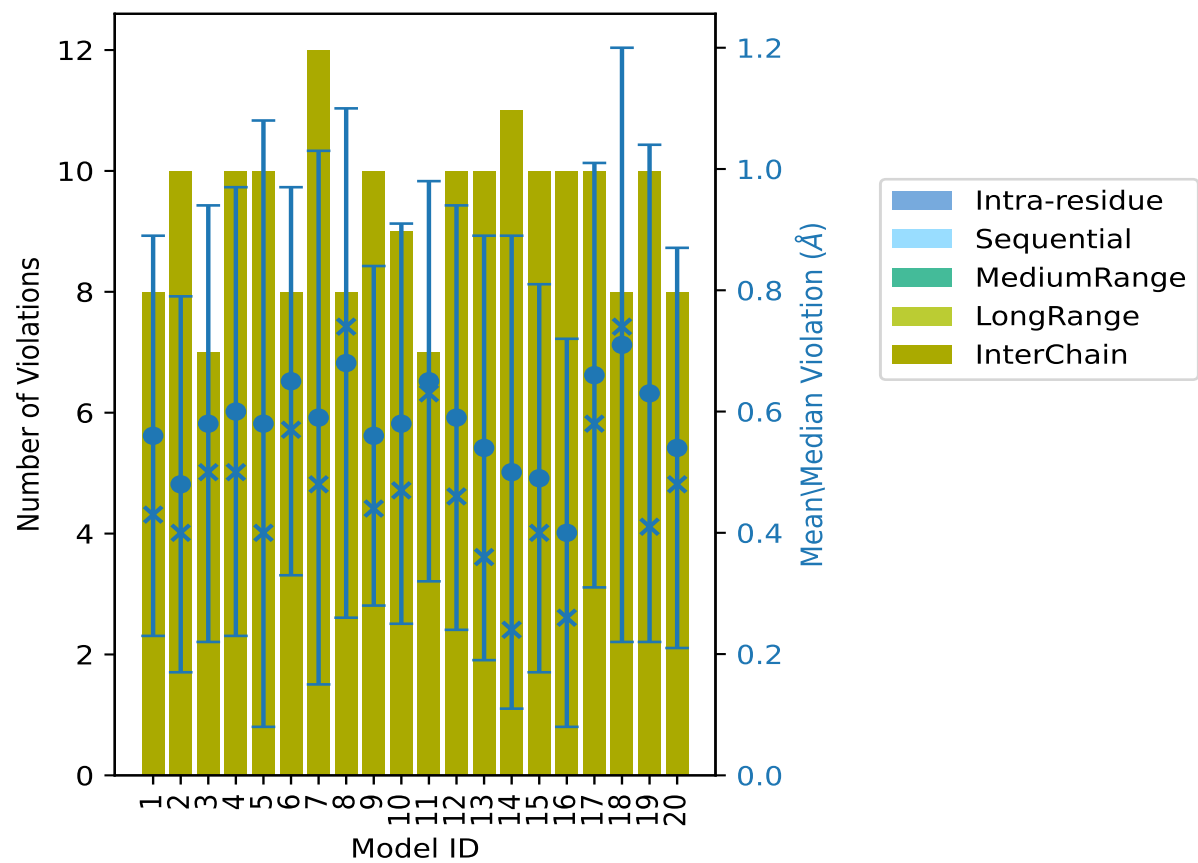
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	7	7	0.65	1.22	0.33	0.63
12	0	0	0	0	10	10	0.59	1.17	0.35	0.46
13	0	0	0	0	10	10	0.54	1.09	0.35	0.36
14	0	0	0	0	11	11	0.5	1.16	0.39	0.24
15	0	0	0	0	10	10	0.49	1.2	0.32	0.4
16	0	0	0	0	10	10	0.4	1.05	0.32	0.26
17	0	0	0	0	10	10	0.66	1.2	0.35	0.58
18	0	0	0	0	8	8	0.71	1.47	0.49	0.74
19	0	0	0	0	10	10	0.63	1.2	0.41	0.41
20	0	0	0	0	8	8	0.54	1.12	0.33	0.48

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

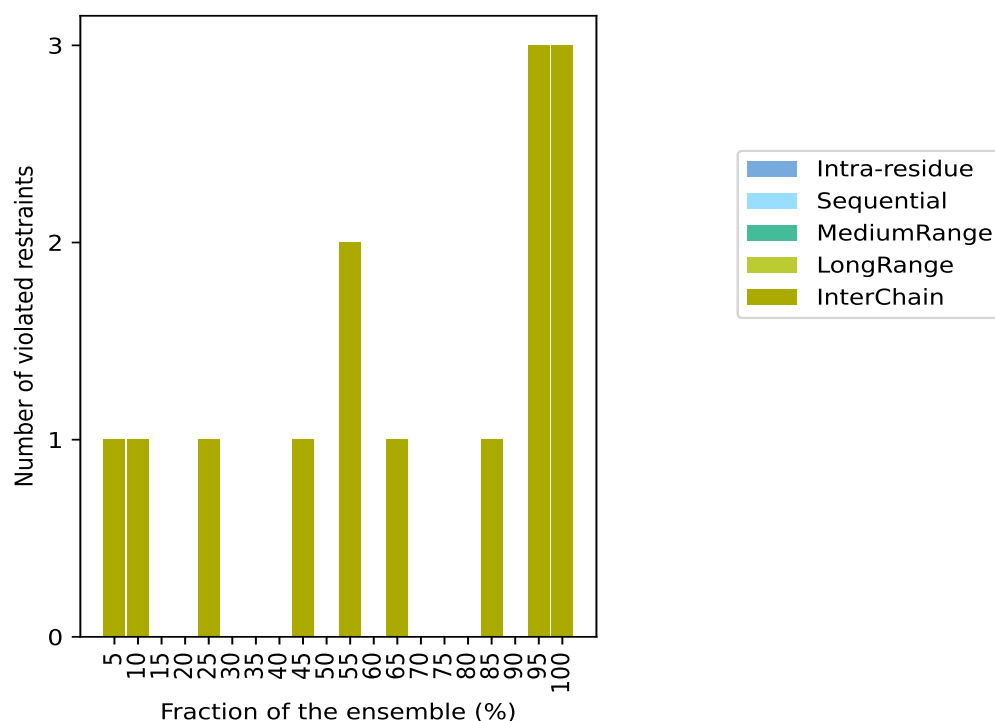
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 0(IR:0, SQ:0, MR:0, LR:0, IC:0) restraints are not violated 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	1	1	1	5.0
0	0	0	0	1	1	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	1	1	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	0	0	8	40.0
0	0	0	0	1	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	2	2	11	55.0
0	0	0	0	0	0	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	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	1	1	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	3	3	20	100.0

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

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

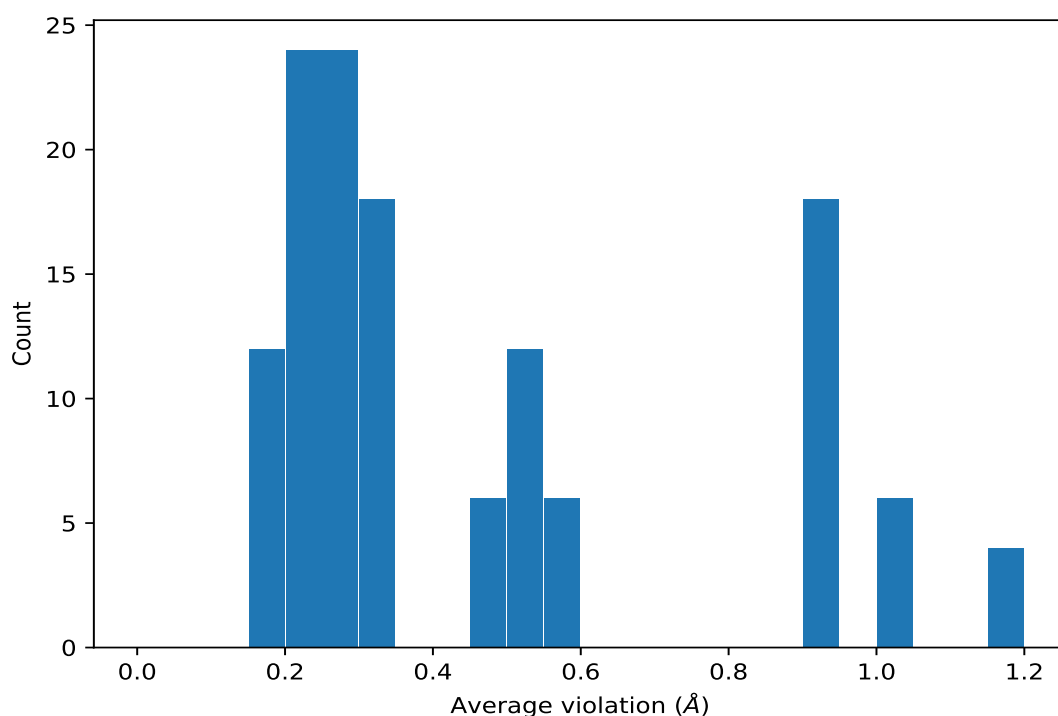
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	20	1.15	0.08	1.15
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	20	1.15	0.08	1.15
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	20	1.15	0.08	1.15
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	20	1.15	0.08	1.15
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	20	1.03	0.11	1.04
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	20	0.34	0.1	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	20	0.34	0.1	0.36
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	19	0.91	0.41	0.93
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	19	0.53	0.1	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	19	0.24	0.09	0.25
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	17	0.56	0.24	0.48
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	13	0.25	0.06	0.27

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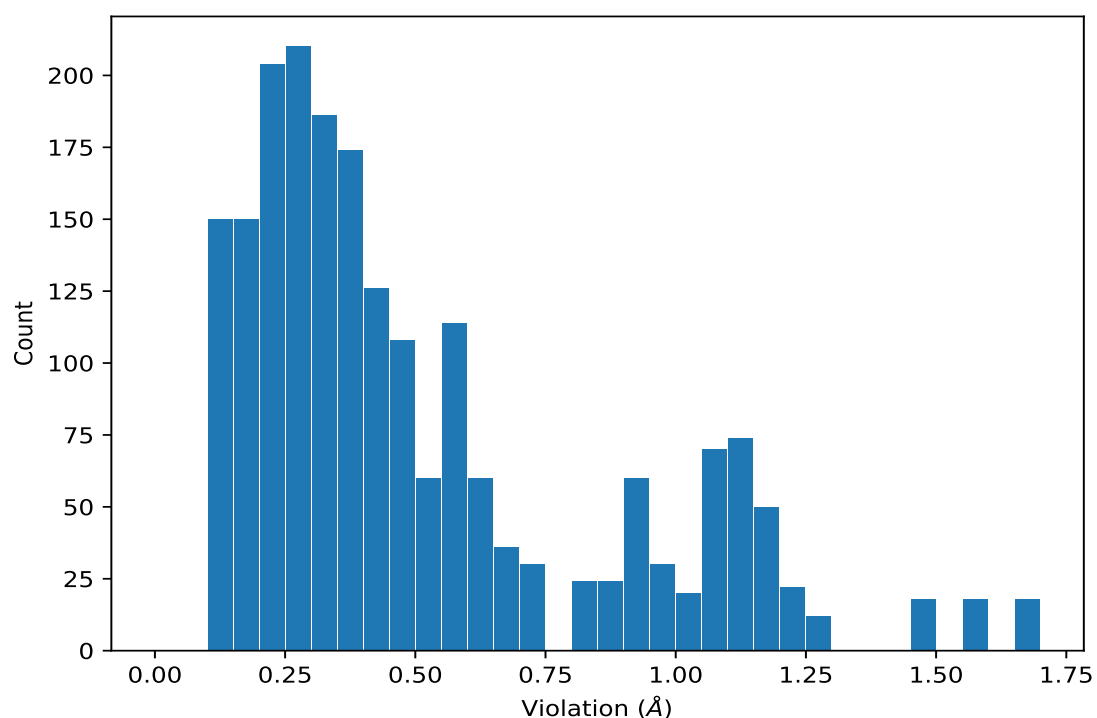
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	11	0.49	0.15	0.55
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	11	0.22	0.05	0.22
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	11	0.22	0.05	0.22
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	11	0.22	0.05	0.22
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	11	0.22	0.05	0.22
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	11	0.22	0.05	0.22
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	11	0.22	0.05	0.22
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	9	0.29	0.13	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	9	0.29	0.13	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	9	0.29	0.13	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	9	0.29	0.13	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	9	0.29	0.13	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	9	0.29	0.13	0.21
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD2	5	0.19	0.09	0.13
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD3	5	0.19	0.09	0.13
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD2	5	0.19	0.09	0.13
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD3	5	0.19	0.09	0.13
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD2	5	0.19	0.09	0.13
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD3	5	0.19	0.09	0.13
(1,3)	2:96:B:MET:HE1	1:42:A:ARG:HD2	2	0.17	0.06	0.17
(1,3)	2:96:B:MET:HE1	1:42:A:ARG:HD3	2	0.17	0.06	0.17
(1,3)	2:96:B:MET:HE2	1:42:A:ARG:HD2	2	0.17	0.06	0.17
(1,3)	2:96:B:MET:HE2	1:42:A:ARG:HD3	2	0.17	0.06	0.17
(1,3)	2:96:B:MET:HE3	1:42:A:ARG:HD2	2	0.17	0.06	0.17
(1,3)	2:96:B:MET:HE3	1:42:A:ARG:HD3	2	0.17	0.06	0.17

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)
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	5	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	18	1.47
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	8	1.29
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	8	1.29
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	8	1.29
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	8	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	10	1.27
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	10	1.27
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	10	1.27
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	10	1.27
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	18	1.26
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	18	1.26
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	18	1.26
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	18	1.26
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	5	1.23
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	5	1.23
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	5	1.23
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	5	1.23
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	11	1.22
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	11	1.22
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	11	1.22
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	11	1.22
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	15	1.2
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	15	1.2
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	15	1.2
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	15	1.2
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	17	1.2
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	17	1.2
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	17	1.2
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	17	1.2
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	19	1.2
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	19	1.2
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	19	1.2
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	19	1.2
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	19	1.2
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	19	1.2
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	4	1.19
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	4	1.19
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	4	1.19
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	4	1.19
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	7	1.19
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	7	1.19
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	7	1.19
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	7	1.19
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	12	1.17
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	12	1.17
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	12	1.17
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	12	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	12	1.17
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	12	1.17
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	19	1.17
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	19	1.17
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	19	1.17
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	19	1.17
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	19	1.17
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	19	1.17
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	19	1.17
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	19	1.17
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	19	1.17
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	19	1.17
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	19	1.17
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	19	1.17
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	19	1.17
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	19	1.17
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	19	1.17
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	19	1.17
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	19	1.17
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	19	1.17
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	14	1.16
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	14	1.16
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	14	1.16
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	14	1.16
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	1	1.15
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	1	1.15
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	1	1.15
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	1	1.15
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	6	1.15
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	6	1.15
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	6	1.15
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	6	1.15
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	17	1.15
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	17	1.15
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	17	1.15
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	17	1.15
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	17	1.15
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	17	1.15
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	4	1.14
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	4	1.14
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	4	1.14
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	4	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	4	1.14
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	4	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	8	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	8	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	8	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	8	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	8	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	8	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	8	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	8	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	8	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	8	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	8	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	8	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	8	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	8	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	8	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	8	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	8	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	8	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	17	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	17	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	17	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	17	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	17	1.14
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	17	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	17	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	17	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	17	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	17	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	17	1.14
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	17	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	17	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	17	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	17	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	17	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	17	1.14
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	17	1.14
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	6	1.13
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	6	1.13
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	6	1.13
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	6	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	6	1.13
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	6	1.13
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	2	1.12
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	2	1.12
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	2	1.12
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	2	1.12
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	20	1.12
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	20	1.12
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	20	1.12
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	20	1.12
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	20	1.12
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	20	1.12
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	3	1.1
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	3	1.1
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	3	1.1
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	3	1.1
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	3	1.1
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	3	1.1
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	3	1.1
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	3	1.1
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	3	1.1
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	3	1.1
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	14	1.1
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	14	1.1
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	14	1.1
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	14	1.1
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	14	1.1
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	14	1.1
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	13	1.09
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	13	1.09
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	13	1.09
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	13	1.09
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	13	1.09
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	13	1.09
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	19	1.09
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	19	1.09
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	19	1.09
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	19	1.09
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	19	1.09
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	19	1.09
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	12	1.07
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	12	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	12	1.07
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	12	1.07
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	13	1.07
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	13	1.07
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	13	1.07
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	13	1.07
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	19	1.06
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	19	1.06
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	19	1.06
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	19	1.06
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	12	1.06
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	12	1.06
