



Full wwPDB NMR Structure Validation Report ⓘ

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BMRB ID : 25923
Title : ULD complex
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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

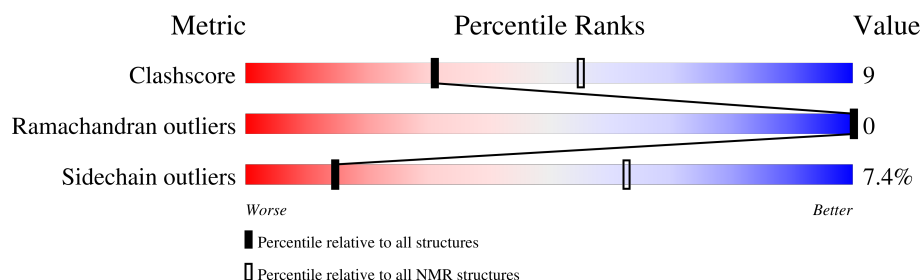
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 50%.

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	155	

2 Ensemble composition and analysis

This entry contains 10 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:128-A:140 (13)	0.06	6
2	A:160-A:231 (72)	0.06	4

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

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

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

Cluster number	Models
1	1, 4, 5, 6, 7, 8, 9, 10
2	2, 3

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2424 atoms, of which 1222 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polycomb complex protein BMI-1, Polyhomeotic-like 2.

Mol	Chain	Residues	Atoms						Trace
1	A	145	Total	C	H	N	O	S	0
			2424	768	1222	208	219	7	

There are 5 discrepancies between the modelled and reference sequences:

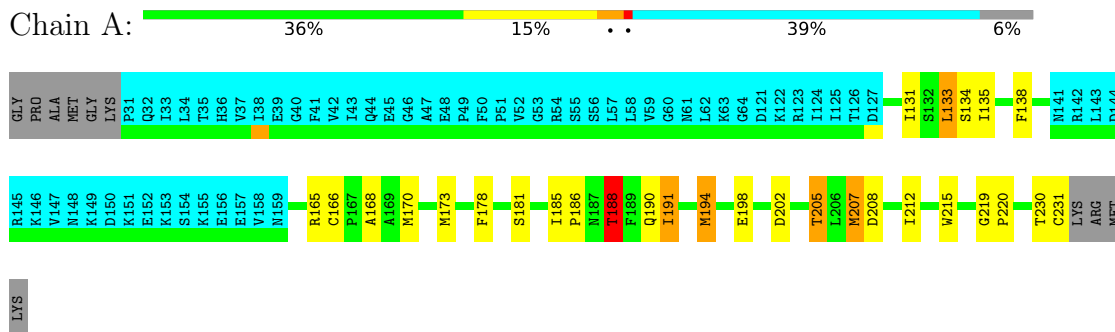
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP B1ASA2
A	26	PRO	-	expression tag	UNP B1ASA2
A	27	ALA	-	expression tag	UNP B1ASA2
A	28	MET	-	expression tag	UNP B1ASA2
A	29	GLY	-	expression tag	UNP B1ASA2

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: Polycomb complex protein BMI-1, Polyhomeotic-like 2

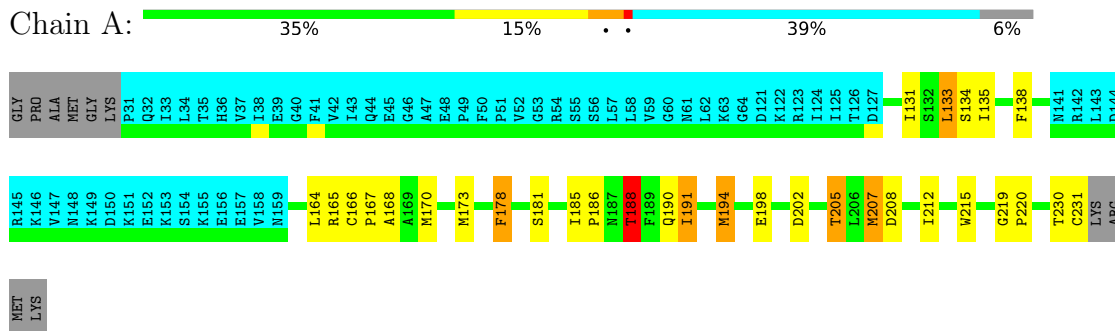


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

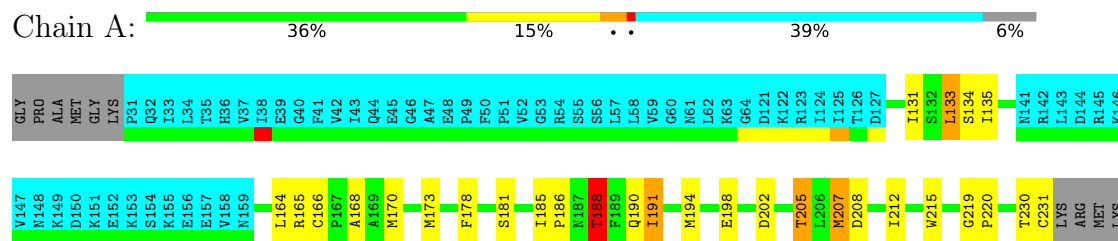
4.2.1 Score per residue for model 1

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2



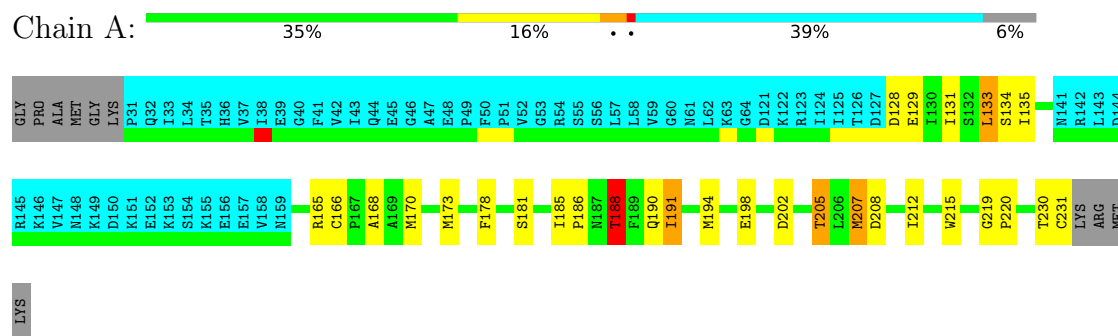
4.2.2 Score per residue for model 2

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2



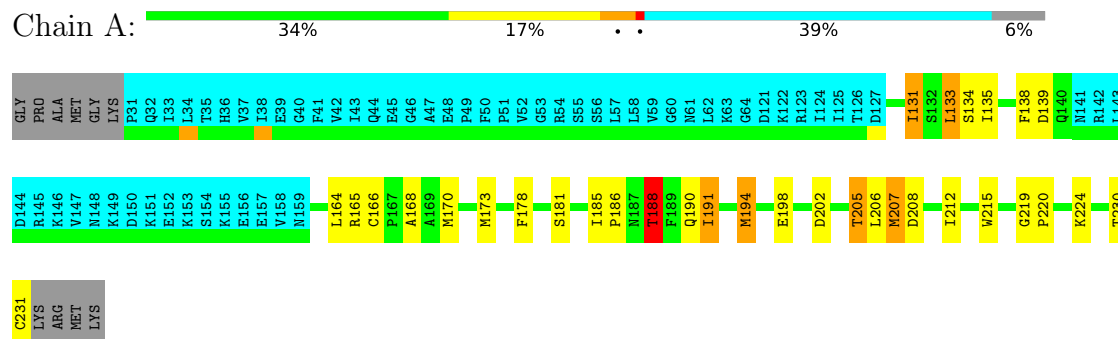
4.2.3 Score per residue for model 3

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2



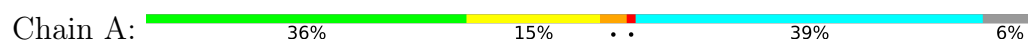
4.2.4 Score per residue for model 4 (medoid)

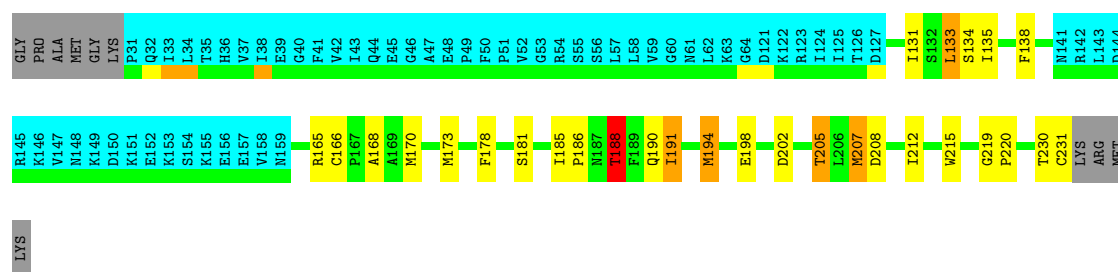
- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2



4.2.5 Score per residue for model 5

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2

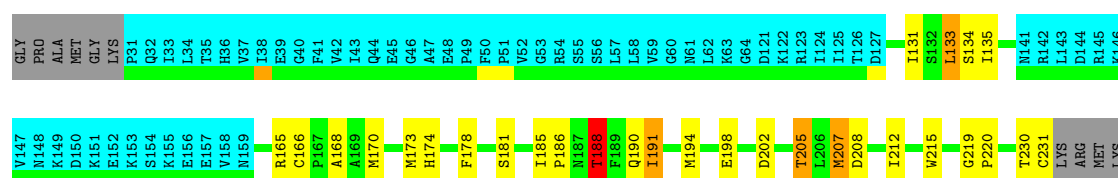




4.2.6 Score per residue for model 6

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2

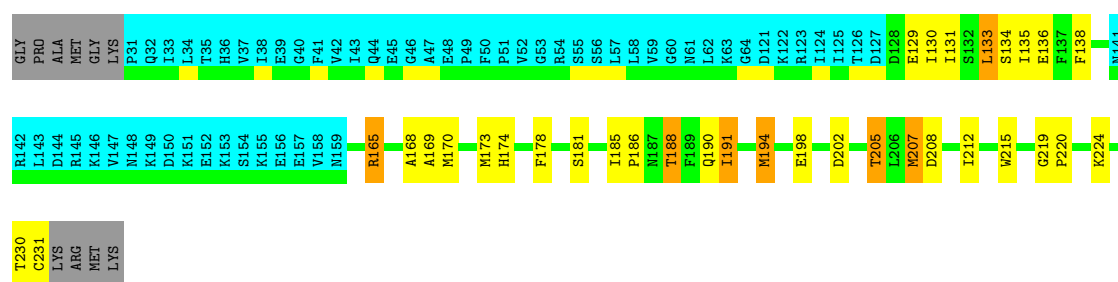
Chain A: 36% 15% 39% 6%



4.2.7 Score per residue for model 7

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2

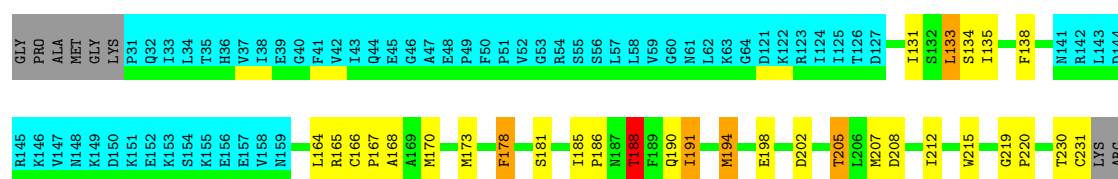
Chain A: 33% 17% 5% 39% 6%



4.2.8 Score per residue for model 8

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2

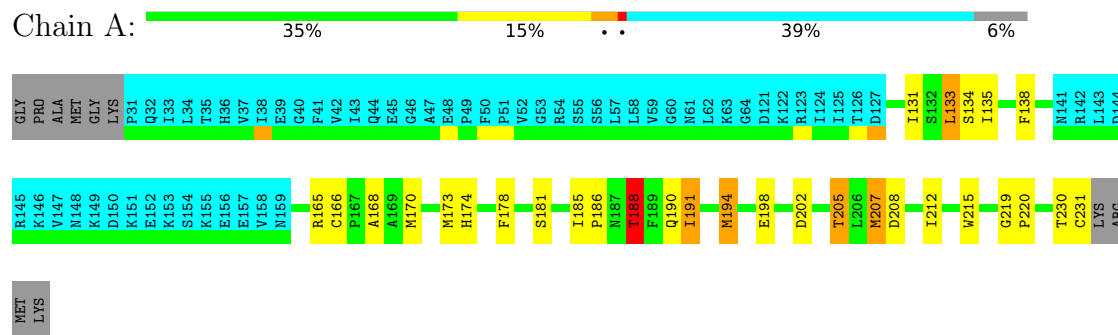
Chain A: 35% 16% 39% 6%



MET
LYS

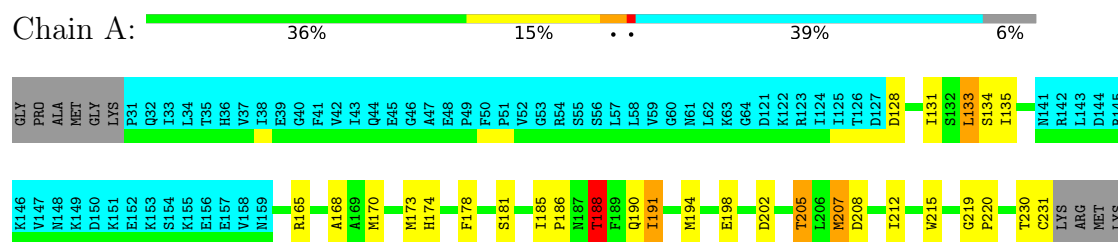
4.2.9 Score per residue for model 9

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2

MET
LYS

4.2.10 Score per residue for model 10

- Molecule 1: Polycomb complex protein BMI-1, Polyhomeotic-like 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *conformational sampling*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
Rosetta	refinement	
TALOS	geometry optimization	

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	1157
Number of shifts mapped to atoms	1132
Number of unparsed shifts	0
Number of shifts with mapping errors	25
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	50%

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	1.62±0.00	8±0/746 (1.1± 0.1%)	1.50±0.00	8±0/1008 (0.8± 0.0%)
All	All	1.62	80/7460 (1.1%)	1.50	80/10080 (0.8%)

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	212	ILE	CA-C	-8.10	1.42	1.52	8	10
1	A	181	SER	C-O	-6.36	1.16	1.24	10	10
1	A	168	ALA	N-CA	6.32	1.54	1.46	9	10
1	A	178	PHE	N-CA	-6.30	1.38	1.46	6	10
1	A	134	SER	C-O	6.16	1.31	1.23	6	10
1	A	194	MET	N-CA	-5.17	1.39	1.45	5	10
1	A	202	ASP	CA-C	5.14	1.59	1.52	7	10
1	A	188	THR	CB-CG2	-5.06	1.35	1.52	9	9
1	A	207	MET	N-CA	5.02	1.52	1.46	8	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	165	ARG	N-CA-C	-8.17	95.92	109.24	10	10
1	A	133	LEU	N-CA-C	7.00	118.82	108.60	3	10
1	A	212	ILE	N-CA-C	6.67	117.42	110.62	9	10
1	A	181	SER	N-CA-C	6.04	117.55	110.97	3	10
1	A	207	MET	CB-CA-C	-6.00	101.22	110.81	9	10
1	A	207	MET	CG-SD-CE	-5.49	88.83	100.90	7	10
1	A	173	MET	CA-C-O	-5.42	115.10	120.90	9	10
1	A	178	PHE	N-CA-C	-5.22	105.03	111.40	3	10

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	727	728	728	13±2
All	All	7270	7280	7280	128

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ILE:HG22	1:A:166:CYS:O	0.65	1.91	4	1
1:A:205:THR:CG2	1:A:208:ASP:H	0.61	2.08	4	10
1:A:166:CYS:SG	1:A:170:MET:HE2	0.60	2.37	6	6
1:A:205:THR:HG22	1:A:208:ASP:CG	0.59	2.22	9	10
1:A:190:GLN:HG2	1:A:230:THR:HB	0.56	1.78	10	10
1:A:135:ILE:O	1:A:135:ILE:HG23	0.52	2.04	9	10
1:A:185:ILE:HG21	1:A:191:ILE:HD11	0.52	1.81	2	10
1:A:133:LEU:HA	1:A:220:PRO:HB2	0.51	1.82	5	10
1:A:170:MET:SD	1:A:174:HIS:CG	0.51	3.03	10	2
1:A:139:ASP:HB3	1:A:224:LYS:HZ1	0.50	1.67	4	1
1:A:186:PRO:HG2	1:A:188:THR:HG22	0.46	1.86	4	10
1:A:138:PHE:HB2	1:A:194:MET:HE1	0.46	1.86	4	6
1:A:205:THR:HG22	1:A:208:ASP:H	0.45	1.70	4	10
1:A:136:GLU:O	1:A:224:LYS:HA	0.44	2.12	7	1
1:A:166:CYS:SG	1:A:170:MET:CE	0.43	3.06	6	2
1:A:164:LEU:HG	1:A:166:CYS:HB2	0.42	1.90	2	4
1:A:205:THR:HG23	1:A:208:ASP:H	0.42	1.73	10	10
1:A:167:PRO:HD2	1:A:170:MET:HG3	0.41	1.92	1	2
1:A:215:TRP:HZ2	1:A:219:GLY:O	0.41	1.99	1	10
1:A:131:ILE:HG23	1:A:166:CYS:HB3	0.40	1.93	4	1
1:A:130:ILE:CG2	1:A:165:ARG:CG	0.40	2.99	7	1
1:A:131:ILE:HG21	1:A:206:LEU:HD13	0.40	1.93	4	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	84/155 (54%)	79±0 (94±1%)	5±0 (6±1%)	0±0 (0±0%)	100	100
All	All	840/1550 (54%)	786 (94%)	54 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	81/142 (57%)	75±0 (93±0%)	6±0 (7±0%)	15	63
All	All	810/1420 (57%)	750 (93%)	60 (7%)	15	63

All 6 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	131	ILE	10
1	A	188	THR	10
1	A	191	ILE	10
1	A	198	GLU	10
1	A	205	THR	10
1	A	231	CYS	10

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 50% for the well-defined parts and 54% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

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	1157
Number of shifts mapped to atoms	1132
Number of unparsed shifts	0
Number of shifts with mapping errors	25
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 25 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	232	LYS	H	8.352	.	1
1	A	232	LYS	C	173.281	.	1
1	A	232	LYS	CA	56.42	.	1
1	A	232	LYS	CB	33.194	.	1
1	A	232	LYS	N	124.226	.	1
1	A	233	ARG	H	8.343	.	1
1	A	233	ARG	HA	4.349	.	1
1	A	233	ARG	C	173.321	.	1
1	A	233	ARG	CA	56.149	.	1
1	A	233	ARG	CB	30.94	.	1
1	A	233	ARG	N	122.896	.	1
1	A	234	MET	H	8.459	.	1
1	A	234	MET	HA	4.494	.	1
1	A	234	MET	C	172.353	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	234	MET	CA	55.576	.	1
1	A	234	MET	CB	33.023	.	1
1	A	234	MET	N	122.76	.	1
1	A	235	LYS	H	7.849	.	1
1	A	235	LYS	HA	4.144	.	1
1	A	235	LYS	HB2	1.753	.	.
1	A	235	LYS	HB3	1.753	.	.
1	A	235	LYS	C	178.173	.	1
1	A	235	LYS	CA	58.001	.	1
1	A	235	LYS	CB	33.6	.	1
1	A	235	LYS	N	126.795	.	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	-0.17 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.19 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	137	2.60 ± 0.20	Should be applied
^{15}N	128	0.30 ± 0.13	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 50%, i.e. 633 atoms were assigned a chemical shift out of a possible 1267. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	350/414 (85%)	128/165 (78%)	153/170 (90%)	69/79 (87%)
Sidechain	279/731 (38%)	174/474 (37%)	105/224 (47%)	0/33 (0%)
Aromatic	4/122 (3%)	3/58 (5%)	0/62 (0%)	1/2 (50%)
Overall	633/1267 (50%)	305/697 (44%)	258/456 (57%)	70/114 (61%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 54%, i.e. 1132 atoms were assigned a chemical shift out of a possible 2114. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	634/713 (89%)	241/287 (84%)	269/290 (93%)	124/136 (91%)
Sidechain	492/1251 (39%)	304/807 (38%)	188/386 (49%)	0/58 (0%)
Aromatic	6/150 (4%)	5/72 (7%)	0/74 (0%)	1/4 (25%)
Overall	1132/2114 (54%)	550/1166 (47%)	457/750 (61%)	125/198 (63%)

