



Full wwPDB NMR Structure Validation Report ⓘ

Jul 3, 2026 – 01:47 AM JST

PDB ID : 9X70 / pdb_00009x70
BMRB ID : 36796
Title : Hsp90a T36E N-terminal domain
Authors : Wan, C.J.
Deposited on : 2025-10-16

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) : 2.50

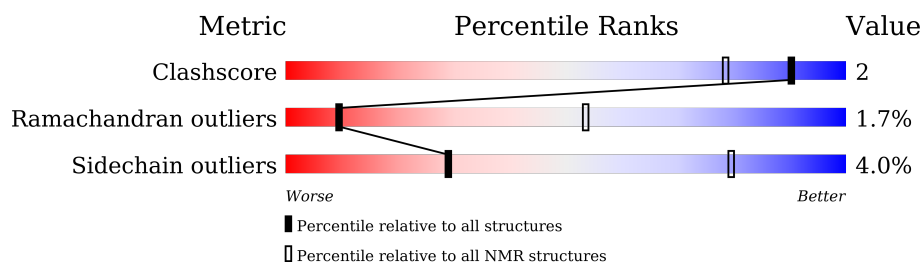
1 Overall quality at a glance

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	237	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:16-A:222 (207)	1.83	5

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 8, 9
2	1, 2, 7
Single-model clusters	6; 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3260 atoms, of which 1632 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms						Trace
1	A	207	Total	C	H	N	O	S	0
			3260	1034	1632	268	321	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLU	THR	engineered mutation	UNP P07900

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: Heat shock protein HSP 90-alpha

Chain A: 



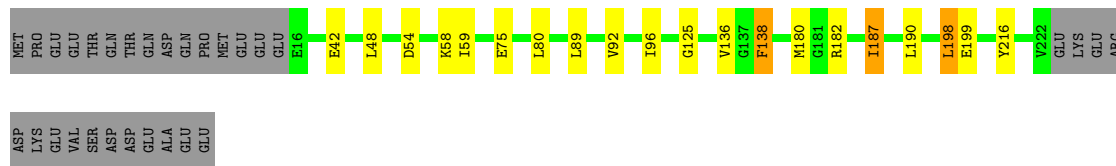
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Heat shock protein HSP 90-alpha

Chain A: 

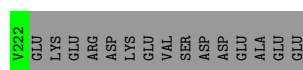


4.2.2 Score per residue for model 2

- Molecule 1: Heat shock protein HSP 90-alpha

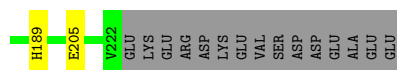
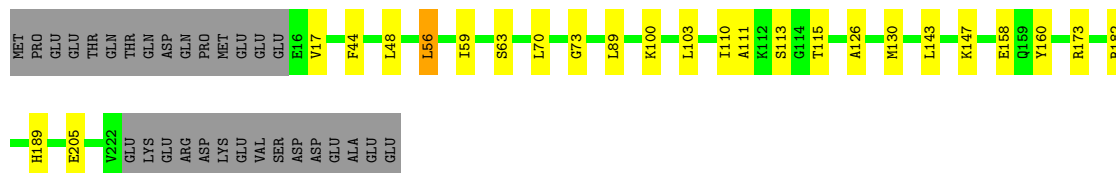
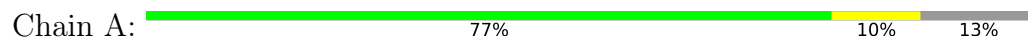
Chain A: 





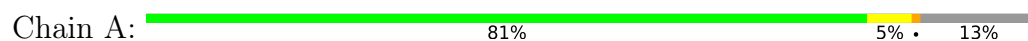
4.2.3 Score per residue for model 3

- Molecule 1: Heat shock protein HSP 90-alpha



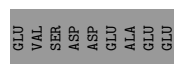
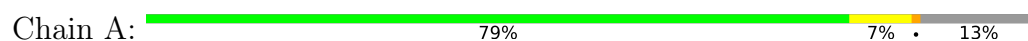
4.2.4 Score per residue for model 4

- Molecule 1: Heat shock protein HSP 90-alpha



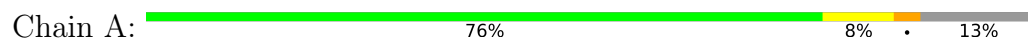
4.2.5 Score per residue for model 5 (medoid)

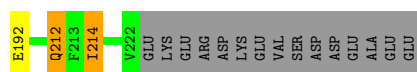
- Molecule 1: Heat shock protein HSP 90-alpha



4.2.6 Score per residue for model 6

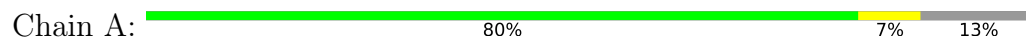
- Molecule 1: Heat shock protein HSP 90-alpha





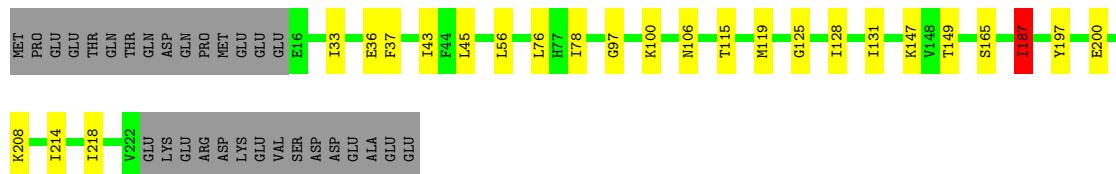
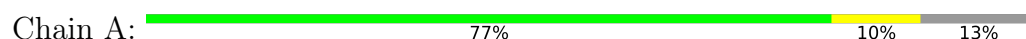
4.2.7 Score per residue for model 7

- Molecule 1: Heat shock protein HSP 90-alpha



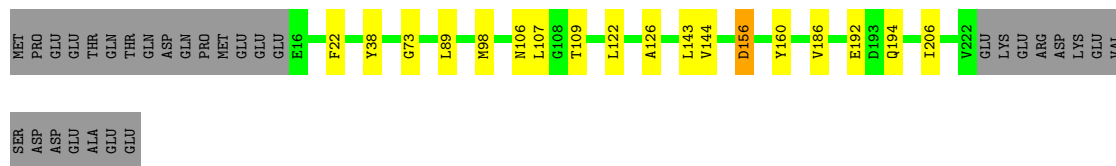
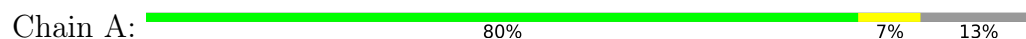
4.2.8 Score per residue for model 8

- Molecule 1: Heat shock protein HSP 90-alpha



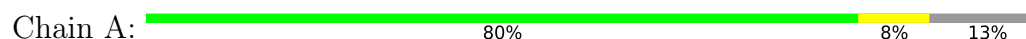
4.2.9 Score per residue for model 9

- Molecule 1: Heat shock protein HSP 90-alpha



4.2.10 Score per residue for model 10

- Molecule 1: Heat shock protein HSP 90-alpha



MET	PRO	GLU	GLU	THR	GLN	THR	GLN	ASP	GLN	PRO	MET	GLU	GLU	E16	I26	N35	L48	A55	D71	S72	G73	L89	I96	G97	N98	L107	I151	E158	K185	L190	L198	K208	V222	GLU	LYS	GLU	ARG	ASP	LYS	GLU	VAL	SER	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP	GLU	ALA	GLU	GLU
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum*.

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

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

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	440
Number of shifts mapped to atoms	440
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	1.26±0.02	1±1/1654 (0.1± 0.1%)	0.97±0.01	0±0/2230 (0.0± 0.0%)
All	All	1.26	13/16540 (0.1%)	0.97	0/22300 (0.0%)

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	187	ILE	CA-CB	6.06	1.60	1.53	5	3
1	A	136	VAL	CA-CB	5.95	1.61	1.54	5	2
1	A	214	ILE	CA-CB	5.83	1.61	1.54	6	2
1	A	150	VAL	CA-CB	5.48	1.60	1.53	6	1
1	A	206	ILE	CA-CB	5.16	1.61	1.54	9	1
1	A	92	VAL	CA-CB	5.12	1.60	1.53	1	1
1	A	59	ILE	CA-CB	5.10	1.60	1.54	6	1
1	A	186	VAL	CA-CB	5.08	1.59	1.53	9	1
1	A	17	VAL	CA-CB	5.05	1.58	1.53	2	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1628	1632	1627	6±2
All	All	16280	16320	16270	55

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:GLU:HB3	1:A:69:LYS:HD3	0.59	1.74	6	1
1:A:141:ALA:HB1	1:A:165:SER:HA	0.57	1.76	4	1
1:A:126:ALA:HB1	1:A:130:MET:SD	0.56	2.40	3	1
1:A:149:THR:HB	1:A:187:ILE:HG23	0.53	1.80	8	1
1:A:159:GLN:HG3	1:A:175:ASP:HB2	0.53	1.80	6	1
1:A:151:ILE:HD11	1:A:185:LYS:HE2	0.51	1.81	10	1
1:A:143:LEU:HG	1:A:144:VAL:HG13	0.51	1.82	4	1
1:A:44:PHE:HB2	1:A:143:LEU:HD23	0.50	1.83	3	1
1:A:212:GLN:HG3	1:A:214:ILE:HB	0.49	1.83	6	1
1:A:151:ILE:HB	1:A:185:LYS:HB2	0.49	1.85	2	1
1:A:115:THR:HG22	1:A:119:MET:SD	0.49	2.47	8	1
1:A:32:LEU:HA	1:A:35:ASN:ND2	0.48	2.24	2	1
1:A:47:GLU:HG2	1:A:129:SER:HA	0.48	1.84	2	1
1:A:56:LEU:HD11	1:A:76:LEU:HG	0.48	1.84	5	2
1:A:98:MET:SD	1:A:107:LEU:HD22	0.47	2.49	9	1
1:A:147:LYS:HG2	1:A:189:HIS:HB3	0.47	1.85	2	1
1:A:207:VAL:HG21	1:A:220:LEU:HD11	0.47	1.85	2	1
1:A:153:LYS:HD2	1:A:180:MET:HE3	0.47	1.85	6	1
1:A:103:LEU:HD13	1:A:160:TYR:HB2	0.47	1.86	3	1
1:A:48:LEU:HD21	1:A:139:TYR:HB3	0.47	1.87	7	1
1:A:33:ILE:HG23	1:A:128:ILE:HD11	0.47	1.87	8	1
1:A:55:ALA:O	1:A:96:ILE:HG21	0.47	2.09	10	1
1:A:147:LYS:HB3	1:A:189:HIS:HB3	0.47	1.85	3	1
1:A:54:ASP:O	1:A:58:LYS:HG2	0.47	2.10	1	1
1:A:79:ASN:HB2	1:A:92:VAL:HG13	0.46	1.87	7	1
1:A:144:VAL:HA	1:A:194:GLN:HG3	0.46	1.86	9	1
1:A:100:LYS:HG2	1:A:158:GLU:H	0.46	1.70	3	1
1:A:140:SER:HA	1:A:143:LEU:HB3	0.46	1.87	4	1
1:A:149:THR:HB	1:A:187:ILE:HG12	0.45	1.89	5	1
1:A:59:ILE:HB	1:A:96:ILE:HA	0.45	1.87	7	1
1:A:159:GLN:NE2	1:A:178:GLU:HB3	0.45	2.27	5	1
1:A:207:VAL:HA	1:A:210:HIS:CE1	0.45	2.47	5	1
1:A:59:ILE:HB	1:A:96:ILE:HB	0.44	1.88	1	1
1:A:190:LEU:HD11	1:A:198:LEU:HB2	0.44	1.90	10	2
1:A:153:LYS:HG2	1:A:180:MET:HB2	0.44	1.88	5	1
1:A:111:ALA:HA	1:A:115:THR:HG22	0.44	1.88	3	1
1:A:53:SER:HB3	1:A:214:ILE:HD11	0.43	1.89	6	1
1:A:17:VAL:HA	1:A:173:ARG:HB3	0.43	1.89	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLU:HG3	1:A:112:LYS:H	0.43	1.74	6	1
1:A:22:PHE:HB3	1:A:26:ILE:HG21	0.42	1.89	7	1
1:A:59:ILE:HD13	1:A:96:ILE:HA	0.42	1.90	2	1
1:A:60:ARG:HA	1:A:60:ARG:NE	0.42	2.29	2	1
1:A:128:ILE:O	1:A:131:ILE:HG13	0.42	2.14	6	1
1:A:56:LEU:O	1:A:59:ILE:HG22	0.42	2.15	3	1
1:A:82:PRO:HA	1:A:89:LEU:HA	0.41	1.92	5	1
1:A:98:MET:SD	1:A:107:LEU:HD23	0.41	2.55	10	1
1:A:45:LEU:HD22	1:A:197:TYR:HB3	0.41	1.91	8	1
1:A:122:LEU:HA	1:A:126:ALA:O	0.41	2.15	9	1
1:A:63:SER:HB3	1:A:70:LEU:HB2	0.41	1.91	3	1
1:A:47:GLU:HB3	1:A:129:SER:HA	0.41	1.92	5	1
1:A:111:ALA:HB1	1:A:115:THR:OG1	0.41	2.16	4	1
1:A:19:THR:HB	1:A:171:THR:HG22	0.40	1.92	6	1
1:A:78:ILE:O	1:A:218:ILE:HA	0.40	2.15	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/237 (86%)	186±4 (91±2%)	16±3 (8±2%)	4±1 (2±1%)	9	53
All	All	2050/2370 (86%)	1857 (91%)	158 (8%)	35 (2%)	9	53

All 23 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	73	GLY	5
1	A	97	GLY	4
1	A	125	GLY	3
1	A	165	SER	2
1	A	110	ILE	2
1	A	156	ASP	2
1	A	136	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	138	PHE	1
1	A	107	LEU	1
1	A	178	GLU	1
1	A	113	SER	1
1	A	111	ALA	1
1	A	108	GLY	1
1	A	112	LYS	1
1	A	179	PRO	1
1	A	212	GLN	1
1	A	17	VAL	1
1	A	139	TYR	1
1	A	36	GLU	1
1	A	37	PHE	1
1	A	106	ASN	1
1	A	38	TYR	1
1	A	109	THR	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/207 (86%)	171±2 (96±1%)	7±2 (4±1%)	29	79
All	All	1780/2070 (86%)	1708 (96%)	72 (4%)	29	79

All 52 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	89	LEU	6
1	A	48	LEU	4
1	A	150	VAL	3
1	A	80	LEU	2
1	A	182	ARG	2
1	A	187	ILE	2
1	A	198	LEU	2
1	A	147	LYS	2
1	A	100	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	154	HIS	2
1	A	192	GLU	2
1	A	131	ILE	2
1	A	208	LYS	2
1	A	42	GLU	1
1	A	75	GLU	1
1	A	138	PHE	1
1	A	180	MET	1
1	A	199	GLU	1
1	A	216	TYR	1
1	A	45	LEU	1
1	A	92	VAL	1
1	A	153	LYS	1
1	A	184	THR	1
1	A	202	ARG	1
1	A	56	LEU	1
1	A	110	ILE	1
1	A	205	GLU	1
1	A	17	VAL	1
1	A	136	VAL	1
1	A	206	ILE	1
1	A	16	GLU	1
1	A	25	GLU	1
1	A	59	ILE	1
1	A	159	GLN	1
1	A	191	LYS	1
1	A	28	GLN	1
1	A	36	GLU	1
1	A	58	LYS	1
1	A	94	THR	1
1	A	105	ASN	1
1	A	43	ILE	1
1	A	200	GLU	1
1	A	22	PHE	1
1	A	106	ASN	1
1	A	143	LEU	1
1	A	156	ASP	1
1	A	160	TYR	1
1	A	26	ILE	1
1	A	35	ASN	1
1	A	71	ASP	1
1	A	158	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	222	VAL	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: *starch_output*

7.1.1 Bookkeeping

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

Total number of shifts	440
Number of shifts mapped to atoms	440
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

- Can not parse the chemical shift value. All 224 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	VAL	HG11	0.76	.	.
1	A	17	VAL	HG12	0.76	.	.
1	A	17	VAL	HG13	0.76	.	.
1	A	17	VAL	HG21	0.78	.	.
1	A	17	VAL	HG22	0.78	.	.
1	A	17	VAL	HG23	0.78	.	.
1	A	17	VAL	CG1	18.22	.	.
1	A	17	VAL	CG2	18.02	.	.
1	A	29	LEU	HD11	0.77	.	.
1	A	29	LEU	HD12	0.77	.	.
1	A	29	LEU	HD13	0.77	.	.
1	A	29	LEU	HD21	0.89	.	.
1	A	29	LEU	HD22	0.89	.	.
1	A	29	LEU	HD23	0.89	.	.
1	A	29	LEU	CD1	23.65	.	.
1	A	29	LEU	CD2	20.97	.	.
1	A	32	LEU	HD11	0.71	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	LEU	HD12	0.71	.	.
1	A	32	LEU	HD13	0.71	.	.
1	A	32	LEU	HD21	0.74	.	.
1	A	32	LEU	HD22	0.74	.	.
1	A	32	LEU	HD23	0.74	.	.
1	A	32	LEU	CD1	22.67	.	.
1	A	32	LEU	CD2	21.7	.	.
1	A	45	LEU	HD11	0.65	.	.
1	A	45	LEU	HD12	0.65	.	.
1	A	45	LEU	HD13	0.65	.	.
1	A	45	LEU	HD21	0.6	.	.
1	A	45	LEU	HD22	0.6	.	.
1	A	45	LEU	HD23	0.6	.	.
1	A	45	LEU	CD1	20.79	.	.
1	A	45	LEU	CD2	22.93	.	.
1	A	48	LEU	HD11	0.79	.	.
1	A	48	LEU	HD12	0.79	.	.
1	A	48	LEU	HD13	0.79	.	.
1	A	48	LEU	HD21	0.81	.	.
1	A	48	LEU	HD22	0.81	.	.
1	A	48	LEU	HD23	0.81	.	.
1	A	48	LEU	CD1	19.77	.	.
1	A	48	LEU	CD2	24.99	.	.
1	A	56	LEU	HD11	0.3	.	.
1	A	56	LEU	HD12	0.3	.	.
1	A	56	LEU	HD13	0.3	.	.
1	A	56	LEU	HD21	-0.03	.	.
1	A	56	LEU	HD22	-0.03	.	.
1	A	56	LEU	HD23	-0.03	.	.
1	A	56	LEU	CD1	23.4	.	.
1	A	56	LEU	CD2	22.7	.	.
1	A	64	LEU	HD11	0.85	.	.
1	A	64	LEU	HD12	0.85	.	.
1	A	64	LEU	HD13	0.85	.	.
1	A	64	LEU	HD21	0.75	.	.
1	A	64	LEU	HD22	0.75	.	.
1	A	64	LEU	HD23	0.75	.	.
1	A	64	LEU	CD1	22.46	.	.
1	A	64	LEU	CD2	19.35	.	.
1	A	70	LEU	HD11	0.9	.	.
1	A	70	LEU	HD12	0.9	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	70	LEU	HD13	0.9	.	.
1	A	70	LEU	HD21	0.68	.	.
1	A	70	LEU	HD22	0.68	.	.
1	A	70	LEU	HD23	0.68	.	.
1	A	70	LEU	CD1	22.75	.	.
1	A	70	LEU	CD2	19.56	.	.
1	A	76	LEU	HD11	0.86	.	.
1	A	76	LEU	HD12	0.86	.	.
1	A	76	LEU	HD13	0.86	.	.
1	A	76	LEU	HD21	0.48	.	.
1	A	76	LEU	HD22	0.48	.	.
1	A	76	LEU	HD23	0.48	.	.
1	A	76	LEU	CD1	23.07	.	.
1	A	76	LEU	CD2	20.85	.	.
1	A	80	LEU	HD11	0.73	.	.
1	A	80	LEU	HD12	0.73	.	.
1	A	80	LEU	HD13	0.73	.	.
1	A	80	LEU	HD21	0.63	.	.
1	A	80	LEU	HD22	0.63	.	.
1	A	80	LEU	HD23	0.63	.	.
1	A	80	LEU	CD1	22.84	.	.
1	A	80	LEU	CD2	23.88	.	.
1	A	89	LEU	HD11	1.03	.	.
1	A	89	LEU	HD12	1.03	.	.
1	A	89	LEU	HD13	1.03	.	.
1	A	89	LEU	HD21	0.79	.	.
1	A	89	LEU	HD22	0.79	.	.
1	A	89	LEU	HD23	0.79	.	.
1	A	89	LEU	CD1	22.9	.	.
1	A	89	LEU	CD2	19.39	.	.
1	A	92	VAL	HG11	0.84	.	.
1	A	92	VAL	HG12	0.84	.	.
1	A	92	VAL	HG13	0.84	.	.
1	A	92	VAL	HG21	0.82	.	.
1	A	92	VAL	HG22	0.82	.	.
1	A	92	VAL	HG23	0.82	.	.
1	A	92	VAL	CG1	18.39	.	.
1	A	92	VAL	CG2	19.42	.	.
1	A	103	LEU	HD11	0.68	.	.
1	A	103	LEU	HD12	0.68	.	.
1	A	103	LEU	HD13	0.68	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	LEU	HD21	0.6	.	.
1	A	103	LEU	HD22	0.6	.	.
1	A	103	LEU	HD23	0.6	.	.
1	A	103	LEU	CD1	22.28	.	.
1	A	103	LEU	CD2	22.28	.	.
1	A	107	LEU	HD11	-0.96	.	.
1	A	107	LEU	HD12	-0.96	.	.
1	A	107	LEU	HD13	-0.96	.	.
1	A	107	LEU	HD21	-0.73	.	.
1	A	107	LEU	HD22	-0.73	.	.
1	A	107	LEU	HD23	-0.73	.	.
1	A	107	LEU	CD1	18.77	.	.
1	A	107	LEU	CD2	20.98	.	.
1	A	122	LEU	HD11	0.37	.	.
1	A	122	LEU	HD12	0.37	.	.
1	A	122	LEU	HD13	0.37	.	.
1	A	122	LEU	HD21	0.29	.	.
1	A	122	LEU	HD22	0.29	.	.
1	A	122	LEU	HD23	0.29	.	.
1	A	122	LEU	CD1	19.98	.	.
1	A	122	LEU	CD2	22.04	.	.
1	A	136	VAL	HG11	0.45	.	.
1	A	136	VAL	HG12	0.45	.	.
1	A	136	VAL	HG13	0.45	.	.
1	A	136	VAL	HG21	0.86	.	.
1	A	136	VAL	HG22	0.86	.	.
1	A	136	VAL	HG23	0.86	.	.
1	A	136	VAL	CG1	14.84	.	.
1	A	136	VAL	CG2	19.78	.	.
1	A	143	LEU	HD11	0.87	.	.
1	A	143	LEU	HD12	0.87	.	.
1	A	143	LEU	HD13	0.87	.	.
1	A	143	LEU	HD21	0.81	.	.
1	A	143	LEU	HD22	0.81	.	.
1	A	143	LEU	HD23	0.81	.	.
1	A	143	LEU	CD1	24	.	.
1	A	143	LEU	CD2	21.58	.	.
1	A	144	VAL	HG11	0.3	.	.
1	A	144	VAL	HG12	0.3	.	.
1	A	144	VAL	HG13	0.3	.	.
1	A	144	VAL	HG21	-0.71	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	144	VAL	HG22	-0.71	.	.
1	A	144	VAL	HG23	-0.71	.	.
1	A	144	VAL	CG1	19.46	.	.
1	A	144	VAL	CG2	12.69	.	.
1	A	148	VAL	HG11	0.04	.	.
1	A	148	VAL	HG12	0.04	.	.
1	A	148	VAL	HG13	0.04	.	.
1	A	148	VAL	HG21	0.84	.	.
1	A	148	VAL	HG22	0.84	.	.
1	A	148	VAL	HG23	0.84	.	.
1	A	148	VAL	CG1	19.91	.	.
1	A	148	VAL	CG2	19.42	.	.
1	A	150	VAL	HG11	0.75	.	.
1	A	150	VAL	HG12	0.75	.	.
1	A	150	VAL	HG13	0.75	.	.
1	A	150	VAL	HG21	0.49	.	.
1	A	150	VAL	HG22	0.49	.	.
1	A	150	VAL	HG23	0.49	.	.
1	A	150	VAL	CG1	19.4	.	.
1	A	150	VAL	CG2	18.3	.	.
1	A	172	VAL	HG11	1.14	.	.
1	A	172	VAL	HG12	1.14	.	.
1	A	172	VAL	HG13	1.14	.	.
1	A	172	VAL	HG21	0.9	.	.
1	A	172	VAL	HG22	0.9	.	.
1	A	172	VAL	HG23	0.9	.	.
1	A	172	VAL	CG1	20.39	.	.
1	A	172	VAL	CG2	19.43	.	.
1	A	186	VAL	HG11	0.97	.	.
1	A	186	VAL	HG12	0.97	.	.
1	A	186	VAL	HG13	0.97	.	.
1	A	186	VAL	HG21	0.77	.	.
1	A	186	VAL	HG22	0.77	.	.
1	A	186	VAL	HG23	0.77	.	.
1	A	186	VAL	CG1	18.31	.	.
1	A	186	VAL	CG2	19.37	.	.
1	A	188	LEU	HD11	0.67	.	.
1	A	188	LEU	HD12	0.67	.	.
1	A	188	LEU	HD13	0.67	.	.
1	A	188	LEU	HD21	0.45	.	.
1	A	188	LEU	HD22	0.45	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	188	LEU	HD23	0.45	.	.
1	A	188	LEU	CD1	23.98	.	.
1	A	188	LEU	CD2	23.93	.	.
1	A	190	LEU	HD11	0.7	.	.
1	A	190	LEU	HD12	0.7	.	.
1	A	190	LEU	HD13	0.7	.	.
1	A	190	LEU	HD21	0.49	.	.
1	A	190	LEU	HD22	0.49	.	.
1	A	190	LEU	HD23	0.49	.	.
1	A	190	LEU	CD1	23.87	.	.
1	A	190	LEU	CD2	20.1	.	.
1	A	198	LEU	HD11	0.87	.	.
1	A	198	LEU	HD12	0.87	.	.
1	A	198	LEU	HD13	0.87	.	.
1	A	198	LEU	HD21	0.59	.	.
1	A	198	LEU	HD22	0.59	.	.
1	A	198	LEU	HD23	0.59	.	.
1	A	198	LEU	CD1	24.22	.	.
1	A	198	LEU	CD2	22.15	.	.
1	A	207	VAL	HG11	0.78	.	.
1	A	207	VAL	HG12	0.78	.	.
1	A	207	VAL	HG13	0.78	.	.
1	A	207	VAL	HG21	0.74	.	.
1	A	207	VAL	HG22	0.74	.	.
1	A	207	VAL	HG23	0.74	.	.
1	A	207	VAL	CG1	20.58	.	.
1	A	207	VAL	CG2	18.95	.	.
1	A	220	LEU	HD11	0.8	.	.
1	A	220	LEU	HD12	0.8	.	.
1	A	220	LEU	HD13	0.8	.	.
1	A	220	LEU	HD21	0.78	.	.
1	A	220	LEU	HD22	0.78	.	.
1	A	220	LEU	HD23	0.78	.	.
1	A	220	LEU	CD1	21.96	.	.
1	A	220	LEU	CD2	24.05	.	.
1	A	222	VAL	HG11	0.83	.	.
1	A	222	VAL	HG12	0.83	.	.
1	A	222	VAL	HG13	0.83	.	.
1	A	222	VAL	HG21	0.77	.	.
1	A	222	VAL	HG22	0.77	.	.
1	A	222	VAL	HG23	0.77	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	222	VAL	CG1	18.63	.	.
1	A	222	VAL	CG2	17.41	.	.

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 216 atoms were assigned a chemical shift out of a possible 2823. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1042 (0%)	0/425 (0%)	0/414 (0%)	0/203 (0%)
Sidechain	216/1574 (14%)	162/1024 (16%)	54/498 (11%)	0/52 (0%)
Aromatic	0/207 (0%)	0/100 (0%)	0/98 (0%)	0/9 (0%)
Overall	216/2823 (8%)	162/1549 (10%)	54/1010 (5%)	0/264 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 216 atoms were assigned a chemical shift out of a possible 2823. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1042 (0%)	0/425 (0%)	0/414 (0%)	0/203 (0%)
Sidechain	216/1574 (14%)	162/1024 (16%)	54/498 (11%)	0/52 (0%)
Aromatic	0/207 (0%)	0/100 (0%)	0/98 (0%)	0/9 (0%)
Overall	216/2823 (8%)	162/1549 (10%)	54/1010 (5%)	0/264 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

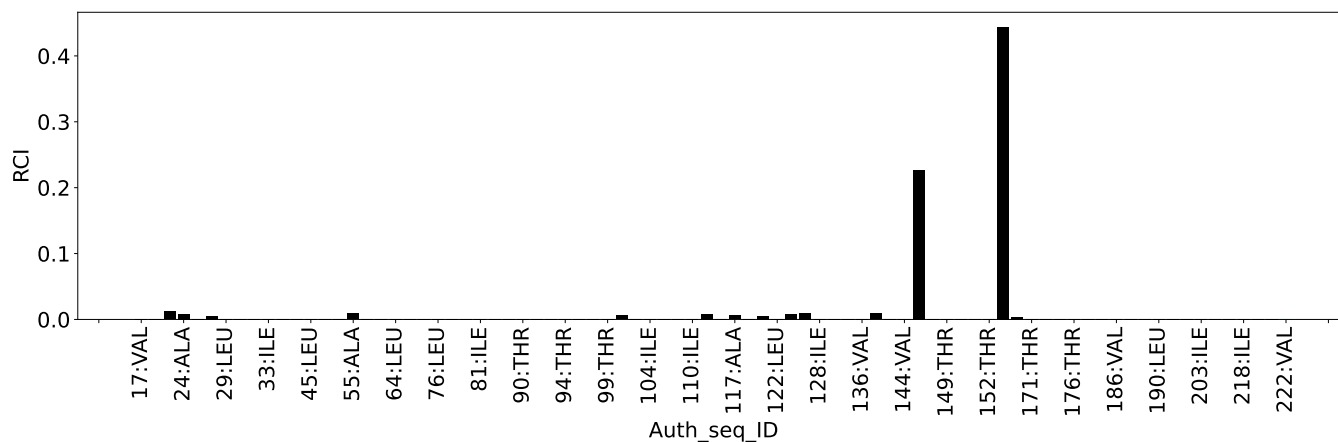
There are no statistically unusual chemical shifts.

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:



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	1891
Intra-residue ($ i-j =0$)	282
Sequential ($ i-j =1$)	441
Medium range ($ i-j >1$ and $ i-j <5$)	554
Long range ($ i-j \geq 5$)	614
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	315
Number of unmapped restraints	0
Number of restraints per residue	9.3
Number of long range restraints per residue ¹	2.6

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)	61.7	0.2
0.2-0.5 (Medium)	11.1	0.43
>0.5 (Large)	0.3	0.72

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	21.0	4.35
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

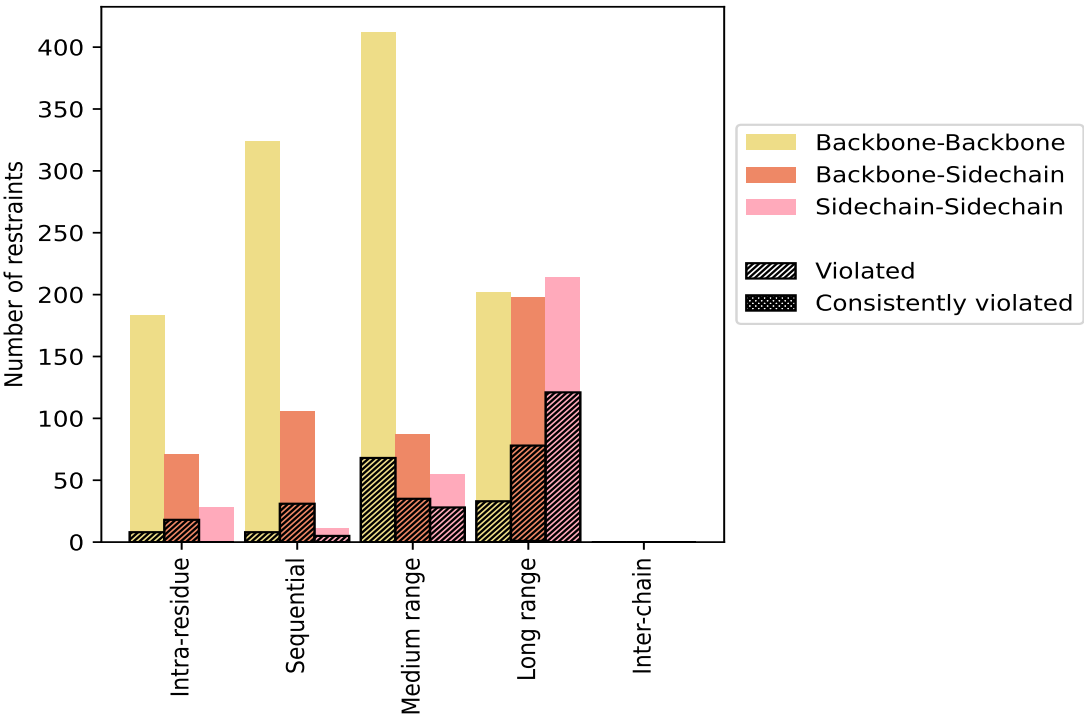
9.1 Summary of distance violations ⓘ

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)	282	14.9	26	9.2	1.4	0	0.0	0.0
Backbone-Backbone	183	9.7	8	4.4	0.4	0	0.0	0.0
Backbone-Sidechain	71	3.8	18	25.4	1.0	0	0.0	0.0
Sidechain-Sidechain	28	1.5	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	441	23.3	44	10.0	2.3	0	0.0	0.0
Backbone-Backbone	324	17.1	8	2.5	0.4	0	0.0	0.0
Backbone-Sidechain	106	5.6	31	29.2	1.6	0	0.0	0.0
Sidechain-Sidechain	11	0.6	5	45.5	0.3	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	554	29.3	131	23.6	6.9	0	0.0	0.0
Backbone-Backbone	412	21.8	68	16.5	3.6	0	0.0	0.0
Backbone-Sidechain	87	4.6	35	40.2	1.9	0	0.0	0.0
Sidechain-Sidechain	55	2.9	28	50.9	1.5	0	0.0	0.0
Long range (i-j ≥5)	614	32.5	232	37.8	12.3	1	0.2	0.1
Backbone-Backbone	202	10.7	33	16.3	1.7	0	0.0	0.0
Backbone-Sidechain	198	10.5	78	39.4	4.1	1	0.5	0.1
Sidechain-Sidechain	214	11.3	121	56.5	6.4	0	0.0	0.0
Inter-chain	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
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	1891	100.0	433	22.9	22.9	1	0.1	0.1
Backbone-Backbone	1121	59.3	117	10.4	6.2	0	0.0	0.0
Backbone-Sidechain	462	24.4	162	35.1	8.6	1	0.2	0.1
Sidechain-Sidechain	308	16.3	154	50.0	8.1	0	0.0	0.0

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

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



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

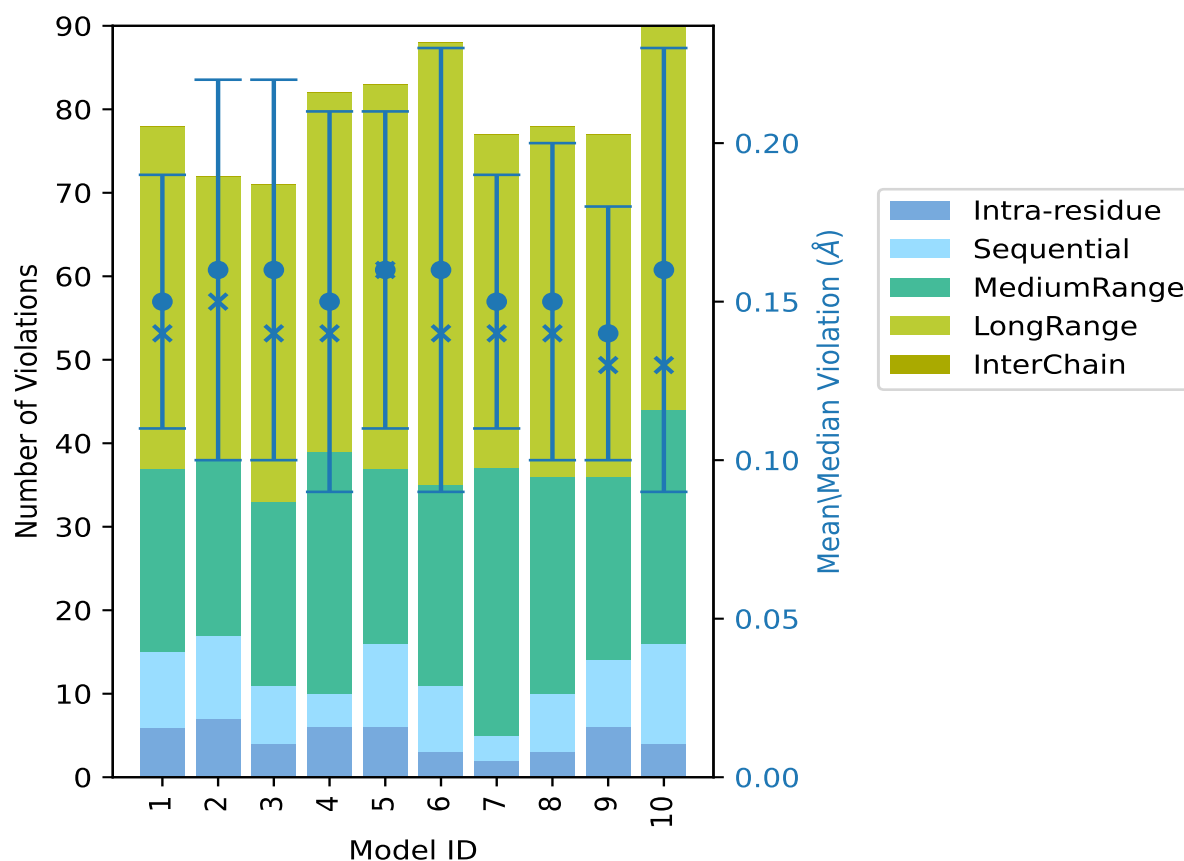
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	6	9	22	41	0	78	0.15	0.3	0.04	0.14
2	7	10	21	34	0	72	0.16	0.34	0.06	0.15
3	4	7	22	38	0	71	0.16	0.42	0.06	0.14
4	6	4	29	43	0	82	0.15	0.58	0.06	0.14
5	6	10	21	46	0	83	0.16	0.35	0.05	0.16
6	3	8	24	53	0	88	0.16	0.72	0.07	0.14
7	2	3	32	40	0	77	0.15	0.26	0.04	0.14
8	3	7	26	42	0	78	0.15	0.43	0.05	0.14
9	6	8	22	41	0	77	0.14	0.28	0.04	0.13
10	4	12	28	46	0	90	0.16	0.54	0.07	0.13