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	12	1.06
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	12	1.06
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	12	1.06
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	12	1.06
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	12	1.06
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	12	1.06
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	12	1.06
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	12	1.06
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	12	1.06
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	12	1.06
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	12	1.06
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	12	1.06
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	12	1.06
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	12	1.06
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	12	1.06
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	12	1.06
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	16	1.05
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	16	1.05
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	16	1.05
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	16	1.05
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	10	1.05
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	10	1.05
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	10	1.05
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	10	1.05
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	10	1.05
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	10	1.05
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	13	1.05
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	13	1.05
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	13	1.05
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	13	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	13	1.05
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	13	1.05
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	13	1.05
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	13	1.05
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	13	1.05
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	13	1.05
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	13	1.05
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	13	1.05
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	13	1.05
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	13	1.05
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	13	1.05
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	13	1.05
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	13	1.05
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	13	1.05
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	9	1.02
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	9	1.02
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	9	1.02
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	9	1.02
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	20	1.02
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	20	1.02
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	20	1.02
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	20	1.02
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	18	1.02
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	18	1.02
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	18	1.02
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	18	1.02
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	18	1.02
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	18	1.02
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	11	1.0
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	11	1.0
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	11	1.0
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	11	1.0
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	11	1.0
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	11	1.0
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	1	0.99
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	1	0.99
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	1	0.99
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	1	0.99
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	1	0.99
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	1	0.99
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	4	0.99
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	4	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	4	0.99
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	4	0.99
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	4	0.99
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	4	0.99
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	4	0.99
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	4	0.99
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	4	0.99
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	4	0.99
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	4	0.99
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	4	0.99
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	4	0.99
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	4	0.99
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	4	0.99
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	4	0.99
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	4	0.99
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	4	0.99
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	9	0.97
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	9	0.97
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	9	0.97
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	9	0.97
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	9	0.97
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	9	0.97
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	2	0.94
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	2	0.94
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	2	0.94
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	2	0.94
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	2	0.94
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	2	0.94
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	9	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	9	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	9	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	9	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	9	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	9	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	9	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	9	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	9	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	9	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	9	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	9	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	9	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	9	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	9	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	9	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	9	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	9	0.93
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	8	0.92
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	8	0.92
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	8	0.92
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	8	0.92
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	8	0.92
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	8	0.92
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	7	0.92
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	7	0.92
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	7	0.92
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	7	0.92
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	7	0.92
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	7	0.92
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	14	0.92
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	14	0.92
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	14	0.92
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	14	0.92
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	14	0.92
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	14	0.92
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	14	0.92
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	14	0.92
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	14	0.92
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	14	0.92
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	14	0.92
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	14	0.92
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	14	0.92
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	14	0.92
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	14	0.92
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	14	0.92
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	14	0.92
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	14	0.92
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	16	0.91
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	16	0.91
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	16	0.91
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	16	0.91
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	16	0.91
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	16	0.91
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	15	0.89
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	15	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	15	0.89
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	15	0.89
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	15	0.89
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	15	0.89
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	8	0.89
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	8	0.89
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	8	0.89
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	8	0.89
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	8	0.89
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	8	0.89
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	7	0.87
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	7	0.87
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	7	0.87
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	7	0.87
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	7	0.87
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	7	0.87
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	5	0.86
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	5	0.86
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	5	0.86
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	5	0.86
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	5	0.86
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	5	0.86
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	18	0.84
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	18	0.84
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	18	0.84
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	18	0.84
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	18	0.84
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	18	0.84
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	6	0.81
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	6	0.81
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	6	0.81
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	6	0.81
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	6	0.81
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	6	0.81
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	6	0.81
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	6	0.81
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	6	0.81
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	6	0.81
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	6	0.81
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	6	0.81
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	6	0.81
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	6	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	6	0.81
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	6	0.81
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	6	0.81
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	6	0.81
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	11	0.73
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	11	0.73
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	11	0.73
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	11	0.73
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	11	0.73
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	11	0.73
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	11	0.73
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	11	0.73
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	11	0.73
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	11	0.73
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	11	0.73
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	11	0.73
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	11	0.73
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	11	0.73
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	11	0.73
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	11	0.73
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	11	0.73
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	11	0.73
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	14	0.7
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	14	0.7
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	14	0.7
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	14	0.7
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	14	0.7
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	14	0.7
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	14	0.7
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	14	0.7
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	14	0.7
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	14	0.7
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	14	0.7
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	14	0.7
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	10	0.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	10	0.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	10	0.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	10	0.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	10	0.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	10	0.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	10	0.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	10	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	10	0.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	10	0.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	10	0.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	10	0.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	10	0.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	10	0.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	10	0.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	10	0.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	10	0.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	10	0.68