7.1.4 Statistically unusual chemical shifts [i](#)

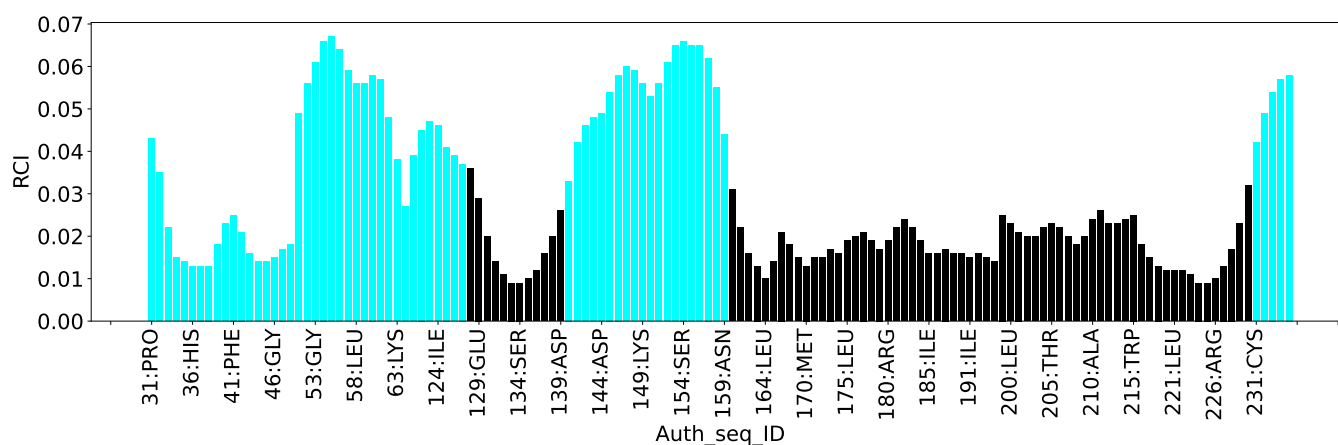
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	215	TRP	NE1	113.11	118.53 – 139.98	-7.5

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	300
Intra-residue ($ i-j =0$)	70
Sequential ($ i-j =1$)	86
Medium range ($ i-j >1$ and $ i-j <5$)	24
Long range ($ i-j \geq 5$)	97
Inter-chain	0
Hydrogen bond restraints	23
Disulfide bond restraints	0
Total dihedral-angle restraints	26
Number of unmapped restraints	0
Number of restraints per residue	2.1
Number of long range restraints per residue ¹	0.7

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)	9.4	0.2
0.2-0.5 (Medium)	20.2	0.5
>0.5 (Large)	120.8	4.69

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)	0.2	9.4
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

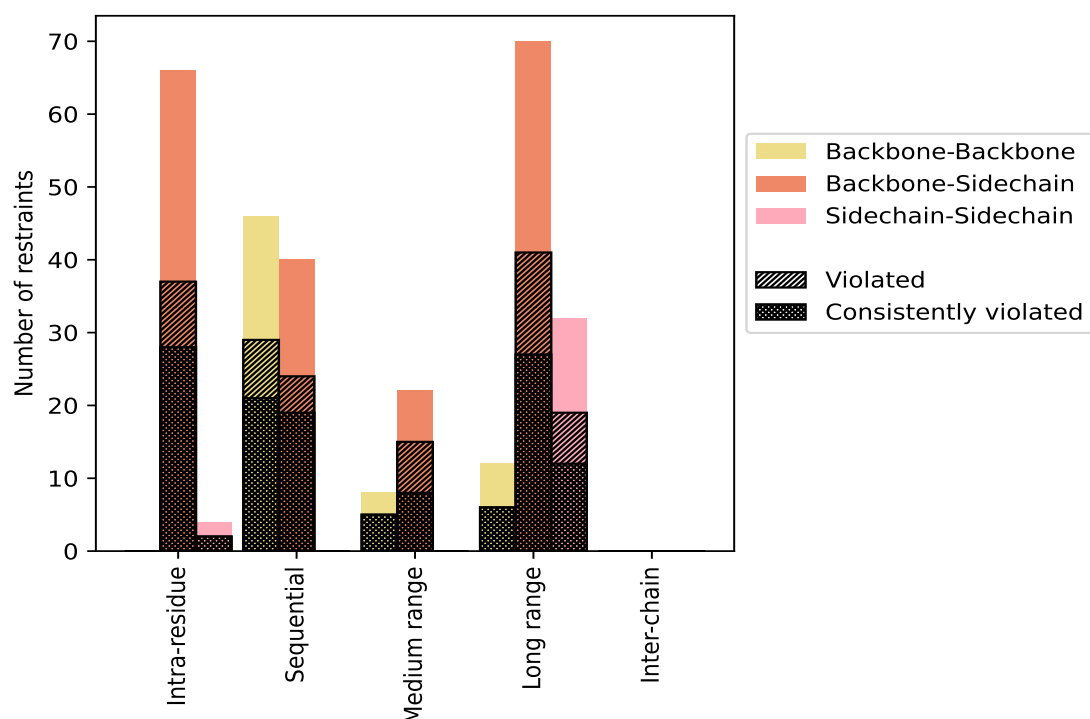
9.1 Summary of distance violations ⓘ

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)	70	23.3	39	55.7	13.0	30	42.9	10.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	66	22.0	37	56.1	12.3	28	42.4	9.3
Sidechain-Sidechain	4	1.3	2	50.0	0.7	2	50.0	0.7
Sequential (i-j =1)	86	28.7	53	61.6	17.7	40	46.5	13.3
Backbone-Backbone	46	15.3	29	63.0	9.7	21	45.7	7.0
Backbone-Sidechain	40	13.3	24	60.0	8.0	19	47.5	6.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	24	8.0	15	62.5	5.0	12	50.0	4.0
Backbone-Backbone	8	2.7	5	62.5	1.7	5	62.5	1.7
Backbone-Sidechain	16	5.3	10	62.5	3.3	7	43.8	2.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	97	32.3	56	57.7	18.7	44	45.4	14.7
Backbone-Backbone	12	4.0	6	50.0	2.0	6	50.0	2.0
Backbone-Sidechain	53	17.7	31	58.5	10.3	26	49.1	8.7
Sidechain-Sidechain	32	10.7	19	59.4	6.3	12	37.5	4.0
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	23	7.7	15	65.2	5.0	2	8.7	0.7
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	300	100.0	178	59.3	59.3	128	42.7	42.7
Backbone-Backbone	66	22.0	40	60.6	13.3	32	48.5	10.7
Backbone-Sidechain	198	66.0	117	59.1	39.0	82	41.4	27.3
Sidechain-Sidechain	36	12.0	21	58.3	7.0	14	38.9	4.7

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 disulfid bonds are counted in their appropriate category on the x-axis

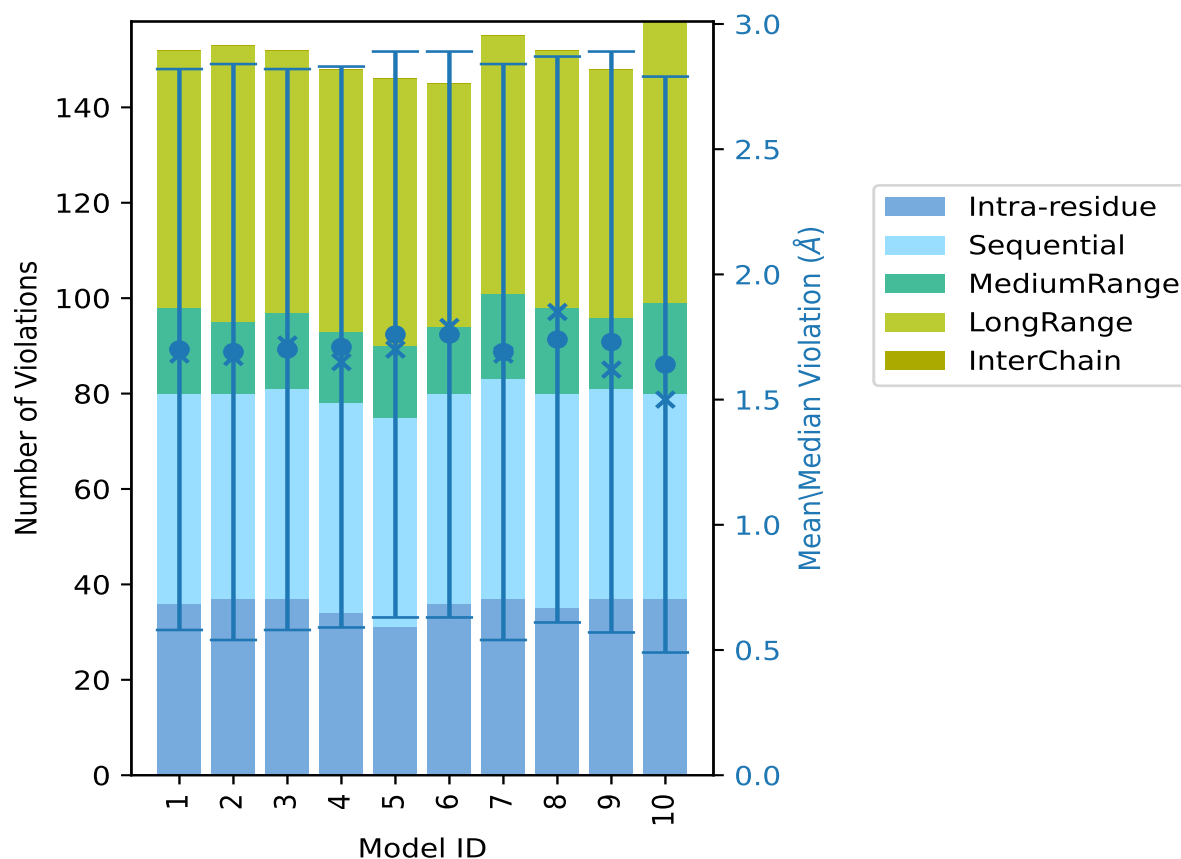
9.2 Distance violation statistics for each model [i](#)

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	36	44	18	54	0	152	1.7	4.36	1.12	1.68
2	37	43	15	58	0	153	1.69	4.57	1.15	1.67
3	37	44	16	55	0	152	1.7	4.57	1.12	1.72
4	34	44	15	55	0	148	1.71	4.56	1.12	1.65
5	31	44	15	56	0	146	1.76	4.57	1.13	1.7
6	36	44	14	51	0	145	1.76	4.57	1.13	1.79
7	37	46	18	54	0	155	1.69	4.69	1.15	1.68
8	35	45	18	54	0	152	1.74	4.29	1.13	1.85
9	37	44	15	52	0	148	1.73	4.55	1.16	1.62
10	37	43	19	59	0	158	1.64	4.62	1.15	1.5

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, 114(IR:31, SQ:33, MR:9, LR:41, 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	%
2	6	1	2	0	11	1	10.0
0	2	0	1	0	3	2	20.0
0	2	0	0	0	2	3	30.0

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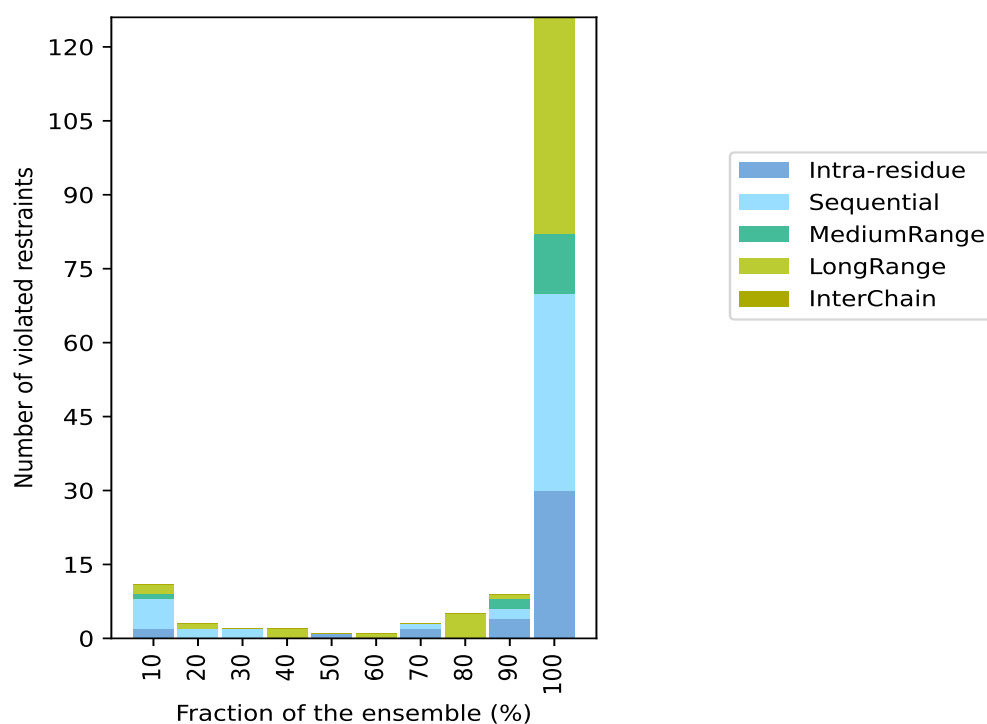
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	2	0	2	4	40.0
1	0	0	0	0	1	5	50.0
0	0	0	1	0	1	6	60.0
2	1	0	0	0	3	7	70.0
0	0	0	5	0	5	8	80.0
4	2	2	1	0	9	9	90.0
30	40	12	44	0	126	10	100.0

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 [i](#)

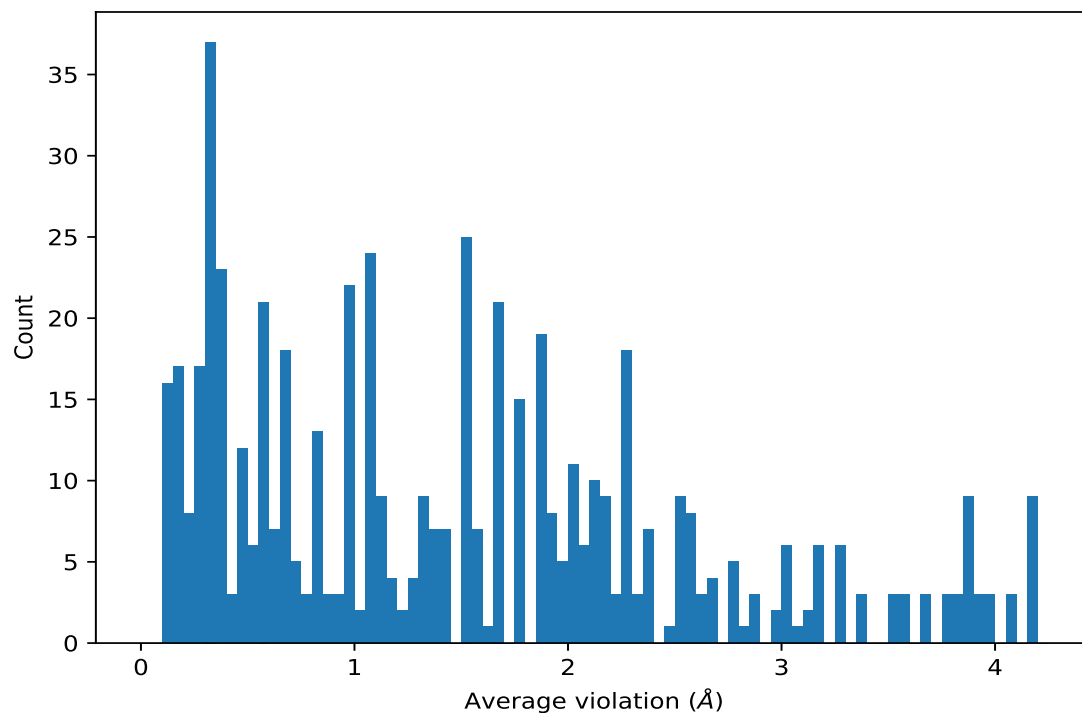


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	10	4.19	0.34	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	10	4.19	0.34	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	10	4.19	0.34	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	10	4.19	0.34	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	10	4.19	0.34	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	10	4.19	0.34	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	10	4.19	0.34	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	10	4.19	0.34	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	10	4.19	0.34	4.17
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	10	4.06	0.18	4.06
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	10	4.06	0.18	4.06
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	10	4.06	0.18	4.06
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	10	3.95	0.04	3.95
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	10	3.95	0.04	3.95
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	10	3.95	0.04	3.95

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	10	3.94	0.31	3.8
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	10	3.94	0.31	3.8
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	10	3.94	0.31	3.8
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	10	3.86	0.35	3.9
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	10	3.86	0.35	3.9
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	10	3.86	0.35	3.9
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	10	3.85	0.84	4.02
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	10	3.85	0.84	4.02
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	10	3.85	0.84	4.02
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	10	3.85	0.84	4.02
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	10	3.85	0.84	4.02
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	10	3.85	0.84	4.02
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	10	3.84	0.04	3.85
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	10	3.84	0.04	3.85
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	10	3.84	0.04	3.85
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	10	3.8	0.07	3.8
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	10	3.8	0.07	3.8
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	10	3.8	0.07	3.8
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	10	3.68	0.27	3.8
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	10	3.68	0.27	3.8
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	10	3.68	0.27	3.8
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	10	3.58	0.38	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	10	3.58	0.38	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	10	3.58	0.38	3.5
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	10	3.54	0.21	3.54
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	10	3.5	0.25	3.38
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	10	3.5	0.25	3.38
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	10	3.35	0.13	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	10	3.35	0.13	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	10	3.35	0.13	3.44
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	10	3.28	0.11	3.29
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	10	3.28	0.11	3.29
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	10	3.28	0.11	3.29
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	10	3.26	0.51	3.61
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	10	3.26	0.51	3.61
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	10	3.26	0.51	3.61
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	10	3.17	0.1	3.14
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	10	3.17	0.1	3.14
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	10	3.17	0.1	3.14
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	10	3.17	0.1	3.14
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	10	3.17	0.1	3.14
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	10	3.17	0.1	3.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	10	3.12	0.7	3.36
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	10	3.12	0.7	3.36
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	10	3.06	0.03	3.08
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	10	3.04	0.38	2.99
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	10	3.04	0.38	2.99
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	10	3.04	0.38	2.99
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	10	3.0	0.07	2.96
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	10	3.0	0.07	2.96
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	10	3.0	0.07	2.96
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	10	2.96	0.26	2.96
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	10	2.96	0.26	2.96
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	10	2.88	0.89	3.01
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	10	2.88	0.89	3.01
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	10	2.88	0.89	3.01
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	10	2.81	0.49	2.76
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	10	2.78	0.26	2.72
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	10	2.77	0.25	2.8
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	10	2.77	0.25	2.8
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	10	2.77	0.25	2.8
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	10	2.77	0.01	2.77
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	10	2.69	0.04	2.7
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	10	2.69	0.04	2.68
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	10	2.68	0.03	2.68
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	10	2.66	0.03	2.65
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	10	2.63	0.03	2.64
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	10	2.61	0.02	2.62
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	10	2.6	0.01	2.6
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	10	2.59	0.02	2.59
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	10	2.58	0.13	2.6
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	10	2.57	0.07	2.6
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	10	2.57	0.07	2.6
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	10	2.57	0.07	2.6
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	10	2.57	0.07	2.6
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	10	2.57	0.07	2.6
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	10	2.57	0.07	2.6
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	10	2.51	0.24	2.62
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	10	2.51	0.24	2.62
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	10	2.51	0.24	2.62
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	10	2.5	0.83	2.99
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	10	2.5	0.83	2.99
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	10	2.5	0.83	2.99
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	10	2.5	0.83	2.99