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 [i](#)



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 [i](#)

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, 1458(IR:256, SQ:397, MR:423, LR:382, 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	%
12	29	77	127	0	245	1	10.0
8	8	26	61	0	103	2	20.0
5	2	12	22	0	41	3	30.0

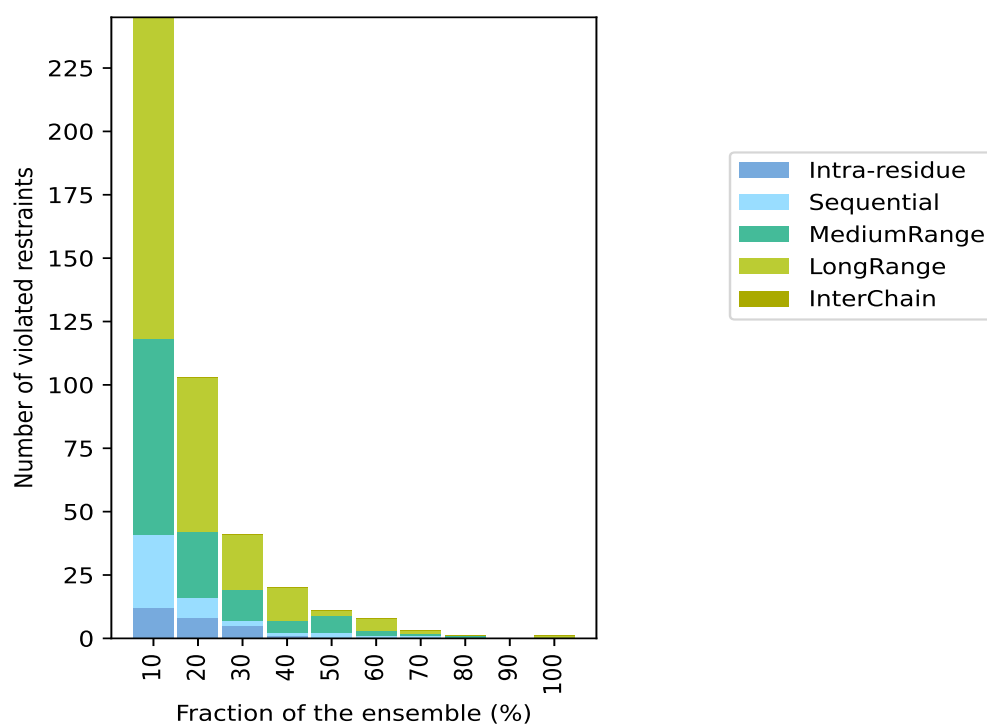
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	1	5	13	0	20	4	40.0
0	2	7	2	0	11	5	50.0
0	1	2	5	0	8	6	60.0
0	1	1	1	0	3	7	70.0
0	0	1	0	0	1	8	80.0
0	0	0	0	0	0	9	90.0
0	0	0	1	0	1	10	100.0

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 ⓘ

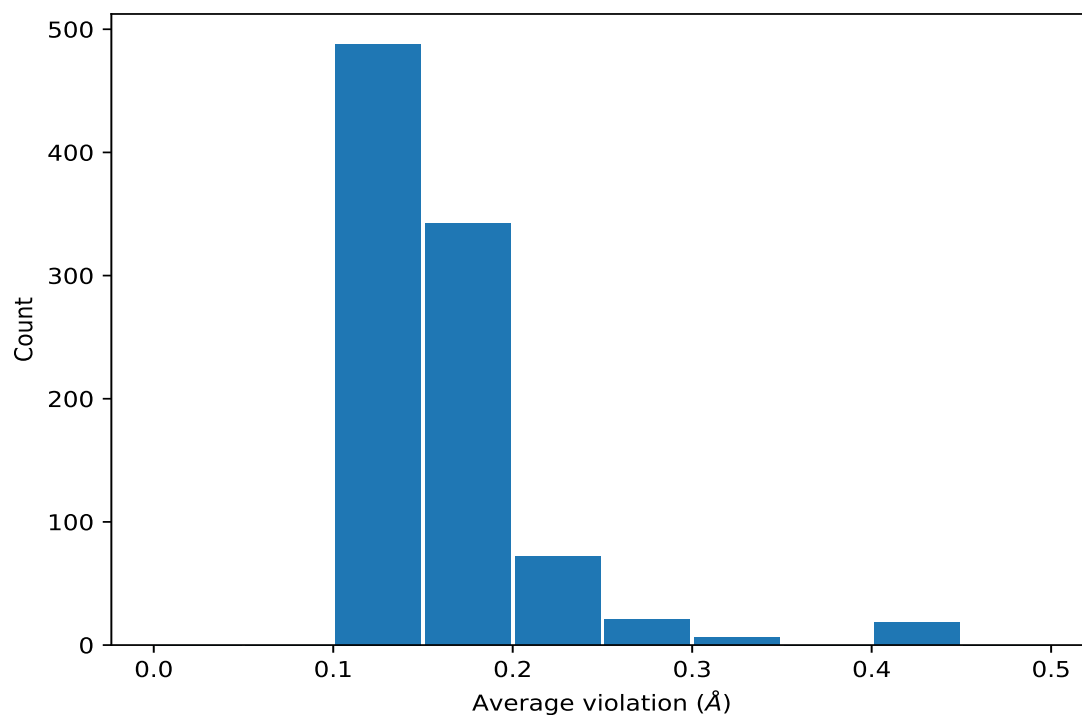


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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)
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	10	0.17	0.03	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	10	0.17	0.03	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	10	0.17	0.03	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	10	0.17	0.03	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	10	0.17	0.03	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	10	0.17	0.03	0.16
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	8	0.15	0.03	0.16
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	8	0.15	0.03	0.16
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	8	0.15	0.03	0.16
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD11	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD12	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD13	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD11	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD12	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD13	7	0.41	0.21	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD11	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD12	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD13	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD21	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD22	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD23	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD21	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD22	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD23	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD21	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD22	7	0.41	0.21	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD23	7	0.41	0.21	0.43
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG21	7	0.18	0.05	0.18
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG22	7	0.18	0.05	0.18
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG23	7	0.18	0.05	0.18
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD11	7	0.17	0.06	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD12	7	0.17	0.06	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD13	7	0.17	0.06	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD21	7	0.17	0.06	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD22	7	0.17	0.06	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD23	7	0.17	0.06	0.17
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD11	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD12	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD13	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD11	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD12	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD13	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD11	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD12	6	0.28	0.08	0.28
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD13	6	0.28	0.08	0.28
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD21	6	0.18	0.05	0.16
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD22	6	0.18	0.05	0.16
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD23	6	0.18	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD21	6	0.18	0.05	0.16
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD22	6	0.18	0.05	0.16
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD23	6	0.18	0.05	0.16
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD21	6	0.18	0.05	0.16
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD22	6	0.18	0.05	0.16
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD23	6	0.18	0.05	0.16
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD21	6	0.17	0.04	0.19
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD22	6	0.17	0.04	0.19
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD23	6	0.17	0.04	0.19
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB1	6	0.15	0.04	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB2	6	0.15	0.04	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB3	6	0.15	0.04	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB1	6	0.15	0.04	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB2	6	0.15	0.04	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB3	6	0.15	0.04	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB1	6	0.15	0.04	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB2	6	0.15	0.04	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB3	6	0.15	0.04	0.14
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB1	6	0.15	0.03	0.14
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB2	6	0.15	0.03	0.14
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB3	6	0.15	0.03	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG21	6	0.15	0.02	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG22	6	0.15	0.02	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG23	6	0.15	0.02	0.14
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD21	6	0.14	0.03	0.13
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD22	6	0.14	0.03	0.13
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD23	6	0.14	0.03	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG11	6	0.13	0.02	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG12	6	0.13	0.02	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG13	6	0.13	0.02	0.13
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD21	5	0.24	0.06	0.23
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD22	5	0.24	0.06	0.23
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD23	5	0.24	0.06	0.23
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG21	5	0.18	0.04	0.21
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG22	5	0.18	0.04	0.21
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG23	5	0.18	0.04	0.21
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB1	5	0.18	0.06	0.14
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB2	5	0.18	0.06	0.14
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB3	5	0.18	0.06	0.14
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB1	5	0.18	0.06	0.14
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB2	5	0.18	0.06	0.14
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB3	5	0.18	0.06	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB1	5	0.18	0.06	0.14
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB2	5	0.18	0.06	0.14
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB3	5	0.18	0.06	0.14
(1,1641)	1:211:A:SER:H	1:207:A:VAL:HA	5	0.17	0.05	0.17
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG21	5	0.16	0.04	0.16
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG22	5	0.16	0.04	0.16
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG23	5	0.16	0.04	0.16
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG21	5	0.16	0.04	0.16
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG22	5	0.16	0.04	0.16
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG23	5	0.16	0.04	0.16
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG21	5	0.16	0.04	0.16
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG22	5	0.16	0.04	0.16
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG23	5	0.16	0.04	0.16
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB1	5	0.16	0.03	0.16
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB2	5	0.16	0.03	0.16
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB3	5	0.16	0.03	0.16
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD11	5	0.15	0.04	0.13
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD12	5	0.15	0.04	0.13
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD13	5	0.15	0.04	0.13
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD11	5	0.15	0.04	0.13
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD12	5	0.15	0.04	0.13
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD13	5	0.15	0.04	0.13
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD11	5	0.15	0.04	0.13
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD12	5	0.15	0.04	0.13
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD13	5	0.15	0.04	0.13
(1,1605)	1:36:A:GLU:H	1:32:A:LEU:HA	5	0.13	0.02	0.12
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG11	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG12	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG13	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG11	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG12	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG13	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG11	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG12	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG13	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	5	0.13	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	5	0.13	0.03	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	5	0.13	0.03	0.13
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA2	5	0.13	0.02	0.14
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA3	5	0.13	0.02	0.14
(1,419)	1:103:A:LEU:H	1:107:A:LEU:H	5	0.12	0.01	0.12
(1,1647)	1:98:A:MET:H	1:154:A:HIS:H	4	0.2	0.06	0.19
(1,1760)	1:184:A:THR:H	1:152:A:THR:HA	4	0.2	0.05	0.2
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD11	4	0.19	0.04	0.18
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD12	4	0.19	0.04	0.18
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD13	4	0.19	0.04	0.18
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD11	4	0.19	0.04	0.18
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD12	4	0.19	0.04	0.18
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD13	4	0.19	0.04	0.18
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD11	4	0.19	0.04	0.18
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD12	4	0.19	0.04	0.18
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD13	4	0.19	0.04	0.18
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD11	4	0.17	0.03	0.17
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD12	4	0.17	0.03	0.17
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD13	4	0.17	0.03	0.17
(1,1709)	1:152:A:THR:H	1:184:A:THR:HA	4	0.16	0.02	0.16
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD11	4	0.15	0.03	0.15
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD12	4	0.15	0.03	0.15
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD13	4	0.15	0.03	0.15
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD11	4	0.15	0.03	0.15
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD12	4	0.15	0.03	0.15
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD13	4	0.15	0.03	0.15
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD11	4	0.15	0.03	0.15
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD12	4	0.15	0.03	0.15
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD13	4	0.15	0.03	0.15
(1,1873)	1:126:A:ALA:H	1:122:A:LEU:HA	4	0.15	0.01	0.16
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG21	4	0.15	0.04	0.16
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG22	4	0.15	0.04	0.16
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG23	4	0.15	0.04	0.16
(1,1672)	1:83:A:ASN:H	1:84:A:LYS:HA	4	0.15	0.04	0.16
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	4	0.15	0.03	0.16
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	4	0.15	0.03	0.16
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	4	0.15	0.03	0.16
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	4	0.15	0.03	0.16
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	4	0.15	0.03	0.16
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	4	0.15	0.03	0.16
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	4	0.15	0.03	0.16
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	4	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	4	0.15	0.03	0.16
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG21	4	0.15	0.04	0.15
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG22	4	0.15	0.04	0.15
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG23	4	0.15	0.04	0.15
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG21	4	0.15	0.04	0.15
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG22	4	0.15	0.04	0.15
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG23	4	0.15	0.04	0.15
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG21	4	0.15	0.04	0.15
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG22	4	0.15	0.04	0.15
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG23	4	0.15	0.04	0.15
(1,1584)	1:197:A:TYR:H	1:194:A:GLN:HA	4	0.15	0.01	0.15
(1,1504)	1:143:A:LEU:H	1:141:A:ALA:HA	4	0.14	0.02	0.15
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG21	4	0.14	0.01	0.14
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG22	4	0.14	0.01	0.14
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG23	4	0.14	0.01	0.14
(1,1505)	1:144:A:VAL:H	1:142:A:TYR:HA	4	0.14	0.03	0.14
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD21	4	0.14	0.02	0.14
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD22	4	0.14	0.02	0.14
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD23	4	0.14	0.02	0.14
(1,1575)	1:106:A:ASN:H	1:103:A:LEU:HA	4	0.12	0.01	0.12
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA2	4	0.11	0.01	0.11
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA3	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE1	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE2	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE3	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE1	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE2	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE3	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE1	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE2	4	0.11	0.01	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE3	4	0.11	0.01	0.11
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD11	4	0.11	0.01	0.11
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD12	4	0.11	0.01	0.11
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD13	4	0.11	0.01	0.11
(1,1789)	1:98:A:MET:H	1:153:A:LYS:HA	3	0.22	0.02	0.23
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG21	3	0.21	0.04	0.23
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG22	3	0.21	0.04	0.23
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG23	3	0.21	0.04	0.23
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG21	3	0.21	0.04	0.23
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG22	3	0.21	0.04	0.23
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG23	3	0.21	0.04	0.23
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG21	3	0.21	0.04	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG22	3	0.21	0.04	0.23
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG23	3	0.21	0.04	0.23
(1,335)	1:62:A:GLU:H	1:65:A:THR:H	3	0.2	0.02	0.21
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	3	0.2	0.05	0.23
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	3	0.2	0.05	0.23
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	3	0.2	0.05	0.23
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	3	0.2	0.05	0.23
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	3	0.2	0.05	0.23
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	3	0.2	0.05	0.23
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	3	0.2	0.05	0.23
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	3	0.2	0.05	0.23
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	3	0.2	0.05	0.23
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG11	3	0.2	0.06	0.17
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG12	3	0.2	0.06	0.17
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG13	3	0.2	0.06	0.17
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG11	3	0.2	0.06	0.17
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG12	3	0.2	0.06	0.17
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG13	3	0.2	0.06	0.17
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG11	3	0.2	0.06	0.17
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG12	3	0.2	0.06	0.17
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG13	3	0.2	0.06	0.17
(1,1544)	1:45:A:LEU:H	1:42:A:GLU:HA	3	0.19	0.05	0.2
(1,1860)	1:125:A:GLY:H	1:122:A:LEU:HA	3	0.19	0.05	0.21
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB1	3	0.18	0.03	0.2
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB2	3	0.18	0.03	0.2
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB3	3	0.18	0.03	0.2
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB1	3	0.18	0.03	0.2
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB2	3	0.18	0.03	0.2
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB3	3	0.18	0.03	0.2
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB1	3	0.18	0.03	0.2
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB2	3	0.18	0.03	0.2
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB3	3	0.18	0.03	0.2
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD11	3	0.18	0.02	0.18
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD12	3	0.18	0.02	0.18
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD13	3	0.18	0.02	0.18
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD11	3	0.18	0.06	0.17
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD12	3	0.18	0.06	0.17
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD13	3	0.18	0.06	0.17
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD11	3	0.18	0.04	0.2
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD12	3	0.18	0.04	0.2
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD13	3	0.18	0.04	0.2
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD21	3	0.17	0.08	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD22	3	0.17	0.08	0.12
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD23	3	0.17	0.08	0.12
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD21	3	0.17	0.08	0.12
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD22	3	0.17	0.08	0.12
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD23	3	0.17	0.08	0.12
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD21	3	0.17	0.08	0.12
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD22	3	0.17	0.08	0.12
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD23	3	0.17	0.08	0.12
(1,1788)	1:97:A:GLY:H	1:183:A:GLY:HA2	3	0.17	0.01	0.16
(1,1788)	1:97:A:GLY:H	1:183:A:GLY:HA3	3	0.17	0.01	0.16
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG21	3	0.17	0.04	0.17
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG22	3	0.17	0.04	0.17
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG23	3	0.17	0.04	0.17
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG21	3	0.16	0.02	0.15
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG22	3	0.16	0.02	0.15
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG23	3	0.16	0.02	0.15
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE1	3	0.16	0.05	0.15
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE2	3	0.16	0.05	0.15
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE3	3	0.16	0.05	0.15
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG21	3	0.16	0.02	0.15
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG22	3	0.16	0.02	0.15
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG23	3	0.16	0.02	0.15
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG21	3	0.16	0.02	0.15
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG22	3	0.16	0.02	0.15
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG23	3	0.16	0.02	0.15
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG21	3	0.16	0.02	0.15
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG22	3	0.16	0.02	0.15
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG23	3	0.16	0.02	0.15
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG21	3	0.15	0.02	0.16
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG22	3	0.15	0.02	0.16
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG23	3	0.15	0.02	0.16
(1,391)	1:58:A:LYS:H	1:96:A:ILE:H	3	0.15	0.04	0.13
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD11	3	0.15	0.02	0.14
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD12	3	0.15	0.02	0.14
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD13	3	0.15	0.02	0.14
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB1	3	0.15	0.03	0.15
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB2	3	0.15	0.03	0.15
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB3	3	0.15	0.03	0.15
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG11	3	0.14	0.01	0.13
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG12	3	0.14	0.01	0.13
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG13	3	0.14	0.01	0.13
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	3	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	3	0.14	0.02	0.14
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	3	0.14	0.02	0.14
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	3	0.14	0.02	0.14
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	3	0.14	0.02	0.14
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	3	0.14	0.02	0.14
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	3	0.14	0.02	0.14
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	3	0.14	0.02	0.14
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	3	0.14	0.02	0.14
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD11	3	0.13	0.04	0.11
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD12	3	0.13	0.04	0.11
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD13	3	0.13	0.04	0.11
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG11	3	0.13	0.02	0.13
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG12	3	0.13	0.02	0.13
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG13	3	0.13	0.02	0.13
(1,1564)	1:65:A:THR:H	1:62:A:GLU:HA	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD21	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD22	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD23	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD21	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD22	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD23	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD21	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD22	3	0.13	0.01	0.13
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD23	3	0.13	0.01	0.13
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD11	3	0.13	0.02	0.13
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD12	3	0.13	0.02	0.13
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD13	3	0.13	0.02	0.13
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD11	3	0.13	0.02	0.13
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD12	3	0.13	0.02	0.13
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD13	3	0.13	0.02	0.13
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD11	3	0.13	0.02	0.13
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD12	3	0.13	0.02	0.13
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD13	3	0.13	0.02	0.13
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE1	3	0.13	0.03	0.12
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE2	3	0.13	0.03	0.12
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE3	3	0.13	0.03	0.12
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE1	3	0.13	0.03	0.12
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE2	3	0.13	0.03	0.12
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE3	3	0.13	0.03	0.12
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE1	3	0.13	0.03	0.12
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE2	3	0.13	0.03	0.12
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE3	3	0.13	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD11	3	0.13	0.01	0.14
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD12	3	0.13	0.01	0.14
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD13	3	0.13	0.01	0.14
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD11	3	0.13	0.01	0.13
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD12	3	0.13	0.01	0.13
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD13	3	0.13	0.01	0.13
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD21	3	0.13	0.03	0.11
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD22	3	0.13	0.03	0.11
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD23	3	0.13	0.03	0.11
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD21	3	0.13	0.03	0.11
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD22	3	0.13	0.03	0.11
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD23	3	0.13	0.03	0.11
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD21	3	0.13	0.03	0.11
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD22	3	0.13	0.03	0.11
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD23	3	0.13	0.03	0.11
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD11	3	0.13	0.01	0.13
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD12	3	0.13	0.01	0.13
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD13	3	0.13	0.01	0.13
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD11	3	0.13	0.01	0.13
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD12	3	0.13	0.01	0.13
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD13	3	0.13	0.01	0.13
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD11	3	0.13	0.01	0.13
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD12	3	0.13	0.01	0.13
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD13	3	0.13	0.01	0.13
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD11	3	0.13	0.01	0.12
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD12	3	0.13	0.01	0.12
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD13	3	0.13	0.01	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD11	3	0.13	0.01	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD12	3	0.13	0.01	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD13	3	0.13	0.01	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD11	3	0.13	0.01	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD12	3	0.13	0.01	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD13	3	0.13	0.01	0.12
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD11	3	0.13	0.01	0.13
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD12	3	0.13	0.01	0.13
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD13	3	0.13	0.01	0.13
(1,1597)	1:214:A:ILE:H	1:211:A:SER:HA	3	0.13	0.02	0.11
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG21	3	0.12	0.02	0.11
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG22	3	0.12	0.02	0.11
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG23	3	0.12	0.02	0.11
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG21	3	0.12	0.02	0.11
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG22	3	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG23	3	0.12	0.02	0.11
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG21	3	0.12	0.02	0.11
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG22	3	0.12	0.02	0.11
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG23	3	0.12	0.02	0.11
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD11	3	0.12	0.01	0.13
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD12	3	0.12	0.01	0.13
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD13	3	0.12	0.01	0.13
(1,1642)	1:212:A:GLN:H	1:208:A:LYS:HA	3	0.12	0.02	0.11
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD11	3	0.11	0.01	0.11
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD12	3	0.11	0.01	0.11
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD13	3	0.11	0.01	0.11
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD11	3	0.11	0.01	0.11
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD12	3	0.11	0.01	0.11
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD13	3	0.11	0.01	0.11
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD11	3	0.11	0.01	0.11
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD12	3	0.11	0.01	0.11
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD13	3	0.11	0.01	0.11
(1,1254)	1:181:A:GLY:H	1:181:A:GLY:HA2	3	0.1	0.0	0.1
(1,1254)	1:181:A:GLY:H	1:181:A:GLY:HA3	3	0.1	0.0	0.1
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE1	2	0.32	0.1	0.32
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE2	2	0.32	0.1	0.32
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE3	2	0.32	0.1	0.32
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE1	2	0.32	0.1	0.32
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE2	2	0.32	0.1	0.32
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE3	2	0.32	0.1	0.32
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD11	2	0.26	0.02	0.26
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD12	2	0.26	0.02	0.26
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD13	2	0.26	0.02	0.26
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG11	2	0.24	0.02	0.24
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG12	2	0.24	0.02	0.24
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG13	2	0.24	0.02	0.24
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG11	2	0.24	0.02	0.24
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG12	2	0.24	0.02	0.24
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG13	2	0.24	0.02	0.24
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG11	2	0.24	0.02	0.24
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG12	2	0.24	0.02	0.24
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG13	2	0.24	0.02	0.24
(1,317)	1:211:A:SER:H	1:213:A:PHE:H	2	0.21	0.0	0.21
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG11	2	0.2	0.03	0.2
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG12	2	0.2	0.03	0.2
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG13	2	0.2	0.03	0.2
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG21	2	0.2	0.03	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG22	2	0.2	0.03	0.2
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG23	2	0.2	0.03	0.2
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD11	2	0.2	0.06	0.2
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD12	2	0.2	0.06	0.2
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD13	2	0.2	0.06	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD11	2	0.2	0.0	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD12	2	0.2	0.0	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD13	2	0.2	0.0	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD11	2	0.2	0.0	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD12	2	0.2	0.0	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD13	2	0.2	0.0	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD11	2	0.2	0.0	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD12	2	0.2	0.0	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD13	2	0.2	0.0	0.2
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD11	2	0.2	0.02	0.2
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD12	2	0.2	0.02	0.2
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD13	2	0.2	0.02	0.2
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD11	2	0.2	0.04	0.2
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD12	2	0.2	0.04	0.2
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD13	2	0.2	0.04	0.2
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG11	2	0.2	0.04	0.2
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG12	2	0.2	0.04	0.2
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG13	2	0.2	0.04	0.2
(1,1577)	1:139:A:TYR:H	1:136:A:VAL:HA	2	0.2	0.02	0.2
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD11	2	0.19	0.04	0.19
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD12	2	0.19	0.04	0.19
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD13	2	0.19	0.04	0.19
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD11	2	0.19	0.04	0.19
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD12	2	0.19	0.04	0.19
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD13	2	0.19	0.04	0.19
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD11	2	0.19	0.04	0.19
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD12	2	0.19	0.04	0.19
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD13	2	0.19	0.04	0.19
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	2	0.19	0.07	0.19
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	2	0.19	0.07	0.19
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	2	0.19	0.07	0.19
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	2	0.19	0.07	0.19
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	2	0.19	0.07	0.19
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	2	0.19	0.07	0.19
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	2	0.19	0.07	0.19
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	2	0.19	0.07	0.19
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	2	0.19	0.07	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD11	2	0.18	0.08	0.18
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD12	2	0.18	0.08	0.18
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD13	2	0.18	0.08	0.18
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD11	2	0.18	0.08	0.18
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD12	2	0.18	0.08	0.18
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD13	2	0.18	0.08	0.18
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD11	2	0.18	0.08	0.18
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD12	2	0.18	0.08	0.18
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD13	2	0.18	0.08	0.18
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD21	2	0.18	0.02	0.18
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD22	2	0.18	0.02	0.18
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD23	2	0.18	0.02	0.18
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD21	2	0.18	0.02	0.18
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD22	2	0.18	0.02	0.18
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD23	2	0.18	0.02	0.18
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD21	2	0.18	0.02	0.18
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD22	2	0.18	0.02	0.18
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD23	2	0.18	0.02	0.18
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG21	2	0.18	0.04	0.18
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG22	2	0.18	0.04	0.18
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG23	2	0.18	0.04	0.18
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG21	2	0.18	0.04	0.18
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG22	2	0.18	0.04	0.18
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG23	2	0.18	0.04	0.18
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG21	2	0.18	0.04	0.18
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG22	2	0.18	0.04	0.18
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG23	2	0.18	0.04	0.18
(1,1875)	1:111:A:ALA:H	1:114:A:GLY:H	2	0.18	0.02	0.18
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG21	2	0.18	0.05	0.18
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG22	2	0.18	0.05	0.18
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG23	2	0.18	0.05	0.18
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG21	2	0.18	0.05	0.18
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG22	2	0.18	0.05	0.18
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG23	2	0.18	0.05	0.18
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG21	2	0.18	0.05	0.18
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG22	2	0.18	0.05	0.18
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG23	2	0.18	0.05	0.18
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD11	2	0.18	0.04	0.18
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD12	2	0.18	0.04	0.18
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD13	2	0.18	0.04	0.18
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	2	0.18	0.0	0.18
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	2	0.18	0.0	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	2	0.18	0.0	0.18
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	2	0.18	0.0	0.18
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	2	0.18	0.0	0.18
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	2	0.18	0.0	0.18
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	2	0.18	0.0	0.18
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	2	0.18	0.0	0.18
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	2	0.18	0.0	0.18
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	2	0.18	0.03	0.18
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	2	0.18	0.03	0.18
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	2	0.18	0.03	0.18
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	2	0.18	0.03	0.18
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	2	0.18	0.03	0.18
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	2	0.18	0.03	0.18
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	2	0.18	0.03	0.18
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	2	0.18	0.03	0.18
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	2	0.18	0.03	0.18
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG11	2	0.18	0.06	0.18
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG12	2	0.18	0.06	0.18
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG13	2	0.18	0.06	0.18
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG11	2	0.18	0.06	0.18
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG12	2	0.18	0.06	0.18
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG13	2	0.18	0.06	0.18
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG11	2	0.18	0.06	0.18
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG12	2	0.18	0.06	0.18
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG13	2	0.18	0.06	0.18
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD21	2	0.18	0.02	0.18
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD22	2	0.18	0.02	0.18
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD23	2	0.18	0.02	0.18
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG11	2	0.18	0.0	0.18
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG12	2	0.18	0.0	0.18
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG13	2	0.18	0.0	0.18
(1,1456)	1:41:A:LYS:H	1:39:A:SER:HA	2	0.18	0.03	0.18
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD21	2	0.17	0.03	0.17
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD22	2	0.17	0.03	0.17
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD23	2	0.17	0.03	0.17
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD21	2	0.17	0.03	0.17
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD22	2	0.17	0.03	0.17
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD23	2	0.17	0.03	0.17
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD21	2	0.17	0.03	0.17
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD22	2	0.17	0.03	0.17
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD23	2	0.17	0.03	0.17
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG11	2	0.17	0.01	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG12	2	0.17	0.01	0.17
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG13	2	0.17	0.01	0.17
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD11	2	0.17	0.04	0.17
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD12	2	0.17	0.04	0.17
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD13	2	0.17	0.04	0.17
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG21	2	0.16	0.04	0.16
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG22	2	0.16	0.04	0.16
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG23	2	0.16	0.04	0.16
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG21	2	0.16	0.04	0.16
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG22	2	0.16	0.04	0.16
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG23	2	0.16	0.04	0.16
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG21	2	0.16	0.04	0.16
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG22	2	0.16	0.04	0.16
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG23	2	0.16	0.04	0.16
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG21	2	0.16	0.01	0.16
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG22	2	0.16	0.01	0.16
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG23	2	0.16	0.01	0.16
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD11	2	0.16	0.01	0.16
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD12	2	0.16	0.01	0.16
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD13	2	0.16	0.01	0.16
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD11	2	0.16	0.02	0.16
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD12	2	0.16	0.02	0.16
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD13	2	0.16	0.02	0.16
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD11	2	0.16	0.01	0.16
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD12	2	0.16	0.01	0.16
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD13	2	0.16	0.01	0.16
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD11	2	0.16	0.01	0.16
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD12	2	0.16	0.01	0.16
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD13	2	0.16	0.01	0.16
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD11	2	0.16	0.01	0.16
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD12	2	0.16	0.01	0.16
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD13	2	0.16	0.01	0.16
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD11	2	0.16	0.06	0.16
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD12	2	0.16	0.06	0.16
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD13	2	0.16	0.06	0.16
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD11	2	0.16	0.06	0.16
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD12	2	0.16	0.06	0.16
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD13	2	0.16	0.06	0.16
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD11	2	0.16	0.06	0.16
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD12	2	0.16	0.06	0.16
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD13	2	0.16	0.06	0.16
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	2	0.16	0.06	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	2	0.16	0.06	0.16
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	2	0.16	0.06	0.16
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	2	0.16	0.06	0.16
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	2	0.16	0.06	0.16
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	2	0.16	0.06	0.16
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	2	0.16	0.06	0.16
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	2	0.16	0.06	0.16
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	2	0.16	0.06	0.16
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD21	2	0.16	0.03	0.16
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD22	2	0.16	0.03	0.16
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD23	2	0.16	0.03	0.16
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD21	2	0.16	0.03	0.16
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD22	2	0.16	0.03	0.16
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD23	2	0.16	0.03	0.16
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD21	2	0.16	0.03	0.16
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD22	2	0.16	0.03	0.16
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD23	2	0.16	0.03	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD11	2	0.16	0.0	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD12	2	0.16	0.0	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD13	2	0.16	0.0	0.16
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG21	2	0.16	0.0	0.16
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG22	2	0.16	0.0	0.16
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG23	2	0.16	0.0	0.16
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD21	2	0.16	0.01	0.16
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD22	2	0.16	0.01	0.16
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD23	2	0.16	0.01	0.16
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD21	2	0.16	0.05	0.16
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD22	2	0.16	0.05	0.16
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD23	2	0.16	0.05	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG21	2	0.16	0.0	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG22	2	0.16	0.0	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG23	2	0.16	0.0	0.16
(1,1664)	1:79:A:ASN:H	1:93:A:ASP:HA	2	0.16	0.04	0.16
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD11	2	0.16	0.02	0.16
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD12	2	0.16	0.02	0.16
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD13	2	0.16	0.02	0.16
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD11	2	0.16	0.02	0.16
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD12	2	0.16	0.02	0.16
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD13	2	0.16	0.02	0.16
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD11	2	0.16	0.02	0.16
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD12	2	0.16	0.02	0.16
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD13	2	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	2	0.16	0.02	0.16
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	2	0.16	0.02	0.16
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	2	0.16	0.02	0.16
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	2	0.16	0.02	0.16
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	2	0.16	0.02	0.16
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	2	0.16	0.02	0.16
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	2	0.16	0.02	0.16
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	2	0.16	0.02	0.16
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	2	0.16	0.02	0.16
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD11	2	0.16	0.04	0.16
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD12	2	0.16	0.04	0.16
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD13	2	0.16	0.04	0.16
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD11	2	0.16	0.04	0.16
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD12	2	0.16	0.04	0.16
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD13	2	0.16	0.04	0.16
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD11	2	0.16	0.04	0.16
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD12	2	0.16	0.04	0.16
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD13	2	0.16	0.04	0.16
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	2	0.16	0.01	0.16
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	2	0.16	0.01	0.16
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	2	0.16	0.01	0.16
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	2	0.16	0.01	0.16
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	2	0.16	0.01	0.16
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	2	0.16	0.01	0.16
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	2	0.16	0.01	0.16
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	2	0.16	0.01	0.16
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	2	0.16	0.01	0.16
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD21	2	0.16	0.02	0.16
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD22	2	0.16	0.02	0.16
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD23	2	0.16	0.02	0.16
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD21	2	0.16	0.02	0.16
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD22	2	0.16	0.02	0.16
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD23	2	0.16	0.02	0.16
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD21	2	0.16	0.02	0.16
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD22	2	0.16	0.02	0.16
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD23	2	0.16	0.02	0.16
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG21	2	0.16	0.05	0.16
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG22	2	0.16	0.05	0.16
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG23	2	0.16	0.05	0.16
(1,980)	1:152:A:THR:H	1:184:A:THR:HG21	2	0.16	0.01	0.16
(1,980)	1:152:A:THR:H	1:184:A:THR:HG22	2	0.16	0.01	0.16
(1,980)	1:152:A:THR:H	1:184:A:THR:HG23	2	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG21	2	0.15	0.01	0.15
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG22	2	0.15	0.01	0.15
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG23	2	0.15	0.01	0.15
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG21	2	0.15	0.01	0.15
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG22	2	0.15	0.01	0.15
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG23	2	0.15	0.01	0.15
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG21	2	0.15	0.01	0.15
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG22	2	0.15	0.01	0.15
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG23	2	0.15	0.01	0.15
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD11	2	0.15	0.01	0.15
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD12	2	0.15	0.01	0.15
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD13	2	0.15	0.01	0.15
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD11	2	0.15	0.01	0.15
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD12	2	0.15	0.01	0.15
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD13	2	0.15	0.01	0.15
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD11	2	0.15	0.04	0.15
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD12	2	0.15	0.04	0.15
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD13	2	0.15	0.04	0.15
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD11	2	0.15	0.04	0.15
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD12	2	0.15	0.04	0.15
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD13	2	0.15	0.04	0.15
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD11	2	0.15	0.04	0.15
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD12	2	0.15	0.04	0.15
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD13	2	0.15	0.04	0.15
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD11	2	0.15	0.0	0.15
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD12	2	0.15	0.0	0.15
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD13	2	0.15	0.0	0.15
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD11	2	0.15	0.0	0.15
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD12	2	0.15	0.0	0.15
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD13	2	0.15	0.0	0.15
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD11	2	0.15	0.0	0.15
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD12	2	0.15	0.0	0.15
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD13	2	0.15	0.0	0.15
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	2	0.15	0.03	0.15
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	2	0.15	0.03	0.15
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	2	0.15	0.03	0.15
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	2	0.15	0.03	0.15
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	2	0.15	0.03	0.15
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	2	0.15	0.03	0.15
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	2	0.15	0.03	0.15
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	2	0.15	0.03	0.15
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	2	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	2	0.15	0.04	0.15
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	2	0.15	0.04	0.15
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	2	0.15	0.04	0.15
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	2	0.15	0.04	0.15
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	2	0.15	0.04	0.15
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	2	0.15	0.04	0.15
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	2	0.15	0.04	0.15
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	2	0.15	0.04	0.15
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	2	0.15	0.04	0.15
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	2	0.15	0.02	0.15
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	2	0.15	0.02	0.15
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	2	0.15	0.02	0.15
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	2	0.15	0.02	0.15
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	2	0.15	0.02	0.15
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	2	0.15	0.02	0.15
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	2	0.15	0.02	0.15
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	2	0.15	0.02	0.15
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG21	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG22	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG23	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG21	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG22	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG23	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG21	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG22	2	0.15	0.02	0.15
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG23	2	0.15	0.02	0.15
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD11	2	0.15	0.0	0.15
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD12	2	0.15	0.0	0.15
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD13	2	0.15	0.0	0.15
(1,1361)	1:96:A:ILE:H	1:95:A:GLY:HA2	2	0.15	0.0	0.15
(1,1361)	1:96:A:ILE:H	1:95:A:GLY:HA3	2	0.15	0.0	0.15
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG11	2	0.14	0.02	0.14
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG12	2	0.14	0.02	0.14
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG13	2	0.14	0.02	0.14
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG11	2	0.14	0.02	0.14
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG12	2	0.14	0.02	0.14
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG13	2	0.14	0.02	0.14
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG11	2	0.14	0.02	0.14
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG12	2	0.14	0.02	0.14
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG13	2	0.14	0.02	0.14
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB1	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB2	2	0.14	0.02	0.14
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB3	2	0.14	0.02	0.14
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB1	2	0.14	0.02	0.14
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB2	2	0.14	0.02	0.14
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB3	2	0.14	0.02	0.14
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB1	2	0.14	0.02	0.14
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB2	2	0.14	0.02	0.14
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB3	2	0.14	0.02	0.14
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG11	2	0.14	0.02	0.14
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG12	2	0.14	0.02	0.14
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG13	2	0.14	0.02	0.14
(1,1240)	1:166:A:ALA:H	1:166:A:ALA:HA	2	0.14	0.01	0.14
(1,1583)	1:195:A:THR:H	1:192:A:GLU:HA	2	0.14	0.02	0.14
(1,1823)	1:126:A:ALA:H	1:125:A:GLY:HA2	2	0.14	0.02	0.14
(1,1823)	1:126:A:ALA:H	1:125:A:GLY:HA3	2	0.14	0.02	0.14
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	2	0.14	0.01	0.14
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	2	0.14	0.01	0.14
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	2	0.14	0.01	0.14
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	2	0.14	0.01	0.14
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	2	0.14	0.01	0.14
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	2	0.14	0.01	0.14
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	2	0.14	0.01	0.14
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	2	0.14	0.01	0.14
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	2	0.14	0.01	0.14
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD11	2	0.14	0.01	0.14
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD12	2	0.14	0.01	0.14
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD13	2	0.14	0.01	0.14
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG21	2	0.14	0.01	0.14
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG22	2	0.14	0.01	0.14
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG23	2	0.14	0.01	0.14
(1,1790)	1:182:A:ARG:H	1:94:A:THR:HA	2	0.14	0.04	0.14
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD21	2	0.13	0.03	0.13
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD22	2	0.13	0.03	0.13
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD23	2	0.13	0.03	0.13
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD21	2	0.13	0.03	0.13
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD22	2	0.13	0.03	0.13
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD23	2	0.13	0.03	0.13
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD21	2	0.13	0.03	0.13
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD22	2	0.13	0.03	0.13
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD23	2	0.13	0.03	0.13
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD11	2	0.13	0.02	0.13
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD12	2	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD13	2	0.13	0.02	0.13
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD11	2	0.13	0.02	0.13
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD12	2	0.13	0.02	0.13
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD13	2	0.13	0.02	0.13
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD11	2	0.13	0.02	0.13
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD12	2	0.13	0.02	0.13
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD13	2	0.13	0.02	0.13
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE1	2	0.13	0.03	0.13
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE2	2	0.13	0.03	0.13
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE3	2	0.13	0.03	0.13
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE1	2	0.13	0.03	0.13
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE2	2	0.13	0.03	0.13
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE3	2	0.13	0.03	0.13
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE1	2	0.13	0.03	0.13
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE2	2	0.13	0.03	0.13
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE3	2	0.13	0.03	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD21	2	0.13	0.0	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD22	2	0.13	0.0	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD23	2	0.13	0.0	0.13
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD11	2	0.13	0.01	0.13
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD12	2	0.13	0.01	0.13
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD13	2	0.13	0.01	0.13
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD11	2	0.13	0.01	0.13
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD12	2	0.13	0.01	0.13
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD13	2	0.13	0.01	0.13
(1,1668)	1:80:A:LEU:H	1:220:A:LEU:HA	2	0.13	0.01	0.13
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD11	2	0.12	0.02	0.12
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD12	2	0.12	0.02	0.12
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD13	2	0.12	0.02	0.12
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD11	2	0.12	0.02	0.12
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD12	2	0.12	0.02	0.12
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD13	2	0.12	0.02	0.12
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD11	2	0.12	0.02	0.12
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD12	2	0.12	0.02	0.12
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD13	2	0.12	0.02	0.12
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	2	0.12	0.01	0.12
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	2	0.12	0.01	0.12
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG21	2	0.12	0.02	0.12
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG22	2	0.12	0.02	0.12
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG23	2	0.12	0.02	0.12
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG21	2	0.12	0.02	0.12
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG22	2	0.12	0.02	0.12
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG23	2	0.12	0.02	0.12
(1,1752)	1:175:A:ASP:H	1:160:A:TYR:HA	2	0.12	0.02	0.12
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD11	2	0.12	0.01	0.12
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD12	2	0.12	0.01	0.12
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD13	2	0.12	0.01	0.12
(1,1657)	1:22:A:PHE:H	1:168:A:GLY:HA2	2	0.12	0.01	0.12
(1,1657)	1:22:A:PHE:H	1:168:A:GLY:HA3	2	0.12	0.01	0.12
(1,1708)	1:152:A:THR:H	1:161:A:ALA:HA	2	0.12	0.0	0.12
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD11	2	0.12	0.02	0.12
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD12	2	0.12	0.02	0.12
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD13	2	0.12	0.02	0.12
(1,1455)	1:36:A:GLU:H	1:34:A:ILE:HA	2	0.12	0.02	0.12
(1,347)	1:104:A:ILE:H	1:107:A:LEU:H	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG11	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG12	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG13	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG11	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG12	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG13	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG11	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG12	2	0.12	0.0	0.12
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG13	2	0.12	0.0	0.12
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD11	2	0.11	0.0	0.11
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD12	2	0.11	0.0	0.11
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD13	2	0.11	0.0	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD11	2	0.11	0.0	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD12	2	0.11	0.0	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD13	2	0.11	0.0	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD11	2	0.11	0.0	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD12	2	0.11	0.0	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD13	2	0.11	0.0	0.11
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD11	2	0.11	0.01	0.11
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD12	2	0.11	0.01	0.11
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD13	2	0.11	0.01	0.11
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD11	2	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD12	2	0.11	0.01	0.11
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD13	2	0.11	0.01	0.11
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD11	2	0.11	0.01	0.11
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD12	2	0.11	0.01	0.11
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD13	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	2	0.11	0.01	0.11
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	2	0.11	0.01	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD11	2	0.11	0.0	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD12	2	0.11	0.0	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD13	2	0.11	0.0	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD11	2	0.11	0.0	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD12	2	0.11	0.0	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD13	2	0.11	0.0	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD11	2	0.11	0.0	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD12	2	0.11	0.0	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD13	2	0.11	0.0	0.11
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG21	2	0.11	0.01	0.11
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG22	2	0.11	0.01	0.11
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG23	2	0.11	0.01	0.11
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG21	2	0.11	0.01	0.11
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG22	2	0.11	0.01	0.11
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG23	2	0.11	0.01	0.11
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG21	2	0.11	0.01	0.11
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG22	2	0.11	0.01	0.11
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG23	2	0.11	0.01	0.11
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE1	2	0.11	0.01	0.11
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE2	2	0.11	0.01	0.11
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE3	2	0.11	0.01	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG21	2	0.11	0.0	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG22	2	0.11	0.0	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG23	2	0.11	0.0	0.11
(1,1251)	1:177:A:GLY:H	1:177:A:GLY:HA2	2	0.11	0.0	0.11
(1,1251)	1:177:A:GLY:H	1:177:A:GLY:HA3	2	0.11	0.0	0.11
(1,1502)	1:139:A:TYR:H	1:137:A:GLY:HA2	2	0.11	0.01	0.11
(1,1502)	1:139:A:TYR:H	1:137:A:GLY:HA3	2	0.11	0.01	0.11