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	17	0.67
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	17	0.67
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	17	0.67
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	17	0.67
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	17	0.67
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	17	0.67
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	1	0.65
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	1	0.65
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	1	0.65
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	1	0.65
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	1	0.65
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	1	0.65
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	1	0.65
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	1	0.65
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	1	0.65
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	1	0.65
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	1	0.65
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	1	0.65
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	7	0.64
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	7	0.64
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	7	0.64
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	7	0.64
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	7	0.64
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	7	0.64
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	3	0.64
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	3	0.64
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	3	0.64
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	3	0.64
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	3	0.64
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	3	0.64
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	3	0.64
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	3	0.64
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	3	0.64
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	3	0.64
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	3	0.64
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	3	0.64
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	3	0.64
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	3	0.64
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	3	0.64
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	3	0.64
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	3	0.64
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	11	0.63
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	11	0.63
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	11	0.63
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	11	0.63
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	11	0.63
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	11	0.63
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	11	0.63
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	11	0.63
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	11	0.63
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	11	0.63
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	11	0.63
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	11	0.63
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	18	0.63
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	18	0.63
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	18	0.63
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	18	0.63
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	18	0.63
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	18	0.63
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	4	0.62
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	4	0.62
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	4	0.62
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	4	0.62
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	4	0.62
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	4	0.62
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	8	0.6
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	8	0.6
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	8	0.6
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	8	0.6
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	8	0.6
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	8	0.6
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	8	0.6
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	8	0.6
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	8	0.6
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	8	0.6
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	8	0.6
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	6	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	6	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	6	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	6	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	6	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	6	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	6	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	6	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	6	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	6	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	6	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	6	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	15	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	15	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	15	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	15	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	15	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	15	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	15	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	15	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	15	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	15	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	15	0.59
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	15	0.59
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	17	0.58
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	17	0.58
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	17	0.58
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	17	0.58
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	17	0.58
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	17	0.58
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	17	0.58
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	17	0.58
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	17	0.58
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	17	0.58
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	17	0.58
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	17	0.58
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	17	0.58
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	17	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	17	0.58
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	17	0.58
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	17	0.58
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	17	0.58
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	2	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	2	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	2	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	2	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	2	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	2	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	2	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	2	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	2	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	2	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	2	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	2	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	4	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	4	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	4	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	4	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	4	0.57
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	4	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	4	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	4	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	4	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	4	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	4	0.57
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	4	0.57
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	20	0.57
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	20	0.57
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	20	0.57
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	20	0.57
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	20	0.57
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	20	0.57
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	14	0.56
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	14	0.56
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	14	0.56
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	14	0.56
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	14	0.56
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	14	0.56
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	15	0.56
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	15	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	15	0.56
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	15	0.56
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	15	0.56
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	15	0.56
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	7	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	7	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	7	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	7	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	7	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	7	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	7	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	7	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	7	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	7	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	7	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	7	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	12	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	12	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	12	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	12	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	12	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	12	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	12	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	12	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	12	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	12	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	12	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	12	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	6	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	6	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	6	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	6	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	6	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	6	0.55
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	9	0.53
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	9	0.53
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	9	0.53
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	9	0.53
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	9	0.53
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	9	0.53
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	2	0.52
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	2	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	2	0.52
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	2	0.52
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	2	0.52
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	2	0.52
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	5	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	5	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	5	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	5	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	5	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	5	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	5	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	5	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	5	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	5	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	5	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	5	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	16	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	16	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	16	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	16	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	16	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	16	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	16	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	16	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	16	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	16	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	16	0.51
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	16	0.51
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	15	0.51
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	15	0.51
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	15	0.51
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	15	0.51
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	15	0.51
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	15	0.51
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	12	0.51
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	12	0.51
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	12	0.51
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	12	0.51
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	12	0.51
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	12	0.51
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	3	0.5
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	3	0.5
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	3	0.5
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	3	0.5
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	3	0.5
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	3	0.5
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	3	0.5
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	3	0.5
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	3	0.5
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	3	0.5
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	3	0.5
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	20	0.49
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	20	0.49
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	20	0.49
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	20	0.49
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	20	0.49
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	20	0.49