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	10	2.5	0.83	2.99
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	10	2.5	0.83	2.99
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	10	2.46	0.08	2.46
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	10	2.37	0.19	2.46
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	10	2.37	0.19	2.46
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	10	2.37	0.19	2.46
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	10	2.36	0.01	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	10	2.36	0.01	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	10	2.36	0.01	2.35
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	10	2.35	0.37	2.5
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	10	2.31	0.55	2.33
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	10	2.31	0.55	2.33
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	10	2.31	0.55	2.33
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	10	2.3	0.25	2.32
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	10	2.3	0.25	2.32
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	10	2.3	0.25	2.32
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	10	2.3	0.25	2.32
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	10	2.3	0.25	2.32
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	10	2.3	0.25	2.32
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	10	2.29	0.16	2.36
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	10	2.29	0.16	2.36
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	10	2.29	0.16	2.36
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	10	2.28	0.91	2.74
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	10	2.28	0.91	2.74
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	10	2.28	0.91	2.74
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	10	2.28	0.91	2.74
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	10	2.28	0.91	2.74
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	10	2.28	0.91	2.74
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	10	2.24	0.54	2.48
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	10	2.24	0.54	2.48
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	10	2.2	0.18	2.12
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	10	2.16	0.47	2.28
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	10	2.16	0.47	2.28
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	10	2.16	0.47	2.28
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	10	2.16	0.47	2.28
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	10	2.16	0.47	2.28
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	10	2.16	0.47	2.28
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	10	2.15	0.4	1.99
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	10	2.15	0.4	1.99
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	10	2.15	0.4	1.99
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	10	2.12	0.03	2.12
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	10	2.12	0.03	2.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	10	2.12	0.03	2.12
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	10	2.11	0.3	2.16
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	10	2.11	0.3	2.16
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	10	2.11	0.3	2.16
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	10	2.11	0.3	2.16
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	10	2.11	0.3	2.16
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	10	2.11	0.3	2.16
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	10	2.11	0.65	2.51
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	10	2.08	0.42	1.94
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	10	2.08	0.42	1.94
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	10	2.08	0.42	1.94
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	10	2.07	0.57	1.81
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	10	2.07	0.57	1.81
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	10	2.07	0.57	1.81
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	10	2.03	0.55	1.81
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	10	2.03	0.55	1.81
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	10	2.03	0.56	2.32
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	10	2.03	0.56	2.32
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	10	2.03	0.56	2.32
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	10	2.03	0.56	2.32
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	10	2.03	0.56	2.32
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	10	2.03	0.56	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	10	2.03	0.56	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	10	2.03	0.56	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	10	2.03	0.56	2.32
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	10	1.98	0.4	1.78
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	10	1.98	0.4	1.78
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	10	1.97	0.57	2.14
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	10	1.97	0.57	2.14
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	10	1.97	0.57	2.14
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	10	1.95	0.22	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	10	1.95	0.22	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	10	1.95	0.22	2.03
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	10	1.94	0.39	1.97
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	10	1.94	0.39	1.97
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	10	1.91	0.93	2.52
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	10	1.91	0.48	1.91
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	10	1.91	0.48	1.91
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	10	1.88	0.13	1.92
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	10	1.88	0.13	1.92
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	10	1.88	0.13	1.92
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	10	1.88	0.13	1.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	10	1.88	0.13	1.92
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	10	1.88	0.13	1.92
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	10	1.88	0.18	1.9
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	10	1.85	0.04	1.85
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	10	1.85	0.04	1.85
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	10	1.85	0.04	1.85
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	10	1.85	0.04	1.85
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	10	1.85	0.04	1.85
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	10	1.85	0.04	1.85
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	10	1.79	0.07	1.76
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	10	1.79	0.07	1.76
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	10	1.79	0.07	1.76
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	10	1.78	1.19	1.12
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	10	1.78	1.19	1.12
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	10	1.78	1.19	1.12
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	10	1.77	0.6	1.58
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	10	1.77	0.6	1.58
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	10	1.77	0.6	1.58
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	10	1.76	0.09	1.74
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	10	1.76	0.09	1.74
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	10	1.76	0.09	1.74
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	10	1.76	0.09	1.74
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	10	1.76	0.09	1.74
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	10	1.76	0.09	1.74
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	10	1.7	0.32	1.54
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	10	1.7	0.32	1.54
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	10	1.7	0.32	1.54
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	10	1.7	0.32	1.54
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	10	1.7	0.32	1.54
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	10	1.7	0.32	1.54
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	10	1.68	0.38	1.85
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	10	1.68	0.38	1.85
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	10	1.68	0.38	1.85
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	10	1.66	0.1	1.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	10	1.66	0.1	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	10	1.66	0.1	1.69
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	10	1.58	0.8	2.04
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	10	1.57	0.14	1.48
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	10	1.57	0.14	1.48
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	10	1.57	0.14	1.48
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	10	1.57	0.14	1.48
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	10	1.57	0.14	1.48
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	10	1.57	0.14	1.48
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	10	1.53	0.5	1.75
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	10	1.53	0.5	1.75
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	10	1.53	0.5	1.75
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	10	1.52	0.25	1.5
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	10	1.52	0.25	1.5
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	10	1.52	0.25	1.5
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	10	1.52	0.25	1.5
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	10	1.52	0.25	1.5
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	10	1.52	0.25	1.5
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	10	1.51	0.2	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	10	1.51	0.2	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	10	1.51	0.2	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	10	1.51	0.2	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	10	1.51	0.2	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	10	1.51	0.2	1.42
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	10	1.5	0.68	1.29
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	10	1.5	0.68	1.29
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	10	1.5	0.68	1.29
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	10	1.5	0.61	1.58
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	10	1.44	0.12	1.41
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	10	1.36	0.04	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	10	1.36	0.04	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	10	1.36	0.04	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	10	1.36	0.04	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	10	1.36	0.04	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	10	1.36	0.04	1.37
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	10	1.32	0.48	1.53
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	10	1.32	0.48	1.53
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	10	1.32	0.48	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	10	1.32	0.48	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	10	1.32	0.48	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	10	1.32	0.48	1.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	10	1.32	0.48	1.53
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	10	1.32	0.48	1.53
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	10	1.32	0.48	1.53
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	10	1.28	0.67	0.92
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	10	1.26	0.64	1.3
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	10	1.26	0.64	1.3
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	10	1.26	0.64	1.3
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	10	1.24	0.48	1.22
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	10	1.24	0.48	1.22
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	10	1.2	0.47	1.42
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	10	1.17	0.35	1.35
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	10	1.17	0.35	1.35
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	10	1.17	0.35	1.35
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	10	1.13	0.46	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	10	1.13	0.46	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	10	1.13	0.46	1.43
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	10	1.11	0.31	1.14
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	10	1.11	0.31	1.14
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	10	1.11	0.31	1.14
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	10	1.11	0.31	1.14
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	10	1.11	0.31	1.14
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	10	1.11	0.31	1.14
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	10	1.05	0.08	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	10	1.05	0.08	1.1
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	10	1.05	0.25	1.08
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	10	1.05	0.25	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	10	1.05	0.25	1.08
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	10	1.05	0.25	1.08
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	10	1.05	0.25	1.08
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	10	1.05	0.25	1.08
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	10	1.01	0.51	0.94
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	10	1.01	0.51	0.94
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	10	0.99	0.1	1.04
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	10	0.99	0.1	1.04
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	10	0.99	0.1	1.04
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	10	0.99	0.1	1.04
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	10	0.99	0.1	1.04
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	10	0.99	0.1	1.04
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	10	0.98	0.46	0.83
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	10	0.97	0.38	0.79
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	10	0.97	0.38	0.79
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	10	0.96	0.91	0.34
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	10	0.96	0.91	0.34
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	10	0.96	0.91	0.34
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	10	0.96	0.91	0.34
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	10	0.96	0.91	0.34
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	10	0.96	0.91	0.34
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	10	0.96	0.91	0.34
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	10	0.96	0.91	0.34
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	10	0.96	0.91	0.34
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	10	0.96	0.5	0.62
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	10	0.96	0.05	0.96
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	10	0.96	0.05	0.96
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	10	0.96	0.05	0.96
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	10	0.94	0.55	0.96
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	10	0.93	0.49	0.67
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	10	0.93	0.23	0.86
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	10	0.88	0.31	0.78
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	10	0.84	0.29	1.0
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	10	0.84	0.29	1.0
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	10	0.84	0.29	1.0
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	10	0.84	0.29	1.0
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	10	0.84	0.29	1.0
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	10	0.84	0.29	1.0
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	10	0.82	0.07	0.86
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	10	0.82	0.07	0.86
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	10	0.82	0.07	0.86
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	10	0.82	0.07	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	10	0.82	0.07	0.86
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	10	0.82	0.07	0.86
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	10	0.81	0.05	0.78
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	10	0.76	0.59	0.42
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	10	0.76	0.59	0.42
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	10	0.76	0.59	0.42
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	10	0.74	0.31	0.62
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	10	0.74	0.31	0.62
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	10	0.74	0.31	0.62
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	10	0.71	0.19	0.66
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	10	0.71	0.19	0.66
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	10	0.7	0.76	0.22
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	10	0.7	0.76	0.22
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	10	0.7	0.76	0.22
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	10	0.66	0.23	0.52
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	10	0.66	0.23	0.52
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	10	0.66	0.23	0.52
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	10	0.63	0.08	0.61
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	10	0.63	0.08	0.61
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	10	0.61	0.31	0.44
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	10	0.61	0.31	0.44
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	10	0.6	0.02	0.6
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	10	0.6	0.02	0.6
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	10	0.6	0.02	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	10	0.6	0.02	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	10	0.6	0.02	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	10	0.6	0.02	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	10	0.6	0.02	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	10	0.6	0.02	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	10	0.6	0.02	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	10	0.6	0.02	0.6
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	10	0.46	0.04	0.46
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	10	0.46	0.04	0.46
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	10	0.46	0.04	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	10	0.44	0.04	0.44
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	10	0.44	0.04	0.44
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	10	0.39	0.21	0.4
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	10	0.37	0.18	0.25
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	10	0.36	0.07	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	10	0.36	0.07	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	10	0.36	0.07	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	10	0.36	0.07	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	10	0.36	0.07	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	10	0.36	0.07	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	10	0.34	0.05	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	10	0.34	0.05	0.33
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	10	0.34	0.04	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	10	0.34	0.04	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	10	0.34	0.04	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	10	0.34	0.04	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	10	0.34	0.04	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	10	0.34	0.04	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	10	0.34	0.04	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	10	0.34	0.04	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	10	0.34	0.04	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	10	0.34	0.09	0.34
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	10	0.34	0.09	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	10	0.34	0.09	0.34
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	10	0.29	0.04	0.29
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	10	0.28	0.13	0.2
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	10	0.28	0.13	0.2
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	10	0.28	0.13	0.2
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	10	0.28	0.13	0.2
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	10	0.28	0.13	0.2
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	10	0.28	0.13	0.2
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	10	0.28	0.13	0.2
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	10	0.28	0.13	0.2
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	10	0.28	0.13	0.2
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	10	0.23	0.1	0.2
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	10	0.23	0.1	0.2
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	10	0.23	0.1	0.2
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	9	2.28	0.76	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	9	2.28	0.76	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	9	2.28	0.76	2.57
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	9	1.85	0.62	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	9	1.85	0.62	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	9	1.85	0.62	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	9	1.85	0.62	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	9	1.85	0.62	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	9	1.85	0.62	2.13
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	9	1.62	0.7	1.97
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	9	1.51	0.55	1.63
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	9	1.51	0.55	1.63
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	9	1.51	0.55	1.63
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	9	1.51	0.55	1.63
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	9	1.51	0.55	1.63
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	9	1.51	0.55	1.63
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	9	1.35	0.65	1.15
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	9	0.87	0.21	0.8
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	9	0.87	0.21	0.8
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	9	0.55	0.25	0.64
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	9	0.55	0.25	0.64
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	9	0.55	0.25	0.64
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	9	0.46	0.22	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	9	0.46	0.22	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	9	0.46	0.22	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	9	0.46	0.22	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	9	0.46	0.22	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	9	0.46	0.22	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	9	0.39	0.17	0.39
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	9	0.39	0.17	0.39
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	9	0.39	0.17	0.39
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	8	0.7	0.2	0.6
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	8	0.7	0.2	0.6
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	8	0.7	0.2	0.6
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	8	0.7	0.2	0.6
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	8	0.7	0.2	0.6
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	8	0.7	0.2	0.6
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	8	0.7	0.2	0.6
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	8	0.7	0.2	0.6
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	8	0.7	0.2	0.6
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	8	0.54	0.33	0.6
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	8	0.54	0.33	0.6
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	8	0.54	0.33	0.6
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	8	0.54	0.33	0.6
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	8	0.54	0.33	0.6
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	8	0.54	0.33	0.6
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	8	0.29	0.1	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	8	0.29	0.1	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	8	0.29	0.1	0.34
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	8	0.23	0.07	0.24
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	8	0.19	0.08	0.16
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	8	0.16	0.03	0.16
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	8	0.16	0.03	0.16
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	8	0.16	0.03	0.16
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	8	0.16	0.03	0.16
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	8	0.16	0.03	0.16
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	8	0.16	0.03	0.16
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	8	0.16	0.03	0.16
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	8	0.16	0.03	0.16
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	8	0.16	0.03	0.16
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	8	0.15	0.02	0.16
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	8	0.15	0.02	0.16
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	8	0.15	0.02	0.16
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG21	7	0.32	0.14	0.25
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG22	7	0.32	0.14	0.25
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG23	7	0.32	0.14	0.25
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD21	7	0.29	0.02	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD22	7	0.29	0.02	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD23	7	0.29	0.02	0.3
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD11	7	0.24	0.01	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD12	7	0.24	0.01	0.24
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD13	7	0.24	0.01	0.24
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE1	6	0.13	0.02	0.12
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE2	6	0.13	0.02	0.12
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE3	6	0.13	0.02	0.12
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE1	6	0.13	0.02	0.12
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE2	6	0.13	0.02	0.12
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE3	6	0.13	0.02	0.12
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE1	6	0.13	0.02	0.12
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE2	6	0.13	0.02	0.12
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE3	6	0.13	0.02	0.12
(1,9)	1:38:A:ILE:H	1:41:A:PHE:O	5	0.43	0.15	0.49
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	5	0.38	0.16	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	5	0.38	0.16	0.46
(3,65)	1:38:A:ILE:HG21	1:174:A:HIS:H	4	0.48	0.38	0.48
(3,65)	1:38:A:ILE:HG22	1:174:A:HIS:H	4	0.48	0.38	0.48
(3,65)	1:38:A:ILE:HG23	1:174:A:HIS:H	4	0.48	0.38	0.48
(1,22)	1:38:A:ILE:O	1:41:A:PHE:N	4	0.32	0.01	0.32
(1,10)	1:38:A:ILE:N	1:41:A:PHE:O	4	0.29	0.05	0.3
(3,97)	1:43:A:ILE:HG21	1:165:A:ARG:H	4	0.17	0.04	0.17
(3,97)	1:43:A:ILE:HG22	1:165:A:ARG:H	4	0.17	0.04	0.17
(3,97)	1:43:A:ILE:HG23	1:165:A:ARG:H	4	0.17	0.04	0.17
(1,7)	1:36:A:HIS:O	1:43:A:ILE:H	4	0.15	0.01	0.15
(3,165)	1:34:A:LEU:HD11	1:35:A:THR:H	3	1.45	0.17	1.42
(3,165)	1:34:A:LEU:HD12	1:35:A:THR:H	3	1.45	0.17	1.42
(3,165)	1:34:A:LEU:HD13	1:35:A:THR:H	3	1.45	0.17	1.42
(3,165)	1:34:A:LEU:HD21	1:35:A:THR:H	3	1.45	0.17	1.42
(3,165)	1:34:A:LEU:HD22	1:35:A:THR:H	3	1.45	0.17	1.42
(3,165)	1:34:A:LEU:HD23	1:35:A:THR:H	3	1.45	0.17	1.42
(3,74)	1:40:A:GLY:H	1:41:A:PHE:HD1	3	0.17	0.02	0.18
(3,74)	1:40:A:GLY:H	1:41:A:PHE:HD2	3	0.17	0.02	0.18
(3,68)	1:38:A:ILE:HG21	1:178:A:PHE:H	2	0.7	0.0	0.7