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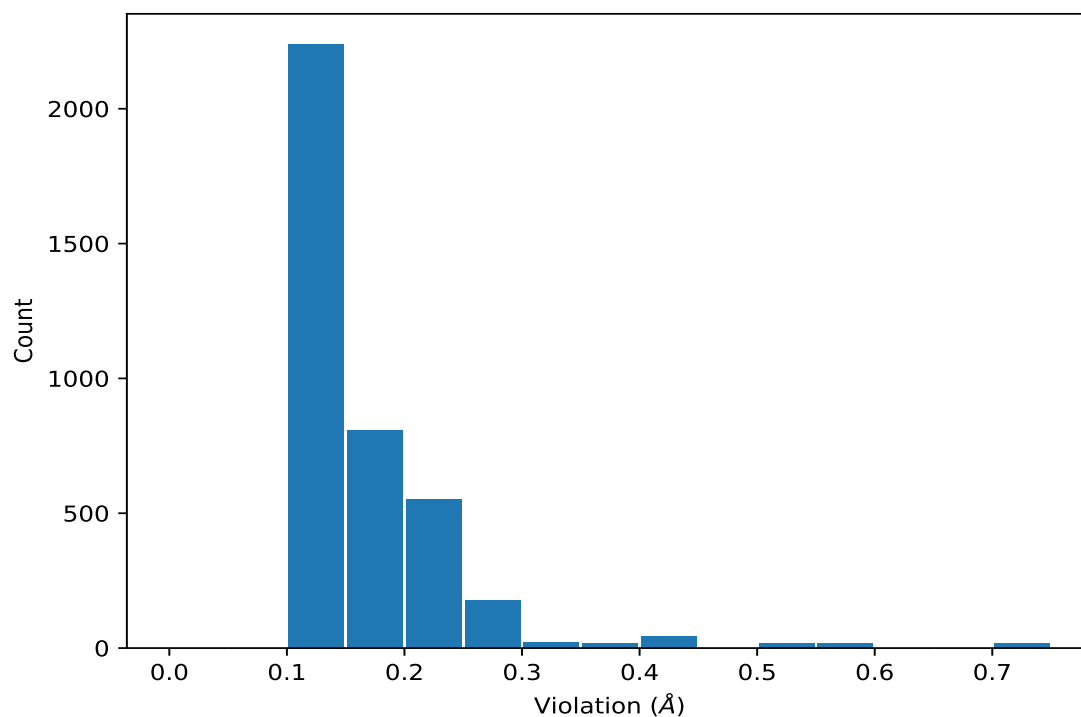
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1842)	1:125:A:GLY:H	1:123:A:GLN:HA	2	0.11	0.01	0.11
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD21	2	0.11	0.0	0.11
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD22	2	0.11	0.0	0.11
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD23	2	0.11	0.0	0.11
(1,1218)	1:137:A:GLY:H	1:137:A:GLY:HA2	2	0.11	0.0	0.11
(1,1218)	1:137:A:GLY:H	1:137:A:GLY:HA3	2	0.11	0.0	0.11
(1,1792)	1:114:A:GLY:H	1:114:A:GLY:HA2	2	0.11	0.0	0.11
(1,1792)	1:114:A:GLY:H	1:114:A:GLY:HA3	2	0.11	0.0	0.11