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	20	0.49
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	20	0.49
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	20	0.49
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	20	0.49
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	20	0.49
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	20	0.49
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	9	0.49
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	9	0.49
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	9	0.49
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	9	0.49
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	9	0.49
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	9	0.49
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	9	0.49
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	9	0.49
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	9	0.49
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	9	0.49
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	9	0.49
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	9	0.49
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	9	0.49
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	9	0.49
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	9	0.49
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	9	0.49
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	9	0.49
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	9	0.49
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	10	0.48
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	10	0.48
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	10	0.48
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	10	0.48
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	10	0.48
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	10	0.48
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	10	0.48
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	10	0.48
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	10	0.48
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	10	0.48
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	10	0.48
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	10	0.48
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	10	0.48
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	10	0.48
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	10	0.48
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	10	0.48
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	10	0.48
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	16	0.48
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	16	0.48
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	16	0.48
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	16	0.48
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	16	0.48
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	16	0.48
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	10	0.47
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	10	0.47
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	10	0.47
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	10	0.47
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	10	0.47
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	10	0.47
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	10	0.47
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	10	0.47
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	10	0.47
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	10	0.47
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	10	0.47
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	10	0.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	20	0.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	20	0.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	20	0.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	20	0.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	20	0.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	20	0.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	20	0.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	20	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	20	0.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	20	0.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	20	0.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	20	0.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	20	0.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	20	0.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	20	0.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	20	0.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	20	0.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	20	0.47
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	5	0.46
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	5	0.46
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	5	0.46
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	5	0.46
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	5	0.46
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	5	0.46
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	5	0.46
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	5	0.46
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	5	0.46
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	5	0.46
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	5	0.46
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	5	0.46
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	5	0.46
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	5	0.46
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	5	0.46
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	5	0.46
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	5	0.46
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	5	0.46
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	1	0.45
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	1	0.45
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	1	0.45
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	1	0.45
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	1	0.45
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	1	0.45
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	19	0.44
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	19	0.44
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	19	0.44
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	19	0.44
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	19	0.44
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	19	0.44
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	19	0.44
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	19	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	19	0.44
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	19	0.44
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	19	0.44
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	19	0.44
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	13	0.43
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	13	0.43
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	13	0.43
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	13	0.43
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	13	0.43
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	13	0.43
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	4	0.43
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	4	0.43
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	4	0.43
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	4	0.43
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	4	0.43
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	4	0.43
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	12	0.42
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	12	0.42
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	12	0.42
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	12	0.42
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	12	0.42
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	12	0.42
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	6	0.41
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	6	0.41
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	6	0.41
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	6	0.41
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	6	0.41
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	6	0.41
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	6	0.41
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	6	0.41
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	6	0.41
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	6	0.41
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	6	0.41
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	6	0.41
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	6	0.41
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	6	0.41
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	6	0.41
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	6	0.41
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	6	0.41
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	6	0.41
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	2	0.41
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	2	0.41
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	2	0.41
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	2	0.41
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	2	0.41
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	2	0.41
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	2	0.41
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	2	0.41
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	2	0.41
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	2	0.41
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	2	0.41
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	2	0.41
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	2	0.41
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	2	0.41
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	2	0.41
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	2	0.41
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	2	0.41
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	1	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	1	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	1	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	1	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	1	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	1	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	1	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	1	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	1	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	1	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	1	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	1	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	1	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	1	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	1	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	1	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	1	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	1	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	7	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	7	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	7	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	7	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	7	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	7	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	7	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	7	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	7	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	7	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	7	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	7	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	7	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	7	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	7	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	7	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	7	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	12	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	12	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	12	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	12	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	12	0.4
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	12	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	12	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	12	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	12	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	12	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	12	0.4
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	12	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	12	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	12	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	12	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	12	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	12	0.4
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	12	0.4
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	13	0.4
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	13	0.4
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	13	0.4
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	13	0.4
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	13	0.4
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	13	0.4
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	9	0.39
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	9	0.39
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	9	0.39
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	9	0.39
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	9	0.39
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	9	0.39
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	17	0.39
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	17	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	17	0.39
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	17	0.39
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	17	0.39
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	17	0.39
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	17	0.39
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	17	0.39
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	17	0.39
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	17	0.39
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	17	0.39
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	17	0.39
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	17	0.39
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	17	0.39
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	17	0.39
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	17	0.39
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	17	0.39
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	17	0.39
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	2	0.39
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	2	0.39
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	2	0.39
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	2	0.39