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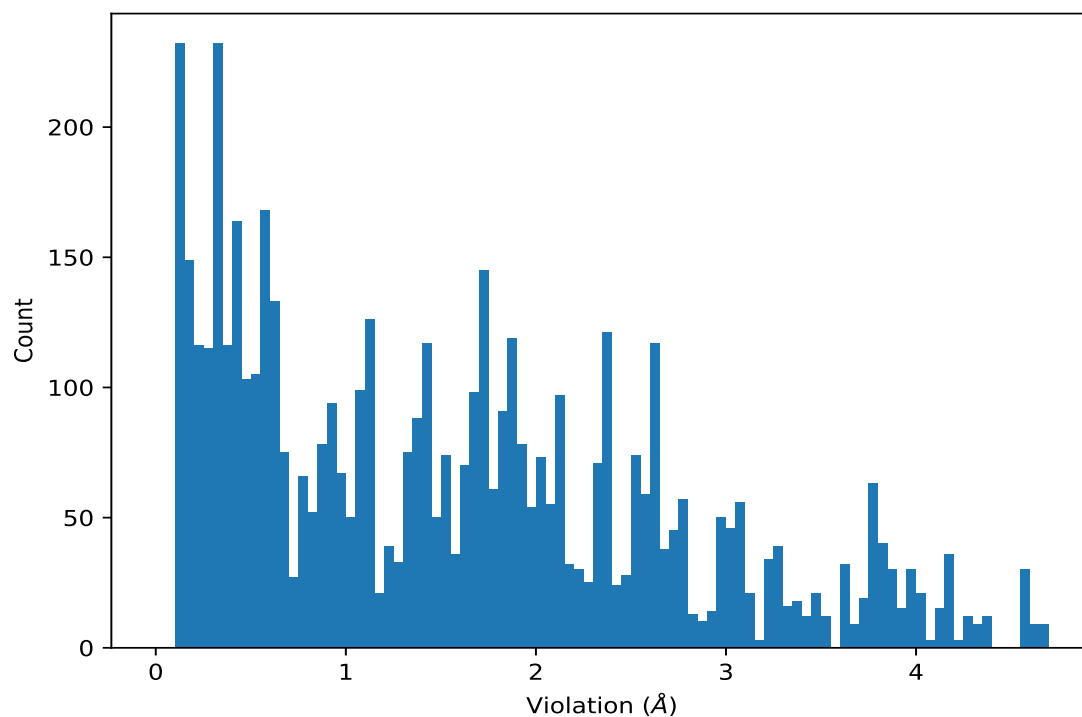
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,68)	1:38:A:ILE:HG22	1:178:A:PHE:H	2	0.7	0.0	0.7
(3,68)	1:38:A:ILE:HG23	1:178:A:PHE:H	2	0.7	0.0	0.7
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD11	2	0.62	0.01	0.62
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD12	2	0.62	0.01	0.62
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD13	2	0.62	0.01	0.62
(1,18)	1:34:A:LEU:O	1:45:A:GLU:N	2	0.24	0.08	0.24
(1,13)	1:46:A:GLY:H	1:163:A:TYR:O	2	0.16	0.01	0.16
(1,15)	1:46:A:GLY:H	1:163:A:TYR:O	2	0.16	0.01	0.16
(3,7)	1:32:A:GLN:HA	1:33:A:ILE:H	2	0.14	0.02	0.14
(1,14)	1:46:A:GLY:N	1:163:A:TYR:O	2	0.11	0.01	0.11
(1,16)	1:46:A:GLY:N	1:163:A:TYR:O	2	0.11	0.01	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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	7	4.69
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	7	4.69
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	7	4.69
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	7	4.69
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	7	4.69
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	7	4.69
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	7	4.69
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	7	4.69
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	7	4.69
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	10	4.62
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	10	4.62
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	10	4.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	10	4.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	10	4.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	10	4.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	10	4.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	10	4.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	10	4.62
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	6	4.57
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	6	4.57
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	6	4.57
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	2	4.57
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	2	4.57
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	2	4.57
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	2	4.57
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	2	4.57
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	2	4.57
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	3	4.57
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	3	4.57
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	3	4.57
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	3	4.57
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	3	4.57
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	3	4.57
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	5	4.57
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	5	4.57
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	5	4.57
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	5	4.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	5	4.57
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	5	4.57
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	4	4.56
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	4	4.56
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	4	4.56
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	4	4.56
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	4	4.56
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	4	4.56
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	9	4.55
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	9	4.55
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	9	4.55
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	1	4.36
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	1	4.36
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	1	4.36
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	1	4.36
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	1	4.36
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	1	4.36
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	1	4.36
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	1	4.36
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	1	4.36
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	3	4.36
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	3	4.36
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	3	4.36
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	6	4.32
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	6	4.32
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	6	4.32
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	9	4.31
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	9	4.31
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	9	4.31
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	2	4.3
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	2	4.3
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	2	4.3
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	8	4.29
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	8	4.29
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	8	4.29
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	8	4.29
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	8	4.29
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	8	4.29
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	8	4.29
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	8	4.29
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	8	4.29
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	4	4.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	4	4.27
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	4	4.27
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	4	4.21
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	4	4.21
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	4	4.21
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	2	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	2	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	2	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	2	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	2	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	2	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	2	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	2	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	2	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	3	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	3	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	3	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	3	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	3	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	3	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	3	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	3	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	3	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	4	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	4	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	4	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	4	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	4	4.17
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	4	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	4	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	4	4.17
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	4	4.17
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	5	4.15
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	5	4.15
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	5	4.15
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	5	4.15
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	5	4.15
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	5	4.15
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	5	4.15
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	5	4.15
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	5	4.15
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	6	4.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	6	4.14
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	6	4.14
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	9	4.14
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	9	4.14
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	9	4.14
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	9	4.13
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	9	4.13
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	9	4.13
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	10	4.11
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	10	4.11
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	10	4.11
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	6	4.11
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	6	4.11
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	6	4.11
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	5	4.09
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	5	4.09
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	5	4.09
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	10	4.03
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	10	4.03
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	10	4.03
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	10	4.03
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	10	4.03
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	10	4.03
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	10	4.03
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	10	4.03
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	10	4.03
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	1	4.03
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	1	4.03
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	1	4.03
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	7	4.0
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	7	4.0
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	7	4.0
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	7	4.0
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	7	4.0
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	7	4.0
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	6	4.0
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	6	4.0
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	6	4.0
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	7	3.99
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	7	3.99
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	7	3.99
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	9	3.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	9	3.99
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	9	3.99
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	6	3.97
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	6	3.97
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	6	3.97
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	8	3.97
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	8	3.97
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	8	3.97
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	4	3.96
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	4	3.96
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	4	3.96
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	1	3.95
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	1	3.95
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	1	3.95
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	9	3.95
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	9	3.95
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	9	3.95
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	7	3.95
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	7	3.95
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	7	3.95
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	1	3.95
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	1	3.95
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	1	3.95
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	10	3.95
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	10	3.95
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	10	3.95
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	3	3.93
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	3	3.93
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	3	3.93
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	5	3.93
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	5	3.93
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	5	3.93
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	8	3.92
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	8	3.92
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	8	3.92
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	1	3.91
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	1	3.91
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	1	3.91
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	8	3.91
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	8	3.91
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	8	3.91
(3,237)	1:43:A:ILE:HG21	1:170:A:MET:HA	2	3.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,237)	1:43:A:ILE:HG22	1:170:A:MET:HA	2	3.9
(3,237)	1:43:A:ILE:HG23	1:170:A:MET:HA	2	3.9
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	7	3.89
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	7	3.89
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	4	3.88
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	4	3.88
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	4	3.88
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	8	3.88
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	8	3.88
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	8	3.88
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	1	3.88
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	1	3.88
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	1	3.86
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	1	3.86
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	1	3.86
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	2	3.86
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	2	3.86
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	2	3.86
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	5	3.86
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	5	3.86
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	5	3.86
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	7	3.86
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	7	3.86
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	7	3.86
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	8	3.85
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	8	3.85
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	8	3.85
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	8	3.85
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	8	3.85
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	3	3.84
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	3	3.84
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	3	3.84
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	8	3.84
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	8	3.84
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	8	3.84
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	8	3.84
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	8	3.84
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	8	3.84
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	7	3.83
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	7	3.83
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	7	3.83
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	10	3.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	10	3.83
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	10	3.83
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	7	3.83
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	7	3.82
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	7	3.82
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	7	3.82
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	10	3.82
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	10	3.82
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	10	3.82
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	3	3.82
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	3	3.82
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	3	3.82
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	5	3.82
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	5	3.82
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	5	3.82
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	7	3.81
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	7	3.81
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	2	3.81
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	2	3.81
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	2	3.81
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	3	3.81
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	3	3.81
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	3	3.81
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	2	3.81
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	2	3.81
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	2	3.81
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	8	3.81
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	4	3.8
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	4	3.8
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	4	3.8
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	5	3.8
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	5	3.8
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	5	3.8
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	10	3.8
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	10	3.8
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	10	3.8
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	1	3.8
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	1	3.8
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	1	3.8
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	1	3.8
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	1	3.8
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	1	3.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	4	3.8
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	4	3.8
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	4	3.8
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	9	3.8
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	9	3.8
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	9	3.8
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	2	3.8
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	2	3.8
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	2	3.8
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	6	3.79
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	6	3.79
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	6	3.79
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	2	3.79
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	2	3.79
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	2	3.79
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	4	3.79
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	4	3.79
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	4	3.79
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG21	6	3.79
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG22	6	3.79
(3,173)	1:36:A:HIS:H	1:38:A:ILE:HG23	6	3.79
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	9	3.78
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	9	3.78
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	9	3.78
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	5	3.78
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	5	3.78
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	5	3.78
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	6	3.78
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	6	3.78
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	6	3.78
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	1	3.78
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	3	3.77
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	3	3.77
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	3	3.77
(3,231)	1:43:A:ILE:HD11	1:165:A:ARG:H	9	3.77
(3,231)	1:43:A:ILE:HD12	1:165:A:ARG:H	9	3.77
(3,231)	1:43:A:ILE:HD13	1:165:A:ARG:H	9	3.77
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	5	3.77
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	5	3.77
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	5	3.77
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	7	3.76
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	7	3.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	7	3.76
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	10	3.75
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	10	3.75
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	8	3.75
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	8	3.75
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	8	3.75
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	5	3.74
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	5	3.74
(3,200)	1:38:A:ILE:HG21	1:174:A:HIS:H	1	3.74
(3,200)	1:38:A:ILE:HG22	1:174:A:HIS:H	1	3.74
(3,200)	1:38:A:ILE:HG23	1:174:A:HIS:H	1	3.74
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	3	3.73
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	3	3.73
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	3	3.73
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	9	3.72
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	9	3.72
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	9	3.72
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	2	3.72
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	2	3.72
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	2	3.72
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	9	3.71
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	9	3.71
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	3	3.7
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	3	3.7
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	3	3.7
(3,232)	1:43:A:ILE:HG21	1:165:A:ARG:H	6	3.69
(3,232)	1:43:A:ILE:HG22	1:165:A:ARG:H	6	3.69
(3,232)	1:43:A:ILE:HG23	1:165:A:ARG:H	6	3.69
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	10	3.68
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	10	3.68
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	10	3.68
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	8	3.68
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	8	3.68
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	8	3.68
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	3	3.65
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	3	3.65
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	3	3.65
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	9	3.64
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	2	3.62
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	2	3.62
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	2	3.62
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	4	3.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	4	3.62
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	4	3.62
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	6	3.62
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	6	3.62
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	6	3.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	6	3.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	6	3.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	6	3.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	6	3.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	6	3.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	6	3.62
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	9	3.62
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	9	3.62
(3,206)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	9	3.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	9	3.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	9	3.62
(3,206)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	9	3.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	9	3.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	9	3.62
(3,206)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	9	3.62
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	6	3.62
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	5	3.6
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	5	3.6
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	5	3.6
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	10	3.53
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	10	3.53
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	10	3.53
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	1	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	1	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	1	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	7	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	7	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	7	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	8	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	8	3.5
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	8	3.5
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	5	3.49
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	9	3.49
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	5	3.49
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	5	3.49
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	5	3.49
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	7	3.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	5	3.48
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	5	3.48
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	5	3.48
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	6	3.47
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	6	3.47
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	6	3.47
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	10	3.47
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	2	3.46
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	2	3.46
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	9	3.46
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	9	3.46
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	9	3.46
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	9	3.45
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	9	3.45
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	9	3.45
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	2	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	2	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	2	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	3	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	3	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	3	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	4	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	4	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	4	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	6	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	6	3.44
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	6	3.44
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	10	3.4
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	10	3.4
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	7	3.39
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	7	3.39
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	7	3.39
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	9	3.39
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	9	3.39
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	9	3.39
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	9	3.39
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	9	3.39
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	6	3.36
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	6	3.36
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	7	3.35
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	7	3.35
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	7	3.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	7	3.35
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	7	3.35
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	7	3.35
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	10	3.34
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	10	3.34
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	10	3.34
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	10	3.34
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	10	3.34
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	10	3.34
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	2	3.33
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	2	3.33
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	2	3.32
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	10	3.31
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	10	3.31
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	2	3.31
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	2	3.31
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	3	3.31
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	3	3.31
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	3	3.31
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	3	3.3
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	3	3.3
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	3	3.3
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	8	3.3
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	8	3.3
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	8	3.3
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	1	3.3
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	1	3.3
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	1	3.3
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	5	3.3
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	5	3.29
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	5	3.29
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	8	3.29
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	8	3.29
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	8	3.29
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	3	3.29
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	3	3.29
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	3	3.29
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	5	3.29
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	1	3.28
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	1	3.28
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	1	3.28
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD1	4	3.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,209)	1:40:A:GLY:H	1:41:A:PHE:HD2	4	3.28
(3,183)	1:37:A:VAL:HA	1:41:A:PHE:H	4	3.28
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	4	3.28
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	4	3.28
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	4	3.28
(3,193)	1:38:A:ILE:HD11	1:41:A:PHE:H	7	3.26
(3,193)	1:38:A:ILE:HD12	1:41:A:PHE:H	7	3.26
(3,193)	1:38:A:ILE:HD13	1:41:A:PHE:H	7	3.26
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	2	3.26
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	2	3.26
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	2	3.26
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD11	5	3.26
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD12	5	3.26
(3,177)	1:37:A:VAL:HA	1:38:A:ILE:HD13	5	3.26
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	3	3.25
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	3	3.25
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	10	3.24
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	10	3.24
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	10	3.24
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	1	3.23
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	1	3.23
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	1	3.23
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	1	3.23
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	1	3.23
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	1	3.23
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	1	3.23
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	1	3.23
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	1	3.23
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	5	3.23
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	5	3.23
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	8	3.22
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	8	3.22
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	8	3.22
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	7	3.21
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	7	3.21
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	8	3.21
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	8	3.21
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	8	3.21
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	8	3.21
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	8	3.21
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	8	3.21
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	4	3.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	4	3.21
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	4	3.21
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	10	3.2
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	10	3.2
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	10	3.2
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	8	3.2
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	8	3.2
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	8	3.2
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	2	3.16
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	2	3.16
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	2	3.16
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	9	3.15
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	9	3.15
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	9	3.15
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	9	3.15
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	9	3.15
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	9	3.15
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	4	3.15
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	4	3.15
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	4	3.15
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	7	3.15
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE1	7	3.13
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE2	7	3.13
(3,236)	1:43:A:ILE:HA	1:170:A:MET:HE3	7	3.13
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	6	3.12
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	6	3.12
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	6	3.12
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	6	3.12
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	6	3.12
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	6	3.12
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	6	3.11
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	6	3.11
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	5	3.09
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	5	3.09
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	5	3.09
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	5	3.09
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	5	3.09
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	5	3.09
(3,222)	1:43:A:ILE:HD11	1:45:A:GLU:H	5	3.09
(3,222)	1:43:A:ILE:HD12	1:45:A:GLU:H	5	3.09
(3,222)	1:43:A:ILE:HD13	1:45:A:GLU:H	5	3.09
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	6	3.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	6	3.09
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	6	3.09
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	9	3.09
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	9	3.09
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	9	3.09
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	6	3.09
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	10	3.09
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	10	3.09
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	10	3.09
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	2	3.08
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	7	3.08
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	8	3.08
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	9	3.08
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	8	3.08
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	8	3.08
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	8	3.08
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	2	3.07
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	2	3.07
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	2	3.07
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	3	3.07
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	3	3.07
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	3	3.07
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	2	3.07
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	2	3.07
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	2	3.07
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	3	3.07
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	3	3.07
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	3	3.07
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	10	3.07
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	10	3.07
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	10	3.07
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	10	3.07
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	1	3.07
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	1	3.07
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	1	3.07
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD21	4	3.06
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD22	4	3.06
(3,229)	1:43:A:ILE:HA	1:164:A:LEU:HD23	4	3.06
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD21	4	3.06
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD22	4	3.06
(3,225)	1:43:A:ILE:HA	1:164:A:LEU:HD23	4	3.06
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	1	3.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	5	3.06
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	1	3.06
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	1	3.06
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	1	3.06
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	9	3.05
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	9	3.05
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	1	3.05
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	1	3.05
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	1	3.05
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	2	3.04
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	2	3.04
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	2	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	2	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	2	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	2	3.04
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	3	3.04
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	3	3.04
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	3	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	3	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	3	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	3	3.04
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	5	3.04
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	5	3.04
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	5	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	5	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	5	3.04
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	5	3.04
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	3	3.04
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	7	3.03
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	7	3.03
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	7	3.03
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	4	3.02
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	4	3.02
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	4	3.02
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	4	3.02
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	4	3.02
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	4	3.02
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	2	3.02
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	2	3.02
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	2	3.02
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	3	3.02
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	3	3.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	3	3.02
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	4	3.02
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	4	3.02
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	4	3.02
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	10	3.02
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	10	3.02
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	10	3.02
(3,164)	1:34:A:LEU:H	1:35:A:THR:HA	4	3.0
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	9	2.99
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	9	2.99
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	9	2.99
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	9	2.99
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	9	2.99
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	9	2.99
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	4	2.99
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	4	2.99
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	6	2.99
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	6	2.99
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	6	2.99
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	9	2.99
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	9	2.99
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	9	2.99
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	6	2.98
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	6	2.98
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	6	2.98
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	6	2.98
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	6	2.98
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	6	2.98
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	5	2.98
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	5	2.98
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	5	2.98
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	3	2.97
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	3	2.97
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	3	2.97
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	2	2.96
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	2	2.96
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	2	2.96
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	4	2.96
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	4	2.96
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	4	2.96
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	5	2.96
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	5	2.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	5	2.96
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	6	2.96
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	6	2.96
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	6	2.96
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	1	2.95
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	1	2.95
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	1	2.95
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	6	2.95
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	6	2.95
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	6	2.95
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	9	2.95
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	9	2.95
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	9	2.95
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	7	2.95
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	7	2.95
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	7	2.95
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	1	2.93
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	1	2.93
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	4	2.93
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	4	2.93
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	4	2.93
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	5	2.92
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	5	2.92
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	5	2.92
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG21	5	2.92
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG22	5	2.92
(3,139)	1:32:A:GLN:HA	1:33:A:ILE:HG23	5	2.92
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	7	2.92
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	7	2.92
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	7	2.92
(3,201)	1:38:A:ILE:HD11	1:174:A:HIS:H	8	2.88
(3,201)	1:38:A:ILE:HD12	1:174:A:HIS:H	8	2.88
(3,201)	1:38:A:ILE:HD13	1:174:A:HIS:H	8	2.88
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	4	2.87
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	4	2.87
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	5	2.86
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	5	2.86
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	10	2.86
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	10	2.86
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	10	2.86
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	2	2.83
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	7	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	7	2.83
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	7	2.83
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	7	2.83
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	7	2.83
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	7	2.83
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	8	2.82
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	8	2.82
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	7	2.82
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	7	2.82
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	7	2.82
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	8	2.81
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	1	2.8
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	1	2.8
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	1	2.8
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	7	2.8
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	7	2.8
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	7	2.8
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	1	2.8
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	2	2.8
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	2	2.8
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	2	2.8
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	2	2.79
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	4	2.79
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	5	2.79
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	10	2.78
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	8	2.78
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	6	2.78
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	9	2.78
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	10	2.78
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	10	2.78
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	10	2.78
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	1	2.78
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	1	2.78
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	1	2.78
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	1	2.78
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	1	2.78
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	1	2.78
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	8	2.78
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	8	2.78
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	8	2.78
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	8	2.78
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	8	2.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	8	2.78
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	9	2.77
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	9	2.77
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	2	2.77
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	3	2.77
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	4	2.77
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	5	2.77
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	1	2.76
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	7	2.76
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	8	2.76
(3,207)	1:39:A:GLU:H	1:40:A:GLY:H	10	2.76
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	9	2.76
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	9	2.76
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	9	2.76
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	9	2.76
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	9	2.76
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	9	2.76
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	6	2.75
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	6	2.75
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	6	2.75
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	6	2.75
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	6	2.75
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	6	2.75
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	3	2.75
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	3	2.75
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	3	2.75
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	4	2.74
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	4	2.74
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	7	2.74
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	10	2.74
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	10	2.74
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	10	2.74
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	10	2.74
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	8	2.73
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	8	2.73
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	10	2.73
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	5	2.73
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	8	2.73
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	8	2.73
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	8	2.73
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	10	2.73
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	10	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	10	2.73
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	10	2.73
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	10	2.73
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	10	2.73
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	6	2.73
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	6	2.72