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)
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD11	6	0.72
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD12	6	0.72
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD13	6	0.72
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD11	6	0.72
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD12	6	0.72
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD13	6	0.72
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD11	6	0.72
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD12	6	0.72
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD13	6	0.72
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD21	6	0.72
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD22	6	0.72
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD23	6	0.72
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD21	6	0.72
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD22	6	0.72
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD23	6	0.72
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD21	6	0.72
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD22	6	0.72
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD23	6	0.72
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD11	4	0.58
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD12	4	0.58
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD13	4	0.58
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD11	4	0.58
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD12	4	0.58
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD13	4	0.58
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD11	4	0.58
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD12	4	0.58
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD13	4	0.58
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD21	4	0.58
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD22	4	0.58
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD23	4	0.58
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD21	4	0.58
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD22	4	0.58
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD23	4	0.58
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD21	4	0.58
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD22	4	0.58
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD23	4	0.58
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD11	10	0.54
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD12	10	0.54
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD13	10	0.54
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD11	10	0.54
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD12	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD13	10	0.54
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD11	10	0.54
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD12	10	0.54
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD13	10	0.54
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD21	10	0.54
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD22	10	0.54
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD23	10	0.54
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD21	10	0.54
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD22	10	0.54
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD23	10	0.54
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD21	10	0.54
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD22	10	0.54
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD23	10	0.54
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD11	8	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD12	8	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD13	8	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD11	8	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD12	8	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD13	8	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD11	8	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD12	8	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD13	8	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD21	8	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD22	8	0.43
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD23	8	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD21	8	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD22	8	0.43
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD23	8	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD21	8	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD22	8	0.43
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD23	8	0.43
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE1	3	0.42
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE2	3	0.42
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE3	3	0.42
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE1	3	0.42
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE2	3	0.42
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE3	3	0.42
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	3	0.42
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	3	0.42
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	3	0.42
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	3	0.42
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	3	0.42
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	3	0.42
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	3	0.42
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	3	0.42
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD11	3	0.42
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD12	3	0.42
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD13	3	0.42
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD11	3	0.42
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD12	3	0.42
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD13	3	0.42
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD11	3	0.42
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD12	3	0.42
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD13	3	0.42
(1,607)	1:104:A:ILE:HD11	1:172:A:VAL:HG11	10	0.37
(1,607)	1:104:A:ILE:HD11	1:172:A:VAL:HG12	10	0.37
(1,607)	1:104:A:ILE:HD11	1:172:A:VAL:HG13	10	0.37
(1,607)	1:104:A:ILE:HD12	1:172:A:VAL:HG11	10	0.37
(1,607)	1:104:A:ILE:HD12	1:172:A:VAL:HG12	10	0.37
(1,607)	1:104:A:ILE:HD12	1:172:A:VAL:HG13	10	0.37
(1,607)	1:104:A:ILE:HD13	1:172:A:VAL:HG11	10	0.37
(1,607)	1:104:A:ILE:HD13	1:172:A:VAL:HG12	10	0.37
(1,607)	1:104:A:ILE:HD13	1:172:A:VAL:HG13	10	0.37
(1,607)	1:104:A:ILE:HD11	1:172:A:VAL:HG21	10	0.37
(1,607)	1:104:A:ILE:HD11	1:172:A:VAL:HG22	10	0.37
(1,607)	1:104:A:ILE:HD11	1:172:A:VAL:HG23	10	0.37
(1,607)	1:104:A:ILE:HD12	1:172:A:VAL:HG21	10	0.37
(1,607)	1:104:A:ILE:HD12	1:172:A:VAL:HG22	10	0.37
(1,607)	1:104:A:ILE:HD12	1:172:A:VAL:HG23	10	0.37
(1,607)	1:104:A:ILE:HD13	1:172:A:VAL:HG21	10	0.37
(1,607)	1:104:A:ILE:HD13	1:172:A:VAL:HG22	10	0.37
(1,607)	1:104:A:ILE:HD13	1:172:A:VAL:HG23	10	0.37
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	5	0.35
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	5	0.35
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	5	0.35
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	5	0.35
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	5	0.35
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	5	0.35
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	5	0.35
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	5	0.35
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	5	0.35
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD11	5	0.35
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD12	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD13	5	0.35
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD11	5	0.35
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD12	5	0.35
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD13	5	0.35
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD11	5	0.35
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD12	5	0.35
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD13	5	0.35
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD21	2	0.34
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD22	2	0.34
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD23	2	0.34
(1,1123)	1:221:A:PHE:H	1:222:A:VAL:HG11	2	0.3
(1,1123)	1:221:A:PHE:H	1:222:A:VAL:HG12	2	0.3
(1,1123)	1:221:A:PHE:H	1:222:A:VAL:HG13	2	0.3
(1,1123)	1:221:A:PHE:H	1:222:A:VAL:HG21	2	0.3
(1,1123)	1:221:A:PHE:H	1:222:A:VAL:HG22	2	0.3
(1,1123)	1:221:A:PHE:H	1:222:A:VAL:HG23	2	0.3
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD11	2	0.3
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD12	2	0.3
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD13	2	0.3
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD21	2	0.3
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD22	2	0.3
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD23	2	0.3
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD11	1	0.3
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD12	1	0.3
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD13	1	0.3
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD11	1	0.3
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD12	1	0.3
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD13	1	0.3
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD11	1	0.3
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD12	1	0.3
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD13	1	0.3
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD21	1	0.3
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD22	1	0.3
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD23	1	0.3
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD21	1	0.3
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD22	1	0.3
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD23	1	0.3
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD21	1	0.3
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD22	1	0.3
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD23	1	0.3
(1,1647)	1:98:A:MET:H	1:154:A:HIS:H	4	0.29
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB1	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB2	10	0.29
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB3	10	0.29
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB1	10	0.29
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB2	10	0.29
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB3	10	0.29
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB1	10	0.29
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB2	10	0.29
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB3	10	0.29
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD11	10	0.28
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD12	10	0.28
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD13	10	0.28
(1,725)	1:203:A:ILE:H	1:203:A:ILE:HD11	2	0.28
(1,725)	1:203:A:ILE:H	1:203:A:ILE:HD12	2	0.28
(1,725)	1:203:A:ILE:H	1:203:A:ILE:HD13	2	0.28
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	9	0.28
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	9	0.28
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	9	0.28
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	9	0.28
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	9	0.28
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	9	0.28
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	9	0.28
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	9	0.28
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	9	0.28
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD11	9	0.28
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD12	9	0.28
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD13	9	0.28
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD11	9	0.28
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD12	9	0.28
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD13	9	0.28
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD11	9	0.28
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD12	9	0.28
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD13	9	0.28
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG11	5	0.28
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG12	5	0.28
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG13	5	0.28
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG11	5	0.28
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG12	5	0.28
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG13	5	0.28
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG11	5	0.28
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG12	5	0.28
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG13	5	0.28
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD21	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD22	10	0.28
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD23	10	0.28
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD21	10	0.28
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD22	10	0.28
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD23	10	0.28
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD21	10	0.28
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD22	10	0.28
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD23	10	0.28
(1,1760)	1:184:A:THR:H	1:152:A:THR:HA	2	0.27
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD11	5	0.27
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD12	5	0.27
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD13	5	0.27
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG21	6	0.27
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG22	6	0.27
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG23	6	0.27
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	6	0.27
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	6	0.27
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	6	0.27
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	6	0.27
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	6	0.27
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	6	0.27
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	6	0.27
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	6	0.27
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	6	0.27
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD11	6	0.27
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD12	6	0.27
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD13	6	0.27
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD11	6	0.27
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD12	6	0.27
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD13	6	0.27
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD11	6	0.27
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD12	6	0.27
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD13	6	0.27
(1,577)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	10	0.27
(1,577)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	10	0.27
(1,577)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	10	0.27
(1,577)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	10	0.27
(1,577)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	10	0.27
(1,577)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	10	0.27
(1,577)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	10	0.27
(1,577)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	10	0.27
(1,577)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD11	4	0.27
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD12	4	0.27
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD13	4	0.27
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD11	4	0.27
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD12	4	0.27
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD13	4	0.27
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD11	4	0.27
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD12	4	0.27
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD13	4	0.27
(1,1503)	1:141:A:ALA:H	1:139:A:TYR:HA	2	0.26
(1,997)	1:163:A:GLU:H	1:171:A:THR:HG21	10	0.26
(1,997)	1:163:A:GLU:H	1:171:A:THR:HG22	10	0.26
(1,997)	1:163:A:GLU:H	1:171:A:THR:HG23	10	0.26
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD11	8	0.26
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD12	8	0.26
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD13	8	0.26
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	2	0.26
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	2	0.26
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	2	0.26
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	2	0.26
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	2	0.26
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	2	0.26
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	2	0.26
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	2	0.26
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	2	0.26
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG11	7	0.26
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG12	7	0.26
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG13	7	0.26
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG11	7	0.26
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG12	7	0.26
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG13	7	0.26
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG11	7	0.26
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG12	7	0.26
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG13	7	0.26
(1,503)	1:32:A:LEU:HD11	1:119:A:MET:HE1	4	0.26
(1,503)	1:32:A:LEU:HD11	1:119:A:MET:HE2	4	0.26
(1,503)	1:32:A:LEU:HD11	1:119:A:MET:HE3	4	0.26
(1,503)	1:32:A:LEU:HD12	1:119:A:MET:HE1	4	0.26
(1,503)	1:32:A:LEU:HD12	1:119:A:MET:HE2	4	0.26
(1,503)	1:32:A:LEU:HD12	1:119:A:MET:HE3	4	0.26
(1,503)	1:32:A:LEU:HD13	1:119:A:MET:HE1	4	0.26
(1,503)	1:32:A:LEU:HD13	1:119:A:MET:HE2	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:32:A:LEU:HD13	1:119:A:MET:HE3	4	0.26
(1,1789)	1:98:A:MET:H	1:153:A:LYS:HA	10	0.25
(1,1641)	1:211:A:SER:H	1:207:A:VAL:HA	6	0.25
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD21	10	0.25
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD22	10	0.25
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD23	10	0.25
(1,832)	1:77:A:HIS:H	1:56:A:LEU:HD21	3	0.25
(1,832)	1:77:A:HIS:H	1:56:A:LEU:HD22	3	0.25
(1,832)	1:77:A:HIS:H	1:56:A:LEU:HD23	3	0.25
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD21	2	0.25
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD22	2	0.25
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD23	2	0.25
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD21	2	0.25
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD22	2	0.25
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD23	2	0.25
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD21	2	0.25
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD22	2	0.25
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD23	2	0.25
(1,1544)	1:45:A:LEU:H	1:42:A:GLU:HA	10	0.24
(1,1040)	1:188:A:LEU:H	1:89:A:LEU:HD21	5	0.24
(1,1040)	1:188:A:LEU:H	1:89:A:LEU:HD22	5	0.24
(1,1040)	1:188:A:LEU:H	1:89:A:LEU:HD23	5	0.24
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG11	9	0.24
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG12	9	0.24
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG13	9	0.24
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG21	8	0.24
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG22	8	0.24
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG23	8	0.24
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD11	8	0.24
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD12	8	0.24
(1,903)	1:111:A:ALA:H	1:26:A:ILE:HD13	8	0.24
(1,788)	1:49:A:ILE:H	1:91:A:ILE:HD11	5	0.24
(1,788)	1:49:A:ILE:H	1:91:A:ILE:HD12	5	0.24
(1,788)	1:49:A:ILE:H	1:91:A:ILE:HD13	5	0.24
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG11	10	0.24
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG12	10	0.24
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG13	10	0.24
(1,659)	1:207:A:VAL:HG21	1:218:A:ILE:HD11	1	0.24
(1,659)	1:207:A:VAL:HG21	1:218:A:ILE:HD12	1	0.24
(1,659)	1:207:A:VAL:HG21	1:218:A:ILE:HD13	1	0.24
(1,659)	1:207:A:VAL:HG22	1:218:A:ILE:HD11	1	0.24
(1,659)	1:207:A:VAL:HG22	1:218:A:ILE:HD12	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:207:A:VAL:HG22	1:218:A:ILE:HD13	1	0.24
(1,659)	1:207:A:VAL:HG23	1:218:A:ILE:HD11	1	0.24
(1,659)	1:207:A:VAL:HG23	1:218:A:ILE:HD12	1	0.24
(1,659)	1:207:A:VAL:HG23	1:218:A:ILE:HD13	1	0.24
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	5	0.24
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	5	0.24
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	5	0.24
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	5	0.24
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	5	0.24
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	5	0.24
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	5	0.24
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	5	0.24
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	5	0.24
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG21	3	0.24
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG22	3	0.24
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG23	3	0.24
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG21	3	0.24
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG22	3	0.24
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG23	3	0.24
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG21	3	0.24
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG22	3	0.24
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG23	3	0.24
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD11	4	0.24
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD12	4	0.24
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD13	4	0.24
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD11	4	0.24
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD12	4	0.24
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD13	4	0.24
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD11	4	0.24
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD12	4	0.24
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD13	4	0.24
(1,542)	1:49:A:ILE:HD11	1:80:A:LEU:HD21	2	0.24
(1,542)	1:49:A:ILE:HD11	1:80:A:LEU:HD22	2	0.24
(1,542)	1:49:A:ILE:HD11	1:80:A:LEU:HD23	2	0.24
(1,542)	1:49:A:ILE:HD12	1:80:A:LEU:HD21	2	0.24
(1,542)	1:49:A:ILE:HD12	1:80:A:LEU:HD22	2	0.24
(1,542)	1:49:A:ILE:HD12	1:80:A:LEU:HD23	2	0.24
(1,542)	1:49:A:ILE:HD13	1:80:A:LEU:HD21	2	0.24
(1,542)	1:49:A:ILE:HD13	1:80:A:LEU:HD22	2	0.24
(1,542)	1:49:A:ILE:HD13	1:80:A:LEU:HD23	2	0.24
(1,530)	1:45:A:LEU:HD21	1:206:A:ILE:HD11	5	0.24
(1,530)	1:45:A:LEU:HD21	1:206:A:ILE:HD12	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:45:A:LEU:HD21	1:206:A:ILE:HD13	5	0.24
(1,530)	1:45:A:LEU:HD22	1:206:A:ILE:HD11	5	0.24
(1,530)	1:45:A:LEU:HD22	1:206:A:ILE:HD12	5	0.24
(1,530)	1:45:A:LEU:HD22	1:206:A:ILE:HD13	5	0.24
(1,530)	1:45:A:LEU:HD23	1:206:A:ILE:HD11	5	0.24
(1,530)	1:45:A:LEU:HD23	1:206:A:ILE:HD12	5	0.24
(1,530)	1:45:A:LEU:HD23	1:206:A:ILE:HD13	5	0.24
(1,388)	1:55:A:ALA:H	1:96:A:ILE:H	10	0.24
(1,77)	1:33:A:ILE:HD11	1:43:A:ILE:HD11	5	0.24
(1,77)	1:33:A:ILE:HD11	1:43:A:ILE:HD12	5	0.24
(1,77)	1:33:A:ILE:HD11	1:43:A:ILE:HD13	5	0.24
(1,77)	1:33:A:ILE:HD12	1:43:A:ILE:HD11	5	0.24
(1,77)	1:33:A:ILE:HD12	1:43:A:ILE:HD12	5	0.24
(1,77)	1:33:A:ILE:HD12	1:43:A:ILE:HD13	5	0.24
(1,77)	1:33:A:ILE:HD13	1:43:A:ILE:HD11	5	0.24
(1,77)	1:33:A:ILE:HD13	1:43:A:ILE:HD12	5	0.24
(1,77)	1:33:A:ILE:HD13	1:43:A:ILE:HD13	5	0.24
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB1	10	0.24
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB2	10	0.24
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB3	10	0.24
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB1	10	0.24
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB2	10	0.24
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB3	10	0.24
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB1	10	0.24
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB2	10	0.24
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB3	10	0.24
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD21	6	0.24
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD22	6	0.24
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD23	6	0.24
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD21	6	0.24
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD22	6	0.24
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD23	6	0.24
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD21	6	0.24
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD22	6	0.24
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD23	6	0.24
(1,1860)	1:125:A:GLY:H	1:122:A:LEU:HA	1	0.23
(1,1789)	1:98:A:MET:H	1:153:A:LYS:HA	4	0.23
(1,1647)	1:98:A:MET:H	1:154:A:HIS:H	6	0.23
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD21	6	0.23
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD22	6	0.23
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD23	6	0.23
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD21	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD22	8	0.23
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD23	8	0.23
(1,941)	1:139:A:TYR:H	1:33:A:ILE:HD11	6	0.23
(1,941)	1:139:A:TYR:H	1:33:A:ILE:HD12	6	0.23
(1,941)	1:139:A:TYR:H	1:33:A:ILE:HD13	6	0.23
(1,731)	1:220:A:LEU:H	1:220:A:LEU:HD11	2	0.23
(1,731)	1:220:A:LEU:H	1:220:A:LEU:HD12	2	0.23
(1,731)	1:220:A:LEU:H	1:220:A:LEU:HD13	2	0.23
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD11	1	0.23
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD12	1	0.23
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD13	1	0.23
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG11	8	0.23
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG12	8	0.23
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG13	8	0.23
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG11	8	0.23
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG12	8	0.23
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG13	8	0.23
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG11	8	0.23
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG12	8	0.23
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG13	8	0.23
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	4	0.23
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	4	0.23
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	4	0.23
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	4	0.23
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	4	0.23
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	4	0.23
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	4	0.23
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	4	0.23
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	4	0.23
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD11	4	0.23
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD12	4	0.23
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD13	4	0.23
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD11	4	0.23
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD12	4	0.23
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD13	4	0.23
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD11	4	0.23
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD12	4	0.23
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD13	4	0.23
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	8	0.23
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	8	0.23
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	8	0.23
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	8	0.23
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	8	0.23
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	8	0.23
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	8	0.23
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	8	0.23
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG21	6	0.23
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG22	6	0.23
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG23	6	0.23
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG21	6	0.23
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG22	6	0.23
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG23	6	0.23
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG21	6	0.23
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG22	6	0.23
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG23	6	0.23
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD11	5	0.23
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD12	5	0.23
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD13	5	0.23
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD11	5	0.23
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD12	5	0.23
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD13	5	0.23
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD11	5	0.23
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD12	5	0.23
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD13	5	0.23
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG21	2	0.23
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG22	2	0.23
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG23	2	0.23
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG21	2	0.23
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG22	2	0.23
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG23	2	0.23
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG21	2	0.23
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG22	2	0.23
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG23	2	0.23
(1,335)	1:62:A:GLU:H	1:65:A:THR:H	2	0.23
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG21	7	0.22
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG22	7	0.22
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG23	7	0.22
(1,1014)	1:175:A:ASP:H	1:176:A:THR:HG21	5	0.22
(1,1014)	1:175:A:ASP:H	1:176:A:THR:HG22	5	0.22
(1,1014)	1:175:A:ASP:H	1:176:A:THR:HG23	5	0.22
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	5	0.22
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	5	0.22
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	5	0.22
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	5	0.22
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	5	0.22
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD11	7	0.22
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD12	7	0.22
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD13	7	0.22
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE1	5	0.22
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE2	5	0.22
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE3	5	0.22
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG21	6	0.22
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG22	6	0.22
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG23	6	0.22
(1,885)	1:93:A:ASP:H	1:92:A:VAL:HG21	10	0.22
(1,885)	1:93:A:ASP:H	1:92:A:VAL:HG22	10	0.22
(1,885)	1:93:A:ASP:H	1:92:A:VAL:HG23	10	0.22
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD11	5	0.22
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD12	5	0.22
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD13	5	0.22
(1,610)	1:107:A:LEU:HD21	1:150:A:VAL:HG11	10	0.22
(1,610)	1:107:A:LEU:HD21	1:150:A:VAL:HG12	10	0.22
(1,610)	1:107:A:LEU:HD21	1:150:A:VAL:HG13	10	0.22
(1,610)	1:107:A:LEU:HD22	1:150:A:VAL:HG11	10	0.22
(1,610)	1:107:A:LEU:HD22	1:150:A:VAL:HG12	10	0.22
(1,610)	1:107:A:LEU:HD22	1:150:A:VAL:HG13	10	0.22
(1,610)	1:107:A:LEU:HD23	1:150:A:VAL:HG11	10	0.22
(1,610)	1:107:A:LEU:HD23	1:150:A:VAL:HG12	10	0.22
(1,610)	1:107:A:LEU:HD23	1:150:A:VAL:HG13	10	0.22
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG21	10	0.22
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG22	10	0.22
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG23	10	0.22
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG21	10	0.22
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG22	10	0.22
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG23	10	0.22
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG21	10	0.22
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG22	10	0.22
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG23	10	0.22
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG11	2	0.22
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG12	2	0.22
(1,568)	1:81:A:ILE:HD11	1:92:A:VAL:HG13	2	0.22
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG11	2	0.22
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG12	2	0.22
(1,568)	1:81:A:ILE:HD12	1:92:A:VAL:HG13	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG11	2	0.22
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG12	2	0.22
(1,568)	1:81:A:ILE:HD13	1:92:A:VAL:HG13	2	0.22
(1,557)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	4	0.22
(1,557)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	4	0.22
(1,557)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	4	0.22
(1,557)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	4	0.22
(1,557)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	4	0.22
(1,557)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	4	0.22
(1,557)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	4	0.22
(1,557)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	4	0.22
(1,557)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	4	0.22
(1,499)	1:29:A:LEU:HD21	1:136:A:VAL:HG21	5	0.22
(1,499)	1:29:A:LEU:HD21	1:136:A:VAL:HG22	5	0.22
(1,499)	1:29:A:LEU:HD21	1:136:A:VAL:HG23	5	0.22
(1,499)	1:29:A:LEU:HD22	1:136:A:VAL:HG21	5	0.22
(1,499)	1:29:A:LEU:HD22	1:136:A:VAL:HG22	5	0.22
(1,499)	1:29:A:LEU:HD22	1:136:A:VAL:HG23	5	0.22
(1,499)	1:29:A:LEU:HD23	1:136:A:VAL:HG21	5	0.22
(1,499)	1:29:A:LEU:HD23	1:136:A:VAL:HG22	5	0.22
(1,499)	1:29:A:LEU:HD23	1:136:A:VAL:HG23	5	0.22
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	3	0.22
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	3	0.22
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	3	0.22
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	3	0.22
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	3	0.22
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	3	0.22
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	3	0.22
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	3	0.22
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	3	0.22
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD11	5	0.22
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD12	5	0.22
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD13	5	0.22
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD11	5	0.22
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD12	5	0.22
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD13	5	0.22
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD11	5	0.22
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD12	5	0.22
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD13	5	0.22
(1,1860)	1:125:A:GLY:H	1:122:A:LEU:HA	8	0.21
(1,1760)	1:184:A:THR:H	1:152:A:THR:HA	1	0.21
(1,1577)	1:139:A:TYR:H	1:136:A:VAL:HA	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE1	10	0.21
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE2	10	0.21
(1,1134)	1:133:A:GLN:HE21	1:130:A:MET:HE3	10	0.21
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE1	10	0.21
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE2	10	0.21
(1,1134)	1:133:A:GLN:HE22	1:130:A:MET:HE3	10	0.21
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD11	9	0.21
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD12	9	0.21
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD13	9	0.21
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG21	1	0.21
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG22	1	0.21
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG23	1	0.21
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG21	10	0.21
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG22	10	0.21
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG23	10	0.21
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	6	0.21
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	6	0.21
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	6	0.21
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	6	0.21
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	6	0.21
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	6	0.21
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	3	0.21
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	3	0.21
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	3	0.21
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD11	1	0.21
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD12	1	0.21
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD13	1	0.21
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG21	2	0.21
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG22	2	0.21
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG23	2	0.21
(1,935)	1:134:A:PHE:H	1:136:A:VAL:HG21	4	0.21
(1,935)	1:134:A:PHE:H	1:136:A:VAL:HG22	4	0.21
(1,935)	1:134:A:PHE:H	1:136:A:VAL:HG23	4	0.21
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD21	6	0.21
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD22	6	0.21
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD23	6	0.21
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD21	9	0.21
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD22	9	0.21
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD23	9	0.21
(1,772)	1:42:A:GLU:H	1:144:A:VAL:HG11	8	0.21
(1,772)	1:42:A:GLU:H	1:144:A:VAL:HG12	8	0.21
(1,772)	1:42:A:GLU:H	1:144:A:VAL:HG13	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:80:A:LEU:H	1:80:A:LEU:HD11	6	0.21
(1,685)	1:80:A:LEU:H	1:80:A:LEU:HD12	6	0.21
(1,685)	1:80:A:LEU:H	1:80:A:LEU:HD13	6	0.21
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD11	1	0.21
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD12	1	0.21
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD13	1	0.21
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	4	0.21
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	4	0.21
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	4	0.21
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	4	0.21
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	4	0.21
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	4	0.21
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	4	0.21
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	4	0.21
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	4	0.21
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD11	6	0.21
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD12	6	0.21
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD13	6	0.21
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD11	6	0.21
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD12	6	0.21
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD13	6	0.21
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD11	6	0.21
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD12	6	0.21
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD13	6	0.21
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD21	5	0.21
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD22	5	0.21
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD23	5	0.21
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD21	5	0.21
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD22	5	0.21
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD23	5	0.21
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD21	5	0.21
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD22	5	0.21
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD23	5	0.21
(1,515)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	8	0.21
(1,515)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	8	0.21
(1,515)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	8	0.21
(1,515)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	8	0.21
(1,515)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	8	0.21
(1,515)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	8	0.21
(1,515)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	8	0.21
(1,515)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	8	0.21
(1,515)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:32:A:LEU:HD11	1:122:A:LEU:HD21	6	0.21
(1,505)	1:32:A:LEU:HD11	1:122:A:LEU:HD22	6	0.21
(1,505)	1:32:A:LEU:HD11	1:122:A:LEU:HD23	6	0.21
(1,505)	1:32:A:LEU:HD12	1:122:A:LEU:HD21	6	0.21
(1,505)	1:32:A:LEU:HD12	1:122:A:LEU:HD22	6	0.21
(1,505)	1:32:A:LEU:HD12	1:122:A:LEU:HD23	6	0.21
(1,505)	1:32:A:LEU:HD13	1:122:A:LEU:HD21	6	0.21
(1,505)	1:32:A:LEU:HD13	1:122:A:LEU:HD22	6	0.21
(1,505)	1:32:A:LEU:HD13	1:122:A:LEU:HD23	6	0.21
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG21	2	0.21
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG22	2	0.21
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG23	2	0.21
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG21	2	0.21
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG22	2	0.21
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG23	2	0.21
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG21	2	0.21
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG22	2	0.21
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG23	2	0.21
(1,392)	1:59:A:ILE:H	1:96:A:ILE:H	10	0.21
(1,391)	1:58:A:LYS:H	1:96:A:ILE:H	9	0.21
(1,335)	1:62:A:GLU:H	1:65:A:THR:H	6	0.21
(1,317)	1:211:A:SER:H	1:213:A:PHE:H	1	0.21
(1,317)	1:211:A:SER:H	1:213:A:PHE:H	7	0.21
(1,82)	1:110:A:ILE:HD11	1:109:A:THR:HG21	10	0.21
(1,82)	1:110:A:ILE:HD11	1:109:A:THR:HG22	10	0.21
(1,82)	1:110:A:ILE:HD11	1:109:A:THR:HG23	10	0.21
(1,82)	1:110:A:ILE:HD12	1:109:A:THR:HG21	10	0.21
(1,82)	1:110:A:ILE:HD12	1:109:A:THR:HG22	10	0.21
(1,82)	1:110:A:ILE:HD12	1:109:A:THR:HG23	10	0.21
(1,82)	1:110:A:ILE:HD13	1:109:A:THR:HG21	10	0.21
(1,82)	1:110:A:ILE:HD13	1:109:A:THR:HG22	10	0.21
(1,82)	1:110:A:ILE:HD13	1:109:A:THR:HG23	10	0.21
(1,56)	1:55:A:ALA:HB1	1:56:A:LEU:HD21	3	0.21
(1,56)	1:55:A:ALA:HB1	1:56:A:LEU:HD22	3	0.21
(1,56)	1:55:A:ALA:HB1	1:56:A:LEU:HD23	3	0.21
(1,56)	1:55:A:ALA:HB2	1:56:A:LEU:HD21	3	0.21
(1,56)	1:55:A:ALA:HB2	1:56:A:LEU:HD22	3	0.21
(1,56)	1:55:A:ALA:HB2	1:56:A:LEU:HD23	3	0.21
(1,56)	1:55:A:ALA:HB3	1:56:A:LEU:HD21	3	0.21
(1,56)	1:55:A:ALA:HB3	1:56:A:LEU:HD22	3	0.21
(1,56)	1:55:A:ALA:HB3	1:56:A:LEU:HD23	3	0.21
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB1	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB2	3	0.21
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB3	3	0.21
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB1	3	0.21
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB2	3	0.21
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB3	3	0.21
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB1	3	0.21
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB2	3	0.21
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB3	3	0.21
(1,1875)	1:111:A:ALA:H	1:114:A:GLY:H	6	0.2
(1,1727)	1:163:A:GLU:H	1:170:A:PHE:HA	2	0.2
(1,1672)	1:83:A:ASN:H	1:84:A:LYS:HA	3	0.2
(1,1664)	1:79:A:ASN:H	1:93:A:ASP:HA	4	0.2
(1,1544)	1:45:A:LEU:H	1:42:A:GLU:HA	7	0.2
(1,1456)	1:41:A:LYS:H	1:39:A:SER:HA	10	0.2
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG21	1	0.2
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG22	1	0.2
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG23	1	0.2
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	3	0.2
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	3	0.2
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	3	0.2
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	3	0.2
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	3	0.2
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	3	0.2
(1,975)	1:151:A:ILE:H	1:149:A:THR:HG21	8	0.2
(1,975)	1:151:A:ILE:H	1:149:A:THR:HG22	8	0.2
(1,975)	1:151:A:ILE:H	1:149:A:THR:HG23	8	0.2
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD11	8	0.2
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD12	8	0.2
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD13	8	0.2
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB1	7	0.2
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB2	7	0.2
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB3	7	0.2
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD11	5	0.2
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD12	5	0.2
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD13	5	0.2
(1,839)	1:79:A:ASN:H	1:81:A:ILE:HD11	5	0.2
(1,839)	1:79:A:ASN:H	1:81:A:ILE:HD12	5	0.2
(1,839)	1:79:A:ASN:H	1:81:A:ILE:HD13	5	0.2
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD11	3	0.2
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD12	3	0.2
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD13	3	0.2
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD21	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD22	3	0.2
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD23	3	0.2
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD21	1	0.2
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD22	1	0.2
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD23	1	0.2
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD21	7	0.2
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD22	7	0.2
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD23	7	0.2
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG21	5	0.2
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG22	5	0.2
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG23	5	0.2
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB1	2	0.2
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB2	2	0.2
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB3	2	0.2
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB1	5	0.2
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB2	5	0.2
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB3	5	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD11	7	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD12	7	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD13	7	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD11	7	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD12	7	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD13	7	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD11	7	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD12	7	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD13	7	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD11	8	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD12	8	0.2
(1,652)	1:190:A:LEU:HD11	1:198:A:LEU:HD13	8	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD11	8	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD12	8	0.2
(1,652)	1:190:A:LEU:HD12	1:198:A:LEU:HD13	8	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD11	8	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD12	8	0.2
(1,652)	1:190:A:LEU:HD13	1:198:A:LEU:HD13	8	0.2
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG21	1	0.2
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG22	1	0.2
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG23	1	0.2
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG21	1	0.2
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG22	1	0.2
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG23	1	0.2
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG21	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG22	1	0.2
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG23	1	0.2
(1,586)	1:98:A:MET:HE1	1:103:A:LEU:HD21	8	0.2
(1,586)	1:98:A:MET:HE1	1:103:A:LEU:HD22	8	0.2
(1,586)	1:98:A:MET:HE1	1:103:A:LEU:HD23	8	0.2
(1,586)	1:98:A:MET:HE2	1:103:A:LEU:HD21	8	0.2
(1,586)	1:98:A:MET:HE2	1:103:A:LEU:HD22	8	0.2
(1,586)	1:98:A:MET:HE2	1:103:A:LEU:HD23	8	0.2
(1,586)	1:98:A:MET:HE3	1:103:A:LEU:HD21	8	0.2
(1,586)	1:98:A:MET:HE3	1:103:A:LEU:HD22	8	0.2
(1,586)	1:98:A:MET:HE3	1:103:A:LEU:HD23	8	0.2
(1,584)	1:94:A:THR:HG21	1:180:A:MET:HE1	1	0.2
(1,584)	1:94:A:THR:HG21	1:180:A:MET:HE2	1	0.2
(1,584)	1:94:A:THR:HG21	1:180:A:MET:HE3	1	0.2
(1,584)	1:94:A:THR:HG22	1:180:A:MET:HE1	1	0.2
(1,584)	1:94:A:THR:HG22	1:180:A:MET:HE2	1	0.2
(1,584)	1:94:A:THR:HG22	1:180:A:MET:HE3	1	0.2
(1,584)	1:94:A:THR:HG23	1:180:A:MET:HE1	1	0.2
(1,584)	1:94:A:THR:HG23	1:180:A:MET:HE2	1	0.2
(1,584)	1:94:A:THR:HG23	1:180:A:MET:HE3	1	0.2
(1,512)	1:33:A:ILE:HD11	1:131:A:ILE:HD11	1	0.2
(1,512)	1:33:A:ILE:HD11	1:131:A:ILE:HD12	1	0.2
(1,512)	1:33:A:ILE:HD11	1:131:A:ILE:HD13	1	0.2
(1,512)	1:33:A:ILE:HD12	1:131:A:ILE:HD11	1	0.2
(1,512)	1:33:A:ILE:HD12	1:131:A:ILE:HD12	1	0.2
(1,512)	1:33:A:ILE:HD12	1:131:A:ILE:HD13	1	0.2
(1,512)	1:33:A:ILE:HD13	1:131:A:ILE:HD11	1	0.2
(1,512)	1:33:A:ILE:HD13	1:131:A:ILE:HD12	1	0.2
(1,512)	1:33:A:ILE:HD13	1:131:A:ILE:HD13	1	0.2
(1,482)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	4	0.2
(1,482)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	4	0.2
(1,482)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	4	0.2
(1,482)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	4	0.2
(1,482)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	4	0.2
(1,482)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	4	0.2
(1,482)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	4	0.2
(1,482)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	4	0.2
(1,482)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	4	0.2
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG21	7	0.2
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG22	7	0.2
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG23	7	0.2
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG21	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG22	7	0.2
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG23	7	0.2
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG21	7	0.2
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG22	7	0.2
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG23	7	0.2
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB1	6	0.2
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB2	6	0.2
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB3	6	0.2
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB1	6	0.2
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB2	6	0.2
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB3	6	0.2
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB1	6	0.2
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB2	6	0.2
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB3	6	0.2
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD21	1	0.2
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD22	1	0.2
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD23	1	0.2
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD21	1	0.2
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD22	1	0.2
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD23	1	0.2
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD21	1	0.2
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD22	1	0.2
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD23	1	0.2
(1,1789)	1:98:A:MET:H	1:153:A:LYS:HA	3	0.19
(1,1788)	1:97:A:GLY:H	1:183:A:GLY:HA2	9	0.19
(1,1788)	1:97:A:GLY:H	1:183:A:GLY:HA3	9	0.19
(1,1672)	1:83:A:ASN:H	1:84:A:LYS:HA	2	0.19
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD11	9	0.19
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD12	9	0.19
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD13	9	0.19
(1,1046)	1:189:A:HIS:H	1:88:A:THR:HG21	7	0.19
(1,1046)	1:189:A:HIS:H	1:88:A:THR:HG22	7	0.19
(1,1046)	1:189:A:HIS:H	1:88:A:THR:HG23	7	0.19
(1,1006)	1:172:A:VAL:H	1:171:A:THR:HG21	5	0.19
(1,1006)	1:172:A:VAL:H	1:171:A:THR:HG22	5	0.19
(1,1006)	1:172:A:VAL:H	1:171:A:THR:HG23	5	0.19
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG21	2	0.19
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG22	2	0.19
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG23	2	0.19
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	7	0.19
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	7	0.19
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	7	0.19
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	7	0.19
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	7	0.19
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	8	0.19
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	8	0.19
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	8	0.19
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD11	8	0.19
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD12	8	0.19
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD13	8	0.19
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD21	2	0.19
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD22	2	0.19
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD23	2	0.19
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD11	8	0.19
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD12	8	0.19
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD13	8	0.19
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG11	6	0.19
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG12	6	0.19
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG13	6	0.19
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG11	6	0.19
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG12	6	0.19
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG13	6	0.19
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG11	6	0.19
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG12	6	0.19
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG13	6	0.19
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	6	0.19
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	6	0.19
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	6	0.19
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	6	0.19
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	6	0.19
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	6	0.19
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	6	0.19
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	6	0.19
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	6	0.19
(1,634)	1:148:A:VAL:HG11	1:188:A:LEU:HD11	8	0.19
(1,634)	1:148:A:VAL:HG11	1:188:A:LEU:HD12	8	0.19
(1,634)	1:148:A:VAL:HG11	1:188:A:LEU:HD13	8	0.19
(1,634)	1:148:A:VAL:HG12	1:188:A:LEU:HD11	8	0.19
(1,634)	1:148:A:VAL:HG12	1:188:A:LEU:HD12	8	0.19
(1,634)	1:148:A:VAL:HG12	1:188:A:LEU:HD13	8	0.19
(1,634)	1:148:A:VAL:HG13	1:188:A:LEU:HD11	8	0.19
(1,634)	1:148:A:VAL:HG13	1:188:A:LEU:HD12	8	0.19
(1,634)	1:148:A:VAL:HG13	1:188:A:LEU:HD13	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD21	2	0.19
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD22	2	0.19
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD23	2	0.19
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD21	2	0.19
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD22	2	0.19
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD23	2	0.19
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD21	2	0.19
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD22	2	0.19
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD23	2	0.19
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD11	7	0.19
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD12	7	0.19
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD13	7	0.19
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD11	7	0.19
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD12	7	0.19
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD13	7	0.19
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD11	7	0.19
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD12	7	0.19
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD13	7	0.19
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	5	0.19
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	5	0.19
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	5	0.19
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	5	0.19
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	5	0.19
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	5	0.19
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	5	0.19
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	5	0.19
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	5	0.19
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD11	2	0.19
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD12	2	0.19
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD13	2	0.19
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD11	2	0.19
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD12	2	0.19
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD13	2	0.19
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD11	2	0.19
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD12	2	0.19
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD13	2	0.19
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD11	7	0.19
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD12	7	0.19
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD13	7	0.19
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD11	7	0.19
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD12	7	0.19
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD13	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD11	7	0.19
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD12	7	0.19
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD13	7	0.19
(1,533)	1:48:A:LEU:HD11	1:186:A:VAL:HG11	3	0.19
(1,533)	1:48:A:LEU:HD11	1:186:A:VAL:HG12	3	0.19
(1,533)	1:48:A:LEU:HD11	1:186:A:VAL:HG13	3	0.19
(1,533)	1:48:A:LEU:HD12	1:186:A:VAL:HG11	3	0.19
(1,533)	1:48:A:LEU:HD12	1:186:A:VAL:HG12	3	0.19
(1,533)	1:48:A:LEU:HD12	1:186:A:VAL:HG13	3	0.19
(1,533)	1:48:A:LEU:HD13	1:186:A:VAL:HG11	3	0.19
(1,533)	1:48:A:LEU:HD13	1:186:A:VAL:HG12	3	0.19
(1,533)	1:48:A:LEU:HD13	1:186:A:VAL:HG13	3	0.19
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG21	9	0.19
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG22	9	0.19
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG23	9	0.19
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG21	9	0.19
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG22	9	0.19
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG23	9	0.19
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG21	9	0.19
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG22	9	0.19
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG23	9	0.19
(1,295)	1:164:A:SER:H	1:166:A:ALA:H	4	0.19
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB1	3	0.19
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB2	3	0.19
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB3	3	0.19
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB1	3	0.19
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB2	3	0.19
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB3	3	0.19
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB1	3	0.19
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB2	3	0.19
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB3	3	0.19
(1,43)	1:48:A:LEU:HD21	1:144:A:VAL:HG11	5	0.19
(1,43)	1:48:A:LEU:HD21	1:144:A:VAL:HG12	5	0.19
(1,43)	1:48:A:LEU:HD21	1:144:A:VAL:HG13	5	0.19
(1,43)	1:48:A:LEU:HD22	1:144:A:VAL:HG11	5	0.19
(1,43)	1:48:A:LEU:HD22	1:144:A:VAL:HG12	5	0.19
(1,43)	1:48:A:LEU:HD22	1:144:A:VAL:HG13	5	0.19
(1,43)	1:48:A:LEU:HD23	1:144:A:VAL:HG11	5	0.19
(1,43)	1:48:A:LEU:HD23	1:144:A:VAL:HG12	5	0.19
(1,43)	1:48:A:LEU:HD23	1:144:A:VAL:HG13	5	0.19
(1,17)	1:70:A:LEU:HD11	1:59:A:ILE:HD11	1	0.19
(1,17)	1:70:A:LEU:HD11	1:59:A:ILE:HD12	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:70:A:LEU:HD11	1:59:A:ILE:HD13	1	0.19
(1,17)	1:70:A:LEU:HD12	1:59:A:ILE:HD11	1	0.19
(1,17)	1:70:A:LEU:HD12	1:59:A:ILE:HD12	1	0.19
(1,17)	1:70:A:LEU:HD12	1:59:A:ILE:HD13	1	0.19
(1,17)	1:70:A:LEU:HD13	1:59:A:ILE:HD11	1	0.19
(1,17)	1:70:A:LEU:HD13	1:59:A:ILE:HD12	1	0.19
(1,17)	1:70:A:LEU:HD13	1:59:A:ILE:HD13	1	0.19
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD11	3	0.19
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD12	3	0.19
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD13	3	0.19
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD11	3	0.19
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD12	3	0.19
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD13	3	0.19
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD11	3	0.19
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD12	3	0.19
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD13	3	0.19
(1,1760)	1:184:A:THR:H	1:152:A:THR:HA	10	0.18
(1,1709)	1:152:A:THR:H	1:184:A:THR:HA	1	0.18
(1,1641)	1:211:A:SER:H	1:207:A:VAL:HA	7	0.18
(1,1605)	1:36:A:GLU:H	1:32:A:LEU:HA	7	0.18
(1,1577)	1:139:A:TYR:H	1:136:A:VAL:HA	6	0.18
(1,1505)	1:144:A:VAL:H	1:142:A:TYR:HA	4	0.18
(1,1501)	1:138:A:PHE:H	1:136:A:VAL:HA	1	0.18
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB1	9	0.18
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB2	9	0.18
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB3	9	0.18
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG21	5	0.18
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG22	5	0.18
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG23	5	0.18
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	2	0.18
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	2	0.18
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	2	0.18
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD21	3	0.18
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD22	3	0.18
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD23	3	0.18
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD21	5	0.18
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD22	5	0.18
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD23	5	0.18
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG21	5	0.18
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG22	5	0.18
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG23	5	0.18
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG21	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG22	7	0.18
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG23	7	0.18
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG11	3	0.18
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG12	3	0.18
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG13	3	0.18
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD11	9	0.18
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD12	9	0.18
(1,859)	1:85:A:GLN:H	1:198:A:LEU:HD13	9	0.18
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD21	5	0.18
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD22	5	0.18
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD23	5	0.18
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD11	6	0.18
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD12	6	0.18
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD13	6	0.18
(1,768)	1:35:A:ASN:H	1:32:A:LEU:HD11	3	0.18
(1,768)	1:35:A:ASN:H	1:32:A:LEU:HD12	3	0.18
(1,768)	1:35:A:ASN:H	1:32:A:LEU:HD13	3	0.18
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG11	6	0.18
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG12	6	0.18
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG13	6	0.18
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG11	10	0.18
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG12	10	0.18
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG13	10	0.18
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD11	5	0.18
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD12	5	0.18
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD13	5	0.18
(1,631)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	10	0.18
(1,631)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	10	0.18
(1,631)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	10	0.18
(1,631)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	10	0.18
(1,631)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	10	0.18
(1,631)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	10	0.18
(1,631)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	10	0.18
(1,631)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	10	0.18
(1,631)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	10	0.18
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	3	0.18
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	3	0.18
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	3	0.18
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	3	0.18
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	3	0.18
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	3	0.18
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	3	0.18
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	3	0.18
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD21	4	0.18
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD22	4	0.18
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD23	4	0.18
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD21	4	0.18
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD22	4	0.18
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD23	4	0.18
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD21	4	0.18
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD22	4	0.18
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD23	4	0.18
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	9	0.18
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	9	0.18
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	9	0.18
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	9	0.18
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	9	0.18
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	9	0.18
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	9	0.18
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	9	0.18
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	9	0.18
(1,516)	1:43:A:ILE:HD11	1:128:A:ILE:HD11	10	0.18
(1,516)	1:43:A:ILE:HD11	1:128:A:ILE:HD12	10	0.18
(1,516)	1:43:A:ILE:HD11	1:128:A:ILE:HD13	10	0.18
(1,516)	1:43:A:ILE:HD12	1:128:A:ILE:HD11	10	0.18
(1,516)	1:43:A:ILE:HD12	1:128:A:ILE:HD12	10	0.18
(1,516)	1:43:A:ILE:HD12	1:128:A:ILE:HD13	10	0.18
(1,516)	1:43:A:ILE:HD13	1:128:A:ILE:HD11	10	0.18
(1,516)	1:43:A:ILE:HD13	1:128:A:ILE:HD12	10	0.18
(1,516)	1:43:A:ILE:HD13	1:128:A:ILE:HD13	10	0.18
(1,338)	1:68:A:SER:H	1:71:A:ASP:H	4	0.18
(1,74)	1:33:A:ILE:HD11	1:143:A:LEU:HD11	2	0.18
(1,74)	1:33:A:ILE:HD11	1:143:A:LEU:HD12	2	0.18
(1,74)	1:33:A:ILE:HD11	1:143:A:LEU:HD13	2	0.18
(1,74)	1:33:A:ILE:HD12	1:143:A:LEU:HD11	2	0.18
(1,74)	1:33:A:ILE:HD12	1:143:A:LEU:HD12	2	0.18
(1,74)	1:33:A:ILE:HD12	1:143:A:LEU:HD13	2	0.18
(1,74)	1:33:A:ILE:HD13	1:143:A:LEU:HD11	2	0.18
(1,74)	1:33:A:ILE:HD13	1:143:A:LEU:HD12	2	0.18
(1,74)	1:33:A:ILE:HD13	1:143:A:LEU:HD13	2	0.18
(1,36)	1:80:A:LEU:HD21	1:207:A:VAL:HG21	6	0.18
(1,36)	1:80:A:LEU:HD21	1:207:A:VAL:HG22	6	0.18
(1,36)	1:80:A:LEU:HD21	1:207:A:VAL:HG23	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:80:A:LEU:HD22	1:207:A:VAL:HG21	6	0.18
(1,36)	1:80:A:LEU:HD22	1:207:A:VAL:HG22	6	0.18
(1,36)	1:80:A:LEU:HD22	1:207:A:VAL:HG23	6	0.18
(1,36)	1:80:A:LEU:HD23	1:207:A:VAL:HG21	6	0.18
(1,36)	1:80:A:LEU:HD23	1:207:A:VAL:HG22	6	0.18
(1,36)	1:80:A:LEU:HD23	1:207:A:VAL:HG23	6	0.18
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG21	7	0.18
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG22	7	0.18
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG23	7	0.18
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG21	7	0.18
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG22	7	0.18
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG23	7	0.18
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG21	7	0.18
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG22	7	0.18
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG23	7	0.18
(1,1875)	1:111:A:ALA:H	1:114:A:GLY:H	9	0.17
(1,1873)	1:126:A:ALA:H	1:122:A:LEU:HA	10	0.17
(1,1790)	1:182:A:ARG:H	1:94:A:THR:HA	6	0.17
(1,1709)	1:152:A:THR:H	1:184:A:THR:HA	5	0.17
(1,1658)	1:22:A:PHE:H	1:169:A:SER:HA	9	0.17
(1,1641)	1:211:A:SER:H	1:207:A:VAL:HA	9	0.17
(1,1504)	1:143:A:LEU:H	1:141:A:ALA:HA	4	0.17
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD11	7	0.17
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD12	7	0.17
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD13	7	0.17
(1,1075)	1:198:A:LEU:H	1:203:A:ILE:HD11	1	0.17
(1,1075)	1:198:A:LEU:H	1:203:A:ILE:HD12	1	0.17
(1,1075)	1:198:A:LEU:H	1:203:A:ILE:HD13	1	0.17
(1,1068)	1:197:A:TYR:H	1:190:A:LEU:HD11	4	0.17
(1,1068)	1:197:A:TYR:H	1:190:A:LEU:HD12	4	0.17
(1,1068)	1:197:A:TYR:H	1:190:A:LEU:HD13	4	0.17
(1,979)	1:151:A:ILE:H	1:187:A:ILE:HD11	8	0.17
(1,979)	1:151:A:ILE:H	1:187:A:ILE:HD12	8	0.17
(1,979)	1:151:A:ILE:H	1:187:A:ILE:HD13	8	0.17
(1,953)	1:142:A:TYR:H	1:188:A:LEU:HD21	8	0.17
(1,953)	1:142:A:TYR:H	1:188:A:LEU:HD22	8	0.17
(1,953)	1:142:A:TYR:H	1:188:A:LEU:HD23	8	0.17
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG21	3	0.17
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG22	3	0.17
(1,943)	1:139:A:TYR:H	1:136:A:VAL:HG23	3	0.17
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB1	6	0.17
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB2	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB3	6	0.17
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG21	3	0.17
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG22	3	0.17
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG23	3	0.17
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD11	5	0.17
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD12	5	0.17
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD13	5	0.17
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD21	8	0.17
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD22	8	0.17
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD23	8	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD11	5	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD12	5	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD13	5	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD21	5	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD22	5	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD23	5	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD11	6	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD12	6	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD13	6	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD21	6	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD22	6	0.17
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD23	6	0.17
(1,820)	1:69:A:LYS:H	1:59:A:ILE:HD11	8	0.17
(1,820)	1:69:A:LYS:H	1:59:A:ILE:HD12	8	0.17
(1,820)	1:69:A:LYS:H	1:59:A:ILE:HD13	8	0.17
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG21	5	0.17
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG22	5	0.17
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG23	5	0.17
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG11	9	0.17
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG12	9	0.17
(1,737)	1:18:A:GLU:H	1:172:A:VAL:HG13	9	0.17
(1,722)	1:190:A:LEU:H	1:190:A:LEU:HD21	1	0.17
(1,722)	1:190:A:LEU:H	1:190:A:LEU:HD22	1	0.17
(1,722)	1:190:A:LEU:H	1:190:A:LEU:HD23	1	0.17
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG11	5	0.17
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG12	5	0.17
(1,714)	1:172:A:VAL:H	1:172:A:VAL:HG13	5	0.17
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG21	10	0.17
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG22	10	0.17
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG23	10	0.17
(1,636)	1:149:A:THR:HG21	1:187:A:ILE:HD11	6	0.17
(1,636)	1:149:A:THR:HG21	1:187:A:ILE:HD12	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:149:A:THR:HG21	1:187:A:ILE:HD13	6	0.17
(1,636)	1:149:A:THR:HG22	1:187:A:ILE:HD11	6	0.17
(1,636)	1:149:A:THR:HG22	1:187:A:ILE:HD12	6	0.17
(1,636)	1:149:A:THR:HG22	1:187:A:ILE:HD13	6	0.17
(1,636)	1:149:A:THR:HG23	1:187:A:ILE:HD11	6	0.17
(1,636)	1:149:A:THR:HG23	1:187:A:ILE:HD12	6	0.17
(1,636)	1:149:A:THR:HG23	1:187:A:ILE:HD13	6	0.17
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	10	0.17
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	10	0.17
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	10	0.17
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	10	0.17
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	10	0.17
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	10	0.17
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	10	0.17
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	10	0.17
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	10	0.17
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG11	3	0.17
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG12	3	0.17
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG13	3	0.17
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG11	3	0.17
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG12	3	0.17
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG13	3	0.17
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG11	3	0.17
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG12	3	0.17
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG13	3	0.17
(1,604)	1:103:A:LEU:HD21	1:152:A:THR:HG21	8	0.17
(1,604)	1:103:A:LEU:HD21	1:152:A:THR:HG22	8	0.17
(1,604)	1:103:A:LEU:HD21	1:152:A:THR:HG23	8	0.17
(1,604)	1:103:A:LEU:HD22	1:152:A:THR:HG21	8	0.17
(1,604)	1:103:A:LEU:HD22	1:152:A:THR:HG22	8	0.17
(1,604)	1:103:A:LEU:HD22	1:152:A:THR:HG23	8	0.17
(1,604)	1:103:A:LEU:HD23	1:152:A:THR:HG21	8	0.17
(1,604)	1:103:A:LEU:HD23	1:152:A:THR:HG22	8	0.17
(1,604)	1:103:A:LEU:HD23	1:152:A:THR:HG23	8	0.17
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE1	4	0.17
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE2	4	0.17
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE3	4	0.17
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE1	4	0.17
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE2	4	0.17
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE3	4	0.17
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE1	4	0.17
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE3	4	0.17
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	6	0.17
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	6	0.17
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	6	0.17
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	6	0.17
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	6	0.17
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	6	0.17
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	6	0.17
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	6	0.17
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	6	0.17
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD11	6	0.17
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD12	6	0.17
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD13	6	0.17
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD11	6	0.17
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD12	6	0.17