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	2	0.39
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	2	0.39
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	10	0.39
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	10	0.39
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	10	0.39
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	10	0.39
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	10	0.39
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	10	0.39
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	19	0.38
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	19	0.38
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	19	0.38
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	19	0.38
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	19	0.38
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	19	0.38
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	11	0.38
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	11	0.38
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	11	0.38
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	11	0.38
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	11	0.38
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	11	0.38
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	11	0.38
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	11	0.38
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	11	0.38
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	11	0.38
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	11	0.38
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	11	0.38
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	11	0.38
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	11	0.38
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	11	0.38
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	11	0.38
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	11	0.38
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	4	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	4	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	4	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	4	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	4	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	4	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	4	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	4	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	4	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	4	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	4	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	4	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	4	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	4	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	4	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	4	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	4	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	4	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	6	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	6	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	6	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	6	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	6	0.37
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	6	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	6	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	6	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	6	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	6	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	6	0.37
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	6	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	6	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	6	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	6	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	6	0.37
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	6	0.37
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	2	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	2	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	2	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	2	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	2	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	2	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	2	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	2	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	2	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	2	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	2	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	2	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	2	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	2	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	2	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	2	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	2	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	2	0.36
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	10	0.35
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	10	0.35
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	10	0.35
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	10	0.35
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	10	0.35
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	10	0.35
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	11	0.35
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	11	0.35
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	11	0.35
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	11	0.35
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	11	0.35
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	11	0.35
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	11	0.35
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	11	0.35
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	11	0.35
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	11	0.35
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	11	0.35
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	11	0.35
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	11	0.35
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	11	0.35
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	11	0.35
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	11	0.35
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	11	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	3	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	3	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	3	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	3	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	3	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	3	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	3	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	3	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	3	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	3	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	3	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	3	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	3	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	3	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	3	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	3	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	3	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	3	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	4	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	4	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	4	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	4	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	4	0.35
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	4	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	4	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	4	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	4	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	4	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	4	0.35
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	4	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	4	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	4	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	4	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	4	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	4	0.35
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	4	0.35
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	17	0.34
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	17	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	17	0.34
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	17	0.34
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	17	0.34
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	17	0.34
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	17	0.34
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	17	0.34
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	17	0.34
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	17	0.34
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	17	0.34
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	17	0.34
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	17	0.34
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	17	0.34
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	17	0.34
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	17	0.34
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	17	0.34
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	17	0.34
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD2	5	0.34
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD3	5	0.34
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD2	5	0.34
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD3	5	0.34
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD2	5	0.34
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD3	5	0.34
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	1	0.34
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	1	0.34
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	1	0.34
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	1	0.34
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	1	0.34
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	1	0.34
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	1	0.34
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	1	0.34
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	1	0.34
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	1	0.34
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	1	0.34
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	1	0.34
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	1	0.34
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	1	0.34
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	1	0.34
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	1	0.34
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	1	0.34
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	1	0.34
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	9	0.33
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	9	0.33
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	9	0.33
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	9	0.33
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	9	0.33
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	9	0.33
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	9	0.33
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	9	0.33
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	9	0.33
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	9	0.33
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	9	0.33
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	9	0.33
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	9	0.33
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	9	0.33
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	9	0.33
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	9	0.33
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	9	0.33
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	9	0.33
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	9	0.33
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	9	0.33
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	9	0.33
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	9	0.33
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	9	0.33
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	9	0.33
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	9	0.33
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	9	0.33
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	9	0.33
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	9	0.33
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	9	0.33
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	17	0.32
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	17	0.32
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	17	0.32
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	17	0.32
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	17	0.32
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	17	0.32
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	17	0.32
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	17	0.32
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	17	0.32
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	17	0.32
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	17	0.32
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	17	0.32
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	17	0.32
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	17	0.32
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	17	0.32
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	17	0.32
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	17	0.32
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	13	0.31
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	13	0.31
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	13	0.31
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	13	0.31
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	13	0.31
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	13	0.31
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	13	0.31
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	13	0.31
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	13	0.31
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	13	0.31
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	13	0.31
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	13	0.31
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	13	0.31
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	13	0.31
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	13	0.31
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	13	0.31
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	13	0.31
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	13	0.31
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	9	0.31
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	9	0.31
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	9	0.31
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	9	0.31
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	9	0.31