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	6	2.72
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	2	2.72
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	3	2.72
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	4	2.72
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	5	2.72
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	6	2.72
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	9	2.72
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	9	2.72
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	7	2.71
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	3	2.71
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	3	2.71
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	3	2.71
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	3	2.71
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	3	2.71
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	3	2.71
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	3	2.7
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	3	2.7
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	7	2.7
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	7	2.7
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	7	2.7
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	1	2.7
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	8	2.7
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	3	2.7
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	4	2.69
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	4	2.69
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	4	2.69
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	4	2.69
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	4	2.69
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	4	2.69
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	7	2.69
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	8	2.69
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	4	2.69
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	8	2.69
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	8	2.69
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	8	2.69
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	8	2.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	1	2.68
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	10	2.68
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	10	2.68
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	10	2.68
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	3	2.68
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	10	2.68
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	10	2.68
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	1	2.68
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	4	2.68
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	6	2.68
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	7	2.68
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	9	2.68
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	10	2.68
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	3	2.67
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	7	2.66
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	10	2.66
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	8	2.66
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	2	2.66
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	8	2.66
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	6	2.66
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	8	2.66
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	9	2.66
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	9	2.66
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	9	2.66
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	2	2.66
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	5	2.65
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	2	2.65
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	3	2.65
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	4	2.65
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	9	2.65
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	9	2.65
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	9	2.65
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	9	2.65
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	9	2.65
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	9	2.65
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	1	2.65
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	1	2.65
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	7	2.65
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	9	2.65
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	1	2.65
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	1	2.65
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	1	2.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	3	2.65
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	3	2.65
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	3	2.65
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	6	2.65
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	6	2.65
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	6	2.65
(3,152)	1:33:A:ILE:H	1:34:A:LEU:H	3	2.65
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	5	2.64
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	5	2.64
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	6	2.64
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	6	2.64
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	6	2.64
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	6	2.64
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	6	2.64
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	6	2.64
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	9	2.64
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	1	2.64
(3,170)	1:35:A:THR:H	1:36:A:HIS:H	7	2.64
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	9	2.63
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	2	2.63
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	2	2.63
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	9	2.63
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	6	2.63
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	6	2.63
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	10	2.63
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	4	2.62
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	6	2.62
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	6	2.62
(3,215)	1:42:A:VAL:H	1:43:A:ILE:H	9	2.62
(3,191)	1:38:A:ILE:H	1:39:A:GLU:H	9	2.62
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	5	2.62
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	5	2.62
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	5	2.62
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	5	2.62
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	5	2.62
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	5	2.62
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	2	2.62
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	3	2.62
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	4	2.62
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	2	2.62
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	2	2.62
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	2	2.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	10	2.62
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	10	2.62
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	10	2.62
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	1	2.61
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	10	2.61
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	8	2.61
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	8	2.61
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	8	2.61
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	8	2.61
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	8	2.61
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	8	2.61
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	10	2.61
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	10	2.61
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	10	2.61
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	10	2.61
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	10	2.61
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	10	2.61
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	1	2.61
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	6	2.61
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	9	2.61
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	8	2.61
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	8	2.61
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	8	2.61
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	10	2.61
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	10	2.61
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	10	2.61
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	2	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	2	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	2	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	2	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	2	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	2	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	7	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	7	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	7	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	7	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	7	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	7	2.6
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	8	2.6
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	1	2.6
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	1	2.6
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	4	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	4	2.6
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	4	2.6
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	4	2.6
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	4	2.6
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	4	2.6
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	7	2.6
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	2	2.6
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	5	2.6
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	7	2.6
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	4	2.6
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	5	2.6
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	7	2.6
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	8	2.6
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	3	2.6
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	3	2.6
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	3	2.6
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	6	2.59
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	6	2.59
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	6	2.59
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	6	2.59
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	6	2.59
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	6	2.59
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	2	2.59
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	3	2.59
(3,239)	1:45:A:GLU:H	1:46:A:GLY:H	7	2.59
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	8	2.59
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	8	2.59
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	1	2.59
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	5	2.59
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	8	2.59
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	2	2.59
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	3	2.59
(3,172)	1:36:A:HIS:H	1:37:A:VAL:H	10	2.59
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	2	2.59
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	2	2.59
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	2	2.59
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	8	2.59
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	8	2.59
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	8	2.59
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	6	2.58
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	8	2.58
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	8	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	8	2.58
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	8	2.58
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	8	2.58
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	8	2.58
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	3	2.58
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	4	2.58
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	1	2.58
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	1	2.58
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	1	2.58
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	4	2.58
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	2	2.57
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	10	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	1	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	1	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	1	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	6	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	6	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	6	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	9	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	9	2.57
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	9	2.57
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	6	2.57
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	9	2.57
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	10	2.56
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	10	2.56
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE1	8	2.56
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE2	8	2.56
(3,234)	1:43:A:ILE:H	1:170:A:MET:HE3	8	2.56
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	6	2.56
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	9	2.56
(3,179)	1:37:A:VAL:H	1:38:A:ILE:H	3	2.56
(3,163)	1:34:A:LEU:H	1:35:A:THR:H	5	2.56
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	1	2.56
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA2	1	2.55
(3,264)	1:59:A:VAL:H	1:60:A:GLY:HA3	1	2.55
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	10	2.55
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	8	2.55
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	8	2.55
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	8	2.55
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	8	2.55
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	8	2.55
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	8	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	1	2.54
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	1	2.54
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	7	2.54
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	7	2.54
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	6	2.54
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	6	2.54
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	6	2.54
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	6	2.54
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	6	2.54
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	6	2.54
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	7	2.54
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	7	2.54
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	7	2.54
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	7	2.54
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	7	2.54
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	7	2.54
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	9	2.54
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	9	2.54
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	9	2.54
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	9	2.54
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	9	2.54
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	9	2.54
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	6	2.53
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	6	2.53
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	1	2.53
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	1	2.53
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	1	2.53
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	1	2.53
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	1	2.53
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	1	2.53
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	2	2.53
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	2	2.53
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	2	2.53
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	2	2.53
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	2	2.53
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	2	2.53
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	3	2.53
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	3	2.53
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	3	2.53
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	2	2.53
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	2	2.53
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	2	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	2	2.53
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	2	2.53
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	2	2.53
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	4	2.53
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	8	2.53
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	1	2.52
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	1	2.52
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	1	2.52
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	1	2.52
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	1	2.52
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	1	2.52
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	3	2.52
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	1	2.51
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	3	2.51
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	3	2.51
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	3	2.51
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	3	2.51
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	3	2.51
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	3	2.51
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	2	2.51
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	2	2.51
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	2	2.51
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	10	2.5
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	1	2.49
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	8	2.49
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	4	2.49
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	4	2.49
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	4	2.49
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	9	2.48
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	5	2.48
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	5	2.48
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	5	2.48
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	1	2.47
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	1	2.47
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	1	2.47
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	10	2.47
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	2	2.47
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	7	2.46
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	1	2.46
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	1	2.46
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	1	2.46
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	1	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	1	2.46
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	1	2.46
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	8	2.46
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	8	2.46
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	8	2.46
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	5	2.45
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	8	2.45
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	8	2.45
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	8	2.45
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	3	2.43
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	3	2.43
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	7	2.43
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	8	2.43
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	7	2.43
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	7	2.43
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	7	2.43
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	7	2.43
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	7	2.43
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	7	2.43
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD11	4	2.43
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD12	4	2.43
(3,138)	1:32:A:GLN:HA	1:33:A:ILE:HD13	4	2.43
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	8	2.42
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	1	2.41
(3,181)	1:37:A:VAL:HG11	1:39:A:GLU:H	7	2.41
(3,181)	1:37:A:VAL:HG12	1:39:A:GLU:H	7	2.41
(3,181)	1:37:A:VAL:HG13	1:39:A:GLU:H	7	2.41
(3,181)	1:37:A:VAL:HG21	1:39:A:GLU:H	7	2.41
(3,181)	1:37:A:VAL:HG22	1:39:A:GLU:H	7	2.41
(3,181)	1:37:A:VAL:HG23	1:39:A:GLU:H	7	2.41
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	10	2.41
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	10	2.41
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	10	2.41
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	6	2.4
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	1	2.4
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	6	2.4
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	5	2.4
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	5	2.4
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	5	2.4
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	5	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	1	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	1	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	1	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	7	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	7	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	7	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	8	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	8	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	8	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	10	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	10	2.39
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	10	2.39
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	8	2.39
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	8	2.39
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	8	2.39
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	8	2.39
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	8	2.39
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	8	2.39
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	8	2.39
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	8	2.39
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	8	2.39
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	3	2.38
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	6	2.38
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	6	2.38
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	6	2.38
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	9	2.38
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	9	2.38
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	9	2.38
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	2	2.38
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	7	2.38
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	7	2.38
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	7	2.38
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	7	2.38
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	7	2.38
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	7	2.38
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	7	2.38
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	7	2.38
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	7	2.38
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	3	2.37
(3,211)	1:41:A:PHE:H	1:42:A:VAL:H	4	2.37
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	10	2.37
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	10	2.37
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	10	2.37
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	10	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	10	2.37
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	10	2.37
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	10	2.37
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	10	2.37
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	10	2.37
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	6	2.37
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	6	2.37
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	6	2.37
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	6	2.37
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	6	2.37
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	6	2.37
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	9	2.37
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	9	2.37
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	9	2.37
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	9	2.37
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	9	2.37
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	9	2.37
(3,166)	1:34:A:LEU:HG	1:45:A:GLU:H	2	2.37
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	4	2.37
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	4	2.37
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	4	2.37
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	2	2.37
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	2	2.37
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	2	2.37
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	8	2.36
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	3	2.36
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	3	2.36
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	3	2.36
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	7	2.36
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	7	2.36
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	7	2.36
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	8	2.36
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	8	2.36
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	8	2.36
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	8	2.36
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	8	2.36
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	8	2.36
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	4	2.36
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	4	2.36
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	4	2.36
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	4	2.36
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	4	2.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	5	2.36
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	5	2.36
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	5	2.36
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	1	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	1	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	1	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	2	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	2	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	2	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	4	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	4	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	4	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	5	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	5	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	5	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	8	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	8	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	8	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD11	10	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD12	10	2.35
(3,218)	1:43:A:ILE:HA	1:43:A:ILE:HD13	10	2.35
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	10	2.35
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	2	2.35
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	2	2.35
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	2	2.35
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	3	2.35
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	3	2.35
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	3	2.35
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	1	2.34
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	1	2.34
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	1	2.34
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	1	2.34
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	1	2.34
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	1	2.34
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	4	2.34
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	4	2.34
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	4	2.34
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	4	2.34
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	4	2.34
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	4	2.34
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	4	2.34
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	4	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	4	2.34
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	3	2.34
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	3	2.34
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	4	2.33
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	4	2.33
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	2	2.33
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	2	2.33
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	2	2.33
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	2	2.33
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	2	2.33
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	2	2.33
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	2	2.33
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	2	2.33
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	2	2.33
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	2	2.33
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	2	2.33
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	9	2.33
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	9	2.33
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	9	2.33
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	7	2.33
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	7	2.33
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	7	2.33
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	2	2.33
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	2	2.33
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	6	2.33
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	6	2.33
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	6	2.33
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	8	2.32
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	3	2.32
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	3	2.32
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	3	2.32
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	3	2.32
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	3	2.32
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	3	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	3	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	3	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	3	2.32
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	5	2.32
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	5	2.32
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	5	2.32
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	5	2.32
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	5	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	5	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	5	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	5	2.32
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	5	2.32
(3,190)	1:38:A:ILE:HD11	1:39:A:GLU:H	6	2.32
(3,190)	1:38:A:ILE:HD12	1:39:A:GLU:H	6	2.32
(3,190)	1:38:A:ILE:HD13	1:39:A:GLU:H	6	2.32
(3,175)	1:36:A:HIS:H	1:45:A:GLU:H	9	2.32
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	7	2.32
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	7	2.32
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	7	2.32
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	3	2.31
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	3	2.31
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	5	2.31
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	5	2.31
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	6	2.3
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	6	2.29
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	6	2.29
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	6	2.29
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	6	2.29
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	6	2.29
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	6	2.29
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB2	9	2.29
(3,199)	1:38:A:ILE:HG21	1:170:A:MET:HB3	9	2.29
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB2	9	2.29
(3,199)	1:38:A:ILE:HG22	1:170:A:MET:HB3	9	2.29
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB2	9	2.29
(3,199)	1:38:A:ILE:HG23	1:170:A:MET:HB3	9	2.29
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	4	2.28
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	4	2.28
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	4	2.28
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	1	2.27
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	1	2.27
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	1	2.27
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	7	2.27
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	7	2.27
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	7	2.27
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	4	2.25
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	4	2.25
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	4	2.25
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	7	2.22
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	7	2.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	7	2.22
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	7	2.22
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	7	2.22
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	7	2.22
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	8	2.22
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	8	2.22
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	8	2.22
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	8	2.22
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	8	2.22
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	8	2.22
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	8	2.22
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	8	2.22
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	8	2.22
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	5	2.22
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	5	2.22
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	5	2.22
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	1	2.22
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	1	2.22
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	9	2.22
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	9	2.22
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	9	2.22
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	10	2.21
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	10	2.21
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	10	2.21
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	10	2.21
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	10	2.21
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	10	2.21
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	6	2.2
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	8	2.19
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	1	2.19
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	1	2.19
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	1	2.19
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	1	2.19
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	1	2.19
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	1	2.19
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	1	2.19
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	1	2.19
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	1	2.19
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	8	2.18
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	8	2.18
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	8	2.18
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	2	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,242)	1:46:A:GLY:H	1:48:A:GLU:H	4	2.17
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	4	2.17
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	4	2.17
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	4	2.17
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	5	2.17
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	5	2.17
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	5	2.17
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	1	2.16
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	2	2.15
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	2	2.15
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	2	2.15
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	2	2.15
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	2	2.15
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	2	2.15
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	2	2.15
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	10	2.15
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	10	2.15
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	10	2.15
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	3	2.14
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	3	2.14
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	3	2.14
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	3	2.14
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	3	2.14
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	3	2.14
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	8	2.14
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	8	2.14
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	8	2.14
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	3	2.14
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	3	2.14
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	3	2.14
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	3	2.14
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	3	2.14
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	3	2.14
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	5	2.14
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	5	2.14
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	5	2.14
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	4	2.13
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	3	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	1	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	1	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	1	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	1	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	1	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	1	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	6	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	6	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	6	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	6	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	6	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	6	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	9	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	9	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	9	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	9	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	9	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	9	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	10	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	10	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	10	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	10	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	10	2.13
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	10	2.13
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	1	2.12
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	1	2.12
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	1	2.12
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	2	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	1	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	1	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	1	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	6	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	6	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	6	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	9	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	9	2.12
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	9	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	2	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	2	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	2	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	2	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	2	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	2	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	8	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	8	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	8	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	8	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	8	2.12
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	8	2.12
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	8	2.11
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	8	2.11
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	8	2.11
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	10	2.11
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	10	2.11
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	10	2.11
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	4	2.11
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	5	2.11
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	3	2.1
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	10	2.1
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	6	2.1
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	6	2.1
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	6	2.1
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	9	2.1
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	9	2.1
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	9	2.1
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	2	2.1
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	2	2.1
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	2	2.1
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	2	2.1
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	2	2.1
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	2	2.1
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	3	2.1
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	3	2.1
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	3	2.1
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	3	2.1
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	3	2.1
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	3	2.1
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	5	2.09
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	5	2.09
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	1	2.09
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	1	2.09
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	1	2.09
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	1	2.09
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	1	2.09
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	1	2.09
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	1	2.09
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	1	2.09
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	1	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	8	2.09
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	8	2.09
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	8	2.09
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	8	2.09
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	8	2.09
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	8	2.09
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	8	2.09
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	8	2.09
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	8	2.09
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	5	2.09
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	5	2.09
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	5	2.09
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	5	2.09
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	5	2.09
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	5	2.09
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	4	2.08
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	4	2.08
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD11	7	2.08
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD12	7	2.08
(3,219)	1:43:A:ILE:H	1:43:A:ILE:HD13	7	2.08
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	10	2.08
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	10	2.08
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	7	2.08
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	7	2.08
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	7	2.08
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	4	2.07
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	10	2.07
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	10	2.07
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	10	2.07
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	10	2.07
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	10	2.07
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	10	2.07
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	8	2.07
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	8	2.07
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	8	2.07
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	10	2.06
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	10	2.06
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	10	2.06
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	10	2.06
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	10	2.06
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	10	2.06
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	10	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	10	2.06
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	10	2.06
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	7	2.05
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	7	2.05
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	7	2.05
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	7	2.05
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	7	2.05
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	7	2.05
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	7	2.05
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	7	2.05
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	7	2.05
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	4	2.05
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	2	2.05
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	2	2.05
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	2	2.05
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	7	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	1	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	1	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	1	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	3	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	3	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	3	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	6	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	6	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	6	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	7	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	7	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	7	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	9	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	9	2.03
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	9	2.03
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	1	2.02
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	1	2.02
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	1	2.02
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	6	2.02
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	6	2.02
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	6	2.02
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	4	2.02
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	4	2.02
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	4	2.02
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	6	2.01
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	6	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	6	2.01
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	6	2.01
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	6	2.01
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	6	2.01
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	8	2.01
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	8	2.01
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	8	2.01
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	10	2.01
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	10	2.01
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	10	2.01
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	4	2.01
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	4	2.01
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	4	2.01
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	4	2.01
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	4	2.01
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	4	2.01
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG21	9	2.01
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG22	9	2.01
(3,178)	1:37:A:VAL:HA	1:38:A:ILE:HG23	9	2.01
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	8	2.01
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	8	2.01
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	8	2.01
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	10	2.01
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	10	2.01
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	10	2.01