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD13	6	0.17
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD11	6	0.17
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD12	6	0.17
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD13	6	0.17
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD11	7	0.17
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD12	7	0.17
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD13	7	0.17
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD11	7	0.17
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD12	7	0.17
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD13	7	0.17
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD11	7	0.17
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD12	7	0.17
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD13	7	0.17
(1,536)	1:48:A:LEU:HD21	1:141:A:ALA:HB1	8	0.17
(1,536)	1:48:A:LEU:HD21	1:141:A:ALA:HB2	8	0.17
(1,536)	1:48:A:LEU:HD21	1:141:A:ALA:HB3	8	0.17
(1,536)	1:48:A:LEU:HD22	1:141:A:ALA:HB1	8	0.17
(1,536)	1:48:A:LEU:HD22	1:141:A:ALA:HB2	8	0.17
(1,536)	1:48:A:LEU:HD22	1:141:A:ALA:HB3	8	0.17
(1,536)	1:48:A:LEU:HD23	1:141:A:ALA:HB1	8	0.17
(1,536)	1:48:A:LEU:HD23	1:141:A:ALA:HB2	8	0.17
(1,536)	1:48:A:LEU:HD23	1:141:A:ALA:HB3	8	0.17
(1,531)	1:48:A:LEU:HD11	1:91:A:ILE:HD11	3	0.17
(1,531)	1:48:A:LEU:HD11	1:91:A:ILE:HD12	3	0.17
(1,531)	1:48:A:LEU:HD11	1:91:A:ILE:HD13	3	0.17
(1,531)	1:48:A:LEU:HD12	1:91:A:ILE:HD11	3	0.17
(1,531)	1:48:A:LEU:HD12	1:91:A:ILE:HD12	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:48:A:LEU:HD12	1:91:A:ILE:HD13	3	0.17
(1,531)	1:48:A:LEU:HD13	1:91:A:ILE:HD11	3	0.17
(1,531)	1:48:A:LEU:HD13	1:91:A:ILE:HD12	3	0.17
(1,531)	1:48:A:LEU:HD13	1:91:A:ILE:HD13	3	0.17
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	3	0.17
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	3	0.17
(1,529)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	3	0.17
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	3	0.17
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	3	0.17
(1,529)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	3	0.17
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	3	0.17
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	3	0.17
(1,529)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	3	0.17
(1,506)	1:32:A:LEU:HD11	1:128:A:ILE:HD11	6	0.17
(1,506)	1:32:A:LEU:HD11	1:128:A:ILE:HD12	6	0.17
(1,506)	1:32:A:LEU:HD11	1:128:A:ILE:HD13	6	0.17
(1,506)	1:32:A:LEU:HD12	1:128:A:ILE:HD11	6	0.17
(1,506)	1:32:A:LEU:HD12	1:128:A:ILE:HD12	6	0.17
(1,506)	1:32:A:LEU:HD12	1:128:A:ILE:HD13	6	0.17
(1,506)	1:32:A:LEU:HD13	1:128:A:ILE:HD11	6	0.17
(1,506)	1:32:A:LEU:HD13	1:128:A:ILE:HD12	6	0.17
(1,506)	1:32:A:LEU:HD13	1:128:A:ILE:HD13	6	0.17
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	7	0.17
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	7	0.17
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	7	0.17
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	7	0.17
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	7	0.17
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	7	0.17
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	7	0.17
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	7	0.17
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	7	0.17
(1,355)	1:131:A:ILE:H	1:134:A:PHE:H	7	0.17
(1,335)	1:62:A:GLU:H	1:65:A:THR:H	5	0.17
(1,166)	1:138:A:PHE:H	1:139:A:TYR:H	1	0.17
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG21	9	0.17
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG22	9	0.17
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG23	9	0.17
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG21	9	0.17
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG22	9	0.17
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG23	9	0.17
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG21	9	0.17
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG22	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG23	9	0.17
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD21	8	0.17
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD22	8	0.17
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD23	8	0.17
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD21	8	0.17
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD22	8	0.17
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD23	8	0.17
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD21	8	0.17
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD22	8	0.17
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD23	8	0.17
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD11	9	0.17
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD12	9	0.17
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD13	9	0.17
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD11	9	0.17
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD12	9	0.17
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD13	9	0.17
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD11	9	0.17
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD12	9	0.17
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD13	9	0.17
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD21	8	0.17
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD22	8	0.17
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD23	8	0.17
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD21	8	0.17
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD22	8	0.17
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD23	8	0.17
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD21	8	0.17
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD22	8	0.17
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD23	8	0.17
(1,16)	1:70:A:LEU:HD11	1:76:A:LEU:HD21	2	0.17
(1,16)	1:70:A:LEU:HD11	1:76:A:LEU:HD22	2	0.17
(1,16)	1:70:A:LEU:HD11	1:76:A:LEU:HD23	2	0.17
(1,16)	1:70:A:LEU:HD12	1:76:A:LEU:HD21	2	0.17
(1,16)	1:70:A:LEU:HD12	1:76:A:LEU:HD22	2	0.17
(1,16)	1:70:A:LEU:HD12	1:76:A:LEU:HD23	2	0.17
(1,16)	1:70:A:LEU:HD13	1:76:A:LEU:HD21	2	0.17
(1,16)	1:70:A:LEU:HD13	1:76:A:LEU:HD22	2	0.17
(1,16)	1:70:A:LEU:HD13	1:76:A:LEU:HD23	2	0.17
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD11	5	0.17
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD12	5	0.17
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD13	5	0.17
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD11	5	0.17
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD12	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD13	5	0.17
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD11	5	0.17
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD12	5	0.17
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD13	5	0.17
(1,1873)	1:126:A:ALA:H	1:122:A:LEU:HA	4	0.16
(1,1823)	1:126:A:ALA:H	1:125:A:GLY:HA2	4	0.16
(1,1823)	1:126:A:ALA:H	1:125:A:GLY:HA3	4	0.16
(1,1788)	1:97:A:GLY:H	1:183:A:GLY:HA2	3	0.16
(1,1788)	1:97:A:GLY:H	1:183:A:GLY:HA3	3	0.16
(1,1788)	1:97:A:GLY:H	1:183:A:GLY:HA2	6	0.16
(1,1788)	1:97:A:GLY:H	1:183:A:GLY:HA3	6	0.16
(1,1770)	1:187:A:ILE:H	1:148:A:VAL:HA	1	0.16
(1,1755)	1:183:A:GLY:H	1:153:A:LYS:HA	3	0.16
(1,1641)	1:211:A:SER:H	1:207:A:VAL:HA	2	0.16
(1,1597)	1:214:A:ILE:H	1:211:A:SER:HA	3	0.16
(1,1584)	1:197:A:TYR:H	1:194:A:GLN:HA	9	0.16
(1,1583)	1:195:A:THR:H	1:192:A:GLU:HA	7	0.16
(1,1571)	1:102:A:ASP:H	1:99:A:THR:HA	3	0.16
(1,1548)	1:49:A:ILE:H	1:46:A:ARG:HA	1	0.16
(1,1516)	1:197:A:TYR:H	1:195:A:THR:HA	4	0.16
(1,1504)	1:143:A:LEU:H	1:141:A:ALA:HA	2	0.16
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD11	10	0.16
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD12	10	0.16
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD13	10	0.16
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD21	4	0.16
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD22	4	0.16
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD23	4	0.16
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG21	4	0.16
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG22	4	0.16
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG23	4	0.16
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG11	2	0.16
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG12	2	0.16
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG13	2	0.16
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD11	1	0.16
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD12	1	0.16
(1,1087)	1:203:A:ILE:H	1:206:A:ILE:HD13	1	0.16
(1,1067)	1:196:A:GLU:H	1:198:A:LEU:HD11	5	0.16
(1,1067)	1:196:A:GLU:H	1:198:A:LEU:HD12	5	0.16
(1,1067)	1:196:A:GLU:H	1:198:A:LEU:HD13	5	0.16
(1,1062)	1:194:A:GLN:H	1:190:A:LEU:HD11	10	0.16
(1,1062)	1:194:A:GLN:H	1:190:A:LEU:HD12	10	0.16
(1,1062)	1:194:A:GLN:H	1:190:A:LEU:HD13	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG11	4	0.16
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG12	4	0.16
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG13	4	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG21	4	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG22	4	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG23	4	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG21	5	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG22	5	0.16
(1,1039)	1:188:A:LEU:H	1:88:A:THR:HG23	5	0.16
(1,1011)	1:173:A:ARG:H	1:172:A:VAL:HG21	5	0.16
(1,1011)	1:173:A:ARG:H	1:172:A:VAL:HG22	5	0.16
(1,1011)	1:173:A:ARG:H	1:172:A:VAL:HG23	5	0.16
(1,1003)	1:170:A:PHE:H	1:19:A:THR:HG21	4	0.16
(1,1003)	1:170:A:PHE:H	1:19:A:THR:HG22	4	0.16
(1,1003)	1:170:A:PHE:H	1:19:A:THR:HG23	4	0.16
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG21	6	0.16
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG22	6	0.16
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG23	6	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	9	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	9	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	9	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	9	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	9	0.16
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	9	0.16
(1,980)	1:152:A:THR:H	1:184:A:THR:HG21	10	0.16
(1,980)	1:152:A:THR:H	1:184:A:THR:HG22	10	0.16
(1,980)	1:152:A:THR:H	1:184:A:THR:HG23	10	0.16
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	1	0.16
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	1	0.16
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	1	0.16
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG11	4	0.16
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG12	4	0.16
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG13	4	0.16
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB1	10	0.16
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB2	10	0.16
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB3	10	0.16
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG11	5	0.16
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG12	5	0.16
(1,908)	1:118:A:PHE:H	1:136:A:VAL:HG13	5	0.16
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD11	2	0.16
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD12	2	0.16
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD13	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG21	1	0.16
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG22	1	0.16
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG23	1	0.16
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG21	3	0.16
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG22	3	0.16
(1,834)	1:77:A:HIS:H	1:94:A:THR:HG23	3	0.16
(1,816)	1:63:A:SER:H	1:70:A:LEU:HD21	4	0.16
(1,816)	1:63:A:SER:H	1:70:A:LEU:HD22	4	0.16
(1,816)	1:63:A:SER:H	1:70:A:LEU:HD23	4	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD11	4	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD12	4	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD13	4	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD11	8	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD12	8	0.16
(1,808)	1:61:A:TYR:H	1:64:A:LEU:HD13	8	0.16
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD21	2	0.16
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD22	2	0.16
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD23	2	0.16
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG21	6	0.16
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG22	6	0.16
(1,743)	1:21:A:ALA:H	1:109:A:THR:HG23	6	0.16
(1,702)	1:131:A:ILE:H	1:131:A:ILE:HD11	6	0.16
(1,702)	1:131:A:ILE:H	1:131:A:ILE:HD12	6	0.16
(1,702)	1:131:A:ILE:H	1:131:A:ILE:HD13	6	0.16
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD21	9	0.16
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD22	9	0.16
(1,695)	1:103:A:LEU:H	1:103:A:LEU:HD23	9	0.16
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD11	8	0.16
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD12	8	0.16
(1,677)	1:59:A:ILE:H	1:59:A:ILE:HD13	8	0.16
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD11	5	0.16
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD12	5	0.16
(1,669)	1:33:A:ILE:H	1:33:A:ILE:HD13	5	0.16
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG21	2	0.16
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG22	2	0.16
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG23	2	0.16
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG21	3	0.16
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG22	3	0.16
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG23	3	0.16
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG21	3	0.16
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG22	3	0.16
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG23	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG21	3	0.16
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG22	3	0.16
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG23	3	0.16
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB1	5	0.16
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB2	5	0.16
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB3	5	0.16
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB1	5	0.16
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB2	5	0.16
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB3	5	0.16
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB1	5	0.16
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB2	5	0.16
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB3	5	0.16
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE1	3	0.16
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE2	3	0.16
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE3	3	0.16
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE1	3	0.16
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE2	3	0.16
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE3	3	0.16
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE1	3	0.16
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE2	3	0.16
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE3	3	0.16
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	1	0.16
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	1	0.16
(1,620)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	1	0.16
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	1	0.16
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	1	0.16
(1,620)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	1	0.16
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	1	0.16
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	1	0.16
(1,620)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	1	0.16
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD11	1	0.16
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD12	1	0.16
(1,620)	1:122:A:LEU:HD21	1:128:A:ILE:HD13	1	0.16
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD11	1	0.16
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD12	1	0.16
(1,620)	1:122:A:LEU:HD22	1:128:A:ILE:HD13	1	0.16
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD11	1	0.16
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD12	1	0.16
(1,620)	1:122:A:LEU:HD23	1:128:A:ILE:HD13	1	0.16
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG21	6	0.16
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG22	6	0.16
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG23	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG21	6	0.16
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG22	6	0.16
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG23	6	0.16
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG21	6	0.16
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG22	6	0.16
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG23	6	0.16
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	7	0.16
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	7	0.16
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	7	0.16
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	7	0.16
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	7	0.16
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	7	0.16
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	7	0.16
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	7	0.16
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	7	0.16
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD11	2	0.16
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD12	2	0.16
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD13	2	0.16
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD11	2	0.16
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD12	2	0.16
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD13	2	0.16
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD11	2	0.16
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD12	2	0.16
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD13	2	0.16
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	5	0.16
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	5	0.16
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	5	0.16
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	5	0.16
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	5	0.16
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	5	0.16
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	5	0.16
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	5	0.16
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	5	0.16
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	2	0.16
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	2	0.16
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	2	0.16
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	2	0.16
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	2	0.16
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	2	0.16
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	2	0.16
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	2	0.16
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD21	4	0.16
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD22	4	0.16
(1,524)	1:45:A:LEU:HD21	1:48:A:LEU:HD23	4	0.16
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD21	4	0.16
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD22	4	0.16
(1,524)	1:45:A:LEU:HD22	1:48:A:LEU:HD23	4	0.16
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD21	4	0.16
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD22	4	0.16
(1,524)	1:45:A:LEU:HD23	1:48:A:LEU:HD23	4	0.16
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD21	8	0.16
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD22	8	0.16
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD23	8	0.16
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD21	8	0.16
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD22	8	0.16
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD23	8	0.16
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD21	8	0.16
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD22	8	0.16
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD23	8	0.16
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG11	4	0.16
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG12	4	0.16
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG13	4	0.16
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG11	4	0.16
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG12	4	0.16
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG13	4	0.16
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG11	4	0.16
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG12	4	0.16
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG13	4	0.16
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG21	10	0.16
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG22	10	0.16
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG23	10	0.16
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG21	10	0.16
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG22	10	0.16
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG23	10	0.16
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG21	10	0.16
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG22	10	0.16
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG23	10	0.16
(1,483)	1:26:A:ILE:HD11	1:115:A:THR:HG21	2	0.16
(1,483)	1:26:A:ILE:HD11	1:115:A:THR:HG22	2	0.16
(1,483)	1:26:A:ILE:HD11	1:115:A:THR:HG23	2	0.16
(1,483)	1:26:A:ILE:HD12	1:115:A:THR:HG21	2	0.16
(1,483)	1:26:A:ILE:HD12	1:115:A:THR:HG22	2	0.16
(1,483)	1:26:A:ILE:HD12	1:115:A:THR:HG23	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:26:A:ILE:HD13	1:115:A:THR:HG21	2	0.16
(1,483)	1:26:A:ILE:HD13	1:115:A:THR:HG22	2	0.16
(1,483)	1:26:A:ILE:HD13	1:115:A:THR:HG23	2	0.16
(1,450)	1:210:A:HIS:H	1:214:A:ILE:H	8	0.16
(1,383)	1:22:A:PHE:H	1:170:A:PHE:H	10	0.16
(1,80)	1:203:A:ILE:HD11	1:91:A:ILE:HD11	5	0.16
(1,80)	1:203:A:ILE:HD11	1:91:A:ILE:HD12	5	0.16
(1,80)	1:203:A:ILE:HD11	1:91:A:ILE:HD13	5	0.16
(1,80)	1:203:A:ILE:HD12	1:91:A:ILE:HD11	5	0.16
(1,80)	1:203:A:ILE:HD12	1:91:A:ILE:HD12	5	0.16
(1,80)	1:203:A:ILE:HD12	1:91:A:ILE:HD13	5	0.16
(1,80)	1:203:A:ILE:HD13	1:91:A:ILE:HD11	5	0.16
(1,80)	1:203:A:ILE:HD13	1:91:A:ILE:HD12	5	0.16
(1,80)	1:203:A:ILE:HD13	1:91:A:ILE:HD13	5	0.16
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD11	5	0.16
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD12	5	0.16
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD13	5	0.16
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD11	5	0.16
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD12	5	0.16
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD13	5	0.16
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD11	5	0.16
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD12	5	0.16
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD13	5	0.16
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD21	5	0.16
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD22	5	0.16
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD23	5	0.16
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD21	5	0.16
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD22	5	0.16
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD23	5	0.16
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD21	5	0.16
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD22	5	0.16
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD23	5	0.16
(1,1873)	1:126:A:ALA:H	1:122:A:LEU:HA	9	0.15
(1,1872)	1:125:A:GLY:H	1:121:A:ALA:HA	8	0.15
(1,1863)	1:133:A:GLN:H	1:130:A:MET:HA	8	0.15
(1,1852)	1:114:A:GLY:H	1:111:A:ALA:HA	10	0.15
(1,1647)	1:98:A:MET:H	1:154:A:HIS:H	7	0.15
(1,1595)	1:210:A:HIS:H	1:207:A:VAL:HA	7	0.15
(1,1584)	1:197:A:TYR:H	1:194:A:GLN:HA	3	0.15
(1,1584)	1:197:A:TYR:H	1:194:A:GLN:HA	5	0.15
(1,1574)	1:105:A:ASN:H	1:102:A:ASP:HA	7	0.15
(1,1564)	1:65:A:THR:H	1:62:A:GLU:HA	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1531)	1:213:A:PHE:H	1:211:A:SER:HA	6	0.15
(1,1456)	1:41:A:LYS:H	1:39:A:SER:HA	6	0.15
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA2	5	0.15
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA3	5	0.15
(1,1361)	1:96:A:ILE:H	1:95:A:GLY:HA2	8	0.15
(1,1361)	1:96:A:ILE:H	1:95:A:GLY:HA3	8	0.15
(1,1240)	1:166:A:ALA:H	1:166:A:ALA:HA	4	0.15
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG21	5	0.15
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG22	5	0.15
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG23	5	0.15
(1,1064)	1:196:A:GLU:H	1:190:A:LEU:HD11	1	0.15
(1,1064)	1:196:A:GLU:H	1:190:A:LEU:HD12	1	0.15
(1,1064)	1:196:A:GLU:H	1:190:A:LEU:HD13	1	0.15
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD21	1	0.15
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD22	1	0.15
(1,1038)	1:187:A:ILE:H	1:188:A:LEU:HD23	1	0.15
(1,1025)	1:185:A:LYS:H	1:186:A:VAL:HG21	5	0.15
(1,1025)	1:185:A:LYS:H	1:186:A:VAL:HG22	5	0.15
(1,1025)	1:185:A:LYS:H	1:186:A:VAL:HG23	5	0.15
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG21	5	0.15
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG22	5	0.15
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG23	5	0.15
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG21	8	0.15
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG22	8	0.15
(1,1005)	1:172:A:VAL:H	1:17:A:VAL:HG23	8	0.15
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB1	2	0.15
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB2	2	0.15
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB3	2	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	1	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	1	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	1	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	1	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	1	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	1	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	2	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	2	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	2	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	2	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	2	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	2	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	4	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	4	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	4	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	4	0.15
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	4	0.15
(1,980)	1:152:A:THR:H	1:184:A:THR:HG21	9	0.15
(1,980)	1:152:A:THR:H	1:184:A:THR:HG22	9	0.15
(1,980)	1:152:A:THR:H	1:184:A:THR:HG23	9	0.15
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	10	0.15
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	10	0.15
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	10	0.15
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG11	1	0.15
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG12	1	0.15
(1,969)	1:149:A:THR:H	1:150:A:VAL:HG13	1	0.15
(1,967)	1:147:A:LYS:H	1:148:A:VAL:HG21	3	0.15
(1,967)	1:147:A:LYS:H	1:148:A:VAL:HG22	3	0.15
(1,967)	1:147:A:LYS:H	1:148:A:VAL:HG23	3	0.15
(1,949)	1:142:A:TYR:H	1:143:A:LEU:HD11	1	0.15
(1,949)	1:142:A:TYR:H	1:143:A:LEU:HD12	1	0.15
(1,949)	1:142:A:TYR:H	1:143:A:LEU:HD13	1	0.15
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG21	8	0.15
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG22	8	0.15
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG23	8	0.15
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE1	9	0.15
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE2	9	0.15
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE3	9	0.15
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD11	4	0.15
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD12	4	0.15
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD13	4	0.15
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD11	1	0.15
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD12	1	0.15
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD13	1	0.15
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD21	7	0.15
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD22	7	0.15
(1,866)	1:87:A:ARG:H	1:198:A:LEU:HD23	7	0.15
(1,795)	1:56:A:LEU:H	1:55:A:ALA:HB1	10	0.15
(1,795)	1:56:A:LEU:H	1:55:A:ALA:HB2	10	0.15
(1,795)	1:56:A:LEU:H	1:55:A:ALA:HB3	10	0.15
(1,760)	1:32:A:LEU:H	1:34:A:ILE:HD11	7	0.15
(1,760)	1:32:A:LEU:H	1:34:A:ILE:HD12	7	0.15
(1,760)	1:32:A:LEU:H	1:34:A:ILE:HD13	7	0.15
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG21	5	0.15
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG22	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG23	5	0.15
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG21	7	0.15
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG22	7	0.15
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG23	7	0.15
(1,717)	1:186:A:VAL:H	1:186:A:VAL:HG21	10	0.15
(1,717)	1:186:A:VAL:H	1:186:A:VAL:HG22	10	0.15
(1,717)	1:186:A:VAL:H	1:186:A:VAL:HG23	10	0.15
(1,655)	1:195:A:THR:HG21	1:198:A:LEU:HD21	7	0.15
(1,655)	1:195:A:THR:HG21	1:198:A:LEU:HD22	7	0.15
(1,655)	1:195:A:THR:HG21	1:198:A:LEU:HD23	7	0.15
(1,655)	1:195:A:THR:HG22	1:198:A:LEU:HD21	7	0.15
(1,655)	1:195:A:THR:HG22	1:198:A:LEU:HD22	7	0.15
(1,655)	1:195:A:THR:HG22	1:198:A:LEU:HD23	7	0.15
(1,655)	1:195:A:THR:HG23	1:198:A:LEU:HD21	7	0.15
(1,655)	1:195:A:THR:HG23	1:198:A:LEU:HD22	7	0.15
(1,655)	1:195:A:THR:HG23	1:198:A:LEU:HD23	7	0.15
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG21	9	0.15
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG22	9	0.15
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG23	9	0.15
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG21	9	0.15
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG22	9	0.15
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG23	9	0.15
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG21	9	0.15
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG22	9	0.15
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG23	9	0.15
(1,637)	1:150:A:VAL:HG11	1:152:A:THR:HG21	6	0.15
(1,637)	1:150:A:VAL:HG11	1:152:A:THR:HG22	6	0.15
(1,637)	1:150:A:VAL:HG11	1:152:A:THR:HG23	6	0.15
(1,637)	1:150:A:VAL:HG12	1:152:A:THR:HG21	6	0.15
(1,637)	1:150:A:VAL:HG12	1:152:A:THR:HG22	6	0.15
(1,637)	1:150:A:VAL:HG12	1:152:A:THR:HG23	6	0.15
(1,637)	1:150:A:VAL:HG13	1:152:A:THR:HG21	6	0.15
(1,637)	1:150:A:VAL:HG13	1:152:A:THR:HG22	6	0.15
(1,637)	1:150:A:VAL:HG13	1:152:A:THR:HG23	6	0.15
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	9	0.15
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	9	0.15
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	9	0.15
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	9	0.15
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	9	0.15
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	9	0.15
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	9	0.15
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	9	0.15
(1,597)	1:103:A:LEU:HD11	1:150:A:VAL:HG11	7	0.15
(1,597)	1:103:A:LEU:HD11	1:150:A:VAL:HG12	7	0.15
(1,597)	1:103:A:LEU:HD11	1:150:A:VAL:HG13	7	0.15
(1,597)	1:103:A:LEU:HD12	1:150:A:VAL:HG11	7	0.15
(1,597)	1:103:A:LEU:HD12	1:150:A:VAL:HG12	7	0.15
(1,597)	1:103:A:LEU:HD12	1:150:A:VAL:HG13	7	0.15
(1,597)	1:103:A:LEU:HD13	1:150:A:VAL:HG11	7	0.15
(1,597)	1:103:A:LEU:HD13	1:150:A:VAL:HG12	7	0.15
(1,597)	1:103:A:LEU:HD13	1:150:A:VAL:HG13	7	0.15
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG21	4	0.15
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG22	4	0.15
(1,592)	1:98:A:MET:HE1	1:184:A:THR:HG23	4	0.15
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG21	4	0.15
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG22	4	0.15
(1,592)	1:98:A:MET:HE2	1:184:A:THR:HG23	4	0.15
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG21	4	0.15
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG22	4	0.15
(1,592)	1:98:A:MET:HE3	1:184:A:THR:HG23	4	0.15
(1,589)	1:98:A:MET:HE1	1:150:A:VAL:HG11	6	0.15
(1,589)	1:98:A:MET:HE1	1:150:A:VAL:HG12	6	0.15
(1,589)	1:98:A:MET:HE1	1:150:A:VAL:HG13	6	0.15
(1,589)	1:98:A:MET:HE2	1:150:A:VAL:HG11	6	0.15
(1,589)	1:98:A:MET:HE2	1:150:A:VAL:HG12	6	0.15
(1,589)	1:98:A:MET:HE2	1:150:A:VAL:HG13	6	0.15
(1,589)	1:98:A:MET:HE3	1:150:A:VAL:HG11	6	0.15
(1,589)	1:98:A:MET:HE3	1:150:A:VAL:HG12	6	0.15
(1,589)	1:98:A:MET:HE3	1:150:A:VAL:HG13	6	0.15
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD11	2	0.15
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD12	2	0.15
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD13	2	0.15
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD11	2	0.15
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD12	2	0.15
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD13	2	0.15
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD11	2	0.15
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD12	2	0.15
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD13	2	0.15
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG21	1	0.15
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG22	1	0.15
(1,567)	1:81:A:ILE:HD11	1:90:A:THR:HG23	1	0.15
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG21	1	0.15
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG22	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:81:A:ILE:HD12	1:90:A:THR:HG23	1	0.15
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG21	1	0.15
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG22	1	0.15
(1,567)	1:81:A:ILE:HD13	1:90:A:THR:HG23	1	0.15
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	7	0.15
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	7	0.15
(1,551)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	7	0.15
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	7	0.15
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	7	0.15
(1,551)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	7	0.15
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	7	0.15
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	7	0.15
(1,551)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	7	0.15
(1,545)	1:49:A:ILE:HD11	1:207:A:VAL:HG21	4	0.15
(1,545)	1:49:A:ILE:HD11	1:207:A:VAL:HG22	4	0.15
(1,545)	1:49:A:ILE:HD11	1:207:A:VAL:HG23	4	0.15
(1,545)	1:49:A:ILE:HD12	1:207:A:VAL:HG21	4	0.15
(1,545)	1:49:A:ILE:HD12	1:207:A:VAL:HG22	4	0.15
(1,545)	1:49:A:ILE:HD12	1:207:A:VAL:HG23	4	0.15
(1,545)	1:49:A:ILE:HD13	1:207:A:VAL:HG21	4	0.15
(1,545)	1:49:A:ILE:HD13	1:207:A:VAL:HG22	4	0.15
(1,545)	1:49:A:ILE:HD13	1:207:A:VAL:HG23	4	0.15
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD11	6	0.15
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD12	6	0.15
(1,490)	1:29:A:LEU:HD21	1:122:A:LEU:HD13	6	0.15
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD11	6	0.15
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD12	6	0.15
(1,490)	1:29:A:LEU:HD22	1:122:A:LEU:HD13	6	0.15
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD11	6	0.15
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD12	6	0.15
(1,490)	1:29:A:LEU:HD23	1:122:A:LEU:HD13	6	0.15
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD11	5	0.15
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD12	5	0.15
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD13	5	0.15
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD11	5	0.15
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD12	5	0.15
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD13	5	0.15
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD11	5	0.15
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD12	5	0.15
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD13	5	0.15
(1,265)	1:83:A:ASN:H	1:85:A:GLN:H	1	0.15
(1,193)	1:176:A:THR:H	1:177:A:GLY:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:203:A:ILE:HD11	1:207:A:VAL:HG11	2	0.15
(1,79)	1:203:A:ILE:HD11	1:207:A:VAL:HG12	2	0.15
(1,79)	1:203:A:ILE:HD11	1:207:A:VAL:HG13	2	0.15
(1,79)	1:203:A:ILE:HD12	1:207:A:VAL:HG11	2	0.15
(1,79)	1:203:A:ILE:HD12	1:207:A:VAL:HG12	2	0.15
(1,79)	1:203:A:ILE:HD12	1:207:A:VAL:HG13	2	0.15
(1,79)	1:203:A:ILE:HD13	1:207:A:VAL:HG11	2	0.15
(1,79)	1:203:A:ILE:HD13	1:207:A:VAL:HG12	2	0.15
(1,79)	1:203:A:ILE:HD13	1:207:A:VAL:HG13	2	0.15
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD11	1	0.15
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD12	1	0.15
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD13	1	0.15
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD11	1	0.15
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD12	1	0.15
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD13	1	0.15
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD11	1	0.15
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD12	1	0.15
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD13	1	0.15
(1,37)	1:190:A:LEU:HD21	1:144:A:VAL:HG11	3	0.15
(1,37)	1:190:A:LEU:HD21	1:144:A:VAL:HG12	3	0.15
(1,37)	1:190:A:LEU:HD21	1:144:A:VAL:HG13	3	0.15
(1,37)	1:190:A:LEU:HD22	1:144:A:VAL:HG11	3	0.15
(1,37)	1:190:A:LEU:HD22	1:144:A:VAL:HG12	3	0.15
(1,37)	1:190:A:LEU:HD22	1:144:A:VAL:HG13	3	0.15
(1,37)	1:190:A:LEU:HD23	1:144:A:VAL:HG11	3	0.15
(1,37)	1:190:A:LEU:HD23	1:144:A:VAL:HG12	3	0.15
(1,37)	1:190:A:LEU:HD23	1:144:A:VAL:HG13	3	0.15
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD21	7	0.15
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD22	7	0.15
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD23	7	0.15
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD21	7	0.15
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD22	7	0.15
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD23	7	0.15
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD21	7	0.15
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD22	7	0.15
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD23	7	0.15
(1,30)	1:89:A:LEU:HD11	1:48:A:LEU:HD21	8	0.15
(1,30)	1:89:A:LEU:HD11	1:48:A:LEU:HD22	8	0.15
(1,30)	1:89:A:LEU:HD11	1:48:A:LEU:HD23	8	0.15
(1,30)	1:89:A:LEU:HD12	1:48:A:LEU:HD21	8	0.15
(1,30)	1:89:A:LEU:HD12	1:48:A:LEU:HD22	8	0.15
(1,30)	1:89:A:LEU:HD12	1:48:A:LEU:HD23	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:89:A:LEU:HD13	1:48:A:LEU:HD21	8	0.15
(1,30)	1:89:A:LEU:HD13	1:48:A:LEU:HD22	8	0.15
(1,30)	1:89:A:LEU:HD13	1:48:A:LEU:HD23	8	0.15
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD11	5	0.15
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD12	5	0.15
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD13	5	0.15
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD11	5	0.15
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD12	5	0.15
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD13	5	0.15
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD11	5	0.15
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD12	5	0.15
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD13	5	0.15
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG21	9	0.15
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG22	9	0.15
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG23	9	0.15
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG21	9	0.15
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG22	9	0.15
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG23	9	0.15
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG21	9	0.15
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG22	9	0.15
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG23	9	0.15
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD11	7	0.15
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD12	7	0.15
(1,1)	1:89:A:LEU:HD21	1:198:A:LEU:HD13	7	0.15
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD11	7	0.15
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD12	7	0.15
(1,1)	1:89:A:LEU:HD22	1:198:A:LEU:HD13	7	0.15
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD11	7	0.15
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD12	7	0.15
(1,1)	1:89:A:LEU:HD23	1:198:A:LEU:HD13	7	0.15
(1,1752)	1:175:A:ASP:H	1:160:A:TYR:HA	6	0.14
(1,1749)	1:173:A:ARG:H	1:162:A:TRP:HA	8	0.14
(1,1730)	1:164:A:SER:H	1:147:A:LYS:HA	10	0.14
(1,1709)	1:152:A:THR:H	1:184:A:THR:HA	6	0.14
(1,1687)	1:94:A:THR:H	1:78:A:ILE:HA	9	0.14
(1,1668)	1:80:A:LEU:H	1:220:A:LEU:HA	2	0.14
(1,1642)	1:212:A:GLN:H	1:208:A:LYS:HA	8	0.14
(1,1631)	1:105:A:ASN:H	1:101:A:ALA:HA	2	0.14
(1,1630)	1:104:A:ILE:H	1:100:A:LYS:HA	3	0.14
(1,1584)	1:197:A:TYR:H	1:194:A:GLN:HA	8	0.14
(1,1576)	1:107:A:LEU:H	1:104:A:ILE:HA	8	0.14
(1,1561)	1:62:A:GLU:H	1:59:A:ILE:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:51:A:ASN:H	1:48:A:LEU:HA	7	0.14
(1,1505)	1:144:A:VAL:H	1:142:A:TYR:HA	1	0.14
(1,1479)	1:65:A:THR:H	1:63:A:SER:HA	8	0.14
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA2	1	0.14
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA3	1	0.14
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA2	9	0.14
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA3	9	0.14
(1,1361)	1:96:A:ILE:H	1:95:A:GLY:HA2	2	0.14
(1,1361)	1:96:A:ILE:H	1:95:A:GLY:HA3	2	0.14
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD11	6	0.14
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD12	6	0.14
(1,1121)	1:221:A:PHE:H	1:220:A:LEU:HD13	6	0.14
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD11	1	0.14
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD12	1	0.14
(1,1115)	1:218:A:ILE:H	1:78:A:ILE:HD13	1	0.14
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD11	7	0.14
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD12	7	0.14
(1,1114)	1:216:A:TYR:H	1:218:A:ILE:HD13	7	0.14
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD21	6	0.14
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD22	6	0.14
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD23	6	0.14
(1,1109)	1:213:A:PHE:H	1:218:A:ILE:HD11	6	0.14
(1,1109)	1:213:A:PHE:H	1:218:A:ILE:HD12	6	0.14
(1,1109)	1:213:A:PHE:H	1:218:A:ILE:HD13	6	0.14
(1,1088)	1:203:A:ILE:H	1:220:A:LEU:HD11	9	0.14
(1,1088)	1:203:A:ILE:H	1:220:A:LEU:HD12	9	0.14
(1,1088)	1:203:A:ILE:H	1:220:A:LEU:HD13	9	0.14
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD11	3	0.14
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD12	3	0.14
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD13	3	0.14
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG21	6	0.14
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG22	6	0.14
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG23	6	0.14
(1,1021)	1:185:A:LYS:H	1:150:A:VAL:HG11	1	0.14
(1,1021)	1:185:A:LYS:H	1:150:A:VAL:HG12	1	0.14
(1,1021)	1:185:A:LYS:H	1:150:A:VAL:HG13	1	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG21	4	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG22	4	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG23	4	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG21	8	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG22	8	0.14
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG23	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG21	1	0.14
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG22	1	0.14
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG23	1	0.14
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG21	5	0.14
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG22	5	0.14
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG23	5	0.14
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD21	4	0.14
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD22	4	0.14
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD23	4	0.14
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD11	8	0.14
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD12	8	0.14
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD13	8	0.14
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG21	2	0.14
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG22	2	0.14
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG23	2	0.14
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD11	2	0.14
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD12	2	0.14
(1,944)	1:141:A:ALA:H	1:131:A:ILE:HD13	2	0.14
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG21	3	0.14
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG22	3	0.14
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG23	3	0.14
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD11	7	0.14
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD12	7	0.14
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD13	7	0.14
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD11	8	0.14
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD12	8	0.14
(1,901)	1:107:A:LEU:H	1:103:A:LEU:HD13	8	0.14
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD11	6	0.14
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD12	6	0.14
(1,889)	1:94:A:THR:H	1:56:A:LEU:HD13	6	0.14
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD11	3	0.14
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD12	3	0.14
(1,865)	1:87:A:ARG:H	1:198:A:LEU:HD13	3	0.14
(1,831)	1:77:A:HIS:H	1:56:A:LEU:HD11	10	0.14
(1,831)	1:77:A:HIS:H	1:56:A:LEU:HD12	10	0.14
(1,831)	1:77:A:HIS:H	1:56:A:LEU:HD13	10	0.14
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD11	7	0.14
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD12	7	0.14
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD13	7	0.14
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD21	7	0.14
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD22	7	0.14
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD23	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:63:A:SER:H	1:59:A:ILE:HD11	7	0.14
(1,814)	1:63:A:SER:H	1:59:A:ILE:HD12	7	0.14
(1,814)	1:63:A:SER:H	1:59:A:ILE:HD13	7	0.14
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD11	4	0.14
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD12	4	0.14
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD13	4	0.14
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD11	9	0.14
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD12	9	0.14
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD13	9	0.14
(1,782)	1:47:A:GLU:H	1:48:A:LEU:HD11	1	0.14
(1,782)	1:47:A:GLU:H	1:48:A:LEU:HD12	1	0.14
(1,782)	1:47:A:GLU:H	1:48:A:LEU:HD13	1	0.14
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD11	4	0.14
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD12	4	0.14
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD13	4	0.14
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD11	6	0.14
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD12	6	0.14
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD13	6	0.14
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD11	1	0.14
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD12	1	0.14
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD13	1	0.14
(1,753)	1:29:A:LEU:H	1:115:A:THR:HG21	1	0.14
(1,753)	1:29:A:LEU:H	1:115:A:THR:HG22	1	0.14
(1,753)	1:29:A:LEU:H	1:115:A:THR:HG23	1	0.14
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB1	4	0.14
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB2	4	0.14
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB3	4	0.14
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG11	2	0.14
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG12	2	0.14
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG13	2	0.14
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD11	5	0.14
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD12	5	0.14
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD13	5	0.14
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD11	5	0.14
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD12	5	0.14
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD13	5	0.14
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD11	5	0.14
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD12	5	0.14
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD13	5	0.14
(1,654)	1:195:A:THR:HG21	1:198:A:LEU:HD11	5	0.14
(1,654)	1:195:A:THR:HG21	1:198:A:LEU:HD12	5	0.14
(1,654)	1:195:A:THR:HG21	1:198:A:LEU:HD13	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:195:A:THR:HG22	1:198:A:LEU:HD11	5	0.14
(1,654)	1:195:A:THR:HG22	1:198:A:LEU:HD12	5	0.14
(1,654)	1:195:A:THR:HG22	1:198:A:LEU:HD13	5	0.14
(1,654)	1:195:A:THR:HG23	1:198:A:LEU:HD11	5	0.14
(1,654)	1:195:A:THR:HG23	1:198:A:LEU:HD12	5	0.14
(1,654)	1:195:A:THR:HG23	1:198:A:LEU:HD13	5	0.14
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG11	8	0.14
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG12	8	0.14
(1,614)	1:115:A:THR:HG21	1:136:A:VAL:HG13	8	0.14
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG11	8	0.14
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG12	8	0.14
(1,614)	1:115:A:THR:HG22	1:136:A:VAL:HG13	8	0.14
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG11	8	0.14
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG12	8	0.14
(1,614)	1:115:A:THR:HG23	1:136:A:VAL:HG13	8	0.14
(1,612)	1:109:A:THR:HG21	1:136:A:VAL:HG21	5	0.14
(1,612)	1:109:A:THR:HG21	1:136:A:VAL:HG22	5	0.14
(1,612)	1:109:A:THR:HG21	1:136:A:VAL:HG23	5	0.14
(1,612)	1:109:A:THR:HG22	1:136:A:VAL:HG21	5	0.14
(1,612)	1:109:A:THR:HG22	1:136:A:VAL:HG22	5	0.14
(1,612)	1:109:A:THR:HG22	1:136:A:VAL:HG23	5	0.14
(1,612)	1:109:A:THR:HG23	1:136:A:VAL:HG21	5	0.14
(1,612)	1:109:A:THR:HG23	1:136:A:VAL:HG22	5	0.14
(1,612)	1:109:A:THR:HG23	1:136:A:VAL:HG23	5	0.14
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	9	0.14
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	9	0.14
(1,601)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	9	0.14
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	9	0.14
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	9	0.14
(1,601)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	9	0.14
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	9	0.14
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	9	0.14
(1,601)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	9	0.14
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG21	7	0.14
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG22	7	0.14
(1,599)	1:103:A:LEU:HD11	1:152:A:THR:HG23	7	0.14
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG21	7	0.14
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG22	7	0.14
(1,599)	1:103:A:LEU:HD12	1:152:A:THR:HG23	7	0.14
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG21	7	0.14
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG22	7	0.14
(1,599)	1:103:A:LEU:HD13	1:152:A:THR:HG23	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	4	0.14
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	4	0.14
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	4	0.14
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	4	0.14
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	4	0.14
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	4	0.14
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	4	0.14
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	4	0.14
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	4	0.14
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	3	0.14
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	3	0.14
(1,574)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	3	0.14
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	3	0.14
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	3	0.14
(1,574)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	3	0.14
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	3	0.14
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	3	0.14
(1,574)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	3	0.14
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	8	0.14
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	8	0.14
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	8	0.14
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	8	0.14
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	8	0.14
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	8	0.14
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	8	0.14
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	8	0.14
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	8	0.14
(1,554)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	6	0.14
(1,554)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	6	0.14
(1,554)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	6	0.14
(1,554)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	6	0.14
(1,554)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	6	0.14
(1,554)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	6	0.14
(1,554)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	6	0.14
(1,554)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	6	0.14
(1,554)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	6	0.14
(1,553)	1:59:A:ILE:HD11	1:70:A:LEU:HD21	10	0.14
(1,553)	1:59:A:ILE:HD11	1:70:A:LEU:HD22	10	0.14
(1,553)	1:59:A:ILE:HD11	1:70:A:LEU:HD23	10	0.14
(1,553)	1:59:A:ILE:HD12	1:70:A:LEU:HD21	10	0.14
(1,553)	1:59:A:ILE:HD12	1:70:A:LEU:HD22	10	0.14
(1,553)	1:59:A:ILE:HD12	1:70:A:LEU:HD23	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:59:A:ILE:HD13	1:70:A:LEU:HD21	10	0.14
(1,553)	1:59:A:ILE:HD13	1:70:A:LEU:HD22	10	0.14
(1,553)	1:59:A:ILE:HD13	1:70:A:LEU:HD23	10	0.14
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD11	6	0.14
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD12	6	0.14
(1,552)	1:56:A:LEU:HD21	1:78:A:ILE:HD13	6	0.14
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD11	6	0.14
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD12	6	0.14
(1,552)	1:56:A:LEU:HD22	1:78:A:ILE:HD13	6	0.14
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD11	6	0.14
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD12	6	0.14
(1,552)	1:56:A:LEU:HD23	1:78:A:ILE:HD13	6	0.14
(1,502)	1:30:A:MET:HE1	1:166:A:ALA:HB1	6	0.14
(1,502)	1:30:A:MET:HE1	1:166:A:ALA:HB2	6	0.14
(1,502)	1:30:A:MET:HE1	1:166:A:ALA:HB3	6	0.14
(1,502)	1:30:A:MET:HE2	1:166:A:ALA:HB1	6	0.14
(1,502)	1:30:A:MET:HE2	1:166:A:ALA:HB2	6	0.14
(1,502)	1:30:A:MET:HE2	1:166:A:ALA:HB3	6	0.14
(1,502)	1:30:A:MET:HE3	1:166:A:ALA:HB1	6	0.14
(1,502)	1:30:A:MET:HE3	1:166:A:ALA:HB2	6	0.14
(1,502)	1:30:A:MET:HE3	1:166:A:ALA:HB3	6	0.14
(1,489)	1:29:A:LEU:HD11	1:119:A:MET:HE1	5	0.14
(1,489)	1:29:A:LEU:HD11	1:119:A:MET:HE2	5	0.14
(1,489)	1:29:A:LEU:HD11	1:119:A:MET:HE3	5	0.14
(1,489)	1:29:A:LEU:HD12	1:119:A:MET:HE1	5	0.14
(1,489)	1:29:A:LEU:HD12	1:119:A:MET:HE2	5	0.14
(1,489)	1:29:A:LEU:HD12	1:119:A:MET:HE3	5	0.14
(1,489)	1:29:A:LEU:HD13	1:119:A:MET:HE1	5	0.14
(1,489)	1:29:A:LEU:HD13	1:119:A:MET:HE2	5	0.14
(1,489)	1:29:A:LEU:HD13	1:119:A:MET:HE3	5	0.14
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD11	1	0.14
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD12	1	0.14
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD13	1	0.14
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD11	1	0.14
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD12	1	0.14
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD13	1	0.14
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD11	1	0.14
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD12	1	0.14
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD13	1	0.14
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB1	6	0.14
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB2	6	0.14
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB3	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB1	6	0.14
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB2	6	0.14
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB3	6	0.14
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB1	6	0.14
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB2	6	0.14
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB3	6	0.14
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB1	8	0.14
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB2	8	0.14
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB3	8	0.14
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB1	8	0.14
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB2	8	0.14
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB3	8	0.14
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB1	8	0.14
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB2	8	0.14
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB3	8	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB1	1	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB2	1	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB3	1	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB1	1	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB2	1	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB3	1	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB1	1	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB2	1	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB3	1	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB1	4	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB2	4	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB3	4	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB1	4	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB2	4	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB3	4	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB1	4	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB2	4	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB3	4	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB1	7	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB2	7	0.14
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB3	7	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB1	7	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB2	7	0.14
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB3	7	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB1	7	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB2	7	0.14
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB1	10	0.14
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB2	10	0.14
(1,47)	1:190:A:LEU:HD11	1:145:A:ALA:HB3	10	0.14
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB1	10	0.14
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB2	10	0.14
(1,47)	1:190:A:LEU:HD12	1:145:A:ALA:HB3	10	0.14
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB1	10	0.14
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB2	10	0.14
(1,47)	1:190:A:LEU:HD13	1:145:A:ALA:HB3	10	0.14
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD21	3	0.14
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD22	3	0.14
(1,41)	1:220:A:LEU:HD11	1:89:A:LEU:HD23	3	0.14
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD21	3	0.14
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD22	3	0.14
(1,41)	1:220:A:LEU:HD12	1:89:A:LEU:HD23	3	0.14
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD21	3	0.14
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD22	3	0.14
(1,41)	1:220:A:LEU:HD13	1:89:A:LEU:HD23	3	0.14
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD11	3	0.14
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD12	3	0.14
(1,32)	1:89:A:LEU:HD11	1:49:A:ILE:HD13	3	0.14
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD11	3	0.14
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD12	3	0.14
(1,32)	1:89:A:LEU:HD12	1:49:A:ILE:HD13	3	0.14
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD11	3	0.14
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD12	3	0.14
(1,32)	1:89:A:LEU:HD13	1:49:A:ILE:HD13	3	0.14
(1,27)	1:76:A:LEU:HD21	1:59:A:ILE:HD11	6	0.14
(1,27)	1:76:A:LEU:HD21	1:59:A:ILE:HD12	6	0.14
(1,27)	1:76:A:LEU:HD21	1:59:A:ILE:HD13	6	0.14
(1,27)	1:76:A:LEU:HD22	1:59:A:ILE:HD11	6	0.14
(1,27)	1:76:A:LEU:HD22	1:59:A:ILE:HD12	6	0.14
(1,27)	1:76:A:LEU:HD22	1:59:A:ILE:HD13	6	0.14
(1,27)	1:76:A:LEU:HD23	1:59:A:ILE:HD11	6	0.14
(1,27)	1:76:A:LEU:HD23	1:59:A:ILE:HD12	6	0.14
(1,27)	1:76:A:LEU:HD23	1:59:A:ILE:HD13	6	0.14
(1,18)	1:45:A:LEU:HD21	1:207:A:VAL:HG21	1	0.14
(1,18)	1:45:A:LEU:HD21	1:207:A:VAL:HG22	1	0.14
(1,18)	1:45:A:LEU:HD21	1:207:A:VAL:HG23	1	0.14
(1,18)	1:45:A:LEU:HD22	1:207:A:VAL:HG21	1	0.14
(1,18)	1:45:A:LEU:HD22	1:207:A:VAL:HG22	1	0.14
(1,18)	1:45:A:LEU:HD22	1:207:A:VAL:HG23	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:45:A:LEU:HD23	1:207:A:VAL:HG21	1	0.14
(1,18)	1:45:A:LEU:HD23	1:207:A:VAL:HG22	1	0.14
(1,18)	1:45:A:LEU:HD23	1:207:A:VAL:HG23	1	0.14
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD11	1	0.14
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD12	1	0.14
(1,13)	1:115:A:THR:HG21	1:131:A:ILE:HD13	1	0.14
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD11	1	0.14
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD12	1	0.14
(1,13)	1:115:A:THR:HG22	1:131:A:ILE:HD13	1	0.14
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD11	1	0.14
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD12	1	0.14
(1,13)	1:115:A:THR:HG23	1:131:A:ILE:HD13	1	0.14
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD21	7	0.14
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD22	7	0.14
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD23	7	0.14
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD21	7	0.14
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD22	7	0.14
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD23	7	0.14
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD21	7	0.14
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD22	7	0.14
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD23	7	0.14
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG21	1	0.14
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG22	1	0.14
(1,10)	1:184:A:THR:HG21	1:152:A:THR:HG23	1	0.14
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG21	1	0.14
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG22	1	0.14
(1,10)	1:184:A:THR:HG22	1:152:A:THR:HG23	1	0.14
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG21	1	0.14
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG22	1	0.14
(1,10)	1:184:A:THR:HG23	1:152:A:THR:HG23	1	0.14
(1,1873)	1:126:A:ALA:H	1:122:A:LEU:HA	7	0.13
(1,1709)	1:152:A:THR:H	1:184:A:THR:HA	2	0.13
(1,1657)	1:22:A:PHE:H	1:168:A:GLY:HA2	9	0.13
(1,1657)	1:22:A:PHE:H	1:168:A:GLY:HA3	9	0.13
(1,1647)	1:98:A:MET:H	1:154:A:HIS:H	10	0.13
(1,1629)	1:103:A:LEU:H	1:99:A:THR:HA	4	0.13
(1,1605)	1:36:A:GLU:H	1:32:A:LEU:HA	10	0.13
(1,1575)	1:106:A:ASN:H	1:103:A:LEU:HA	2	0.13
(1,1564)	1:65:A:THR:H	1:62:A:GLU:HA	6	0.13
(1,1517)	1:198:A:LEU:H	1:196:A:GLU:HA	4	0.13
(1,1511)	1:177:A:GLY:H	1:175:A:ASP:HA	2	0.13
(1,1509)	1:169:A:SER:H	1:167:A:GLY:HA2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:169:A:SER:H	1:167:A:GLY:HA3	10	0.13
(1,1505)	1:144:A:VAL:H	1:142:A:TYR:HA	3	0.13
(1,1504)	1:143:A:LEU:H	1:141:A:ALA:HA	1	0.13
(1,1473)	1:59:A:ILE:H	1:57:A:ASP:HA	10	0.13
(1,1455)	1:36:A:GLU:H	1:34:A:ILE:HA	8	0.13
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA2	3	0.13
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA3	3	0.13
(1,1240)	1:166:A:ALA:H	1:166:A:ALA:HA	8	0.13
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA2	9	0.13
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA3	9	0.13
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD21	3	0.13
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD22	3	0.13
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD23	3	0.13
(1,1104)	1:210:A:HIS:H	1:207:A:VAL:HG11	3	0.13
(1,1104)	1:210:A:HIS:H	1:207:A:VAL:HG12	3	0.13
(1,1104)	1:210:A:HIS:H	1:207:A:VAL:HG13	3	0.13
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG11	3	0.13
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG12	3	0.13
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG13	3	0.13
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG11	5	0.13
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG12	5	0.13
(1,1100)	1:208:A:LYS:H	1:207:A:VAL:HG13	5	0.13
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD11	6	0.13
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD12	6	0.13
(1,1093)	1:204:A:LYS:H	1:220:A:LEU:HD13	6	0.13
(1,1071)	1:197:A:TYR:H	1:198:A:LEU:HD11	2	0.13
(1,1071)	1:197:A:TYR:H	1:198:A:LEU:HD12	2	0.13
(1,1071)	1:197:A:TYR:H	1:198:A:LEU:HD13	2	0.13
(1,1045)	1:188:A:LEU:H	1:190:A:LEU:HD21	3	0.13
(1,1045)	1:188:A:LEU:H	1:190:A:LEU:HD22	3	0.13
(1,1045)	1:188:A:LEU:H	1:190:A:LEU:HD23	3	0.13
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG11	5	0.13
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG12	5	0.13
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG13	5	0.13
(1,1026)	1:186:A:VAL:H	1:90:A:THR:HG21	5	0.13
(1,1026)	1:186:A:VAL:H	1:90:A:THR:HG22	5	0.13
(1,1026)	1:186:A:VAL:H	1:90:A:THR:HG23	5	0.13
(1,1012)	1:175:A:ASP:H	1:161:A:ALA:HB1	5	0.13
(1,1012)	1:175:A:ASP:H	1:161:A:ALA:HB2	5	0.13
(1,1012)	1:175:A:ASP:H	1:161:A:ALA:HB3	5	0.13
(1,999)	1:164:A:SER:H	1:148:A:VAL:HG11	3	0.13
(1,999)	1:164:A:SER:H	1:148:A:VAL:HG12	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:164:A:SER:H	1:148:A:VAL:HG13	3	0.13
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG21	1	0.13
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG22	1	0.13
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG23	1	0.13
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG21	7	0.13
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG22	7	0.13
(1,995)	1:163:A:GLU:H	1:149:A:THR:HG23	7	0.13
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	10	0.13
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	10	0.13
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	10	0.13
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	10	0.13
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	10	0.13
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	10	0.13
(1,974)	1:151:A:ILE:H	1:103:A:LEU:HD11	4	0.13
(1,974)	1:151:A:ILE:H	1:103:A:LEU:HD12	4	0.13
(1,974)	1:151:A:ILE:H	1:103:A:LEU:HD13	4	0.13
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	4	0.13
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	4	0.13
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	4	0.13
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD11	6	0.13
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD12	6	0.13
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD13	6	0.13
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG21	6	0.13
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG22	6	0.13
(1,955)	1:143:A:LEU:H	1:144:A:VAL:HG23	6	0.13
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD11	9	0.13
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD12	9	0.13
(1,947)	1:142:A:TYR:H	1:33:A:ILE:HD13	9	0.13
(1,942)	1:139:A:TYR:H	1:131:A:ILE:HD11	2	0.13
(1,942)	1:139:A:TYR:H	1:131:A:ILE:HD12	2	0.13
(1,942)	1:139:A:TYR:H	1:131:A:ILE:HD13	2	0.13
(1,931)	1:131:A:ILE:H	1:43:A:ILE:HD11	5	0.13
(1,931)	1:131:A:ILE:H	1:43:A:ILE:HD12	5	0.13
(1,931)	1:131:A:ILE:H	1:43:A:ILE:HD13	5	0.13
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD11	9	0.13
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD12	9	0.13
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD13	9	0.13
(1,920)	1:125:A:GLY:H	1:124:A:ALA:HB1	9	0.13
(1,920)	1:125:A:GLY:H	1:124:A:ALA:HB2	9	0.13
(1,920)	1:125:A:GLY:H	1:124:A:ALA:HB3	9	0.13
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB1	9	0.13
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB3	9	0.13
(1,888)	1:93:A:ASP:H	1:184:A:THR:HG21	4	0.13
(1,888)	1:93:A:ASP:H	1:184:A:THR:HG22	4	0.13
(1,888)	1:93:A:ASP:H	1:184:A:THR:HG23	4	0.13
(1,877)	1:91:A:ILE:H	1:186:A:VAL:HG11	10	0.13
(1,877)	1:91:A:ILE:H	1:186:A:VAL:HG12	10	0.13
(1,877)	1:91:A:ILE:H	1:186:A:VAL:HG13	10	0.13
(1,857)	1:84:A:LYS:H	1:198:A:LEU:HD11	4	0.13
(1,857)	1:84:A:LYS:H	1:198:A:LEU:HD12	4	0.13
(1,857)	1:84:A:LYS:H	1:198:A:LEU:HD13	4	0.13
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD11	4	0.13
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD12	4	0.13
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD13	4	0.13
(1,838)	1:79:A:ASN:H	1:80:A:LEU:HD21	10	0.13
(1,838)	1:79:A:ASN:H	1:80:A:LEU:HD22	10	0.13
(1,838)	1:79:A:ASN:H	1:80:A:LEU:HD23	10	0.13
(1,836)	1:78:A:ILE:H	1:56:A:LEU:HD21	10	0.13
(1,836)	1:78:A:ILE:H	1:56:A:LEU:HD22	10	0.13
(1,836)	1:78:A:ILE:H	1:56:A:LEU:HD23	10	0.13
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD11	7	0.13
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD12	7	0.13
(1,778)	1:46:A:ARG:H	1:45:A:LEU:HD13	7	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD21	4	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD22	4	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD23	4	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD21	5	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD22	5	0.13
(1,766)	1:34:A:ILE:H	1:32:A:LEU:HD23	5	0.13
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB1	1	0.13
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB2	1	0.13
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB3	1	0.13
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG21	9	0.13
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG22	9	0.13
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG23	9	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG11	3	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG12	3	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG13	3	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG11	7	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG12	7	0.13
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG13	7	0.13
(1,703)	1:136:A:VAL:H	1:136:A:VAL:HG11	4	0.13
(1,703)	1:136:A:VAL:H	1:136:A:VAL:HG12	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:136:A:VAL:H	1:136:A:VAL:HG13	4	0.13
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD11	1	0.13
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD12	1	0.13
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD13	1	0.13
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD11	2	0.13
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD12	2	0.13
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD13	2	0.13
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD11	4	0.13
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD12	4	0.13
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD13	4	0.13
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG21	9	0.13
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG22	9	0.13
(1,665)	1:17:A:VAL:H	1:17:A:VAL:HG23	9	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG11	7	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG12	7	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG13	7	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG11	7	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG12	7	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG13	7	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG11	7	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG12	7	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG13	7	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	7	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	7	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	7	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	7	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	7	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	7	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	7	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	7	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	7	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG11	8	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG12	8	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG13	8	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG11	8	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG12	8	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG13	8	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG11	8	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG12	8	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG13	8	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	8	0.13
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	8	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	8	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	8	0.13
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	8	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	8	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	8	0.13
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	8	0.13
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG21	10	0.13
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG22	10	0.13
(1,640)	1:150:A:VAL:HG21	1:184:A:THR:HG23	10	0.13
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG21	10	0.13
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG22	10	0.13
(1,640)	1:150:A:VAL:HG22	1:184:A:THR:HG23	10	0.13
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG21	10	0.13
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG22	10	0.13
(1,640)	1:150:A:VAL:HG23	1:184:A:THR:HG23	10	0.13
(1,615)	1:115:A:THR:HG21	1:136:A:VAL:HG21	4	0.13
(1,615)	1:115:A:THR:HG21	1:136:A:VAL:HG22	4	0.13
(1,615)	1:115:A:THR:HG21	1:136:A:VAL:HG23	4	0.13
(1,615)	1:115:A:THR:HG22	1:136:A:VAL:HG21	4	0.13
(1,615)	1:115:A:THR:HG22	1:136:A:VAL:HG22	4	0.13
(1,615)	1:115:A:THR:HG22	1:136:A:VAL:HG23	4	0.13
(1,615)	1:115:A:THR:HG23	1:136:A:VAL:HG21	4	0.13
(1,615)	1:115:A:THR:HG23	1:136:A:VAL:HG22	4	0.13
(1,615)	1:115:A:THR:HG23	1:136:A:VAL:HG23	4	0.13
(1,602)	1:103:A:LEU:HD21	1:150:A:VAL:HG11	1	0.13
(1,602)	1:103:A:LEU:HD21	1:150:A:VAL:HG12	1	0.13
(1,602)	1:103:A:LEU:HD21	1:150:A:VAL:HG13	1	0.13
(1,602)	1:103:A:LEU:HD22	1:150:A:VAL:HG11	1	0.13
(1,602)	1:103:A:LEU:HD22	1:150:A:VAL:HG12	1	0.13
(1,602)	1:103:A:LEU:HD22	1:150:A:VAL:HG13	1	0.13
(1,602)	1:103:A:LEU:HD23	1:150:A:VAL:HG11	1	0.13
(1,602)	1:103:A:LEU:HD23	1:150:A:VAL:HG12	1	0.13
(1,602)	1:103:A:LEU:HD23	1:150:A:VAL:HG13	1	0.13
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG21	6	0.13
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG22	6	0.13
(1,598)	1:103:A:LEU:HD11	1:150:A:VAL:HG23	6	0.13
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG21	6	0.13
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG22	6	0.13
(1,598)	1:103:A:LEU:HD12	1:150:A:VAL:HG23	6	0.13
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG21	6	0.13
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG22	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:103:A:LEU:HD13	1:150:A:VAL:HG23	6	0.13
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	4	0.13
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	4	0.13
(1,596)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	4	0.13
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	4	0.13
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	4	0.13
(1,596)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	4	0.13
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	4	0.13
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	4	0.13
(1,596)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	4	0.13
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD21	10	0.13
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD22	10	0.13
(1,588)	1:98:A:MET:HE1	1:107:A:LEU:HD23	10	0.13
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD21	10	0.13
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD22	10	0.13
(1,588)	1:98:A:MET:HE2	1:107:A:LEU:HD23	10	0.13
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD21	10	0.13
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD22	10	0.13
(1,588)	1:98:A:MET:HE3	1:107:A:LEU:HD23	10	0.13
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD21	6	0.13