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	9	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	8	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	8	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	8	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	8	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	8	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	8	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	8	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	8	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	8	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	8	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	8	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	8	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	8	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	8	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	8	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	8	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	8	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	13	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	13	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	13	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	13	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	13	0.31
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	13	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	13	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	13	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	13	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	13	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	13	0.31
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	13	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	13	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	13	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	13	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	13	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	13	0.31
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	13	0.31
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	20	0.3
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	20	0.3
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	20	0.3
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	20	0.3
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	20	0.3
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	20	0.3
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	20	0.3
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	20	0.3
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	20	0.3
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	20	0.3
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	20	0.3
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	20	0.3
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	20	0.3
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	20	0.3
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	20	0.3
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	20	0.3
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	20	0.3
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	20	0.3
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	19	0.3
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	19	0.3
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	19	0.3
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	19	0.3
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	19	0.3
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	19	0.3
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	19	0.3
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	19	0.3
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	19	0.3
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	19	0.3
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	19	0.3
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	19	0.3
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	19	0.3
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	19	0.3
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	19	0.3
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	19	0.3
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	19	0.3
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	13	0.29
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	13	0.29
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	13	0.29
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	13	0.29
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	13	0.29
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	13	0.29
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	13	0.29
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	13	0.29
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	13	0.29
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	13	0.29
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	13	0.29
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	13	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	9	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	9	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	9	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	9	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	9	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	9	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	9	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	9	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	9	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	9	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	9	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	9	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	9	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	9	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	9	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	9	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	9	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	15	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	15	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	15	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	15	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	15	0.29
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	15	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	15	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	15	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	15	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	15	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	15	0.29
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	15	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	15	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	15	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	15	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	15	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	15	0.29
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	15	0.29
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	16	0.28
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	16	0.28
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	16	0.28
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	16	0.28
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	16	0.28
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	16	0.28
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	19	0.28
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	19	0.28
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	19	0.28
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	19	0.28
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	19	0.28
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	19	0.28
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	19	0.28
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	19	0.28
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	19	0.28
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	19	0.28
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	19	0.28
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	19	0.28
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	19	0.28
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	19	0.28
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	19	0.28
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	19	0.28
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	19	0.28
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	10	0.28
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	10	0.28
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	10	0.28
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	10	0.28
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	10	0.28
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	10	0.28
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	10	0.28
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	10	0.28
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	10	0.28
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	10	0.28
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	10	0.28
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	10	0.28
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	10	0.28
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	10	0.28
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	10	0.28
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	10	0.28
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	10	0.28
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	10	0.28
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	11	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	11	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	11	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	11	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	11	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	11	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	11	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	11	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	11	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	11	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	11	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	11	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	11	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	11	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	11	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	11	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	11	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	11	0.27
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	7	0.27
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	7	0.27
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	7	0.27
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	7	0.27
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	7	0.27
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	10	0.27
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	10	0.27
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	10	0.27
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	10	0.27
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	10	0.27
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	10	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	12	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	12	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	12	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	12	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	12	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	12	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	12	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	12	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	12	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	12	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	12	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	12	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	12	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	12	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	12	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	12	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	12	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	12	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	13	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	13	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	13	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	13	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	13	0.27
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	13	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	13	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	13	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	13	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	13	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	13	0.27
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	13	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	13	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	13	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	13	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	13	0.27
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	13	0.27
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	15	0.27
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	15	0.27
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	15	0.27
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	15	0.27
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	15	0.27
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	15	0.27
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	15	0.27
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	15	0.27
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	15	0.27
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	15	0.27
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	15	0.27
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	15	0.27
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	15	0.27
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	15	0.27
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	15	0.27
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	15	0.27
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	15	0.27
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	15	0.27
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD2	15	0.26
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD3	15	0.26
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD2	15	0.26
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD3	15	0.26
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD2	15	0.26
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD3	15	0.26
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	1	0.25
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	1	0.25
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	1	0.25
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	1	0.25
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	1	0.25
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	1	0.25
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	12	0.25
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	12	0.25