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	7	2.01
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	7	2.01
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	9	2.0
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	9	2.0
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	9	2.0
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	9	2.0
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	9	2.0
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	9	2.0
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	7	1.99
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	7	1.99
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	7	1.99
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	7	1.99
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	7	1.99
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	7	1.99
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	7	1.99
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	3	1.98
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	3	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	3	1.98
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	3	1.98
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	3	1.98
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	3	1.98
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	4	1.98
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	6	1.98
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	6	1.98
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	6	1.98
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD11	9	1.98
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD12	9	1.98
(3,188)	1:38:A:ILE:HA	1:38:A:ILE:HD13	9	1.98
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	8	1.98
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	7	1.97
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	6	1.97
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	3	1.97
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	3	1.97
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	3	1.97
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	3	1.97
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	3	1.97
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	3	1.97
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	6	1.97
(3,194)	1:38:A:ILE:H	1:41:A:PHE:H	9	1.97
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	7	1.97
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	7	1.97
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	7	1.97
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	8	1.97
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	5	1.96
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	1	1.96
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	10	1.96
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	10	1.96
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	10	1.96
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	10	1.96
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	10	1.96
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	10	1.96
(3,182)	1:37:A:VAL:HG11	1:40:A:GLY:H	10	1.96
(3,182)	1:37:A:VAL:HG12	1:40:A:GLY:H	10	1.96
(3,182)	1:37:A:VAL:HG13	1:40:A:GLY:H	10	1.96
(3,182)	1:37:A:VAL:HG21	1:40:A:GLY:H	10	1.96
(3,182)	1:37:A:VAL:HG22	1:40:A:GLY:H	10	1.96
(3,182)	1:37:A:VAL:HG23	1:40:A:GLY:H	10	1.96
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	1	1.96
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	8	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	8	1.96
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	8	1.96
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	3	1.96
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	8	1.95
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	8	1.95
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	6	1.94
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	3	1.94
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	3	1.94
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	3	1.94
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	4	1.94
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	4	1.94
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	4	1.94
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	10	1.93
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	10	1.93
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	10	1.93
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	1	1.93
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	1	1.93
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	1	1.93
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	1	1.93
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	1	1.93
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	1	1.93
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	2	1.93
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	2	1.93
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	2	1.93
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	1	1.93
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	1	1.93
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	1	1.93
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	1	1.93
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	1	1.93
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	1	1.93
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	7	1.92
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	7	1.92
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	8	1.92
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	10	1.92
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	10	1.92
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	10	1.92
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	10	1.92
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	10	1.92
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	10	1.92
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	7	1.92
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	7	1.92
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	7	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	7	1.92
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	7	1.92
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	7	1.92
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	7	1.92
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	7	1.92
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	7	1.92
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	7	1.92
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	7	1.92
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	7	1.92
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	5	1.92
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	5	1.92
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	5	1.92
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	5	1.92
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	5	1.92
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	5	1.92
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	2	1.92
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	2	1.92
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	2	1.92
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	7	1.91
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	7	1.91
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	8	1.91
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	8	1.91
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	8	1.91
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	8	1.91
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	8	1.91
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	8	1.91
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	2	1.91
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	2	1.91
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	2	1.91
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	2	1.91
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	2	1.91
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	2	1.91
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	3	1.91
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	3	1.91
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	3	1.91
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	4	1.91
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	4	1.91
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	4	1.91
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	6	1.91
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	3	1.9
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	3	1.9
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	3	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	3	1.9
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	3	1.9
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	3	1.9
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	6	1.9
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	3	1.9
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	3	1.9
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	3	1.9
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	4	1.9
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	4	1.9
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	4	1.9
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	10	1.9
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	10	1.9
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	10	1.9
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	10	1.9
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	10	1.9
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	10	1.9
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	9	1.9
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	9	1.9
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	9	1.9
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD11	2	1.9
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD12	2	1.9
(3,187)	1:38:A:ILE:H	1:38:A:ILE:HD13	2	1.9
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	3	1.9
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	5	1.9
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	5	1.9
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	5	1.9
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	6	1.89
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	6	1.89
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	6	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	1	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	1	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	1	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	1	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	1	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	1	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	7	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	7	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	7	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	7	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	7	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	7	1.89
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	4	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	4	1.89
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	4	1.89
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	4	1.89
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	4	1.89
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	4	1.89
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	6	1.89
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	6	1.89
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	6	1.89
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	8	1.88
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	8	1.88
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	8	1.88
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	8	1.88
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	8	1.88
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	8	1.88
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	8	1.88
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	8	1.88
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	8	1.88
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	8	1.88
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	8	1.88
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	8	1.88
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	1	1.87
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	1	1.87
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	1	1.87
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	3	1.87
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	3	1.87
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	3	1.87
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	3	1.87
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	3	1.87
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	3	1.87
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	5	1.87
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	5	1.87
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	5	1.87
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	5	1.87
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	5	1.87
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	5	1.87
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	7	1.87
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	7	1.87
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	7	1.87
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	9	1.87
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	10	1.87
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	10	1.87
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	10	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	2	1.86
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	2	1.86
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	2	1.86
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	2	1.86
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	2	1.86
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	2	1.86
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	6	1.86
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	6	1.86
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	3	1.86
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	3	1.86
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	3	1.86
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	3	1.86
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	3	1.86
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	3	1.86
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	1	1.85
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	1	1.85
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	1	1.85
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	1	1.85
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	1	1.85
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	1	1.85
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	9	1.85
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	9	1.85
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	9	1.85
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	9	1.85
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	10	1.85
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	10	1.85
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD21	7	1.85
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD22	7	1.85
(3,161)	1:34:A:LEU:H	1:34:A:LEU:HD23	7	1.85
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	5	1.85
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	5	1.85
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	5	1.85
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	5	1.84
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	5	1.84
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	5	1.84
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	5	1.84
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	5	1.84
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	5	1.84
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	9	1.83
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	9	1.83
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	9	1.83
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	4	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	4	1.83
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	4	1.83
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	4	1.83
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	4	1.83
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	4	1.83
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	10	1.83
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	10	1.83
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	10	1.83
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	2	1.83
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	6	1.83
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	6	1.83
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	6	1.83
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	8	1.82
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	7	1.82
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	7	1.82
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	7	1.82
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	7	1.82
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	7	1.82
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	7	1.82
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	6	1.82
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	6	1.82
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	9	1.82
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	9	1.82
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	8	1.82
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	8	1.82
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	3	1.82
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	3	1.82
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	3	1.82
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	5	1.82
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	2	1.81
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	2	1.81
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	2	1.81
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	2	1.81
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	2	1.81
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	2	1.81
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	1	1.81
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	1	1.81
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	1	1.81
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	1	1.81
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	1	1.81
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	1	1.81
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	2	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	2	1.81
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	2	1.81
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	2	1.81
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	2	1.81
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	2	1.81
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	5	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	5	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	5	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	5	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	5	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	5	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	9	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	9	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	9	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	9	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	9	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	9	1.8
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	8	1.8
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	8	1.8
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	8	1.8
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	8	1.8
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	8	1.8
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	8	1.8
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	5	1.8
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	5	1.8
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	5	1.8
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	5	1.8
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	5	1.8
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	5	1.8
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	6	1.8
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	6	1.8
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	7	1.8
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	7	1.8
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	7	1.8
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	9	1.8
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	9	1.8
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	9	1.8
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	5	1.8
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	5	1.8
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD11	6	1.79
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD12	6	1.79
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD13	6	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD21	6	1.79
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD22	6	1.79
(3,240)	1:45:A:GLU:H	1:164:A:LEU:HD23	6	1.79
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	3	1.79
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	3	1.79
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	3	1.79
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	3	1.79
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	3	1.79
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	3	1.79
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	1	1.79
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	1	1.79
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	8	1.78
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	8	1.78
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	8	1.78
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	9	1.78
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	10	1.78
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	10	1.78
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	10	1.78
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	1	1.78
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	1	1.78
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	1	1.78
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	4	1.77
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	4	1.77
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	4	1.77
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	10	1.77
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	10	1.77
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	10	1.77
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	2	1.76
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	2	1.76
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	9	1.76
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	9	1.76
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	9	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	9	1.76
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	9	1.76
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	9	1.76
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	3	1.76
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	3	1.76
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	3	1.76
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	3	1.76
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	3	1.76
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	9	1.76
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	9	1.76
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	9	1.76
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	3	1.75
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	5	1.75
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	5	1.75
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	5	1.75
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	5	1.75
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	5	1.74
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	5	1.74
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	5	1.74
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	5	1.74
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	5	1.74
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	5	1.74
(3,259)	1:58:A:LEU:HB2	1:60:A:GLY:H	8	1.74
(3,259)	1:58:A:LEU:HB3	1:60:A:GLY:H	8	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	4	1.74
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	4	1.74
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	6	1.74
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	6	1.74
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	6	1.74
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	7	1.74
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	7	1.74
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	7	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	1	1.73
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	1	1.73
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	2	1.73
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	2	1.73
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	2	1.73
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	2	1.73
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	2	1.73
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	2	1.73
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	6	1.73
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	6	1.73
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	6	1.73
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	6	1.73
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	6	1.73
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	6	1.73
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	3	1.73
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	3	1.73
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	3	1.73
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	3	1.73
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	3	1.73
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	3	1.73
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	3	1.73
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	3	1.73
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	3	1.73
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	3	1.73
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	3	1.73
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	5	1.73
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	5	1.73
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	5	1.73
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	5	1.73
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	5	1.73
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	5	1.73
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	5	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	5	1.73
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	5	1.73
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	1	1.73
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	1	1.73
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	1	1.73
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	2	1.73
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	2	1.73
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	2	1.73
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	3	1.73
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	3	1.73
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	3	1.73
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	7	1.72
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	7	1.72
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	7	1.72
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	7	1.72
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	7	1.72
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	7	1.72
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	3	1.72
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	4	1.72
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	4	1.72
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	4	1.72
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	4	1.72
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	4	1.72
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	4	1.72
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	3	1.72
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	3	1.72
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	3	1.72
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	3	1.72
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	3	1.72
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	3	1.72
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	2	1.72
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	2	1.72
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	2	1.72
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	2	1.72
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	2	1.72
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	2	1.72
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	2	1.72
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	2	1.72
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	2	1.72
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	4	1.72
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	4	1.72
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	4	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	4	1.72
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	4	1.72
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	4	1.72
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	4	1.72
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	4	1.72
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	4	1.72
(3,192)	1:38:A:ILE:HG21	1:39:A:GLU:H	8	1.72
(3,192)	1:38:A:ILE:HG22	1:39:A:GLU:H	8	1.72
(3,192)	1:38:A:ILE:HG23	1:39:A:GLU:H	8	1.72
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	3	1.72
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	3	1.72
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	3	1.72
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	3	1.72
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	3	1.72
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	3	1.72
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE1	5	1.71
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE2	5	1.71
(3,238)	1:43:A:ILE:HG12	1:170:A:MET:HE3	5	1.71
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE1	5	1.71
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE2	5	1.71
(3,238)	1:43:A:ILE:HG13	1:170:A:MET:HE3	5	1.71
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	2	1.71
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	2	1.71
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	5	1.71
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	5	1.71
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	4	1.71
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	4	1.71
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	4	1.71
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	4	1.71
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	4	1.71
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	4	1.71
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	5	1.71
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	5	1.71
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	5	1.71
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	4	1.71
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	8	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	8	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	9	1.7
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	9	1.7
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	5	1.7
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	5	1.7
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	5	1.7
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	5	1.7
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	5	1.7
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	5	1.7
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	4	1.7
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	4	1.7
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	2	1.7
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	2	1.7
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	7	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	6	1.69
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	6	1.69
(3,184)	1:37:A:VAL:HG11	1:41:A:PHE:H	4	1.68
(3,184)	1:37:A:VAL:HG12	1:41:A:PHE:H	4	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,184)	1:37:A:VAL:HG13	1:41:A:PHE:H	4	1.68
(3,184)	1:37:A:VAL:HG21	1:41:A:PHE:H	4	1.68
(3,184)	1:37:A:VAL:HG22	1:41:A:PHE:H	4	1.68
(3,184)	1:37:A:VAL:HG23	1:41:A:PHE:H	4	1.68
(3,165)	1:34:A:LEU:HD11	1:35:A:THR:H	7	1.68
(3,165)	1:34:A:LEU:HD12	1:35:A:THR:H	7	1.68
(3,165)	1:34:A:LEU:HD13	1:35:A:THR:H	7	1.68
(3,165)	1:34:A:LEU:HD21	1:35:A:THR:H	7	1.68
(3,165)	1:34:A:LEU:HD22	1:35:A:THR:H	7	1.68
(3,165)	1:34:A:LEU:HD23	1:35:A:THR:H	7	1.68
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	3	1.67
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	5	1.67
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	5	1.67
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	5	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	7	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	7	1.67
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	2	1.67
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	2	1.67
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	2	1.67
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	2	1.67
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	2	1.67
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	2	1.67
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	7	1.67
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	7	1.67
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	2	1.67
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	2	1.67
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	2	1.67
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	5	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	5	1.66
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	5	1.66
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	5	1.65
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	5	1.65
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	5	1.65
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	3	1.65
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	3	1.65
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	10	1.63
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	10	1.63
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	10	1.63
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	10	1.63
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	10	1.63
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	10	1.63
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	1	1.63
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	1	1.63
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	1	1.63
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	1	1.63
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	1	1.63
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	1	1.63
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	6	1.63
(3,150)	1:33:A:ILE:HD11	1:34:A:LEU:H	1	1.63
(3,150)	1:33:A:ILE:HD12	1:34:A:LEU:H	1	1.63
(3,150)	1:33:A:ILE:HD13	1:34:A:LEU:H	1	1.63
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	6	1.62
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	6	1.62
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	6	1.62
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	6	1.62
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	6	1.62
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	6	1.62
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD11	4	1.62
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD12	4	1.62
(3,227)	1:43:A:ILE:HA	1:164:A:LEU:HD13	4	1.62
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD11	4	1.62
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD12	4	1.62
(3,223)	1:43:A:ILE:HA	1:164:A:LEU:HD13	4	1.62
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	8	1.62
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	8	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	8	1.62
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	8	1.62
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	8	1.62
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	8	1.62
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	9	1.62
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	9	1.62
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	9	1.62
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	4	1.62
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	4	1.62
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	4	1.62
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	3	1.62
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	3	1.62
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	3	1.62
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	8	1.61
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	1	1.61
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	9	1.61
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	2	1.61
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	2	1.61
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	2	1.61
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	2	1.61
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	2	1.61
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	2	1.61
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	2	1.61
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	2	1.61
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	2	1.61
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	10	1.6
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	7	1.6
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	7	1.6
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	7	1.6
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	7	1.6
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	7	1.6
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	7	1.6
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	1	1.6
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	1	1.6
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	1	1.6
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	1	1.59
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	1	1.59
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	1	1.59
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	1	1.59
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	1	1.59
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	1	1.59
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	5	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	5	1.59
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	5	1.59
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	3	1.57
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	3	1.57
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	3	1.57
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD1	10	1.56
(3,210)	1:41:A:PHE:H	1:41:A:PHE:HD2	10	1.56
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	3	1.56
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	3	1.56
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	3	1.56
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	6	1.55
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	6	1.55
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	6	1.55
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	6	1.55
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	6	1.55
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	6	1.55
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	5	1.55
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	9	1.55
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	9	1.55
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	9	1.55
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	9	1.55
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	9	1.55
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	9	1.55
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	4	1.55
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	4	1.55
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	4	1.55
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	4	1.55
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	4	1.55
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	4	1.55
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	1	1.54
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	10	1.54
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	2	1.54
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	2	1.54
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	2	1.54
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	2	1.54
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	2	1.54
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	2	1.54
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	4	1.54
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	4	1.54
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	4	1.54
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	4	1.54
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	4	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	4	1.54
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	5	1.54
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	5	1.54
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	5	1.54
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	5	1.54
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	5	1.54
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	5	1.54
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	10	1.54
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	10	1.54
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	10	1.54
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	6	1.53
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	6	1.53
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	6	1.53
(3,205)	1:38:A:ILE:HD11	1:178:A:PHE:H	9	1.53
(3,205)	1:38:A:ILE:HD12	1:178:A:PHE:H	9	1.53
(3,205)	1:38:A:ILE:HD13	1:178:A:PHE:H	9	1.53
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	3	1.53
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	3	1.53
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	3	1.53
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	3	1.53
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	3	1.53
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	3	1.53
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	1	1.53
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	1	1.53
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	1	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	1	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	1	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	1	1.53
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	1	1.53
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	1	1.53
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	1	1.53
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	8	1.53
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	8	1.53
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	8	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	8	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	8	1.53
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	8	1.53
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	8	1.53
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	8	1.53
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	8	1.53
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	9	1.52
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG11	5	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG12	5	1.51
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG13	5	1.51
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG21	5	1.51
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG22	5	1.51
(3,258)	1:58:A:LEU:H	1:59:A:VAL:HG23	5	1.51
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	5	1.51
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	1	1.51
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	1	1.51
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	10	1.51
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	10	1.51
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	10	1.5
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	10	1.5
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	3	1.5
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	4	1.5
(3,168)	1:34:A:LEU:HB2	1:45:A:GLU:H	7	1.5
(3,168)	1:34:A:LEU:HB3	1:45:A:GLU:H	7	1.5
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	2	1.5
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	2	1.5
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	2	1.5
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	10	1.49
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	10	1.49
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	10	1.49
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	10	1.49
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	10	1.49
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	10	1.49
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	10	1.49
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	10	1.49
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	4	1.47
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	4	1.47
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	4	1.47
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	4	1.47
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	4	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	4	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	1	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	1	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	1	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	1	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	1	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	1	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	8	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	8	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	8	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	8	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	8	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	8	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	9	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	9	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	9	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	9	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	9	1.47
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	9	1.47
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	10	1.46
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	6	1.46
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	7	1.46
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	7	1.46
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	7	1.46
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	10	1.46
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	10	1.46
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	10	1.46
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	9	1.45
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	9	1.45
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	9	1.45
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	9	1.45
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	9	1.45
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	9	1.45
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	4	1.45
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	6	1.45
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	6	1.45
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	6	1.45
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	6	1.45
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	6	1.45
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	6	1.45
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	5	1.44
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	5	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	5	1.44
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	5	1.44
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	5	1.44
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	5	1.44
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG11	7	1.44
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG12	7	1.44
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG13	7	1.44
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG21	7	1.44
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG22	7	1.44
(3,174)	1:36:A:HIS:H	1:42:A:VAL:HG23	7	1.44
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	9	1.44
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	9	1.44
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	9	1.44
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	4	1.44
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	4	1.44
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	4	1.43
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	4	1.43
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	2	1.43
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	9	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD11	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD12	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD13	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD21	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD22	3	1.43
(3,244)	1:46:A:GLY:H	1:164:A:LEU:HD23	3	1.43
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	4	1.43
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	4	1.43
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	4	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	2	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	2	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	2	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	3	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	3	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	3	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	6	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	6	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	6	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	7	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	7	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	7	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	9	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	9	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	9	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	10	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	10	1.43
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	10	1.43