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD22	6	0.13
(1,580)	1:91:A:ILE:HD11	1:188:A:LEU:HD23	6	0.13
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD21	6	0.13
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD22	6	0.13
(1,580)	1:91:A:ILE:HD12	1:188:A:LEU:HD23	6	0.13
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD21	6	0.13
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD22	6	0.13
(1,580)	1:91:A:ILE:HD13	1:188:A:LEU:HD23	6	0.13
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD11	9	0.13
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD12	9	0.13
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD13	9	0.13
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD11	9	0.13
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD12	9	0.13
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD13	9	0.13
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD11	9	0.13
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD12	9	0.13
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD13	9	0.13
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	7	0.13
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	7	0.13
(1,572)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	7	0.13
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	7	0.13
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	7	0.13
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	7	0.13
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	7	0.13
(1,572)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	7	0.13
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD11	3	0.13
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD12	3	0.13
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD13	3	0.13
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD11	3	0.13
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD12	3	0.13
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD13	3	0.13
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD11	3	0.13
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD12	3	0.13
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD13	3	0.13
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	10	0.13
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	10	0.13
(1,564)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	10	0.13
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	10	0.13
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	10	0.13
(1,564)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	10	0.13
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	10	0.13
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	10	0.13
(1,564)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	10	0.13
(1,547)	1:49:A:ILE:HD11	1:218:A:ILE:HD11	7	0.13
(1,547)	1:49:A:ILE:HD11	1:218:A:ILE:HD12	7	0.13
(1,547)	1:49:A:ILE:HD11	1:218:A:ILE:HD13	7	0.13
(1,547)	1:49:A:ILE:HD12	1:218:A:ILE:HD11	7	0.13
(1,547)	1:49:A:ILE:HD12	1:218:A:ILE:HD12	7	0.13
(1,547)	1:49:A:ILE:HD12	1:218:A:ILE:HD13	7	0.13
(1,547)	1:49:A:ILE:HD13	1:218:A:ILE:HD11	7	0.13
(1,547)	1:49:A:ILE:HD13	1:218:A:ILE:HD12	7	0.13
(1,547)	1:49:A:ILE:HD13	1:218:A:ILE:HD13	7	0.13
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	1	0.13
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	1	0.13
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	1	0.13
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	1	0.13
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	1	0.13
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	1	0.13
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	1	0.13
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	1	0.13
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	1	0.13
(1,523)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	3	0.13
(1,523)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	3	0.13
(1,523)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	3	0.13
(1,523)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	3	0.13
(1,523)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	3	0.13
(1,523)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	3	0.13
(1,523)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	3	0.13
(1,523)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	3	0.13
(1,519)	1:45:A:LEU:HD11	1:49:A:ILE:HD11	7	0.13
(1,519)	1:45:A:LEU:HD11	1:49:A:ILE:HD12	7	0.13
(1,519)	1:45:A:LEU:HD11	1:49:A:ILE:HD13	7	0.13
(1,519)	1:45:A:LEU:HD12	1:49:A:ILE:HD11	7	0.13
(1,519)	1:45:A:LEU:HD12	1:49:A:ILE:HD12	7	0.13
(1,519)	1:45:A:LEU:HD12	1:49:A:ILE:HD13	7	0.13
(1,519)	1:45:A:LEU:HD13	1:49:A:ILE:HD11	7	0.13
(1,519)	1:45:A:LEU:HD13	1:49:A:ILE:HD12	7	0.13
(1,519)	1:45:A:LEU:HD13	1:49:A:ILE:HD13	7	0.13
(1,514)	1:33:A:ILE:HD11	1:143:A:LEU:HD21	5	0.13
(1,514)	1:33:A:ILE:HD11	1:143:A:LEU:HD22	5	0.13
(1,514)	1:33:A:ILE:HD11	1:143:A:LEU:HD23	5	0.13
(1,514)	1:33:A:ILE:HD12	1:143:A:LEU:HD21	5	0.13
(1,514)	1:33:A:ILE:HD12	1:143:A:LEU:HD22	5	0.13
(1,514)	1:33:A:ILE:HD12	1:143:A:LEU:HD23	5	0.13
(1,514)	1:33:A:ILE:HD13	1:143:A:LEU:HD21	5	0.13
(1,514)	1:33:A:ILE:HD13	1:143:A:LEU:HD22	5	0.13
(1,514)	1:33:A:ILE:HD13	1:143:A:LEU:HD23	5	0.13
(1,487)	1:29:A:LEU:HD11	1:33:A:ILE:HD11	9	0.13
(1,487)	1:29:A:LEU:HD11	1:33:A:ILE:HD12	9	0.13
(1,487)	1:29:A:LEU:HD11	1:33:A:ILE:HD13	9	0.13
(1,487)	1:29:A:LEU:HD12	1:33:A:ILE:HD11	9	0.13
(1,487)	1:29:A:LEU:HD12	1:33:A:ILE:HD12	9	0.13
(1,487)	1:29:A:LEU:HD12	1:33:A:ILE:HD13	9	0.13
(1,487)	1:29:A:LEU:HD13	1:33:A:ILE:HD11	9	0.13
(1,487)	1:29:A:LEU:HD13	1:33:A:ILE:HD12	9	0.13
(1,487)	1:29:A:LEU:HD13	1:33:A:ILE:HD13	9	0.13
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD11	3	0.13
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD12	3	0.13
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD13	3	0.13
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD11	3	0.13
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD12	3	0.13
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD13	3	0.13
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD11	3	0.13
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD12	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD13	3	0.13
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG21	1	0.13
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG22	1	0.13
(1,480)	1:19:A:THR:HG21	1:171:A:THR:HG23	1	0.13
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG21	1	0.13
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG22	1	0.13
(1,480)	1:19:A:THR:HG22	1:171:A:THR:HG23	1	0.13
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG21	1	0.13
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG22	1	0.13
(1,480)	1:19:A:THR:HG23	1:171:A:THR:HG23	1	0.13
(1,419)	1:103:A:LEU:H	1:107:A:LEU:H	6	0.13
(1,391)	1:58:A:LYS:H	1:96:A:ILE:H	10	0.13
(1,376)	1:211:A:SER:H	1:214:A:ILE:H	2	0.13
(1,81)	1:151:A:ILE:HD11	1:103:A:LEU:HD11	8	0.13
(1,81)	1:151:A:ILE:HD11	1:103:A:LEU:HD12	8	0.13
(1,81)	1:151:A:ILE:HD11	1:103:A:LEU:HD13	8	0.13
(1,81)	1:151:A:ILE:HD12	1:103:A:LEU:HD11	8	0.13
(1,81)	1:151:A:ILE:HD12	1:103:A:LEU:HD12	8	0.13
(1,81)	1:151:A:ILE:HD12	1:103:A:LEU:HD13	8	0.13
(1,81)	1:151:A:ILE:HD13	1:103:A:LEU:HD11	8	0.13
(1,81)	1:151:A:ILE:HD13	1:103:A:LEU:HD12	8	0.13
(1,81)	1:151:A:ILE:HD13	1:103:A:LEU:HD13	8	0.13
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD11	9	0.13
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD12	9	0.13
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD13	9	0.13
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD11	9	0.13
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD12	9	0.13
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD13	9	0.13
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD11	9	0.13
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD12	9	0.13
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD13	9	0.13
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD21	9	0.13
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD22	9	0.13
(1,72)	1:131:A:ILE:HD11	1:122:A:LEU:HD23	9	0.13
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD21	9	0.13
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD22	9	0.13
(1,72)	1:131:A:ILE:HD12	1:122:A:LEU:HD23	9	0.13
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD21	9	0.13
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD22	9	0.13
(1,72)	1:131:A:ILE:HD13	1:122:A:LEU:HD23	9	0.13
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB1	3	0.13
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB2	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB3	3	0.13
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB1	3	0.13
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB2	3	0.13
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB3	3	0.13
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB1	3	0.13
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB2	3	0.13
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB3	3	0.13
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB1	9	0.13
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB2	9	0.13
(1,62)	1:121:A:ALA:HB1	1:117:A:ALA:HB3	9	0.13
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB1	9	0.13
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB2	9	0.13
(1,62)	1:121:A:ALA:HB2	1:117:A:ALA:HB3	9	0.13
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB1	9	0.13
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB2	9	0.13
(1,62)	1:121:A:ALA:HB3	1:117:A:ALA:HB3	9	0.13
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD11	5	0.13
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD12	5	0.13
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD13	5	0.13
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD11	5	0.13
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD12	5	0.13
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD13	5	0.13
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD11	5	0.13
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD12	5	0.13
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD13	5	0.13
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD21	10	0.13
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD22	10	0.13
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD23	10	0.13
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD21	10	0.13
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD22	10	0.13
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD23	10	0.13
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD21	10	0.13
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD22	10	0.13
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD23	10	0.13
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD11	8	0.13
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD12	8	0.13
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD13	8	0.13
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD11	8	0.13
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD12	8	0.13
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD13	8	0.13
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD11	8	0.13
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD12	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD13	8	0.13
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD21	1	0.13
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD22	1	0.13
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD23	1	0.13
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD21	1	0.13
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD22	1	0.13
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD23	1	0.13
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD21	1	0.13
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD22	1	0.13
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD23	1	0.13
(1,1860)	1:125:A:GLY:H	1:122:A:LEU:HA	2	0.12
(1,1842)	1:125:A:GLY:H	1:123:A:GLN:HA	1	0.12
(1,1823)	1:126:A:ALA:H	1:125:A:GLY:HA2	8	0.12
(1,1823)	1:126:A:ALA:H	1:125:A:GLY:HA3	8	0.12
(1,1784)	1:191:A:LYS:H	1:145:A:ALA:HA	1	0.12
(1,1760)	1:184:A:THR:H	1:152:A:THR:HA	5	0.12
(1,1708)	1:152:A:THR:H	1:161:A:ALA:HA	6	0.12
(1,1708)	1:152:A:THR:H	1:161:A:ALA:HA	9	0.12
(1,1672)	1:83:A:ASN:H	1:84:A:LYS:HA	9	0.12
(1,1671)	1:81:A:ILE:H	1:91:A:ILE:HA	9	0.12
(1,1668)	1:80:A:LEU:H	1:220:A:LEU:HA	6	0.12
(1,1664)	1:79:A:ASN:H	1:93:A:ASP:HA	3	0.12
(1,1627)	1:88:A:THR:H	1:84:A:LYS:HA	6	0.12
(1,1605)	1:36:A:GLU:H	1:32:A:LEU:HA	1	0.12
(1,1605)	1:36:A:GLU:H	1:32:A:LEU:HA	2	0.12
(1,1605)	1:36:A:GLU:H	1:32:A:LEU:HA	6	0.12
(1,1583)	1:195:A:THR:H	1:192:A:GLU:HA	5	0.12
(1,1579)	1:144:A:VAL:H	1:141:A:ALA:HA	5	0.12
(1,1575)	1:106:A:ASN:H	1:103:A:LEU:HA	9	0.12
(1,1564)	1:65:A:THR:H	1:62:A:GLU:HA	5	0.12
(1,1544)	1:45:A:LEU:H	1:42:A:GLU:HA	3	0.12
(1,1502)	1:139:A:TYR:H	1:137:A:GLY:HA2	3	0.12
(1,1502)	1:139:A:TYR:H	1:137:A:GLY:HA3	3	0.12
(1,1129)	1:123:A:GLN:HE21	1:122:A:LEU:HD21	10	0.12
(1,1129)	1:123:A:GLN:HE21	1:122:A:LEU:HD22	10	0.12
(1,1129)	1:123:A:GLN:HE21	1:122:A:LEU:HD23	10	0.12
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD11	6	0.12
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD12	6	0.12
(1,1083)	1:201:A:ARG:H	1:203:A:ILE:HD13	6	0.12
(1,1035)	1:187:A:ILE:H	1:150:A:VAL:HG11	2	0.12
(1,1035)	1:187:A:ILE:H	1:150:A:VAL:HG12	2	0.12
(1,1035)	1:187:A:ILE:H	1:150:A:VAL:HG13	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:173:A:ARG:H	1:103:A:LEU:HD21	7	0.12
(1,1008)	1:173:A:ARG:H	1:103:A:LEU:HD22	7	0.12
(1,1008)	1:173:A:ARG:H	1:103:A:LEU:HD23	7	0.12
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE1	4	0.12
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE2	4	0.12
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE3	4	0.12
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD21	7	0.12
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD22	7	0.12
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD23	7	0.12
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD11	10	0.12
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD12	10	0.12
(1,961)	1:145:A:ALA:H	1:188:A:LEU:HD13	10	0.12
(1,956)	1:144:A:VAL:H	1:148:A:VAL:HG21	9	0.12
(1,956)	1:144:A:VAL:H	1:148:A:VAL:HG22	9	0.12
(1,956)	1:144:A:VAL:H	1:148:A:VAL:HG23	9	0.12
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG21	10	0.12
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG22	10	0.12
(1,939)	1:138:A:PHE:H	1:136:A:VAL:HG23	10	0.12
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG11	9	0.12
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG12	9	0.12
(1,934)	1:134:A:PHE:H	1:136:A:VAL:HG13	9	0.12
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB1	3	0.12
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB2	3	0.12
(1,912)	1:122:A:LEU:H	1:124:A:ALA:HB3	3	0.12
(1,896)	1:104:A:ILE:H	1:101:A:ALA:HB1	2	0.12
(1,896)	1:104:A:ILE:H	1:101:A:ALA:HB2	2	0.12
(1,896)	1:104:A:ILE:H	1:101:A:ALA:HB3	2	0.12
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD11	4	0.12
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD12	4	0.12
(1,890)	1:95:A:GLY:H	1:56:A:LEU:HD13	4	0.12
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD11	1	0.12
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD12	1	0.12
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD13	1	0.12
(1,803)	1:60:A:ARG:H	1:70:A:LEU:HD21	7	0.12
(1,803)	1:60:A:ARG:H	1:70:A:LEU:HD22	7	0.12
(1,803)	1:60:A:ARG:H	1:70:A:LEU:HD23	7	0.12
(1,779)	1:46:A:ARG:H	1:45:A:LEU:HD21	8	0.12
(1,779)	1:46:A:ARG:H	1:45:A:LEU:HD22	8	0.12
(1,779)	1:46:A:ARG:H	1:45:A:LEU:HD23	8	0.12
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD11	1	0.12
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD12	1	0.12
(1,775)	1:44:A:PHE:H	1:43:A:ILE:HD13	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:43:A:ILE:H	1:143:A:LEU:HD11	8	0.12
(1,773)	1:43:A:ILE:H	1:143:A:LEU:HD12	8	0.12
(1,773)	1:43:A:ILE:H	1:143:A:LEU:HD13	8	0.12
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD11	9	0.12
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD12	9	0.12
(1,771)	1:42:A:GLU:H	1:143:A:LEU:HD13	9	0.12
(1,763)	1:33:A:ILE:H	1:32:A:LEU:HD21	4	0.12
(1,763)	1:33:A:ILE:H	1:32:A:LEU:HD22	4	0.12
(1,763)	1:33:A:ILE:H	1:32:A:LEU:HD23	4	0.12
(1,757)	1:31:A:SER:H	1:166:A:ALA:HB1	3	0.12
(1,757)	1:31:A:SER:H	1:166:A:ALA:HB2	3	0.12
(1,757)	1:31:A:SER:H	1:166:A:ALA:HB3	3	0.12
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB1	6	0.12
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB2	6	0.12
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB3	6	0.12
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB1	10	0.12
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB2	10	0.12
(1,752)	1:29:A:LEU:H	1:27:A:ALA:HB3	10	0.12
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG21	10	0.12
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG22	10	0.12
(1,747)	1:26:A:ILE:H	1:115:A:THR:HG23	10	0.12
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG11	4	0.12
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG12	4	0.12
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG13	4	0.12
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG21	4	0.12
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG22	4	0.12
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG23	4	0.12
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG21	4	0.12
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG22	4	0.12
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG23	4	0.12
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG21	4	0.12
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG22	4	0.12
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG23	4	0.12
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD11	4	0.12
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD12	4	0.12
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD13	4	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD11	4	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD12	4	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD13	4	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD11	4	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD12	4	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD13	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD11	8	0.12
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD12	8	0.12
(1,656)	1:203:A:ILE:HD11	1:220:A:LEU:HD13	8	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD11	8	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD12	8	0.12
(1,656)	1:203:A:ILE:HD12	1:220:A:LEU:HD13	8	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD11	8	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD12	8	0.12
(1,656)	1:203:A:ILE:HD13	1:220:A:LEU:HD13	8	0.12
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD11	9	0.12
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD12	9	0.12
(1,644)	1:151:A:ILE:HD11	1:187:A:ILE:HD13	9	0.12
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD11	9	0.12
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD12	9	0.12
(1,644)	1:151:A:ILE:HD12	1:187:A:ILE:HD13	9	0.12
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD11	9	0.12
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD12	9	0.12
(1,644)	1:151:A:ILE:HD13	1:187:A:ILE:HD13	9	0.12
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB1	7	0.12
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB2	7	0.12
(1,635)	1:149:A:THR:HG21	1:161:A:ALA:HB3	7	0.12
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB1	7	0.12
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB2	7	0.12
(1,635)	1:149:A:THR:HG22	1:161:A:ALA:HB3	7	0.12
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB1	7	0.12
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB2	7	0.12
(1,635)	1:149:A:THR:HG23	1:161:A:ALA:HB3	7	0.12
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	10	0.12
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	10	0.12
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	10	0.12
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	10	0.12
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	10	0.12
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	10	0.12
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	10	0.12
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	10	0.12
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	10	0.12
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG11	6	0.12
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG12	6	0.12
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG13	6	0.12
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG11	6	0.12
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG12	6	0.12
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG11	6	0.12
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG12	6	0.12
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG13	6	0.12
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG11	4	0.12
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG12	4	0.12
(1,624)	1:131:A:ILE:HD11	1:136:A:VAL:HG13	4	0.12
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG11	4	0.12
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG12	4	0.12
(1,624)	1:131:A:ILE:HD12	1:136:A:VAL:HG13	4	0.12
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG11	4	0.12
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG12	4	0.12
(1,624)	1:131:A:ILE:HD13	1:136:A:VAL:HG13	4	0.12
(1,616)	1:119:A:MET:HE1	1:122:A:LEU:HD21	4	0.12
(1,616)	1:119:A:MET:HE1	1:122:A:LEU:HD22	4	0.12
(1,616)	1:119:A:MET:HE1	1:122:A:LEU:HD23	4	0.12
(1,616)	1:119:A:MET:HE2	1:122:A:LEU:HD21	4	0.12
(1,616)	1:119:A:MET:HE2	1:122:A:LEU:HD22	4	0.12
(1,616)	1:119:A:MET:HE2	1:122:A:LEU:HD23	4	0.12
(1,616)	1:119:A:MET:HE3	1:122:A:LEU:HD21	4	0.12
(1,616)	1:119:A:MET:HE3	1:122:A:LEU:HD22	4	0.12
(1,616)	1:119:A:MET:HE3	1:122:A:LEU:HD23	4	0.12
(1,613)	1:115:A:THR:HG21	1:119:A:MET:HE1	4	0.12
(1,613)	1:115:A:THR:HG21	1:119:A:MET:HE2	4	0.12
(1,613)	1:115:A:THR:HG21	1:119:A:MET:HE3	4	0.12
(1,613)	1:115:A:THR:HG22	1:119:A:MET:HE1	4	0.12
(1,613)	1:115:A:THR:HG22	1:119:A:MET:HE2	4	0.12
(1,613)	1:115:A:THR:HG22	1:119:A:MET:HE3	4	0.12
(1,613)	1:115:A:THR:HG23	1:119:A:MET:HE1	4	0.12
(1,613)	1:115:A:THR:HG23	1:119:A:MET:HE2	4	0.12
(1,613)	1:115:A:THR:HG23	1:119:A:MET:HE3	4	0.12
(1,603)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	7	0.12
(1,603)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	7	0.12
(1,603)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	7	0.12
(1,603)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	7	0.12
(1,603)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	7	0.12
(1,603)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	7	0.12
(1,603)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	7	0.12
(1,603)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	7	0.12
(1,603)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	7	0.12
(1,591)	1:98:A:MET:HE1	1:152:A:THR:HG21	9	0.12
(1,591)	1:98:A:MET:HE1	1:152:A:THR:HG22	9	0.12
(1,591)	1:98:A:MET:HE1	1:152:A:THR:HG23	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:98:A:MET:HE2	1:152:A:THR:HG21	9	0.12
(1,591)	1:98:A:MET:HE2	1:152:A:THR:HG22	9	0.12
(1,591)	1:98:A:MET:HE2	1:152:A:THR:HG23	9	0.12
(1,591)	1:98:A:MET:HE3	1:152:A:THR:HG21	9	0.12
(1,591)	1:98:A:MET:HE3	1:152:A:THR:HG22	9	0.12
(1,591)	1:98:A:MET:HE3	1:152:A:THR:HG23	9	0.12
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE1	6	0.12
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE2	6	0.12
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE3	6	0.12
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE1	6	0.12
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE2	6	0.12
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE3	6	0.12
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE1	6	0.12
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE2	6	0.12
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE3	6	0.12
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD11	10	0.12
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD12	10	0.12
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD13	10	0.12
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD11	10	0.12
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD12	10	0.12
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD13	10	0.12
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD11	10	0.12
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD12	10	0.12
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD13	10	0.12
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD11	2	0.12
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD12	2	0.12
(1,571)	1:89:A:LEU:HD11	1:203:A:ILE:HD13	2	0.12
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD11	2	0.12
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD12	2	0.12
(1,571)	1:89:A:LEU:HD12	1:203:A:ILE:HD13	2	0.12
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD11	2	0.12
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD12	2	0.12
(1,571)	1:89:A:LEU:HD13	1:203:A:ILE:HD13	2	0.12
(1,555)	1:64:A:LEU:HD11	1:65:A:THR:HG21	10	0.12
(1,555)	1:64:A:LEU:HD11	1:65:A:THR:HG22	10	0.12
(1,555)	1:64:A:LEU:HD11	1:65:A:THR:HG23	10	0.12
(1,555)	1:64:A:LEU:HD12	1:65:A:THR:HG21	10	0.12
(1,555)	1:64:A:LEU:HD12	1:65:A:THR:HG22	10	0.12
(1,555)	1:64:A:LEU:HD12	1:65:A:THR:HG23	10	0.12
(1,555)	1:64:A:LEU:HD13	1:65:A:THR:HG21	10	0.12
(1,555)	1:64:A:LEU:HD13	1:65:A:THR:HG22	10	0.12
(1,555)	1:64:A:LEU:HD13	1:65:A:THR:HG23	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	4	0.12
(1,544)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	4	0.12
(1,544)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	4	0.12
(1,544)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	4	0.12
(1,544)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	4	0.12
(1,544)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	4	0.12
(1,544)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	4	0.12
(1,544)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	4	0.12
(1,544)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	4	0.12
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD11	5	0.12
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD12	5	0.12
(1,543)	1:49:A:ILE:HD11	1:91:A:ILE:HD13	5	0.12
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD11	5	0.12
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD12	5	0.12
(1,543)	1:49:A:ILE:HD12	1:91:A:ILE:HD13	5	0.12
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD11	5	0.12
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD12	5	0.12
(1,543)	1:49:A:ILE:HD13	1:91:A:ILE:HD13	5	0.12
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	7	0.12
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	7	0.12
(1,535)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	7	0.12
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	7	0.12
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	7	0.12
(1,535)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	7	0.12
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	7	0.12
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	7	0.12
(1,535)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	7	0.12
(1,532)	1:48:A:LEU:HD11	1:141:A:ALA:HB1	8	0.12
(1,532)	1:48:A:LEU:HD11	1:141:A:ALA:HB2	8	0.12
(1,532)	1:48:A:LEU:HD11	1:141:A:ALA:HB3	8	0.12
(1,532)	1:48:A:LEU:HD12	1:141:A:ALA:HB1	8	0.12
(1,532)	1:48:A:LEU:HD12	1:141:A:ALA:HB2	8	0.12
(1,532)	1:48:A:LEU:HD12	1:141:A:ALA:HB3	8	0.12
(1,532)	1:48:A:LEU:HD13	1:141:A:ALA:HB1	8	0.12
(1,532)	1:48:A:LEU:HD13	1:141:A:ALA:HB2	8	0.12
(1,532)	1:48:A:LEU:HD13	1:141:A:ALA:HB3	8	0.12
(1,527)	1:45:A:LEU:HD21	1:89:A:LEU:HD21	8	0.12
(1,527)	1:45:A:LEU:HD21	1:89:A:LEU:HD22	8	0.12
(1,527)	1:45:A:LEU:HD21	1:89:A:LEU:HD23	8	0.12
(1,527)	1:45:A:LEU:HD22	1:89:A:LEU:HD21	8	0.12
(1,527)	1:45:A:LEU:HD22	1:89:A:LEU:HD22	8	0.12
(1,527)	1:45:A:LEU:HD22	1:89:A:LEU:HD23	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:45:A:LEU:HD23	1:89:A:LEU:HD21	8	0.12
(1,527)	1:45:A:LEU:HD23	1:89:A:LEU:HD22	8	0.12
(1,527)	1:45:A:LEU:HD23	1:89:A:LEU:HD23	8	0.12
(1,510)	1:32:A:LEU:HD21	1:122:A:LEU:HD21	6	0.12
(1,510)	1:32:A:LEU:HD21	1:122:A:LEU:HD22	6	0.12
(1,510)	1:32:A:LEU:HD21	1:122:A:LEU:HD23	6	0.12
(1,510)	1:32:A:LEU:HD22	1:122:A:LEU:HD21	6	0.12
(1,510)	1:32:A:LEU:HD22	1:122:A:LEU:HD22	6	0.12
(1,510)	1:32:A:LEU:HD22	1:122:A:LEU:HD23	6	0.12
(1,510)	1:32:A:LEU:HD23	1:122:A:LEU:HD21	6	0.12
(1,510)	1:32:A:LEU:HD23	1:122:A:LEU:HD22	6	0.12
(1,510)	1:32:A:LEU:HD23	1:122:A:LEU:HD23	6	0.12
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE1	10	0.12
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE2	10	0.12
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE3	10	0.12
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE1	10	0.12
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE2	10	0.12
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE3	10	0.12
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE1	10	0.12
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE2	10	0.12
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE3	10	0.12
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD11	8	0.12
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD12	8	0.12
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD13	8	0.12
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD11	8	0.12
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD12	8	0.12
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD13	8	0.12
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD11	8	0.12
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD12	8	0.12
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD13	8	0.12
(1,501)	1:30:A:MET:HE1	1:34:A:ILE:HD11	10	0.12
(1,501)	1:30:A:MET:HE1	1:34:A:ILE:HD12	10	0.12
(1,501)	1:30:A:MET:HE1	1:34:A:ILE:HD13	10	0.12
(1,501)	1:30:A:MET:HE2	1:34:A:ILE:HD11	10	0.12
(1,501)	1:30:A:MET:HE2	1:34:A:ILE:HD12	10	0.12
(1,501)	1:30:A:MET:HE2	1:34:A:ILE:HD13	10	0.12
(1,501)	1:30:A:MET:HE3	1:34:A:ILE:HD11	10	0.12
(1,501)	1:30:A:MET:HE3	1:34:A:ILE:HD12	10	0.12
(1,501)	1:30:A:MET:HE3	1:34:A:ILE:HD13	10	0.12
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG11	8	0.12
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG12	8	0.12
(1,498)	1:29:A:LEU:HD21	1:136:A:VAL:HG13	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG11	8	0.12
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG12	8	0.12
(1,498)	1:29:A:LEU:HD22	1:136:A:VAL:HG13	8	0.12
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG11	8	0.12
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG12	8	0.12
(1,498)	1:29:A:LEU:HD23	1:136:A:VAL:HG13	8	0.12
(1,494)	1:29:A:LEU:HD11	1:136:A:VAL:HG21	2	0.12
(1,494)	1:29:A:LEU:HD11	1:136:A:VAL:HG22	2	0.12
(1,494)	1:29:A:LEU:HD11	1:136:A:VAL:HG23	2	0.12
(1,494)	1:29:A:LEU:HD12	1:136:A:VAL:HG21	2	0.12
(1,494)	1:29:A:LEU:HD12	1:136:A:VAL:HG22	2	0.12
(1,494)	1:29:A:LEU:HD12	1:136:A:VAL:HG23	2	0.12
(1,494)	1:29:A:LEU:HD13	1:136:A:VAL:HG21	2	0.12
(1,494)	1:29:A:LEU:HD13	1:136:A:VAL:HG22	2	0.12
(1,494)	1:29:A:LEU:HD13	1:136:A:VAL:HG23	2	0.12
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG21	5	0.12
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG22	5	0.12
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG23	5	0.12
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG21	5	0.12
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG22	5	0.12
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG23	5	0.12
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG21	5	0.12
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG22	5	0.12
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG23	5	0.12
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	1	0.12
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	1	0.12
(1,484)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	1	0.12
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	1	0.12
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	1	0.12
(1,484)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	1	0.12
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	1	0.12
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	1	0.12
(1,484)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	1	0.12
(1,419)	1:103:A:LEU:H	1:107:A:LEU:H	7	0.12
(1,419)	1:103:A:LEU:H	1:107:A:LEU:H	10	0.12
(1,395)	1:77:A:HIS:H	1:95:A:GLY:H	10	0.12
(1,391)	1:58:A:LYS:H	1:96:A:ILE:H	4	0.12
(1,366)	1:199:A:GLU:H	1:202:A:ARG:H	1	0.12
(1,347)	1:104:A:ILE:H	1:107:A:LEU:H	10	0.12
(1,316)	1:210:A:HIS:H	1:212:A:GLN:H	9	0.12
(1,210)	1:197:A:TYR:H	1:198:A:LEU:H	10	0.12
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB1	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB2	1	0.12
(1,63)	1:141:A:ALA:HB1	1:145:A:ALA:HB3	1	0.12
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB1	1	0.12
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB2	1	0.12
(1,63)	1:141:A:ALA:HB2	1:145:A:ALA:HB3	1	0.12
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB1	1	0.12
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB2	1	0.12
(1,63)	1:141:A:ALA:HB3	1:145:A:ALA:HB3	1	0.12
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD21	9	0.12
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD22	9	0.12
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD23	9	0.12
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD21	9	0.12
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD22	9	0.12
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD23	9	0.12
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD21	9	0.12
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD22	9	0.12
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD23	9	0.12
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG21	2	0.12
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG22	2	0.12
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG23	2	0.12
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG21	2	0.12
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG22	2	0.12
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG23	2	0.12
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG21	2	0.12
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG22	2	0.12
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG23	2	0.12
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD21	3	0.12
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD22	3	0.12
(1,33)	1:89:A:LEU:HD11	1:80:A:LEU:HD23	3	0.12
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD21	3	0.12
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD22	3	0.12
(1,33)	1:89:A:LEU:HD12	1:80:A:LEU:HD23	3	0.12
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD21	3	0.12
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD22	3	0.12
(1,33)	1:89:A:LEU:HD13	1:80:A:LEU:HD23	3	0.12
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD21	2	0.12
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD22	2	0.12
(1,11)	1:115:A:THR:HG21	1:122:A:LEU:HD23	2	0.12
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD21	2	0.12
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD22	2	0.12
(1,11)	1:115:A:THR:HG22	1:122:A:LEU:HD23	2	0.12
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD21	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD22	2	0.12
(1,11)	1:115:A:THR:HG23	1:122:A:LEU:HD23	2	0.12
(1,1874)	1:136:A:VAL:H	1:132:A:GLY:HA2	7	0.11
(1,1874)	1:136:A:VAL:H	1:132:A:GLY:HA3	7	0.11
(1,1834)	1:116:A:LYS:H	1:114:A:GLY:HA2	10	0.11
(1,1834)	1:116:A:LYS:H	1:114:A:GLY:HA3	10	0.11
(1,1792)	1:114:A:GLY:H	1:114:A:GLY:HA2	3	0.11
(1,1792)	1:114:A:GLY:H	1:114:A:GLY:HA3	3	0.11
(1,1777)	1:189:A:HIS:H	1:88:A:THR:HA	2	0.11
(1,1752)	1:175:A:ASP:H	1:160:A:TYR:HA	1	0.11
(1,1737)	1:170:A:PHE:H	1:21:A:ALA:HA	1	0.11
(1,1685)	1:94:A:THR:H	1:76:A:LEU:HA	8	0.11
(1,1659)	1:77:A:HIS:H	1:93:A:ASP:HA	5	0.11
(1,1657)	1:22:A:PHE:H	1:168:A:GLY:HA2	3	0.11
(1,1657)	1:22:A:PHE:H	1:168:A:GLY:HA3	3	0.11
(1,1655)	1:20:A:PHE:H	1:171:A:THR:HA	5	0.11
(1,1642)	1:212:A:GLN:H	1:208:A:LYS:HA	7	0.11
(1,1597)	1:214:A:ILE:H	1:211:A:SER:HA	5	0.11
(1,1597)	1:214:A:ILE:H	1:211:A:SER:HA	6	0.11
(1,1589)	1:204:A:LYS:H	1:201:A:ARG:HA	2	0.11
(1,1575)	1:106:A:ASN:H	1:103:A:LEU:HA	8	0.11
(1,1575)	1:106:A:ASN:H	1:103:A:LEU:HA	10	0.11
(1,1558)	1:59:A:ILE:H	1:56:A:LEU:HA	9	0.11
(1,1504)	1:143:A:LEU:H	1:141:A:ALA:HA	7	0.11
(1,1500)	1:137:A:GLY:H	1:135:A:GLY:HA2	9	0.11
(1,1500)	1:137:A:GLY:H	1:135:A:GLY:HA3	9	0.11
(1,1254)	1:181:A:GLY:H	1:181:A:GLY:HA2	4	0.11
(1,1254)	1:181:A:GLY:H	1:181:A:GLY:HA3	4	0.11
(1,1251)	1:177:A:GLY:H	1:177:A:GLY:HA2	7	0.11
(1,1251)	1:177:A:GLY:H	1:177:A:GLY:HA3	7	0.11
(1,1251)	1:177:A:GLY:H	1:177:A:GLY:HA2	9	0.11
(1,1251)	1:177:A:GLY:H	1:177:A:GLY:HA3	9	0.11
(1,1218)	1:137:A:GLY:H	1:137:A:GLY:HA2	5	0.11
(1,1218)	1:137:A:GLY:H	1:137:A:GLY:HA3	5	0.11
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA2	3	0.11
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA3	3	0.11
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD21	9	0.11
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD22	9	0.11
(1,1111)	1:216:A:TYR:H	1:56:A:LEU:HD23	9	0.11
(1,1108)	1:213:A:PHE:H	1:214:A:ILE:HD11	8	0.11
(1,1108)	1:213:A:PHE:H	1:214:A:ILE:HD12	8	0.11
(1,1108)	1:213:A:PHE:H	1:214:A:ILE:HD13	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG21	9	0.11
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG22	9	0.11
(1,1074)	1:198:A:LEU:H	1:195:A:THR:HG23	9	0.11
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG11	2	0.11
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG12	2	0.11
(1,1044)	1:188:A:LEU:H	1:186:A:VAL:HG13	2	0.11
(1,1031)	1:186:A:VAL:H	1:184:A:THR:HG21	9	0.11
(1,1031)	1:186:A:VAL:H	1:184:A:THR:HG22	9	0.11
(1,1031)	1:186:A:VAL:H	1:184:A:THR:HG23	9	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG21	7	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG22	7	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG23	7	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG21	10	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG22	10	0.11
(1,1030)	1:186:A:VAL:H	1:150:A:VAL:HG23	10	0.11
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB1	10	0.11
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB2	10	0.11
(1,1002)	1:169:A:SER:H	1:166:A:ALA:HB3	10	0.11
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG11	8	0.11
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG12	8	0.11
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG13	8	0.11
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG21	8	0.11
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG22	8	0.11
(1,994)	1:162:A:TRP:H	1:172:A:VAL:HG23	8	0.11
(1,991)	1:162:A:TRP:H	1:150:A:VAL:HG11	5	0.11
(1,991)	1:162:A:TRP:H	1:150:A:VAL:HG12	5	0.11
(1,991)	1:162:A:TRP:H	1:150:A:VAL:HG13	5	0.11
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG21	9	0.11
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG22	9	0.11
(1,990)	1:162:A:TRP:H	1:149:A:THR:HG23	9	0.11
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG21	7	0.11
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG22	7	0.11
(1,982)	1:159:A:GLN:H	1:174:A:THR:HG23	7	0.11
(1,973)	1:150:A:VAL:H	1:151:A:ILE:HD11	10	0.11
(1,973)	1:150:A:VAL:H	1:151:A:ILE:HD12	10	0.11
(1,973)	1:150:A:VAL:H	1:151:A:ILE:HD13	10	0.11
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	5	0.11
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	5	0.11
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	5	0.11
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG11	7	0.11
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG12	7	0.11
(1,971)	1:150:A:VAL:H	1:148:A:VAL:HG13	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD21	9	0.11
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD22	9	0.11
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD23	9	0.11
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE1	6	0.11
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE2	6	0.11
(1,932)	1:131:A:ILE:H	1:130:A:MET:HE3	6	0.11
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD11	10	0.11
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD12	10	0.11
(1,929)	1:128:A:ILE:H	1:122:A:LEU:HD13	10	0.11
(1,911)	1:122:A:LEU:H	1:121:A:ALA:HB1	6	0.11
(1,911)	1:122:A:LEU:H	1:121:A:ALA:HB2	6	0.11
(1,911)	1:122:A:LEU:H	1:121:A:ALA:HB3	6	0.11
(1,905)	1:118:A:PHE:H	1:115:A:THR:HG21	9	0.11
(1,905)	1:118:A:PHE:H	1:115:A:THR:HG22	9	0.11
(1,905)	1:118:A:PHE:H	1:115:A:THR:HG23	9	0.11
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG21	10	0.11
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG22	10	0.11
(1,904)	1:111:A:ALA:H	1:109:A:THR:HG23	10	0.11
(1,891)	1:96:A:ILE:H	1:55:A:ALA:HB1	2	0.11
(1,891)	1:96:A:ILE:H	1:55:A:ALA:HB2	2	0.11
(1,891)	1:96:A:ILE:H	1:55:A:ALA:HB3	2	0.11
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD11	3	0.11
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD12	3	0.11
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD13	3	0.11
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD21	10	0.11
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD22	10	0.11
(1,869)	1:89:A:LEU:H	1:188:A:LEU:HD23	10	0.11
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD21	9	0.11
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD22	9	0.11
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD23	9	0.11
(1,861)	1:86:A:ASP:H	1:88:A:THR:HG21	2	0.11
(1,861)	1:86:A:ASP:H	1:88:A:THR:HG22	2	0.11
(1,861)	1:86:A:ASP:H	1:88:A:THR:HG23	2	0.11
(1,849)	1:81:A:ILE:H	1:90:A:THR:HG21	5	0.11
(1,849)	1:81:A:ILE:H	1:90:A:THR:HG22	5	0.11
(1,849)	1:81:A:ILE:H	1:90:A:THR:HG23	5	0.11
(1,841)	1:79:A:ASN:H	1:92:A:VAL:HG11	2	0.11
(1,841)	1:79:A:ASN:H	1:92:A:VAL:HG12	2	0.11
(1,841)	1:79:A:ASN:H	1:92:A:VAL:HG13	2	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD11	4	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD12	4	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD13	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD21	4	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD22	4	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD23	4	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD11	9	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD12	9	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD13	9	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD21	9	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD22	9	0.11
(1,824)	1:71:A:ASP:H	1:70:A:LEU:HD23	9	0.11
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD11	8	0.11
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD12	8	0.11
(1,813)	1:62:A:GLU:H	1:96:A:ILE:HD13	8	0.11
(1,786)	1:49:A:ILE:H	1:48:A:LEU:HD11	10	0.11
(1,786)	1:49:A:ILE:H	1:48:A:LEU:HD12	10	0.11
(1,786)	1:49:A:ILE:H	1:48:A:LEU:HD13	10	0.11
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG21	6	0.11
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG22	6	0.11
(1,774)	1:43:A:ILE:H	1:144:A:VAL:HG23	6	0.11
(1,756)	1:31:A:SER:H	1:34:A:ILE:HD11	8	0.11
(1,756)	1:31:A:SER:H	1:34:A:ILE:HD12	8	0.11
(1,756)	1:31:A:SER:H	1:34:A:ILE:HD13	8	0.11
(1,736)	1:18:A:GLU:H	1:17:A:VAL:HG21	1	0.11
(1,736)	1:18:A:GLU:H	1:17:A:VAL:HG22	1	0.11
(1,736)	1:18:A:GLU:H	1:17:A:VAL:HG23	1	0.11
(1,726)	1:206:A:ILE:H	1:206:A:ILE:HD11	7	0.11
(1,726)	1:206:A:ILE:H	1:206:A:ILE:HD12	7	0.11
(1,726)	1:206:A:ILE:H	1:206:A:ILE:HD13	7	0.11
(1,698)	1:107:A:LEU:H	1:107:A:LEU:HD21	2	0.11
(1,698)	1:107:A:LEU:H	1:107:A:LEU:HD22	2	0.11
(1,698)	1:107:A:LEU:H	1:107:A:LEU:HD23	2	0.11
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD11	10	0.11
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD12	10	0.11
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD13	10	0.11
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD11	2	0.11
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD12	2	0.11
(1,666)	1:26:A:ILE:H	1:26:A:ILE:HD13	2	0.11
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG11	9	0.11
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG12	9	0.11
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG13	9	0.11
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG11	9	0.11
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG12	9	0.11
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG13	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG11	9	0.11
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG12	9	0.11
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG13	9	0.11
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	9	0.11
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	9	0.11
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	9	0.11
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	9	0.11
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	9	0.11
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	9	0.11
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	9	0.11
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	9	0.11
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	9	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD11	3	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD12	3	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD13	3	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD11	3	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD12	3	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD13	3	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD11	3	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD12	3	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD13	3	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD11	6	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD12	6	0.11
(1,653)	1:190:A:LEU:HD21	1:198:A:LEU:HD13	6	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD11	6	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD12	6	0.11
(1,653)	1:190:A:LEU:HD22	1:198:A:LEU:HD13	6	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD11	6	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD12	6	0.11
(1,653)	1:190:A:LEU:HD23	1:198:A:LEU:HD13	6	0.11
(1,647)	1:184:A:THR:HG21	1:186:A:VAL:HG11	10	0.11
(1,647)	1:184:A:THR:HG21	1:186:A:VAL:HG12	10	0.11
(1,647)	1:184:A:THR:HG21	1:186:A:VAL:HG13	10	0.11
(1,647)	1:184:A:THR:HG22	1:186:A:VAL:HG11	10	0.11
(1,647)	1:184:A:THR:HG22	1:186:A:VAL:HG12	10	0.11
(1,647)	1:184:A:THR:HG22	1:186:A:VAL:HG13	10	0.11
(1,647)	1:184:A:THR:HG23	1:186:A:VAL:HG11	10	0.11
(1,647)	1:184:A:THR:HG23	1:186:A:VAL:HG12	10	0.11
(1,647)	1:184:A:THR:HG23	1:186:A:VAL:HG13	10	0.11
(1,645)	1:174:A:THR:HG21	1:176:A:THR:HG21	6	0.11
(1,645)	1:174:A:THR:HG21	1:176:A:THR:HG22	6	0.11
(1,645)	1:174:A:THR:HG21	1:176:A:THR:HG23	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:174:A:THR:HG22	1:176:A:THR:HG21	6	0.11
(1,645)	1:174:A:THR:HG22	1:176:A:THR:HG22	6	0.11
(1,645)	1:174:A:THR:HG22	1:176:A:THR:HG23	6	0.11
(1,645)	1:174:A:THR:HG23	1:176:A:THR:HG21	6	0.11
(1,645)	1:174:A:THR:HG23	1:176:A:THR:HG22	6	0.11
(1,645)	1:174:A:THR:HG23	1:176:A:THR:HG23	6	0.11
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG21	8	0.11
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG22	8	0.11
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG23	8	0.11
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG21	8	0.11
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG22	8	0.11
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG23	8	0.11
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG21	8	0.11
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG22	8	0.11
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG23	8	0.11
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG11	10	0.11
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG12	10	0.11
(1,626)	1:141:A:ALA:HB1	1:148:A:VAL:HG13	10	0.11
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG11	10	0.11
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG12	10	0.11
(1,626)	1:141:A:ALA:HB2	1:148:A:VAL:HG13	10	0.11
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG11	10	0.11
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG12	10	0.11
(1,626)	1:141:A:ALA:HB3	1:148:A:VAL:HG13	10	0.11
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD11	1	0.11
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD12	1	0.11
(1,587)	1:98:A:MET:HE1	1:107:A:LEU:HD13	1	0.11
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD11	1	0.11
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD12	1	0.11
(1,587)	1:98:A:MET:HE2	1:107:A:LEU:HD13	1	0.11
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD11	1	0.11
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD12	1	0.11
(1,587)	1:98:A:MET:HE3	1:107:A:LEU:HD13	1	0.11
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	3	0.11
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	3	0.11
(1,579)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	3	0.11
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	3	0.11
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	3	0.11
(1,579)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	3	0.11
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	3	0.11
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	3	0.11
(1,579)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD11	8	0.11
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD12	8	0.11
(1,576)	1:90:A:THR:HG21	1:187:A:ILE:HD13	8	0.11
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD11	8	0.11
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD12	8	0.11
(1,576)	1:90:A:THR:HG22	1:187:A:ILE:HD13	8	0.11
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD11	8	0.11
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD12	8	0.11
(1,576)	1:90:A:THR:HG23	1:187:A:ILE:HD13	8	0.11
(1,570)	1:89:A:LEU:HD11	1:198:A:LEU:HD21	4	0.11
(1,570)	1:89:A:LEU:HD11	1:198:A:LEU:HD22	4	0.11
(1,570)	1:89:A:LEU:HD11	1:198:A:LEU:HD23	4	0.11
(1,570)	1:89:A:LEU:HD12	1:198:A:LEU:HD21	4	0.11
(1,570)	1:89:A:LEU:HD12	1:198:A:LEU:HD22	4	0.11
(1,570)	1:89:A:LEU:HD12	1:198:A:LEU:HD23	4	0.11
(1,570)	1:89:A:LEU:HD13	1:198:A:LEU:HD21	4	0.11
(1,570)	1:89:A:LEU:HD13	1:198:A:LEU:HD22	4	0.11
(1,570)	1:89:A:LEU:HD13	1:198:A:LEU:HD23	4	0.11
(1,558)	1:78:A:ILE:HD11	1:214:A:ILE:HD11	9	0.11
(1,558)	1:78:A:ILE:HD11	1:214:A:ILE:HD12	9	0.11
(1,558)	1:78:A:ILE:HD11	1:214:A:ILE:HD13	9	0.11
(1,558)	1:78:A:ILE:HD12	1:214:A:ILE:HD11	9	0.11
(1,558)	1:78:A:ILE:HD12	1:214:A:ILE:HD12	9	0.11
(1,558)	1:78:A:ILE:HD12	1:214:A:ILE:HD13	9	0.11
(1,558)	1:78:A:ILE:HD13	1:214:A:ILE:HD11	9	0.11
(1,558)	1:78:A:ILE:HD13	1:214:A:ILE:HD12	9	0.11
(1,558)	1:78:A:ILE:HD13	1:214:A:ILE:HD13	9	0.11
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG11	9	0.11
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG12	9	0.11
(1,537)	1:48:A:LEU:HD21	1:186:A:VAL:HG13	9	0.11
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG11	9	0.11
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG12	9	0.11
(1,537)	1:48:A:LEU:HD22	1:186:A:VAL:HG13	9	0.11
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG11	9	0.11
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG12	9	0.11
(1,537)	1:48:A:LEU:HD23	1:186:A:VAL:HG13	9	0.11
(1,522)	1:45:A:LEU:HD11	1:188:A:LEU:HD11	2	0.11
(1,522)	1:45:A:LEU:HD11	1:188:A:LEU:HD12	2	0.11
(1,522)	1:45:A:LEU:HD11	1:188:A:LEU:HD13	2	0.11
(1,522)	1:45:A:LEU:HD12	1:188:A:LEU:HD11	2	0.11
(1,522)	1:45:A:LEU:HD12	1:188:A:LEU:HD12	2	0.11
(1,522)	1:45:A:LEU:HD12	1:188:A:LEU:HD13	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:45:A:LEU:HD13	1:188:A:LEU:HD11	2	0.11
(1,522)	1:45:A:LEU:HD13	1:188:A:LEU:HD12	2	0.11
(1,522)	1:45:A:LEU:HD13	1:188:A:LEU:HD13	2	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE1	7	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE2	7	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE3	7	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE1	7	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE2	7	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE3	7	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE1	7	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE2	7	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE3	7	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE1	8	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE2	8	0.11
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE3	8	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE1	8	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE2	8	0.11
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE3	8	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE1	8	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE2	8	0.11
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE3	8	0.11
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG21	7	0.11
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG22	7	0.11
(1,488)	1:29:A:LEU:HD11	1:115:A:THR:HG23	7	0.11
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG21	7	0.11
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG22	7	0.11
(1,488)	1:29:A:LEU:HD12	1:115:A:THR:HG23	7	0.11
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG21	7	0.11
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG22	7	0.11
(1,488)	1:29:A:LEU:HD13	1:115:A:THR:HG23	7	0.11
(1,486)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	4	0.11
(1,486)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	4	0.11
(1,486)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	4	0.11
(1,486)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	4	0.11
(1,486)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	4	0.11
(1,486)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	4	0.11
(1,486)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	4	0.11
(1,486)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	4	0.11
(1,486)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	4	0.11
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD11	6	0.11
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD12	6	0.11
(1,481)	1:26:A:ILE:HD11	1:29:A:LEU:HD13	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD11	6	0.11
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD12	6	0.11
(1,481)	1:26:A:ILE:HD12	1:29:A:LEU:HD13	6	0.11
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD11	6	0.11
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD12	6	0.11
(1,481)	1:26:A:ILE:HD13	1:29:A:LEU:HD13	6	0.11
(1,439)	1:159:A:GLN:H	1:175:A:ASP:H	1	0.11
(1,419)	1:103:A:LEU:H	1:107:A:LEU:H	8	0.11
(1,419)	1:103:A:LEU:H	1:107:A:LEU:H	9	0.11
(1,347)	1:104:A:ILE:H	1:107:A:LEU:H	8	0.11
(1,274)	1:114:A:GLY:H	1:116:A:LYS:H	10	0.11
(1,264)	1:72:A:SER:H	1:74:A:LYS:H	1	0.11
(1,228)	1:215:A:GLY:H	1:216:A:TYR:H	8	0.11
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD21	6	0.11
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD22	6	0.11
(1,60)	1:111:A:ALA:HB1	1:29:A:LEU:HD23	6	0.11
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD21	6	0.11
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD22	6	0.11
(1,60)	1:111:A:ALA:HB2	1:29:A:LEU:HD23	6	0.11
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD21	6	0.11
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD22	6	0.11
(1,60)	1:111:A:ALA:HB3	1:29:A:LEU:HD23	6	0.11
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD11	2	0.11
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD12	2	0.11
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD13	2	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD11	2	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD12	2	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD13	2	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD11	2	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD12	2	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD13	2	0.11
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD11	4	0.11
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD12	4	0.11
(1,57)	1:126:A:ALA:HB1	1:122:A:LEU:HD13	4	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD11	4	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD12	4	0.11
(1,57)	1:126:A:ALA:HB2	1:122:A:LEU:HD13	4	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD11	4	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD12	4	0.11
(1,57)	1:126:A:ALA:HB3	1:122:A:LEU:HD13	4	0.11
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG21	10	0.11
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:180:A:MET:HE1	1:152:A:THR:HG23	10	0.11
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG21	10	0.11
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG22	10	0.11
(1,55)	1:180:A:MET:HE2	1:152:A:THR:HG23	10	0.11
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG21	10	0.11
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG22	10	0.11
(1,55)	1:180:A:MET:HE3	1:152:A:THR:HG23	10	0.11
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD11	10	0.11
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD12	10	0.11
(1,45)	1:76:A:LEU:HD11	1:78:A:ILE:HD13	10	0.11
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD11	10	0.11
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD12	10	0.11
(1,45)	1:76:A:LEU:HD12	1:78:A:ILE:HD13	10	0.11
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD11	10	0.11
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD12	10	0.11
(1,45)	1:76:A:LEU:HD13	1:78:A:ILE:HD13	10	0.11
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD11	7	0.11
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD12	7	0.11
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD13	7	0.11
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD11	7	0.11
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD12	7	0.11
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD13	7	0.11
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD11	7	0.11
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD12	7	0.11
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD13	7	0.11
(1,28)	1:70:A:LEU:HD21	1:76:A:LEU:HD21	9	0.11
(1,28)	1:70:A:LEU:HD21	1:76:A:LEU:HD22	9	0.11
(1,28)	1:70:A:LEU:HD21	1:76:A:LEU:HD23	9	0.11
(1,28)	1:70:A:LEU:HD22	1:76:A:LEU:HD21	9	0.11
(1,28)	1:70:A:LEU:HD22	1:76:A:LEU:HD22	9	0.11
(1,28)	1:70:A:LEU:HD22	1:76:A:LEU:HD23	9	0.11
(1,28)	1:70:A:LEU:HD23	1:76:A:LEU:HD21	9	0.11
(1,28)	1:70:A:LEU:HD23	1:76:A:LEU:HD22	9	0.11
(1,28)	1:70:A:LEU:HD23	1:76:A:LEU:HD23	9	0.11
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD21	4	0.11
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD22	4	0.11
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD23	4	0.11
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD21	4	0.11
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD22	4	0.11
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD23	4	0.11
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD21	4	0.11
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD22	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD23	4	0.11
(1,1853)	1:117:A:ALA:H	1:114:A:GLY:HA2	5	0.1
(1,1853)	1:117:A:ALA:H	1:114:A:GLY:HA3	5	0.1
(1,1842)	1:125:A:GLY:H	1:123:A:GLN:HA	8	0.1
(1,1809)	1:132:A:GLY:H	1:132:A:GLY:HA2	3	0.1
(1,1809)	1:132:A:GLY:H	1:132:A:GLY:HA3	3	0.1
(1,1792)	1:114:A:GLY:H	1:114:A:GLY:HA2	1	0.1
(1,1792)	1:114:A:GLY:H	1:114:A:GLY:HA3	1	0.1
(1,1790)	1:182:A:ARG:H	1:94:A:THR:HA	10	0.1
(1,1765)	1:186:A:VAL:H	1:90:A:THR:HA	4	0.1
(1,1705)	1:151:A:ILE:H	1:186:A:VAL:HA	10	0.1
(1,1672)	1:83:A:ASN:H	1:84:A:LYS:HA	6	0.1
(1,1642)	1:212:A:GLN:H	1:208:A:LYS:HA	1	0.1
(1,1641)	1:211:A:SER:H	1:207:A:VAL:HA	4	0.1
(1,1612)	1:52:A:SER:H	1:48:A:LEU:HA	4	0.1
(1,1505)	1:144:A:VAL:H	1:142:A:TYR:HA	6	0.1
(1,1502)	1:139:A:TYR:H	1:137:A:GLY:HA2	4	0.1
(1,1502)	1:139:A:TYR:H	1:137:A:GLY:HA3	4	0.1
(1,1484)	1:72:A:SER:H	1:70:A:LEU:HA	2	0.1
(1,1455)	1:36:A:GLU:H	1:34:A:ILE:HA	7	0.1
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA2	10	0.1
(1,1363)	1:98:A:MET:H	1:97:A:GLY:HA3	10	0.1
(1,1254)	1:181:A:GLY:H	1:181:A:GLY:HA2	1	0.1
(1,1254)	1:181:A:GLY:H	1:181:A:GLY:HA3	1	0.1
(1,1254)	1:181:A:GLY:H	1:181:A:GLY:HA2	3	0.1
(1,1254)	1:181:A:GLY:H	1:181:A:GLY:HA3	3	0.1
(1,1218)	1:137:A:GLY:H	1:137:A:GLY:HA2	4	0.1
(1,1218)	1:137:A:GLY:H	1:137:A:GLY:HA3	4	0.1
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA2	5	0.1
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA3	5	0.1
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA2	6	0.1
(1,1207)	1:97:A:GLY:H	1:97:A:GLY:HA3	6	0.1
(1,1205)	1:95:A:GLY:H	1:95:A:GLY:HA2	9	0.1
(1,1205)	1:95:A:GLY:H	1:95:A:GLY:HA3	9	0.1
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG21	6	0.1
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG22	6	0.1
(1,1107)	1:212:A:GLN:H	1:207:A:VAL:HG23	6	0.1
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE1	7	0.1
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE2	7	0.1
(1,1001)	1:169:A:SER:H	1:30:A:MET:HE3	7	0.1
(1,983)	1:160:A:TYR:H	1:103:A:LEU:HD21	6	0.1
(1,983)	1:160:A:TYR:H	1:103:A:LEU:HD22	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:160:A:TYR:H	1:103:A:LEU:HD23	6	0.1
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD21	6	0.1
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD22	6	0.1
(1,965)	1:146:A:GLU:H	1:190:A:LEU:HD23	6	0.1
(1,913)	1:122:A:LEU:H	1:126:A:ALA:HB1	7	0.1
(1,913)	1:122:A:LEU:H	1:126:A:ALA:HB2	7	0.1
(1,913)	1:122:A:LEU:H	1:126:A:ALA:HB3	7	0.1
(1,900)	1:105:A:ASN:H	1:104:A:ILE:HD11	5	0.1
(1,900)	1:105:A:ASN:H	1:104:A:ILE:HD12	5	0.1
(1,900)	1:105:A:ASN:H	1:104:A:ILE:HD13	5	0.1
(1,883)	1:92:A:VAL:H	1:90:A:THR:HG21	7	0.1
(1,883)	1:92:A:VAL:H	1:90:A:THR:HG22	7	0.1
(1,883)	1:92:A:VAL:H	1:90:A:THR:HG23	7	0.1
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD11	7	0.1
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD12	7	0.1
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD13	7	0.1
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD11	9	0.1
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD12	9	0.1
(1,879)	1:91:A:ILE:H	1:188:A:LEU:HD13	9	0.1
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD21	8	0.1
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD22	8	0.1
(1,863)	1:86:A:ASP:H	1:198:A:LEU:HD23	8	0.1
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD11	7	0.1
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD12	7	0.1
(1,845)	1:80:A:LEU:H	1:220:A:LEU:HD13	7	0.1
(1,828)	1:75:A:GLU:H	1:70:A:LEU:HD11	6	0.1
(1,828)	1:75:A:GLU:H	1:70:A:LEU:HD12	6	0.1
(1,828)	1:75:A:GLU:H	1:70:A:LEU:HD13	6	0.1
(1,812)	1:62:A:GLU:H	1:59:A:ILE:HD11	8	0.1
(1,812)	1:62:A:GLU:H	1:59:A:ILE:HD12	8	0.1
(1,812)	1:62:A:GLU:H	1:59:A:ILE:HD13	8	0.1
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD21	3	0.1
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD22	3	0.1
(1,783)	1:47:A:GLU:H	1:48:A:LEU:HD23	3	0.1
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG11	5	0.1
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG12	5	0.1
(1,741)	1:20:A:PHE:H	1:172:A:VAL:HG13	5	0.1
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD11	4	0.1
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD12	4	0.1
(1,699)	1:122:A:LEU:H	1:122:A:LEU:HD13	4	0.1
(1,683)	1:76:A:LEU:H	1:76:A:LEU:HD21	9	0.1
(1,683)	1:76:A:LEU:H	1:76:A:LEU:HD22	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,683)	1:76:A:LEU:H	1:76:A:LEU:HD23	9	0.1
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD11	5	0.1
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD12	5	0.1
(1,682)	1:76:A:LEU:H	1:76:A:LEU:HD13	5	0.1
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG11	1	0.1
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG12	1	0.1
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG13	1	0.1
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG11	1	0.1
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG12	1	0.1
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG13	1	0.1
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG11	1	0.1
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG12	1	0.1
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG13	1	0.1
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	1	0.1
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	1	0.1
(1,663)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	1	0.1
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	1	0.1
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	1	0.1
(1,663)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	1	0.1
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	1	0.1
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	1	0.1
(1,663)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	1	0.1
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG21	7	0.1
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG22	7	0.1
(1,662)	1:220:A:LEU:HD11	1:222:A:VAL:HG23	7	0.1
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG21	7	0.1
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG22	7	0.1
(1,662)	1:220:A:LEU:HD12	1:222:A:VAL:HG23	7	0.1
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG21	7	0.1
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG22	7	0.1
(1,662)	1:220:A:LEU:HD13	1:222:A:VAL:HG23	7	0.1
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG21	6	0.1
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG22	6	0.1
(1,638)	1:150:A:VAL:HG11	1:186:A:VAL:HG23	6	0.1
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG21	6	0.1
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG22	6	0.1
(1,638)	1:150:A:VAL:HG12	1:186:A:VAL:HG23	6	0.1
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG21	6	0.1
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG22	6	0.1
(1,638)	1:150:A:VAL:HG13	1:186:A:VAL:HG23	6	0.1
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	7	0.1
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	7	0.1
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	7	0.1
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	7	0.1
(1,628)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	7	0.1
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	7	0.1
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	7	0.1
(1,628)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	7	0.1
(1,627)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	6	0.1
(1,627)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	6	0.1
(1,627)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	6	0.1
(1,627)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	6	0.1
(1,627)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	6	0.1
(1,627)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	6	0.1
(1,627)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	6	0.1
(1,627)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	6	0.1
(1,627)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	6	0.1
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE1	10	0.1
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE2	10	0.1
(1,621)	1:126:A:ALA:HB1	1:130:A:MET:HE3	10	0.1
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE1	10	0.1
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE2	10	0.1
(1,621)	1:126:A:ALA:HB2	1:130:A:MET:HE3	10	0.1
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE1	10	0.1
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE2	10	0.1
(1,621)	1:126:A:ALA:HB3	1:130:A:MET:HE3	10	0.1
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	4	0.1
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	4	0.1
(1,617)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	4	0.1
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	4	0.1
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	4	0.1
(1,617)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	4	0.1
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	4	0.1
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	4	0.1
(1,617)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	4	0.1
(1,590)	1:98:A:MET:HE1	1:150:A:VAL:HG21	3	0.1
(1,590)	1:98:A:MET:HE1	1:150:A:VAL:HG22	3	0.1
(1,590)	1:98:A:MET:HE1	1:150:A:VAL:HG23	3	0.1
(1,590)	1:98:A:MET:HE2	1:150:A:VAL:HG21	3	0.1
(1,590)	1:98:A:MET:HE2	1:150:A:VAL:HG22	3	0.1
(1,590)	1:98:A:MET:HE2	1:150:A:VAL:HG23	3	0.1
(1,590)	1:98:A:MET:HE3	1:150:A:VAL:HG21	3	0.1
(1,590)	1:98:A:MET:HE3	1:150:A:VAL:HG22	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:98:A:MET:HE3	1:150:A:VAL:HG23	3	0.1
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE1	2	0.1
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE2	2	0.1
(1,583)	1:92:A:VAL:HG21	1:180:A:MET:HE3	2	0.1
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE1	2	0.1
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE2	2	0.1
(1,583)	1:92:A:VAL:HG22	1:180:A:MET:HE3	2	0.1
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE1	2	0.1
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE2	2	0.1
(1,583)	1:92:A:VAL:HG23	1:180:A:MET:HE3	2	0.1
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	3	0.1
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	3	0.1
(1,559)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	3	0.1
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	3	0.1
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	3	0.1
(1,559)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	3	0.1
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	3	0.1
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	3	0.1
(1,559)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	3	0.1
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD21	1	0.1
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD22	1	0.1
(1,520)	1:45:A:LEU:HD11	1:89:A:LEU:HD23	1	0.1
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD21	1	0.1
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD22	1	0.1
(1,520)	1:45:A:LEU:HD12	1:89:A:LEU:HD23	1	0.1
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD21	1	0.1
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD22	1	0.1
(1,520)	1:45:A:LEU:HD13	1:89:A:LEU:HD23	1	0.1
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE1	6	0.1
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE2	6	0.1
(1,508)	1:32:A:LEU:HD21	1:119:A:MET:HE3	6	0.1
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE1	6	0.1
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE2	6	0.1
(1,508)	1:32:A:LEU:HD22	1:119:A:MET:HE3	6	0.1
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE1	6	0.1
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE2	6	0.1
(1,508)	1:32:A:LEU:HD23	1:119:A:MET:HE3	6	0.1
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD11	2	0.1
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD12	2	0.1
(1,507)	1:32:A:LEU:HD21	1:33:A:ILE:HD13	2	0.1
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD11	2	0.1
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD12	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:32:A:LEU:HD22	1:33:A:ILE:HD13	2	0.1
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD11	2	0.1
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD12	2	0.1
(1,507)	1:32:A:LEU:HD23	1:33:A:ILE:HD13	2	0.1
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD11	3	0.1
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD12	3	0.1
(1,500)	1:30:A:MET:HE1	1:33:A:ILE:HD13	3	0.1
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD11	3	0.1
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD12	3	0.1
(1,500)	1:30:A:MET:HE2	1:33:A:ILE:HD13	3	0.1
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD11	3	0.1
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD12	3	0.1
(1,500)	1:30:A:MET:HE3	1:33:A:ILE:HD13	3	0.1
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	8	0.1
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	8	0.1
(1,497)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	8	0.1
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	8	0.1
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	8	0.1
(1,497)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	8	0.1
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	8	0.1
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	8	0.1
(1,497)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	8	0.1
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD11	6	0.1
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD12	6	0.1
(1,485)	1:29:A:LEU:HD11	1:32:A:LEU:HD13	6	0.1
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD11	6	0.1
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD12	6	0.1
(1,485)	1:29:A:LEU:HD12	1:32:A:LEU:HD13	6	0.1
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD11	6	0.1
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD12	6	0.1
(1,485)	1:29:A:LEU:HD13	1:32:A:LEU:HD13	6	0.1
(1,479)	1:17:A:VAL:HG11	1:171:A:THR:HG21	4	0.1
(1,479)	1:17:A:VAL:HG11	1:171:A:THR:HG22	4	0.1
(1,479)	1:17:A:VAL:HG11	1:171:A:THR:HG23	4	0.1
(1,479)	1:17:A:VAL:HG12	1:171:A:THR:HG21	4	0.1
(1,479)	1:17:A:VAL:HG12	1:171:A:THR:HG22	4	0.1
(1,479)	1:17:A:VAL:HG12	1:171:A:THR:HG23	4	0.1
(1,479)	1:17:A:VAL:HG13	1:171:A:THR:HG21	4	0.1
(1,479)	1:17:A:VAL:HG13	1:171:A:THR:HG22	4	0.1
(1,479)	1:17:A:VAL:HG13	1:171:A:THR:HG23	4	0.1
(1,363)	1:192:A:GLU:H	1:195:A:THR:H	4	0.1
(1,297)	1:180:A:MET:H	1:182:A:ARG:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:104:A:ILE:H	1:106:A:ASN:H	8	0.1
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD11	9	0.1
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD12	9	0.1
(1,68)	1:206:A:ILE:HD11	1:203:A:ILE:HD13	9	0.1
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD11	9	0.1
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD12	9	0.1
(1,68)	1:206:A:ILE:HD12	1:203:A:ILE:HD13	9	0.1
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD11	9	0.1
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD12	9	0.1
(1,68)	1:206:A:ILE:HD13	1:203:A:ILE:HD13	9	0.1
(1,61)	1:121:A:ALA:HB1	1:124:A:ALA:HB1	9	0.1
(1,61)	1:121:A:ALA:HB1	1:124:A:ALA:HB2	9	0.1
(1,61)	1:121:A:ALA:HB1	1:124:A:ALA:HB3	9	0.1
(1,61)	1:121:A:ALA:HB2	1:124:A:ALA:HB1	9	0.1
(1,61)	1:121:A:ALA:HB2	1:124:A:ALA:HB2	9	0.1
(1,61)	1:121:A:ALA:HB2	1:124:A:ALA:HB3	9	0.1
(1,61)	1:121:A:ALA:HB3	1:124:A:ALA:HB1	9	0.1
(1,61)	1:121:A:ALA:HB3	1:124:A:ALA:HB2	9	0.1
(1,61)	1:121:A:ALA:HB3	1:124:A:ALA:HB3	9	0.1
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD11	9	0.1
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD12	9	0.1
(1,31)	1:89:A:LEU:HD11	1:190:A:LEU:HD13	9	0.1
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD11	9	0.1
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD12	9	0.1
(1,31)	1:89:A:LEU:HD12	1:190:A:LEU:HD13	9	0.1
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD11	9	0.1
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD12	9	0.1
(1,31)	1:89:A:LEU:HD13	1:190:A:LEU:HD13	9	0.1
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD21	1	0.1
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD22	1	0.1
(1,23)	1:80:A:LEU:HD11	1:89:A:LEU:HD23	1	0.1
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD21	1	0.1
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD22	1	0.1
(1,23)	1:80:A:LEU:HD12	1:89:A:LEU:HD23	1	0.1
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD21	1	0.1
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD22	1	0.1
(1,23)	1:80:A:LEU:HD13	1:89:A:LEU:HD23	1	0.1
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD11	8	0.1
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD12	8	0.1
(1,7)	1:109:A:THR:HG21	1:104:A:ILE:HD13	8	0.1
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD11	8	0.1
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD12	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:109:A:THR:HG22	1:104:A:ILE:HD13	8	0.1
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD11	8	0.1
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD12	8	0.1
(1,7)	1:109:A:THR:HG23	1:104:A:ILE:HD13	8	0.1