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	12	0.25
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	12	0.25
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	12	0.25
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	12	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	5	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	5	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	5	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	5	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	5	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	5	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	5	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	5	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	5	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	5	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	5	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	5	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	5	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	5	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	5	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	5	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	5	0.25
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	12	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	12	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	12	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	12	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	12	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	12	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	12	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	12	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	12	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	12	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	12	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	12	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	12	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	12	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	12	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	12	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	12	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	12	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	14	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	14	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	14	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	14	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	14	0.24
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	14	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	14	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	14	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	14	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	14	0.24
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	14	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	14	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	14	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	14	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	14	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	14	0.24
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	14	0.24
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	19	0.24
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	19	0.24
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	19	0.24
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	19	0.24
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	19	0.24
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	19	0.24
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	19	0.24
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	19	0.24
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	19	0.24
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	19	0.24
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	19	0.24
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	19	0.24
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	19	0.24
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	19	0.24
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	19	0.24
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	19	0.24
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	19	0.24
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	19	0.24
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	18	0.23
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	18	0.23
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	18	0.23
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	18	0.23
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	18	0.23
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	18	0.23
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	18	0.23
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	18	0.23
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	18	0.23
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	18	0.23
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	18	0.23
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	18	0.23
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	18	0.23
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	18	0.23
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	18	0.23
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	18	0.23
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	18	0.23
(1,3)	2:96:B:MET:HE1	1:42:A:ARG:HD2	7	0.23
(1,3)	2:96:B:MET:HE1	1:42:A:ARG:HD3	7	0.23
(1,3)	2:96:B:MET:HE2	1:42:A:ARG:HD2	7	0.23
(1,3)	2:96:B:MET:HE2	1:42:A:ARG:HD3	7	0.23
(1,3)	2:96:B:MET:HE3	1:42:A:ARG:HD2	7	0.23
(1,3)	2:96:B:MET:HE3	1:42:A:ARG:HD3	7	0.23
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	16	0.23
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	16	0.23
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	16	0.23
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	16	0.23
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	16	0.23
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	16	0.23
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	16	0.23
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	16	0.23
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	16	0.23
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	16	0.23
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	16	0.23
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	16	0.23
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	16	0.23
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	16	0.23
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	16	0.23
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	16	0.23
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	16	0.23
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	16	0.23
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	17	0.22
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	17	0.22
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	17	0.22
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	17	0.22
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	17	0.22
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	17	0.22
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	20	0.22
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	20	0.22
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	20	0.22
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	20	0.22
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	20	0.22
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	20	0.22
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	6	0.22
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	6	0.22
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	6	0.22
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	6	0.22
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	6	0.22
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	2	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	2	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	2	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	2	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	2	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	2	0.21
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	1	0.21
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	1	0.21
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	1	0.21
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	1	0.21
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	1	0.21
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	1	0.21
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	1	0.21
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	1	0.21
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	1	0.21
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	1	0.21
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	1	0.21
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	1	0.21
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	1	0.21
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	1	0.21
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	1	0.21
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	1	0.21
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	1	0.21
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	1	0.21
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	15	0.21
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	15	0.21
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	15	0.21
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	15	0.21
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	15	0.21
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	15	0.21
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	15	0.21
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	15	0.21
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	15	0.21
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	15	0.21
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	15	0.21
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	15	0.21
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	15	0.21
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	15	0.21
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	15	0.21
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	15	0.21
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	15	0.21
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	14	0.21
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	14	0.21
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	14	0.21
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	14	0.21
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	14	0.21
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	14	0.21
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	4	0.2
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	4	0.2
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	4	0.2
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	4	0.2
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	4	0.2
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	4	0.2
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	16	0.2
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	16	0.2
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	16	0.2
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	16	0.2
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	16	0.2
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	16	0.2
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	16	0.2
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	16	0.2
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	16	0.2
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	16	0.2
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	16	0.2
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	16	0.2
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	16	0.2
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	16	0.2
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	16	0.2
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	16	0.2
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	16	0.2
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	16	0.2
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	3	0.2
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	3	0.2
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	3	0.2
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	3	0.2
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	3	0.2
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	3	0.2
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	3	0.2
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	3	0.2
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	3	0.2
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	3	0.2
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	3	0.2
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	3	0.2
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	3	0.2
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	3	0.2
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	3	0.2
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	3	0.2
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	3	0.2
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	3	0.19
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	3	0.19
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	3	0.19
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	3	0.19
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	3	0.19
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	3	0.19
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	13	0.18
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	13	0.18
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	13	0.18
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	13	0.18
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	13	0.18
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	13	0.18
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	19	0.18
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	19	0.18
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	19	0.18
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	19	0.18
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	19	0.18
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	19	0.18
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	5	0.16
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	5	0.16
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	5	0.16
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	5	0.16
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	5	0.16
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	5	0.16
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	5	0.16
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	5	0.16
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	5	0.16
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	5	0.16
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	5	0.16
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	5	0.16
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	5	0.16
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	5	0.16
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	5	0.16