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	4	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	4	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	4	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	4	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	4	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	4	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	10	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	10	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	10	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	10	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	10	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	10	1.42
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	3	1.42
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	3	1.42
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	3	1.42
(3,165)	1:34:A:LEU:HD11	1:35:A:THR:H	5	1.42
(3,165)	1:34:A:LEU:HD12	1:35:A:THR:H	5	1.42
(3,165)	1:34:A:LEU:HD13	1:35:A:THR:H	5	1.42
(3,165)	1:34:A:LEU:HD21	1:35:A:THR:H	5	1.42
(3,165)	1:34:A:LEU:HD22	1:35:A:THR:H	5	1.42
(3,165)	1:34:A:LEU:HD23	1:35:A:THR:H	5	1.42
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	1	1.42
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	1	1.42
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	1	1.42
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	3	1.41
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	3	1.41
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	3	1.41
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	3	1.41
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	3	1.41
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	3	1.41
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	9	1.41
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	9	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	9	1.41
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	9	1.41
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	9	1.41
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	9	1.41
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	10	1.41
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	10	1.41
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	10	1.41
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	10	1.41
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	10	1.41
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	10	1.41
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	2	1.41
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	2	1.41
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	2	1.41
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	2	1.41
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	8	1.41
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	4	1.41
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	4	1.41
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	4	1.41
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	6	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	6	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	6	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	6	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	6	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	6	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	10	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	10	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	10	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	10	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	10	1.4
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	10	1.4
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	5	1.4
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	5	1.4
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	5	1.4
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	1	1.4
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	5	1.4
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	5	1.4
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	5	1.4
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	5	1.4
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	8	1.39
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	8	1.39
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	8	1.39
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	8	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	8	1.39
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	8	1.39
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	3	1.39
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	3	1.39
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	3	1.39
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	3	1.39
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	3	1.39
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	3	1.39
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	10	1.39
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	10	1.39
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	10	1.39
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	10	1.39
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	10	1.39
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	10	1.39
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	4	1.38
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	4	1.38
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	4	1.38
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	1	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	1	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	1	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	1	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	1	1.37
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	1	1.37
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	4	1.37
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	1	1.37
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	1	1.37
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	1	1.37
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	7	1.37
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	7	1.37
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	7	1.37
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	1	1.36
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	1	1.36
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	1	1.36
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	1	1.36
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	1	1.36
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	1	1.36
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	5	1.36
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	5	1.36
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	5	1.36
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	5	1.36
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	5	1.36
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	5	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	1	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	1	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	1	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	1	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	1	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	1	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	8	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	8	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	8	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	8	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	8	1.36
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	8	1.36
(3,171)	1:35:A:THR:HA	1:45:A:GLU:H	5	1.36
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	7	1.35
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	7	1.35
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	7	1.35
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	7	1.35
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	7	1.35
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	7	1.35
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	2	1.35
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	2	1.35
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	2	1.35
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	7	1.34
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	7	1.34
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	7	1.34
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	7	1.34
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	7	1.34
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	7	1.34
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	4	1.34
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	4	1.34
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	4	1.34
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	4	1.34
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	4	1.34
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	4	1.34
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	1	1.34
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	1	1.34
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	1	1.34
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	1	1.34
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	1	1.34
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	1	1.34
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	5	1.34
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	5	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	5	1.34
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	5	1.34
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	5	1.34
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	5	1.34
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	6	1.34
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	6	1.34
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	6	1.34
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD11	4	1.34
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD12	4	1.34
(3,141)	1:32:A:GLN:H	1:33:A:ILE:HD13	4	1.34
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD11	2	1.33
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD12	2	1.33
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD13	2	1.33
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD21	2	1.33
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD22	2	1.33
(3,268)	1:62:A:LEU:H	1:62:A:LEU:HD23	2	1.33
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	7	1.33
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	5	1.33
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	5	1.33
(3,241)	1:46:A:GLY:H	1:47:A:ALA:H	7	1.33
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	8	1.33
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	8	1.33
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	8	1.33
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	7	1.33
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	4	1.33
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	4	1.33
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	8	1.32
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	8	1.32
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	6	1.32
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	6	1.32
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	6	1.32
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	6	1.32
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	6	1.32
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	6	1.32
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD1	9	1.32
(3,204)	1:38:A:ILE:HD11	1:178:A:PHE:HD2	9	1.32
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD1	9	1.32
(3,204)	1:38:A:ILE:HD12	1:178:A:PHE:HD2	9	1.32
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD1	9	1.32
(3,204)	1:38:A:ILE:HD13	1:178:A:PHE:HD2	9	1.32
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	8	1.31
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	8	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	8	1.31
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	8	1.31
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	8	1.31
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	8	1.31
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD21	2	1.3
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD22	2	1.3
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD23	2	1.3
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD11	2	1.3
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD12	2	1.3
(3,255)	1:58:A:LEU:H	1:58:A:LEU:HD13	2	1.3
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG21	5	1.3
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG22	5	1.3
(3,146)	1:33:A:ILE:H	1:33:A:ILE:HG23	5	1.3
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	7	1.29
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	7	1.29
(3,212)	1:41:A:PHE:HD1	1:42:A:VAL:H	1	1.29
(3,212)	1:41:A:PHE:HD2	1:42:A:VAL:H	1	1.29
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	10	1.28
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	10	1.28
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	10	1.28
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	10	1.28
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	10	1.28
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	10	1.28
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	10	1.28
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	10	1.27
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	10	1.27
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	10	1.27
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	6	1.27
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	6	1.27
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	6	1.27
(3,165)	1:34:A:LEU:HD11	1:35:A:THR:H	4	1.26
(3,165)	1:34:A:LEU:HD12	1:35:A:THR:H	4	1.26
(3,165)	1:34:A:LEU:HD13	1:35:A:THR:H	4	1.26
(3,165)	1:34:A:LEU:HD21	1:35:A:THR:H	4	1.26
(3,165)	1:34:A:LEU:HD22	1:35:A:THR:H	4	1.26
(3,165)	1:34:A:LEU:HD23	1:35:A:THR:H	4	1.26
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	9	1.25
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	9	1.25
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	6	1.25
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	6	1.25
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	6	1.25
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	6	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	6	1.25
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	6	1.25
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	6	1.25
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	6	1.25
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	5	1.24
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	3	1.24
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	3	1.24
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	3	1.24
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	6	1.24
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	3	1.23
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	3	1.23
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	3	1.23
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	3	1.23
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	3	1.23
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	3	1.23
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	3	1.23
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	3	1.23
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	3	1.23
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	3	1.23
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	3	1.23
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	3	1.23
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	1	1.23
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	1	1.23
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	1	1.23
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	10	1.23
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	10	1.23
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	10	1.23
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	7	1.22
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	7	1.22
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	7	1.22
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	7	1.22
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	7	1.22
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	7	1.22
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	9	1.22
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	9	1.21
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	9	1.21
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	9	1.21
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	9	1.21
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	9	1.21
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	9	1.21
(3,243)	1:46:A:GLY:HA2	1:48:A:GLU:H	2	1.21
(3,243)	1:46:A:GLY:HA3	1:48:A:GLU:H	2	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	5	1.21
(3,186)	1:37:A:VAL:HA	1:43:A:ILE:H	10	1.2
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	7	1.2
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	7	1.2
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	7	1.2
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	2	1.19
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	2	1.19
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	10	1.17
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	10	1.17
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	10	1.17
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	10	1.17
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	10	1.17
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	10	1.17
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	10	1.17
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	10	1.17
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	10	1.17
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	7	1.17
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	7	1.17
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	7	1.17
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	9	1.16
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	9	1.16
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	9	1.16
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	10	1.15
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	6	1.14
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	6	1.14
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	7	1.14
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	7	1.14
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	7	1.14
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	1	1.14
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	1	1.14
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	1	1.14
(3,156)	1:33:A:ILE:HD11	1:48:A:GLU:H	2	1.14
(3,156)	1:33:A:ILE:HD12	1:48:A:GLU:H	2	1.14
(3,156)	1:33:A:ILE:HD13	1:48:A:GLU:H	2	1.14
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	2	1.13
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	2	1.13
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG12	9	1.13
(3,143)	1:32:A:GLN:H	1:33:A:ILE:HG13	9	1.13
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	7	1.12
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	2	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	2	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	2	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	2	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	2	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	2	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	2	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	2	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	2	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	2	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	2	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	2	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	2	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	2	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	2	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	2	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	2	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	3	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	3	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	3	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	3	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	3	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	3	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	3	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	3	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	3	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	3	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	3	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	3	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	3	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	3	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	3	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	3	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	3	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	3	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	4	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	4	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	4	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	4	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	4	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	4	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	4	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	4	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	4	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	4	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	4	1.11
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	4	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	4	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	4	1.11
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	4	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	4	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	4	1.11
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	4	1.11
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	7	1.11
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	7	1.11
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	7	1.11
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	7	1.11
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	7	1.11
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	7	1.11
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	7	1.11
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	7	1.11
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	7	1.11
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	1	1.11
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	3	1.1
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	3	1.1
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	3	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	5	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	5	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	5	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	5	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	5	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	5	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	5	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	5	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	5	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	5	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	5	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	5	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	5	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	5	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	5	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	5	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	5	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	5	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	9	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	9	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	9	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	9	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	9	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	9	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	9	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	9	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	9	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	9	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	9	1.1
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	9	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	9	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	9	1.1
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	9	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	9	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	9	1.1
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	9	1.1
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	3	1.1
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	3	1.1
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	3	1.1
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	3	1.1
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	3	1.1
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	3	1.1
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	4	1.09
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	4	1.09
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	4	1.09
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	6	1.09
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	6	1.09
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	6	1.09
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	6	1.09
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	6	1.09
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	6	1.09
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	6	1.09
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	6	1.09
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	6	1.09
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	6	1.09
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	6	1.09
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	6	1.09
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	6	1.09
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	6	1.09
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	6	1.09
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	6	1.09
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	6	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	6	1.09
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	9	1.09
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	2	1.08
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	2	1.08
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	2	1.08
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	8	1.08
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	8	1.08
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	8	1.08
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	7	1.08
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	7	1.08
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	7	1.08
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	7	1.08
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	7	1.08
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	7	1.08
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	7	1.08
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	7	1.08
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	7	1.08
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	7	1.08
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	7	1.08
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	7	1.08
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	7	1.08
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	7	1.08
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	7	1.08
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	7	1.08
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	7	1.08
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	7	1.08
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	10	1.08
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	10	1.08
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	10	1.08
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	10	1.08
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	10	1.08
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	10	1.08
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	6	1.07
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	6	1.07
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	6	1.07
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	6	1.07
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	6	1.07
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	6	1.07
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	1	1.07
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	1	1.07
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	1	1.07
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	1	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	1	1.07
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	1	1.07
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	3	1.06
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	3	1.06
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	3	1.06
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	3	1.06
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	3	1.06
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	3	1.06
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	7	1.06
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	7	1.06
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	7	1.06
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	7	1.06
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	7	1.06
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	7	1.06
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	5	1.06
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	5	1.06
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	7	1.06
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	7	1.06
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	7	1.06
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	7	1.06
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	7	1.06
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	7	1.06
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	7	1.06
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	7	1.06
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	7	1.06
(3,203)	1:38:A:ILE:HG21	1:178:A:PHE:H	5	1.05
(3,203)	1:38:A:ILE:HG22	1:178:A:PHE:H	5	1.05
(3,203)	1:38:A:ILE:HG23	1:178:A:PHE:H	5	1.05
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	5	1.05
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	5	1.05
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	5	1.05
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	5	1.05
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	5	1.05
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	5	1.05
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	8	1.05
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	8	1.05
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	8	1.05
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	9	1.04
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	9	1.04
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	9	1.04
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	9	1.04
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	9	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	9	1.04
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	6	1.04
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	6	1.04
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	6	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	2	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	2	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	2	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	2	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	2	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	2	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	9	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	9	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	9	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	9	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	9	1.04
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	9	1.04
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	2	1.04
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	2	1.04
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	2	1.04
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	2	1.04
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	2	1.04
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	2	1.04
(3,158)	1:34:A:LEU:H	1:34:A:LEU:HG	4	1.04
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD11	9	1.03
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD12	9	1.03
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD13	9	1.03
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD21	9	1.03
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD22	9	1.03
(3,251)	1:57:A:LEU:H	1:57:A:LEU:HD23	9	1.03
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	9	1.02
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	9	1.02
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	9	1.02
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	9	1.01
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	5	1.01
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	5	1.01
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	5	1.01
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	5	1.01
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	5	1.01
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	5	1.01
(3,153)	1:33:A:ILE:HG21	1:45:A:GLU:H	4	1.01
(3,153)	1:33:A:ILE:HG22	1:45:A:GLU:H	4	1.01
(3,153)	1:33:A:ILE:HG23	1:45:A:GLU:H	4	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	3	1.0
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	3	1.0
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	2	1.0
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	5	0.99
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	5	0.99
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	5	0.99
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	5	0.99
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	5	0.99
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	5	0.99
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	4	0.99
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	4	0.99
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	4	0.99
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	4	0.99
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	4	0.99
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	4	0.99
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	6	0.99
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	10	0.99
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	10	0.99
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	10	0.99
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	10	0.99
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	10	0.99
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	10	0.99
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	10	0.99
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	10	0.99
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	10	0.99
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	5	0.98
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	5	0.98
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	5	0.98
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	5	0.98
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	5	0.98
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	5	0.98
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	9	0.98
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	2	0.98
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	2	0.98
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	2	0.98
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	3	0.98
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	3	0.98
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	3	0.98
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	10	0.98
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	10	0.98
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	10	0.98
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	10	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	10	0.98
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	10	0.98
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	4	0.97
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	4	0.97
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	4	0.97
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	10	0.97
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	10	0.97
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	10	0.97
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	10	0.97
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	10	0.97
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	10	0.97
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	10	0.97
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	10	0.97
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	10	0.97
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	10	0.97
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	10	0.97
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	10	0.97
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	10	0.97
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	10	0.97
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	10	0.97
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	10	0.97
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	10	0.97
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	10	0.97
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	5	0.96
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	5	0.96
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	5	0.96
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	6	0.96
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	6	0.96
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	7	0.95
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	7	0.95
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	7	0.95
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	6	0.95
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	6	0.95
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	6	0.95
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	6	0.95
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	6	0.95
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	6	0.95
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	9	0.95
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	9	0.95
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	10	0.94
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	10	0.94
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	5	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	7	0.94
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	7	0.94
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	7	0.94
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	7	0.94
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	7	0.94
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	7	0.94
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	9	0.94
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	9	0.94
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	9	0.94
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	9	0.94
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	9	0.94
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	9	0.94
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	1	0.93
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	1	0.93
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	1	0.93
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	1	0.93
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	1	0.93
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	1	0.93
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	1	0.93
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	1	0.93
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	1	0.93
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	1	0.93
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	1	0.93
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	1	0.93
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	1	0.93
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	1	0.93
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	1	0.93
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	1	0.93
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	1	0.93
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	1	0.93
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	9	0.92
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	9	0.92
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	9	0.92
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	9	0.92
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	9	0.92
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	9	0.92
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	9	0.92
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	9	0.92
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	9	0.92
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	10	0.92
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	10	0.92
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	8	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	8	0.91
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	8	0.91
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	8	0.91
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD11	8	0.91
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD12	8	0.91
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD13	8	0.91
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD11	8	0.91
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD12	8	0.91
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD13	8	0.91
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD11	8	0.91
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD12	8	0.91
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD13	8	0.91
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD21	8	0.91
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD22	8	0.91
(3,202)	1:38:A:ILE:HD11	1:175:A:LEU:HD23	8	0.91
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD21	8	0.91
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD22	8	0.91
(3,202)	1:38:A:ILE:HD12	1:175:A:LEU:HD23	8	0.91
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD21	8	0.91
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD22	8	0.91
(3,202)	1:38:A:ILE:HD13	1:175:A:LEU:HD23	8	0.91
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	8	0.91
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	8	0.91
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	10	0.9
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	10	0.9
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	10	0.9
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	1	0.9
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	1	0.9
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	1	0.9
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE1	6	0.9
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE2	6	0.9
(3,198)	1:38:A:ILE:HG21	1:170:A:MET:HE3	6	0.9
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE1	6	0.9
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE2	6	0.9
(3,198)	1:38:A:ILE:HG22	1:170:A:MET:HE3	6	0.9
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE1	6	0.9
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE2	6	0.9
(3,198)	1:38:A:ILE:HG23	1:170:A:MET:HE3	6	0.9
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	5	0.89
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	5	0.89
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	5	0.89
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	5	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	5	0.89
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	5	0.89
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	9	0.89
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	9	0.89
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	9	0.89
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	9	0.89
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	9	0.89
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	9	0.89
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	1	0.89
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	1	0.89
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	1	0.89
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	6	0.88
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	6	0.88
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	6	0.88
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	6	0.88
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	6	0.88
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	6	0.88
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	3	0.88
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	3	0.88
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	3	0.87
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	4	0.87
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	4	0.87
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	4	0.87
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	4	0.87
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	4	0.87
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	4	0.87
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	3	0.87
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	3	0.87
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	3	0.87
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	3	0.87
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	3	0.87
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	3	0.87
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	4	0.87
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	4	0.87
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	4	0.87
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	4	0.87
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	4	0.87
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	4	0.87
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	1	0.87
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	1	0.87
(3,65)	1:38:A:ILE:HG21	1:174:A:HIS:H	6	0.87
(3,65)	1:38:A:ILE:HG22	1:174:A:HIS:H	6	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,65)	1:38:A:ILE:HG23	1:174:A:HIS:H	6	0.87
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	2	0.87
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	2	0.87
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	2	0.87
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	2	0.87
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	2	0.87
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	2	0.87
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	3	0.87
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	3	0.87
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	3	0.87
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	3	0.87
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	3	0.87
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	3	0.87
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	5	0.87
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	5	0.87
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	5	0.87
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	5	0.87
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	5	0.87
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	5	0.87
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG21	10	0.86
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG22	10	0.86
(3,220)	1:43:A:ILE:H	1:43:A:ILE:HG23	10	0.86
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	7	0.86
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	4	0.86
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	4	0.86
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	4	0.86
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	4	0.86
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	4	0.86
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	4	0.86
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	4	0.86
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	4	0.86
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	4	0.86
(3,65)	1:38:A:ILE:HG21	1:174:A:HIS:H	9	0.85
(3,65)	1:38:A:ILE:HG22	1:174:A:HIS:H	9	0.85
(3,65)	1:38:A:ILE:HG23	1:174:A:HIS:H	9	0.85
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	4	0.84
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	10	0.84
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	10	0.84
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	10	0.84
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	10	0.84
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	10	0.84
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	10	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	8	0.83
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	5	0.83
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	5	0.83
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	5	0.83
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	9	0.83
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	9	0.83
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	9	0.83
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	10	0.83
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	2	0.83
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	6	0.83
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	6	0.83
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	6	0.83
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	4	0.82
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	4	0.82
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	4	0.82
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	4	0.82
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	4	0.82
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	4	0.82
(3,180)	1:37:A:VAL:HG11	1:38:A:ILE:H	8	0.82
(3,180)	1:37:A:VAL:HG12	1:38:A:ILE:H	8	0.82
(3,180)	1:37:A:VAL:HG13	1:38:A:ILE:H	8	0.82
(3,180)	1:37:A:VAL:HG21	1:38:A:ILE:H	8	0.82
(3,180)	1:37:A:VAL:HG22	1:38:A:ILE:H	8	0.82
(3,180)	1:37:A:VAL:HG23	1:38:A:ILE:H	8	0.82
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	3	0.82
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	3	0.82
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	9	0.82
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	9	0.82
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	9	0.82
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	6	0.81
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	6	0.81
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	6	0.81
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	6	0.81
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	6	0.81
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	6	0.81
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	9	0.81
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	9	0.81
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	5	0.8
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	5	0.8
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	7	0.8
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	7	0.8