10 Dihedral-angle violation analysis [i](#)

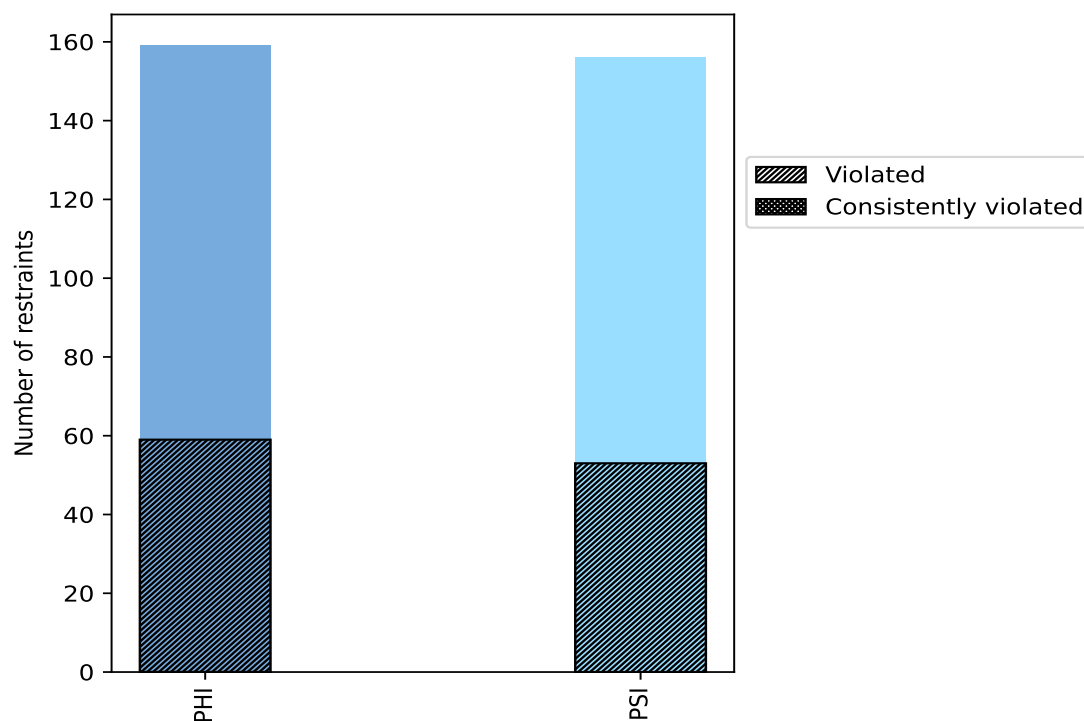
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	159	50.5	59	37.1	18.7	0	0.0	0.0
PSI	156	49.5	53	34.0	16.8	0	0.0	0.0
Total	315	100.0	112	35.6	35.6	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