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	5	0.16
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	5	0.16
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	5	0.16
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	5	0.16
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	5	0.16
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	5	0.16
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	5	0.16
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	5	0.16
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	7	0.16
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	7	0.16
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	7	0.16
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	7	0.16
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	7	0.16
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	7	0.16
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	7	0.16
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	7	0.16
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	7	0.16
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	7	0.16
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	7	0.16
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	7	0.16
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	7	0.16
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	7	0.16
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	7	0.16
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	7	0.16
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	7	0.16
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	7	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	14	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	14	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	14	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	14	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	14	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	14	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	14	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	14	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	14	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	14	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	14	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	14	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	14	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	14	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	14	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	14	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	14	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	16	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	16	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	16	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	16	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	16	0.16
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	16	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	16	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	16	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	16	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	16	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	16	0.16
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	16	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	16	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	16	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	16	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	16	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	16	0.16
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	16	0.16
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	7	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	7	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	7	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	7	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	7	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	7	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG11	14	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG12	14	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG13	14	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG21	14	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG22	14	0.15
(1,12)	2:92:B:GLU:HG2	1:70:A:VAL:HG23	14	0.15
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	8	0.15
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	8	0.15
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	8	0.15
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	8	0.15
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	8	0.15
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	8	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	2	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	2	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	2	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	2	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	2	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	2	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	2	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	2	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	2	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	2	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	2	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	2	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	2	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	2	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	2	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	2	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	2	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	14	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	14	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	14	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	14	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	14	0.15
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	14	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	14	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	14	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	14	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	14	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	14	0.15
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	14	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	14	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	14	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	14	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	14	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	14	0.15
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	14	0.15
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	2	0.14
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG3	2	0.14
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG2	2	0.14
(1,6)	2:114:B:ILE:HD12	1:42:A:ARG:HG3	2	0.14
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG2	2	0.14
(1,6)	2:114:B:ILE:HD13	1:42:A:ARG:HG3	2	0.14
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	20	0.14
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	20	0.14
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	20	0.14
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	20	0.14
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	20	0.14
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	20	0.14
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	20	0.14
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	20	0.14
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	20	0.14
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	20	0.14
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	20	0.14
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	20	0.14
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	20	0.14
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	20	0.14
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	20	0.14
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	20	0.14
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	20	0.14
(1,10)	2:89:B:TYR:HB2	1:70:A:VAL:HG11	7	0.13
(1,10)	2:89:B:TYR:HB2	1:70:A:VAL:HG12	7	0.13
(1,10)	2:89:B:TYR:HB2	1:70:A:VAL:HG13	7	0.13
(1,10)	2:89:B:TYR:HB2	1:70:A:VAL:HG21	7	0.13
(1,10)	2:89:B:TYR:HB2	1:70:A:VAL:HG22	7	0.13
(1,10)	2:89:B:TYR:HB2	1:70:A:VAL:HG23	7	0.13
(1,10)	2:89:B:TYR:HB3	1:70:A:VAL:HG11	7	0.13
(1,10)	2:89:B:TYR:HB3	1:70:A:VAL:HG12	7	0.13
(1,10)	2:89:B:TYR:HB3	1:70:A:VAL:HG13	7	0.13
(1,10)	2:89:B:TYR:HB3	1:70:A:VAL:HG21	7	0.13
(1,10)	2:89:B:TYR:HB3	1:70:A:VAL:HG22	7	0.13
(1,10)	2:89:B:TYR:HB3	1:70:A:VAL:HG23	7	0.13
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD2	14	0.13
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD3	14	0.13
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD2	14	0.13
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD3	14	0.13
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD2	14	0.13
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD3	14	0.13
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	8	0.13
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	8	0.13
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	8	0.13
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	8	0.13
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	8	0.13
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	8	0.13
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	8	0.13
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	8	0.13
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	8	0.13
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	8	0.13
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	8	0.13
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	8	0.13
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	8	0.13
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	8	0.13
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	8	0.13
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	8	0.13
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	8	0.13
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	15	0.13
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	15	0.13
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	15	0.13
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	15	0.13
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	15	0.13
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	15	0.13
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	15	0.13
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	15	0.13
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	15	0.13
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	15	0.13
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	15	0.13
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	15	0.13
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	15	0.13
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	15	0.13
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	15	0.13
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	15	0.13
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	15	0.13
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	15	0.13
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD2	16	0.12
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD3	16	0.12
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD2	16	0.12
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD3	16	0.12
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD2	16	0.12
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD3	16	0.12
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	18	0.11
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	18	0.11
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	18	0.11
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	18	0.11
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	18	0.11
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	18	0.11
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	18	0.11
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	18	0.11
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	18	0.11
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	18	0.11
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	18	0.11
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	18	0.11
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	18	0.11
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	18	0.11
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	18	0.11
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	18	0.11
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	18	0.11
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD2	4	0.11
(1,7)	2:114:B:ILE:HD11	1:42:A:ARG:HD3	4	0.11
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD2	4	0.11
(1,7)	2:114:B:ILE:HD12	1:42:A:ARG:HD3	4	0.11
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD2	4	0.11
(1,7)	2:114:B:ILE:HD13	1:42:A:ARG:HD3	4	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	16	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	16	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	16	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	16	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	16	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	16	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	16	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	16	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	16	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	16	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	16	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	16	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	16	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	16	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	16	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	16	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	16	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	16	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	18	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	18	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	18	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	18	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	18	0.11
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	18	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	18	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	18	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	18	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	18	0.11
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	18	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	18	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	18	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	18	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	18	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	18	0.11
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	18	0.11
(1,3)	2:96:B:MET:HE1	1:42:A:ARG:HD2	5	0.11
(1,3)	2:96:B:MET:HE1	1:42:A:ARG:HD3	5	0.11
(1,3)	2:96:B:MET:HE2	1:42:A:ARG:HD2	5	0.11
(1,3)	2:96:B:MET:HE2	1:42:A:ARG:HD3	5	0.11
(1,3)	2:96:B:MET:HE3	1:42:A:ARG:HD2	5	0.11
(1,3)	2:96:B:MET:HE3	1:42:A:ARG:HD3	5	0.11

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found