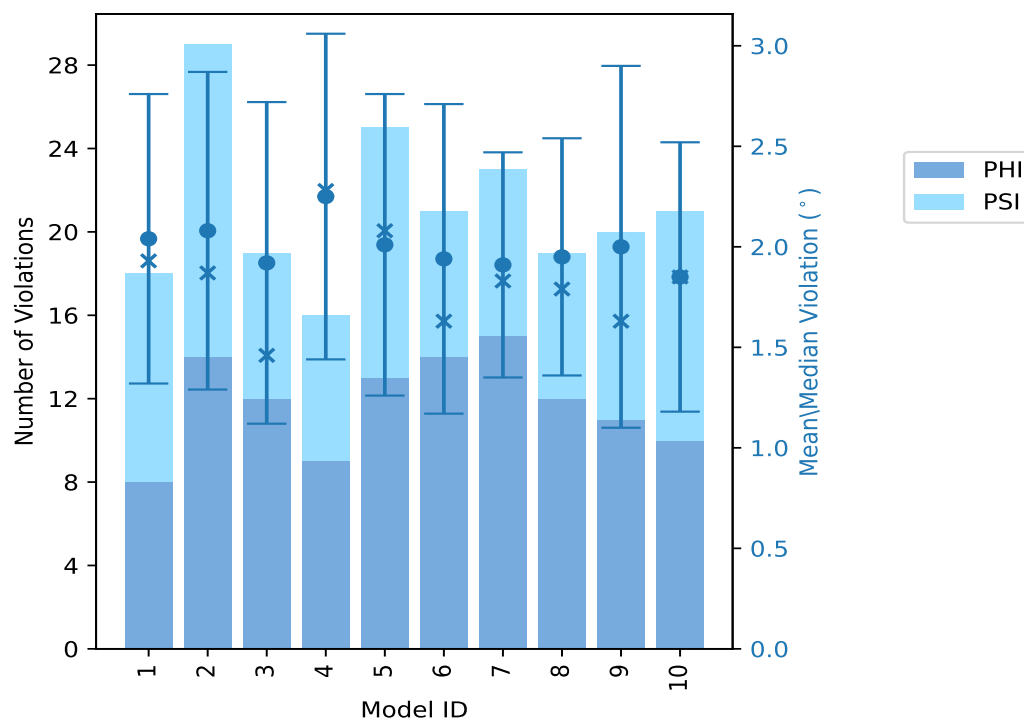
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	8	10	18	2.04	3.68	0.72	1.93
2	14	15	29	2.08	3.95	0.79	1.87
3	12	7	19	1.92	3.8	0.8	1.46
4	9	7	16	2.25	4.21	0.81	2.28
5	13	12	25	2.01	4.35	0.75	2.08
6	14	7	21	1.94	3.81	0.77	1.63
7	15	8	23	1.91	3.05	0.56	1.83
8	12	7	19	1.95	3.3	0.59	1.79
9	11	9	20	2.0	4.24	0.9	1.63
10	10	11	21	1.85	3.13	0.67	1.85

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

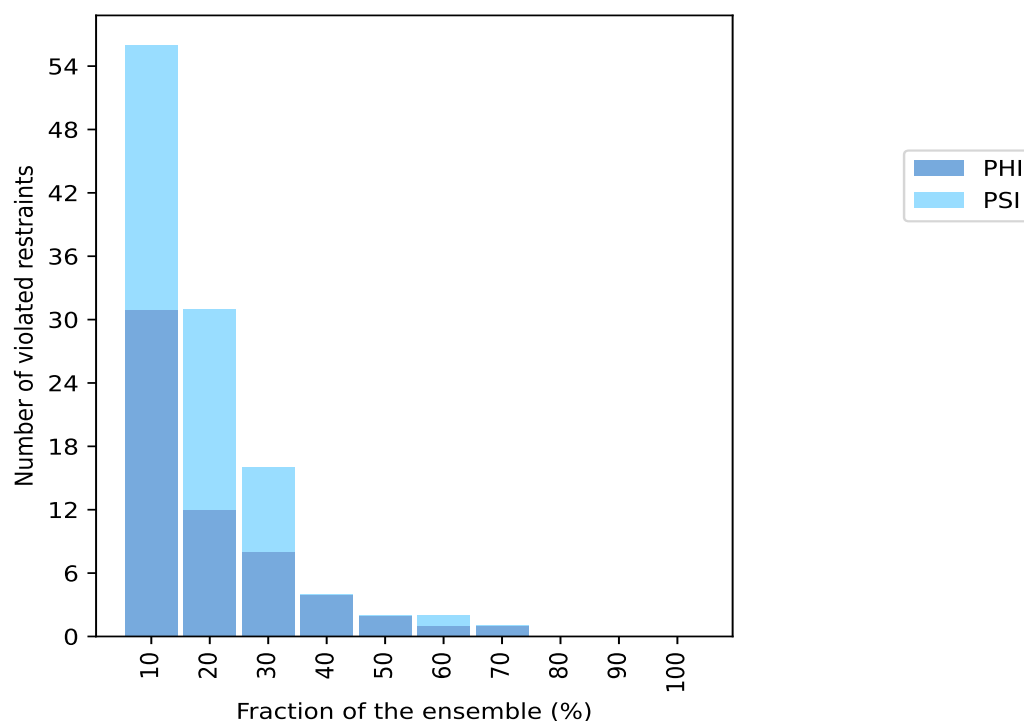
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
31	25	56	1	10.0
12	19	31	2	20.0
8	8	16	3	30.0
4	0	4	4	40.0
2	0	2	5	50.0
1	1	2	6	60.0
1	0	1	7	70.0
0	0	0	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

¹ Number of models with violations

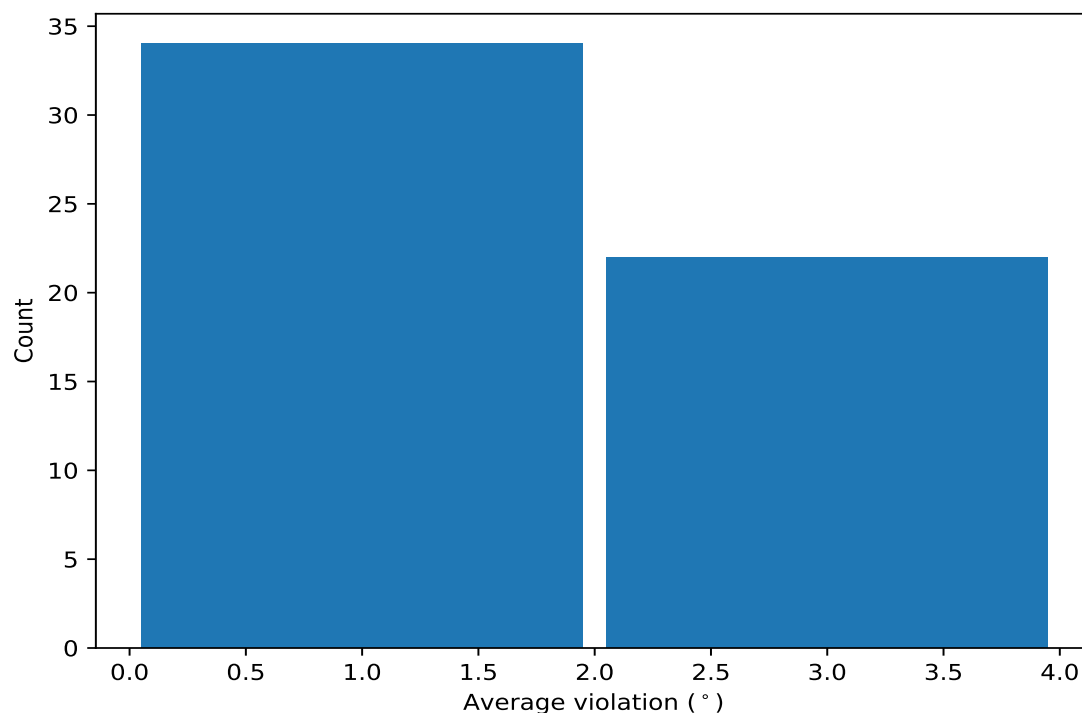
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,13)	1:26:A:ILE:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	7	1.79	0.57	1.58
(1,266)	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	1:189:A:HIS:N	6	2.86	0.81	2.82
(1,269)	1:189:A:HIS:C	1:190:A:LEU:N	1:190:A:LEU:CA	1:190:A:LEU:C	6	1.83	0.47	1.92
(1,255)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	5	2.62	0.36	2.72
(1,315)	1:221:A:PHE:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	5	1.88	0.53	1.81
(1,205)	1:151:A:ILE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	4	2.51	0.55	2.56
(1,179)	1:133:A:GLN:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	4	1.77	0.55	1.54
(1,313)	1:220:A:LEU:C	1:221:A:PHE:N	1:221:A:PHE:CA	1:221:A:PHE:C	4	1.74	0.56	1.49
(1,27)	1:34:A:ILE:C	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	4	1.72	0.71	1.35
(1,228)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:SER:N	3	3.04	0.59	3.38
(1,114)	1:88:A:THR:C	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	3	2.46	0.33	2.65
(1,256)	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1:184:A:THR:N	3	2.42	1.3	1.87
(1,116)	1:89:A:LEU:C	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	3	2.18	0.68	2.09

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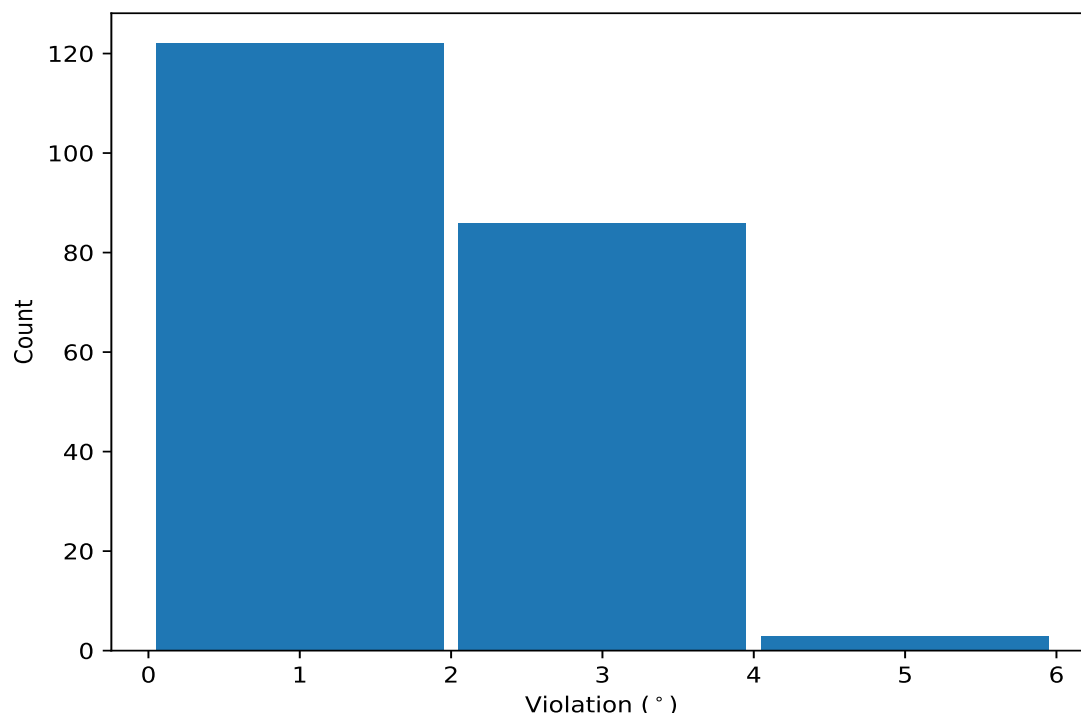
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,117)	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	1:91:A:ILE:N	3	2.1	0.38	2.2
(1,235)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	3	2.02	0.7	1.81
(1,213)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	3	1.98	0.38	1.91
(1,264)	1:187:A:ILE:N	1:187:A:ILE:CA	1:187:A:ILE:C	1:188:A:LEU:N	3	1.97	0.53	1.6
(1,230)	1:166:A:ALA:N	1:166:A:ALA:CA	1:166:A:ALA:C	1:167:A:GLY:N	3	1.93	0.56	2.07
(1,310)	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	1:220:A:LEU:N	3	1.8	0.31	1.85
(1,194)	1:146:A:GLU:N	1:146:A:GLU:CA	1:146:A:GLU:C	1:147:A:LYS:N	3	1.79	0.27	1.68
(1,118)	1:90:A:THR:C	1:91:A:ILE:N	1:91:A:ILE:CA	1:91:A:ILE:C	3	1.78	0.06	1.81
(1,233)	1:167:A:GLY:C	1:168:A:GLY:N	1:168:A:GLY:CA	1:168:A:GLY:C	3	1.7	0.66	1.38
(1,107)	1:83:A:ASN:N	1:83:A:ASN:CA	1:83:A:ASN:C	1:84:A:LYS:N	3	1.47	0.43	1.26
(1,263)	1:186:A:VAL:C	1:187:A:ILE:N	1:187:A:ILE:CA	1:187:A:ILE:C	3	1.37	0.13	1.36
(1,82)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	3	1.17	0.06	1.19
(1,147)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:LYS:N	2	3.66	0.58	3.66
(1,204)	1:151:A:ILE:N	1:151:A:ILE:CA	1:151:A:ILE:C	1:152:A:THR:N	2	3.04	0.12	3.04
(1,97)	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	1:79:A:ASN:N	2	2.53	0.39	2.53
(1,202)	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	1:151:A:ILE:N	2	2.5	1.18	2.5
(1,145)	1:106:A:ASN:N	1:106:A:ASN:CA	1:106:A:ASN:C	1:107:A:LEU:N	2	2.38	0.91	2.38
(1,7)	1:20:A:PHE:C	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	2	2.3	1.22	2.3
(1,87)	1:72:A:SER:N	1:72:A:SER:CA	1:72:A:SER:C	1:73:A:GLY:N	2	2.3	0.2	2.3
(1,236)	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	1:170:A:PHE:N	2	2.26	0.18	2.26
(1,192)	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	1:146:A:GLU:N	2	2.22	0.06	2.22
(1,34)	1:41:A:LYS:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	2	2.21	0.43	2.21
(1,302)	1:214:A:ILE:N	1:214:A:ILE:CA	1:214:A:ILE:C	1:215:A:GLY:N	2	2.07	0.04	2.07
(1,1)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	2	2.0	0.44	2.0
(1,28)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	2	2.0	0.92	2.0
(1,224)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	2	1.96	0.02	1.96
(1,89)	1:73:A:GLY:N	1:73:A:GLY:CA	1:73:A:GLY:C	1:74:A:LYS:N	2	1.93	0.55	1.93
(1,243)	1:172:A:VAL:C	1:173:A:ARG:N	1:173:A:ARG:CA	1:173:A:ARG:C	2	1.92	0.51	1.92
(1,83)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:ASP:N	2	1.92	0.06	1.92
(1,32)	1:40:A:ASN:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	2	1.9	0.44	1.9
(1,80)	1:68:A:SER:C	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	2	1.83	0.79	1.83
(1,309)	1:218:A:ILE:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	2	1.82	0.16	1.82
(1,4)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:PHE:N	2	1.77	0.14	1.77
(1,184)	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1:137:A:GLY:N	2	1.74	0.4	1.74
(1,198)	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	1:149:A:THR:N	2	1.74	0.45	1.74
(1,219)	1:159:A:GLN:C	1:160:A:TYR:N	1:160:A:TYR:CA	1:160:A:TYR:C	2	1.71	0.01	1.71
(1,249)	1:175:A:ASP:C	1:176:A:THR:N	1:176:A:THR:CA	1:176:A:THR:C	2	1.65	0.52	1.65
(1,177)	1:132:A:GLY:C	1:133:A:GLN:N	1:133:A:GLN:CA	1:133:A:GLN:C	2	1.6	0.55	1.6
(1,223)	1:161:A:ALA:C	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	2	1.59	0.45	1.59
(1,8)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:PHE:N	2	1.56	0.16	1.56
(1,251)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	2	1.35	0.28	1.35
(1,105)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	2	1.31	0.09	1.31
(1,135)	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	1:102:A:ASP:N	2	1.14	0.1	1.14

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,88)	1:72:A:SER:C	1:73:A:GLY:N	1:73:A:GLY:CA	1:73:A:GLY:C	5	4.35
(1,147)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:LYS:N	9	4.24
(1,256)	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1:184:A:THR:N	4	4.21
(1,146)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	9	3.99
(1,248)	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	1:176:A:THR:N	2	3.95
(1,266)	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	1:189:A:HIS:N	6	3.81
(1,266)	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	1:189:A:HIS:N	3	3.8
(1,202)	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	1:151:A:ILE:N	1	3.68
(1,228)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:SER:N	2	3.54
(1,7)	1:20:A:PHE:C	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	2	3.53
(1,222)	1:161:A:ALA:N	1:161:A:ALA:CA	1:161:A:ALA:C	1:162:A:TRP:N	2	3.47
(1,228)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:SER:N	9	3.38
(1,187)	1:141:A:ALA:C	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	2	3.36
(1,145)	1:106:A:ASN:N	1:106:A:ASN:CA	1:106:A:ASN:C	1:107:A:LEU:N	8	3.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:22:A:PHE:N	1:22:A:PHE:CA	1:22:A:PHE:C	1:23:A:GLN:N	3	3.24
(1,205)	1:151:A:ILE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	4	3.22
(1,129)	1:98:A:MET:N	1:98:A:MET:CA	1:98:A:MET:C	1:99:A:THR:N	8	3.2
(1,280)	1:197:A:TYR:C	1:198:A:LEU:N	1:198:A:LEU:CA	1:198:A:LEU:C	5	3.18
(1,204)	1:151:A:ILE:N	1:151:A:ILE:CA	1:151:A:ILE:C	1:152:A:THR:N	6	3.17
(1,266)	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	1:189:A:HIS:N	10	3.13
(1,183)	1:135:A:GLY:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	6	3.12
(1,147)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:LYS:N	10	3.09
(1,255)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	10	3.05
(1,116)	1:89:A:LEU:C	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	7	3.05
(1,235)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	1	2.96
(1,305)	1:215:A:GLY:C	1:216:A:TYR:N	1:216:A:TYR:CA	1:216:A:TYR:C	3	2.94
(1,27)	1:34:A:ILE:C	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	4	2.94
(1,204)	1:151:A:ILE:N	1:151:A:ILE:CA	1:151:A:ILE:C	1:152:A:THR:N	1	2.92
(1,97)	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	1:79:A:ASN:N	7	2.92
(1,28)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	8	2.92
(1,255)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1	2.85
(1,13)	1:26:A:ILE:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	4	2.8
(1,205)	1:151:A:ILE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	5	2.74
(1,114)	1:88:A:THR:C	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	6	2.73
(1,315)	1:221:A:PHE:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	5	2.72
(1,264)	1:187:A:ILE:N	1:187:A:ILE:CA	1:187:A:ILE:C	1:188:A:LEU:N	10	2.72
(1,255)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	4	2.72
(1,179)	1:133:A:GLN:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	7	2.7
(1,313)	1:220:A:LEU:C	1:221:A:PHE:N	1:221:A:PHE:CA	1:221:A:PHE:C	3	2.69
(1,114)	1:88:A:THR:C	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	2	2.65
(1,34)	1:41:A:LYS:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	1	2.64
(1,80)	1:68:A:SER:C	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	9	2.62
(1,233)	1:167:A:GLY:C	1:168:A:GLY:N	1:168:A:GLY:CA	1:168:A:GLY:C	4	2.61
(1,230)	1:166:A:ALA:N	1:166:A:ALA:CA	1:166:A:ALA:C	1:167:A:GLY:N	4	2.53
(1,266)	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	1:189:A:HIS:N	5	2.52
(1,36)	1:43:A:ILE:C	1:44:A:PHE:N	1:44:A:PHE:CA	1:44:A:PHE:C	4	2.52
(1,117)	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	1:91:A:ILE:N	7	2.51
(1,269)	1:189:A:HIS:C	1:190:A:LEU:N	1:190:A:LEU:CA	1:190:A:LEU:C	6	2.49
(1,255)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	6	2.49
(1,87)	1:72:A:SER:N	1:72:A:SER:CA	1:72:A:SER:C	1:73:A:GLY:N	6	2.49
(1,89)	1:73:A:GLY:N	1:73:A:GLY:CA	1:73:A:GLY:C	1:74:A:LYS:N	5	2.48
(1,13)	1:26:A:ILE:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	9	2.48
(1,213)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	3	2.47
(1,1)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	5	2.44
(1,243)	1:172:A:VAL:C	1:173:A:ARG:N	1:173:A:ARG:CA	1:173:A:ARG:C	3	2.43
(1,236)	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	1:170:A:PHE:N	3	2.43
(1,205)	1:151:A:ILE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1	2.38
(1,90)	1:73:A:GLY:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	7	2.36
(1,266)	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	1:189:A:HIS:N	2	2.35
(1,32)	1:40:A:ASN:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	9	2.34
(1,122)	1:92:A:VAL:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	7	2.31
(1,143)	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	1:106:A:ASN:N	5	2.3
(1,192)	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	1:146:A:GLU:N	2	2.28
(1,153)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:MET:N	2	2.28
(1,217)	1:158:A:GLU:C	1:159:A:GLN:N	1:159:A:GLN:CA	1:159:A:GLN:C	6	2.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	7	2.26
(1,303)	1:214:A:ILE:C	1:215:A:GLY:N	1:215:A:GLY:CA	1:215:A:GLY:C	8	2.25
(1,228)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:SER:N	5	2.21
(1,117)	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	1:91:A:ILE:N	10	2.2
(1,198)	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	1:149:A:THR:N	5	2.19
(1,269)	1:189:A:HIS:C	1:190:A:LEU:N	1:190:A:LEU:CA	1:190:A:LEU:C	5	2.18
(1,249)	1:175:A:ASP:C	1:176:A:THR:N	1:176:A:THR:CA	1:176:A:THR:C	8	2.17
(1,315)	1:221:A:PHE:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	10	2.16
(1,194)	1:146:A:GLU:N	1:146:A:GLU:CA	1:146:A:GLU:C	1:147:A:LYS:N	1	2.16
(1,192)	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	1:146:A:GLU:N	7	2.16
(1,310)	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	1:220:A:LEU:N	2	2.15
(1,184)	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1:137:A:GLY:N	10	2.15
(1,177)	1:132:A:GLY:C	1:133:A:GLN:N	1:133:A:GLN:CA	1:133:A:GLN:C	2	2.14
(1,97)	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	1:79:A:ASN:N	1	2.14
(1,302)	1:214:A:ILE:N	1:214:A:ILE:CA	1:214:A:ILE:C	1:215:A:GLY:N	5	2.11
(1,87)	1:72:A:SER:N	1:72:A:SER:CA	1:72:A:SER:C	1:73:A:GLY:N	8	2.1
(1,116)	1:89:A:LEU:C	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	2	2.09
(1,236)	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	1:170:A:PHE:N	5	2.08
(1,230)	1:166:A:ALA:N	1:166:A:ALA:CA	1:166:A:ALA:C	1:167:A:GLY:N	7	2.07
(1,107)	1:83:A:ASN:N	1:83:A:ASN:CA	1:83:A:ASN:C	1:84:A:LYS:N	9	2.07
(1,223)	1:161:A:ALA:C	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	4	2.05
(1,302)	1:214:A:ILE:N	1:214:A:ILE:CA	1:214:A:ILE:C	1:215:A:GLY:N	2	2.03
(1,262)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	1	2.03
(1,255)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	2	2.0
(1,114)	1:88:A:THR:C	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	10	1.99
(1,252)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	5	1.98
(1,83)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:ASP:N	3	1.98
(1,309)	1:218:A:ILE:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	7	1.97
(1,224)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	8	1.97
(1,2)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:THR:N	10	1.96
(1,224)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	4	1.94
(1,269)	1:189:A:HIS:C	1:190:A:LEU:N	1:190:A:LEU:CA	1:190:A:LEU:C	3	1.93
(1,269)	1:189:A:HIS:C	1:190:A:LEU:N	1:190:A:LEU:CA	1:190:A:LEU:C	8	1.91
(1,213)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	7	1.91
(1,4)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:PHE:N	9	1.91
(1,95)	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1:78:A:ILE:N	8	1.89
(1,256)	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1:184:A:THR:N	10	1.87
(1,231)	1:166:A:ALA:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	2	1.87
(1,310)	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	1:220:A:LEU:N	10	1.85
(1,83)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:ASP:N	2	1.85
(1,123)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:THR:N	7	1.83
(1,118)	1:90:A:THR:C	1:91:A:ILE:N	1:91:A:ILE:CA	1:91:A:ILE:C	1	1.83
(1,278)	1:195:A:THR:C	1:196:A:GLU:N	1:196:A:GLU:CA	1:196:A:GLU:C	5	1.82
(1,315)	1:221:A:PHE:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	1	1.81
(1,235)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	7	1.81
(1,118)	1:90:A:THR:C	1:91:A:ILE:N	1:91:A:ILE:CA	1:91:A:ILE:C	2	1.81
(1,304)	1:215:A:GLY:N	1:215:A:GLY:CA	1:215:A:GLY:C	1:216:A:TYR:N	8	1.79
(1,34)	1:41:A:LYS:C	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	6	1.78
(1,138)	1:102:A:ASP:C	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	7	1.76
(1,13)	1:26:A:ILE:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	8	1.73
(1,219)	1:159:A:GLN:C	1:160:A:TYR:N	1:160:A:TYR:CA	1:160:A:TYR:C	9	1.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:PHE:N	7	1.72
(1,205)	1:151:A:ILE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	2	1.71
(1,180)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLY:N	7	1.71
(1,219)	1:159:A:GLN:C	1:160:A:TYR:N	1:160:A:TYR:CA	1:160:A:TYR:C	8	1.7
(1,193)	1:145:A:ALA:C	1:146:A:GLU:N	1:146:A:GLU:CA	1:146:A:GLU:C	6	1.69
(1,118)	1:90:A:THR:C	1:91:A:ILE:N	1:91:A:ILE:CA	1:91:A:ILE:C	8	1.69
(1,247)	1:174:A:THR:C	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	5	1.68
(1,194)	1:146:A:GLU:N	1:146:A:GLU:CA	1:146:A:GLU:C	1:147:A:LYS:N	9	1.68
(1,309)	1:218:A:ILE:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	2	1.66
(1,251)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	2	1.63
(1,4)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:PHE:N	6	1.63
(1,311)	1:219:A:THR:C	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	8	1.6
(1,264)	1:187:A:ILE:N	1:187:A:ILE:CA	1:187:A:ILE:C	1:188:A:LEU:N	2	1.6
(1,117)	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	1:91:A:ILE:N	4	1.6
(1,92)	1:74:A:LYS:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	6	1.6
(1,237)	1:169:A:SER:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	8	1.59
(1,313)	1:220:A:LEU:C	1:221:A:PHE:N	1:221:A:PHE:CA	1:221:A:PHE:C	6	1.58
(1,264)	1:187:A:ILE:N	1:187:A:ILE:CA	1:187:A:ILE:C	1:188:A:LEU:N	9	1.58
(1,13)	1:26:A:ILE:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	1	1.58
(1,301)	1:213:A:PHE:C	1:214:A:ILE:N	1:214:A:ILE:CA	1:214:A:ILE:C	7	1.57
(1,179)	1:133:A:GLN:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	5	1.57
(1,1)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	7	1.57
(1,296)	1:208:A:LYS:N	1:208:A:LYS:CA	1:208:A:LYS:C	1:209:A:LYS:N	1	1.56
(1,315)	1:221:A:PHE:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	9	1.55
(1,266)	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	1:189:A:HIS:N	4	1.55
(1,213)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	10	1.55
(1,101)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:ILE:N	9	1.55
(1,124)	1:93:A:ASP:C	1:94:A:THR:N	1:94:A:THR:CA	1:94:A:THR:C	8	1.54
(1,263)	1:186:A:VAL:C	1:187:A:ILE:N	1:187:A:ILE:CA	1:187:A:ILE:C	2	1.53
(1,194)	1:146:A:GLU:N	1:146:A:GLU:CA	1:146:A:GLU:C	1:147:A:LYS:N	5	1.52
(1,179)	1:133:A:GLN:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	10	1.52
(1,145)	1:106:A:ASN:N	1:106:A:ASN:CA	1:106:A:ASN:C	1:107:A:LEU:N	2	1.47
(1,126)	1:95:A:GLY:C	1:96:A:ILE:N	1:96:A:ILE:CA	1:96:A:ILE:C	3	1.46
(1,32)	1:40:A:ASN:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	6	1.46
(1,201)	1:149:A:THR:C	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	3	1.44
(1,13)	1:26:A:ILE:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	6	1.44
(1,243)	1:172:A:VAL:C	1:173:A:ARG:N	1:173:A:ARG:CA	1:173:A:ARG:C	9	1.42
(1,8)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:PHE:N	6	1.41
(1,313)	1:220:A:LEU:C	1:221:A:PHE:N	1:221:A:PHE:CA	1:221:A:PHE:C	8	1.4
(1,116)	1:89:A:LEU:C	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	4	1.4
(1,105)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	3	1.4
(1,310)	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	1:220:A:LEU:N	1	1.39
(1,233)	1:167:A:GLY:C	1:168:A:GLY:N	1:168:A:GLY:CA	1:168:A:GLY:C	10	1.38
(1,89)	1:73:A:GLY:N	1:73:A:GLY:CA	1:73:A:GLY:C	1:74:A:LYS:N	9	1.38
(1,263)	1:186:A:VAL:C	1:187:A:ILE:N	1:187:A:ILE:CA	1:187:A:ILE:C	4	1.36
(1,27)	1:34:A:ILE:C	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	2	1.35
(1,27)	1:34:A:ILE:C	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	10	1.35
(1,184)	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1:137:A:GLY:N	2	1.34
(1,306)	1:216:A:TYR:N	1:216:A:TYR:CA	1:216:A:TYR:C	1:217:A:PRO:N	1	1.33
(1,232)	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	1:168:A:GLY:N	4	1.33
(1,111)	1:86:A:ASP:N	1:86:A:ASP:CA	1:86:A:ASP:C	1:87:A:ARG:N	6	1.33

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,202)	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	1:151:A:ILE:N	9	1.32
(1,259)	1:184:A:THR:C	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	3	1.31
(1,179)	1:133:A:GLN:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1	1.29
(1,313)	1:220:A:LEU:C	1:221:A:PHE:N	1:221:A:PHE:CA	1:221:A:PHE:C	9	1.28
(1,235)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	3	1.28
(1,198)	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	1:149:A:THR:N	2	1.28
(1,107)	1:83:A:ASN:N	1:83:A:ASN:CA	1:83:A:ASN:C	1:84:A:LYS:N	7	1.26
(1,13)	1:26:A:ILE:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	3	1.25
(1,135)	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	1:102:A:ASP:N	5	1.24
(1,128)	1:97:A:GLY:C	1:98:A:MET:N	1:98:A:MET:CA	1:98:A:MET:C	8	1.24
(1,13)	1:26:A:ILE:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	10	1.24
(1,269)	1:189:A:HIS:C	1:190:A:LEU:N	1:190:A:LEU:CA	1:190:A:LEU:C	9	1.23
(1,82)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	5	1.23
(1,27)	1:34:A:ILE:C	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	5	1.23
(1,245)	1:173:A:ARG:C	1:174:A:THR:N	1:174:A:THR:CA	1:174:A:THR:C	2	1.22
(1,105)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	10	1.22
(1,269)	1:189:A:HIS:C	1:190:A:LEU:N	1:190:A:LEU:CA	1:190:A:LEU:C	7	1.21
(1,263)	1:186:A:VAL:C	1:187:A:ILE:N	1:187:A:ILE:CA	1:187:A:ILE:C	5	1.21
(1,29)	1:37:A:PHE:N	1:37:A:PHE:CA	1:37:A:PHE:C	1:38:A:TYR:N	4	1.2
(1,82)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	10	1.19
(1,230)	1:166:A:ALA:N	1:166:A:ALA:CA	1:166:A:ALA:C	1:167:A:GLY:N	3	1.18
(1,256)	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1:184:A:THR:N	5	1.17
(1,106)	1:82:A:PRO:C	1:83:A:ASN:N	1:83:A:ASN:CA	1:83:A:ASN:C	3	1.16
(1,315)	1:221:A:PHE:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	6	1.15
(1,209)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	5	1.15
(1,249)	1:175:A:ASP:C	1:176:A:THR:N	1:176:A:THR:CA	1:176:A:THR:C	9	1.14
(1,223)	1:161:A:ALA:C	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	9	1.14
(1,30)	1:38:A:TYR:C	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	3	1.12
(1,233)	1:167:A:GLY:C	1:168:A:GLY:N	1:168:A:GLY:CA	1:168:A:GLY:C	7	1.1
(1,18)	1:30:A:MET:N	1:30:A:MET:CA	1:30:A:MET:C	1:31:A:SER:N	6	1.09
(1,164)	1:125:A:GLY:C	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	10	1.08
(1,107)	1:83:A:ASN:N	1:83:A:ASN:CA	1:83:A:ASN:C	1:84:A:LYS:N	10	1.08
(1,82)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	7	1.08
(1,28)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	1	1.08
(1,7)	1:20:A:PHE:C	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	8	1.08
(1,251)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	6	1.07
(1,73)	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	1:64:A:LEU:N	10	1.07
(1,284)	1:201:A:ARG:N	1:201:A:ARG:CA	1:201:A:ARG:C	1:202:A:ARG:N	2	1.06
(1,234)	1:168:A:GLY:N	1:168:A:GLY:CA	1:168:A:GLY:C	1:169:A:SER:N	5	1.05
(1,177)	1:132:A:GLY:C	1:133:A:GLN:N	1:133:A:GLN:CA	1:133:A:GLN:C	6	1.05
(1,135)	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	1:102:A:ASP:N	3	1.04
(1,80)	1:68:A:SER:C	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	7	1.04
(1,22)	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1:33:A:ILE:N	1	1.02
(1,155)	1:119:A:MET:N	1:119:A:MET:CA	1:119:A:MET:C	1:120:A:GLU:N	2	1.0