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	1	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	3	0.79
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	6	0.79
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	1	0.79
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	1	0.79
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	6	0.79
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	10	0.79
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	10	0.78
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	10	0.78
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	10	0.78
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	10	0.78
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	10	0.78
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	10	0.78
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	2	0.78
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	2	0.78
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	2	0.78
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	2	0.78
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	2	0.78
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	2	0.78
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	1	0.78
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	1	0.78
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	1	0.78
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	1	0.78
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	1	0.78
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	1	0.78
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	8	0.78
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	8	0.78
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	8	0.78
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	8	0.78
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	8	0.78
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	8	0.78
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	9	0.78
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	6	0.78
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	6	0.78
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	10	0.78
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	10	0.78
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	3	0.78
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	9	0.78
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	5	0.78
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	5	0.78
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	5	0.78
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	1	0.77
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	7	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	7	0.77
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	7	0.77
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	7	0.77
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	7	0.77
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	7	0.77
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	2	0.77
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	4	0.77
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	5	0.77
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	7	0.77
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	8	0.77
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	10	0.77
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	4	0.77
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	7	0.77
(3,118)	1:57:A:LEU:H	1:58:A:LEU:H	2	0.77
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	6	0.76
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	6	0.76
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	2	0.76
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	2	0.76
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	2	0.76
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	2	0.76
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	2	0.76
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	2	0.76
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	10	0.76
(3,208)	1:40:A:GLY:H	1:41:A:PHE:H	3	0.76
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	1	0.74
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	1	0.74
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	3	0.74
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	3	0.74
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	3	0.74
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	8	0.74
(3,148)	1:33:A:ILE:H	1:33:A:ILE:HB	10	0.74
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	9	0.73
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	1	0.73
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	1	0.73
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	1	0.73
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	1	0.73
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	1	0.73
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	1	0.73
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	1	0.73
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	1	0.73
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	1	0.73
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	1	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	1	0.72
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	1	0.72
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	6	0.72
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	6	0.72
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	9	0.72
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	9	0.72
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	1	0.71
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG12	2	0.71
(3,149)	1:33:A:ILE:H	1:33:A:ILE:HG13	2	0.71
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	9	0.7
(3,68)	1:38:A:ILE:HG21	1:178:A:PHE:H	6	0.7
(3,68)	1:38:A:ILE:HG22	1:178:A:PHE:H	6	0.7
(3,68)	1:38:A:ILE:HG23	1:178:A:PHE:H	6	0.7
(3,68)	1:38:A:ILE:HG21	1:178:A:PHE:H	9	0.7
(3,68)	1:38:A:ILE:HG22	1:178:A:PHE:H	9	0.7
(3,68)	1:38:A:ILE:HG23	1:178:A:PHE:H	9	0.7
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	6	0.69
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	6	0.69
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	8	0.69
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	2	0.69
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	2	0.69
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	2	0.69
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	10	0.69
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	10	0.69
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	10	0.69
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	6	0.69
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	6	0.68
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	7	0.68
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	5	0.67
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	5	0.67
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	5	0.67
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	5	0.67
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	5	0.67
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	5	0.67
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	8	0.66
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	8	0.66
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	2	0.66
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	10	0.66
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	5	0.66
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	5	0.66
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	5	0.66
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	8	0.66
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	9	0.66
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	9	0.66
(3,250)	1:52:A:VAL:HG11	1:53:A:GLY:H	8	0.66
(3,250)	1:52:A:VAL:HG12	1:53:A:GLY:H	8	0.66
(3,250)	1:52:A:VAL:HG13	1:53:A:GLY:H	8	0.66
(3,250)	1:52:A:VAL:HG21	1:53:A:GLY:H	8	0.66
(3,250)	1:52:A:VAL:HG22	1:53:A:GLY:H	8	0.66
(3,250)	1:52:A:VAL:HG23	1:53:A:GLY:H	8	0.66
(3,216)	1:42:A:VAL:HG11	1:43:A:ILE:H	2	0.66
(3,216)	1:42:A:VAL:HG12	1:43:A:ILE:H	2	0.66
(3,216)	1:42:A:VAL:HG13	1:43:A:ILE:H	2	0.66
(3,216)	1:42:A:VAL:HG21	1:43:A:ILE:H	2	0.66
(3,216)	1:42:A:VAL:HG22	1:43:A:ILE:H	2	0.66
(3,216)	1:42:A:VAL:HG23	1:43:A:ILE:H	2	0.66
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	8	0.66
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	8	0.66
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	8	0.66
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	8	0.66
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	8	0.66
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	8	0.66
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	8	0.66
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	8	0.66
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	8	0.66
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	8	0.66
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	3	0.66
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	3	0.66
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	3	0.66
(3,263)	1:59:A:VAL:H	1:60:A:GLY:H	1	0.65
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	4	0.65
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	2	0.65
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	2	0.65
(3,247)	1:47:A:ALA:HB1	1:48:A:GLU:H	7	0.65
(3,247)	1:47:A:ALA:HB2	1:48:A:GLU:H	7	0.65
(3,247)	1:47:A:ALA:HB3	1:48:A:GLU:H	7	0.65
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	3	0.65
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	3	0.65
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	3	0.65
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	5	0.65
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	5	0.65
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	5	0.65
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	4	0.64
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	4	0.64
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	2	0.64
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	2	0.64
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	7	0.64
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	7	0.64
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB2	8	0.64
(3,136)	1:32:A:GLN:H	1:32:A:GLN:HB3	8	0.64
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	2	0.64
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	2	0.64
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	2	0.64
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	3	0.63
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	3	0.63
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	1	0.63
(3,261)	1:59:A:VAL:H	1:59:A:VAL:HB	3	0.63
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	10	0.63
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	10	0.63
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	5	0.63
(3,167)	1:34:A:LEU:H	1:45:A:GLU:H	3	0.63
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	7	0.63
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	8	0.63
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	4	0.63
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	4	0.63
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	4	0.63
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	1	0.63
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	4	0.62
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	4	0.62
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	9	0.62
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	9	0.62
(3,265)	1:59:A:VAL:HG11	1:60:A:GLY:H	8	0.62
(3,265)	1:59:A:VAL:HG12	1:60:A:GLY:H	8	0.62
(3,265)	1:59:A:VAL:HG13	1:60:A:GLY:H	8	0.62
(3,265)	1:59:A:VAL:HG21	1:60:A:GLY:H	8	0.62
(3,265)	1:59:A:VAL:HG22	1:60:A:GLY:H	8	0.62
(3,265)	1:59:A:VAL:HG23	1:60:A:GLY:H	8	0.62
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	10	0.62
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	7	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	2	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	2	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	2	0.62
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	2	0.62
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	2	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	2	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	2	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	2	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	4	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	4	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	4	0.62
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	4	0.62
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	4	0.62
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	4	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	4	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	4	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	4	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	8	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	8	0.62
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	8	0.62
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	8	0.62
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	8	0.62
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	8	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	8	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	8	0.62
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	8	0.62
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	2	0.62
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	2	0.62
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	2	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	2	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	2	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	2	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	2	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	2	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	2	0.62
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	4	0.62
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	4	0.62
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	4	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	4	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	4	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	4	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	4	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	4	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	4	0.62
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	8	0.62
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	8	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	8	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	8	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	8	0.62
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	8	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	8	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	8	0.62
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	8	0.62
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	4	0.62
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	4	0.62
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	4	0.62
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	7	0.62
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	7	0.62
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	7	0.62
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	9	0.62
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	9	0.62
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	9	0.62
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD11	6	0.62
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD12	6	0.62
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD13	6	0.62
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	8	0.62
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	3	0.61
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	1	0.61
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	1	0.61
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB2	3	0.61
(3,254)	1:58:A:LEU:H	1:58:A:LEU:HB3	3	0.61
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	3	0.61
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	3	0.61
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	3	0.61
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	3	0.61
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	3	0.61
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	3	0.61
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	3	0.61
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	3	0.61
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	3	0.61
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	3	0.61
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	3	0.61
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	3	0.61
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	3	0.61
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	3	0.61
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	3	0.61
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	3	0.61
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	3	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	3	0.61
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	6	0.61
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	6	0.61
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	6	0.61
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD11	9	0.61
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD12	9	0.61
(3,42)	1:37:A:VAL:HA	1:38:A:ILE:HD13	9	0.61
(3,269)	1:62:A:LEU:HB2	1:63:A:LYS:H	6	0.6
(3,269)	1:62:A:LEU:HB3	1:63:A:LYS:H	6	0.6
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	1	0.6
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	1	0.6
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	10	0.6
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	10	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	1	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	1	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	1	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	1	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	1	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	1	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	1	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	1	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	1	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	7	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	7	0.6
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	7	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	7	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	7	0.6
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	7	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	7	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	7	0.6
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	7	0.6
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	1	0.6
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	1	0.6
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	1	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	1	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	1	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	1	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	1	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	1	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	1	0.6
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	7	0.6
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	7	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	7	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	7	0.6
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	7	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	7	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	7	0.6
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	7	0.6
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	2	0.6
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	2	0.6
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	2	0.6
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	2	0.59
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	2	0.59
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	9	0.59
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	9	0.59
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	9	0.59
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	9	0.59
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	9	0.59
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	9	0.59
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	10	0.59
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	10	0.59
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	10	0.59
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	10	0.59
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	10	0.59
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	10	0.59
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	10	0.59
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	10	0.59
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	10	0.59
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	10	0.59
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	10	0.59
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	10	0.59
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	10	0.59
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	10	0.59
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	10	0.59
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	10	0.59
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	10	0.59
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	10	0.59
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	1	0.59
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	1	0.59
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	1	0.59
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	1	0.59
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	3	0.58
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	2	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	4	0.58
(3,253)	1:57:A:LEU:H	1:58:A:LEU:H	4	0.58
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	6	0.58
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	6	0.58
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	6	0.58
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	6	0.58
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	6	0.58
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	6	0.58
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	6	0.58
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	6	0.58
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	6	0.58
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	9	0.58
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	9	0.58
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	9	0.58
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	9	0.58
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	9	0.58
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	9	0.58
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	9	0.58
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	9	0.58
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	9	0.58
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	6	0.58
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	6	0.58
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	6	0.58
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	6	0.58
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	6	0.58
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	6	0.58
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	6	0.58
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	6	0.58
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	6	0.58
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	9	0.58
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	9	0.58
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	9	0.58
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	9	0.58
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	9	0.58
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	9	0.58
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	9	0.58
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	9	0.58
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	9	0.58
(3,151)	1:33:A:ILE:HG21	1:34:A:LEU:H	8	0.58
(3,151)	1:33:A:ILE:HG22	1:34:A:LEU:H	8	0.58
(3,151)	1:33:A:ILE:HG23	1:34:A:LEU:H	8	0.58
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	8	0.57
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	5	0.57
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	5	0.57
(3,228)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	5	0.57
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	5	0.57
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	5	0.57
(3,228)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	5	0.57
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	5	0.57
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	5	0.57
(3,228)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	5	0.57
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD11	5	0.57
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD12	5	0.57
(3,226)	1:43:A:ILE:HD11	1:164:A:LEU:HD13	5	0.57
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD11	5	0.57
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD12	5	0.57
(3,226)	1:43:A:ILE:HD12	1:164:A:LEU:HD13	5	0.57
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD11	5	0.57
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD12	5	0.57
(3,226)	1:43:A:ILE:HD13	1:164:A:LEU:HD13	5	0.57
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	6	0.57
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	6	0.57
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	6	0.57
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	7	0.57
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	7	0.57
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	7	0.57
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG21	4	0.57
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG22	4	0.57
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG23	4	0.57
(3,257)	1:58:A:LEU:H	1:59:A:VAL:H	9	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	2	0.56
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	2	0.56
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	6	0.55
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	6	0.55
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	6	0.55
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	7	0.55
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	7	0.55
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	8	0.55
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	8	0.55
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	10	0.54
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	10	0.54
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	10	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	2	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	2	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	2	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	2	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	2	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	2	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	2	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	2	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	2	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	3	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	3	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	3	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	3	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	3	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	3	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	3	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	3	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	3	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	4	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	4	0.54
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	4	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	4	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	4	0.54
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	4	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	4	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	4	0.54
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	4	0.54
(1,9)	1:38:A:ILE:H	1:41:A:PHE:O	7	0.54
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG2	2	0.53
(3,137)	1:32:A:GLN:H	1:32:A:GLN:HG3	2	0.53
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	7	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	7	0.52
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	7	0.52
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	2	0.52
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD11	5	0.52
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD12	5	0.52
(3,71)	1:38:A:ILE:HD11	1:179:A:LEU:HD13	5	0.52
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD11	5	0.52
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD12	5	0.52
(3,71)	1:38:A:ILE:HD12	1:179:A:LEU:HD13	5	0.52
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD11	5	0.52
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD12	5	0.52
(3,71)	1:38:A:ILE:HD13	1:179:A:LEU:HD13	5	0.52
(1,9)	1:38:A:ILE:H	1:41:A:PHE:O	8	0.52
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	2	0.51
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	8	0.51
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	8	0.51
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	8	0.51
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	10	0.51
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	10	0.51
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	10	0.51
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	4	0.51
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	4	0.51
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	4	0.51
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	10	0.51
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB2	7	0.5
(3,267)	1:62:A:LEU:H	1:62:A:LEU:HB3	7	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	7	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	7	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	7	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	7	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	7	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	7	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	8	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	8	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	8	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	8	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	8	0.5
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	8	0.5
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	6	0.5
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	2	0.5
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	2	0.5
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	2	0.5
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	4	0.5
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	4	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	2	0.5
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	2	0.5
(3,155)	1:33:A:ILE:HD11	1:47:A:ALA:H	10	0.5
(3,155)	1:33:A:ILE:HD12	1:47:A:ALA:H	10	0.5
(3,155)	1:33:A:ILE:HD13	1:47:A:ALA:H	10	0.5
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	7	0.5
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	7	0.5
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	7	0.5
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	5	0.49
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	5	0.49
(3,122)	1:58:A:LEU:H	1:59:A:VAL:H	7	0.49
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	9	0.49
(1,9)	1:38:A:ILE:H	1:41:A:PHE:O	10	0.49
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	6	0.48
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	6	0.48
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	6	0.48
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG21	9	0.48
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG22	9	0.48
(3,189)	1:38:A:ILE:H	1:38:A:ILE:HG23	9	0.48
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	6	0.48
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	6	0.48
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:38:A:ILE:H	1:41:A:PHE:O	1	0.48
(3,256)	1:58:A:LEU:HA	1:59:A:VAL:H	7	0.47
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	1	0.47
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	1	0.47
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	1	0.47
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	8	0.47
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	8	0.47
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	8	0.47
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	2	0.47
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	2	0.47
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	9	0.47
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	9	0.47
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	9	0.47
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	9	0.47
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	9	0.47
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	9	0.47
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	9	0.47
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	9	0.47
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	9	0.47
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	4	0.47
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	4	0.47
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	4	0.47
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	6	0.47
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	5	0.46
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	5	0.46
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	7	0.46
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	7	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	3	0.46
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	3	0.46
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	3	0.46
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	3	0.46
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB1	4	0.46
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB2	4	0.46
(3,245)	1:47:A:ALA:H	1:47:A:ALA:HB3	4	0.46
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	1	0.46
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	1	0.46
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	1	0.46
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	1	0.46
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	1	0.46
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	1	0.46
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	1	0.46
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	1	0.46
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	1	0.46
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	3	0.46
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	3	0.46
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD11	6	0.46
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD12	6	0.46
(3,196)	1:38:A:ILE:HG21	1:43:A:ILE:HD13	6	0.46
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD11	6	0.46
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD12	6	0.46
(3,196)	1:38:A:ILE:HG22	1:43:A:ILE:HD13	6	0.46
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD11	6	0.46
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD12	6	0.46
(3,196)	1:38:A:ILE:HG23	1:43:A:ILE:HD13	6	0.46
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	1	0.46
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	1	0.46
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	1	0.46
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	9	0.46
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	9	0.46
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	9	0.46
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	1	0.45
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	1	0.45
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	1	0.45
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	1	0.45
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	1	0.45
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	1	0.45
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	1	0.45
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	7	0.45
(3,248)	1:47:A:ALA:HA	1:163:A:TYR:H	10	0.45
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	8	0.45
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	8	0.45
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	8	0.45
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	8	0.45
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	8	0.45
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	8	0.45
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	8	0.45
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	8	0.45
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	3	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	3	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	3	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	3	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	3	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	3	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	10	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	10	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	10	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	10	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	10	0.44
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	10	0.44
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	1	0.44
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	1	0.44
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	2	0.44
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	2	0.44
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	2	0.44
(3,154)	1:33:A:ILE:HG21	1:47:A:ALA:H	5	0.44
(3,154)	1:33:A:ILE:HG22	1:47:A:ALA:H	5	0.44
(3,154)	1:33:A:ILE:HG23	1:47:A:ALA:H	5	0.44
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	3	0.44
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	3	0.44
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	3	0.44
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	5	0.44
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	5	0.44
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	5	0.44
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	3	0.43
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	3	0.43
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	10	0.43
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	10	0.43
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	10	0.43
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	10	0.43
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	10	0.43
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	10	0.43
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	10	0.43
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	10	0.43
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	8	0.43
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	8	0.43
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	10	0.43
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	10	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	6	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	9	0.43
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	9	0.43
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	7	0.43
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	7	0.43
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	7	0.43
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	7	0.43
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	7	0.43
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	7	0.43
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	10	0.43
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	10	0.43
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	10	0.43
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	8	0.43
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	8	0.43
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	8	0.43
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG21	9	0.43
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG22	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG23	9	0.43
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	7	0.42
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	7	0.42
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	7	0.42
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	7	0.42
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	7	0.42
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	7	0.42
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	7	0.42
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	7	0.42
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	7	0.42
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	1	0.42
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	1	0.42
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	1	0.42
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	1	0.42
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	1	0.42
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	1	0.42
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	4	0.42
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	4	0.42
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	4	0.42
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	1	0.41
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	1	0.41
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	9	0.41
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	9	0.41
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	6	0.41
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	6	0.41
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	6	0.41
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	6	0.41
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	6	0.41
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	6	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	4	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	8	0.41
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	8	0.41
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	3	0.41
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	3	0.41
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	3	0.41
(3,102)	1:43:A:ILE:HG21	1:170:A:MET:HA	2	0.41
(3,102)	1:43:A:ILE:HG22	1:170:A:MET:HA	2	0.41
(3,102)	1:43:A:ILE:HG23	1:170:A:MET:HA	2	0.41
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	7	0.41
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	7	0.41
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	7	0.41
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	10	0.41
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	10	0.41
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	10	0.41
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG21	6	0.41
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG22	6	0.41
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG23	6	0.41
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	2	0.4
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	2	0.4
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	2	0.4
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	2	0.4
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	2	0.4
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	2	0.4
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	6	0.4
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	6	0.4
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	9	0.4
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	9	0.4
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	8	0.4
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	8	0.4
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	8	0.4
(3,142)	1:32:A:GLN:HA	1:33:A:ILE:H	3	0.4
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	10	0.4
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	10	0.4
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG12	7	0.39
(3,221)	1:43:A:ILE:H	1:43:A:ILE:HG13	7	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	2	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	2	0.39
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	5	0.39
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	5	0.39
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	5	0.39
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	3	0.38
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	3	0.38
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD11	5	0.38
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD12	5	0.38
(3,147)	1:33:A:ILE:HB	1:33:A:ILE:HD13	5	0.38
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	5	0.38
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	5	0.38
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	5	0.38
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	5	0.38
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	8	0.37
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	8	0.37
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	1	0.37
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	1	0.37
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	1	0.37
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	1	0.37
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	1	0.37
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	1	0.37
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	1	0.37
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	1	0.37
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	8	0.37
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	8	0.37
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	8	0.37
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	8	0.37
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	8	0.37
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	8	0.37
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	8	0.37
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	8	0.37
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	8	0.37
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG11	8	0.37
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG12	8	0.37
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG13	8	0.37
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG21	8	0.37
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG22	8	0.37
(3,185)	1:37:A:VAL:HA	1:42:A:VAL:HG23	8	0.37
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	2	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	2	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	2	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	2	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	2	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	2	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	2	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	2	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	2	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	4	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	4	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	4	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	4	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	4	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	4	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	4	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	4	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	4	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	5	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	5	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	5	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	5	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	5	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	5	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	5	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	5	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	7	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	7	0.36
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	7	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	7	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	7	0.36
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	7	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	7	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	7	0.36
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	7	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	4	0.36
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	4	0.36
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	1	0.36
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	1	0.36
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	1	0.36
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	9	0.36
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	9	0.36
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	9	0.36
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	2	0.35
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	9	0.35
(3,246)	1:47:A:ALA:H	1:48:A:GLU:H	7	0.35
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	6	0.35
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	6	0.35
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	6	0.35
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	6	0.35
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	6	0.35
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	6	0.35
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	6	0.35
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	6	0.35
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	10	0.35
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	10	0.35
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	10	0.35
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	10	0.35
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	10	0.35
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	10	0.35
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	10	0.35
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	10	0.35
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	10	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	3	0.35
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	3	0.35
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	6	0.35
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	6	0.35
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	6	0.35
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD11	9	0.35
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD12	9	0.35
(3,160)	1:34:A:LEU:HA	1:34:A:LEU:HD13	9	0.35
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD11	4	0.35
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD12	4	0.35
(3,144)	1:33:A:ILE:H	1:33:A:ILE:HD13	4	0.35
(1,10)	1:38:A:ILE:N	1:41:A:PHE:O	7	0.35
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	4	0.34
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	4	0.34
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	4	0.34
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	4	0.34
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	4	0.34
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	4	0.34
(3,252)	1:57:A:LEU:HA	1:58:A:LEU:H	2	0.34
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	3	0.34
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	3	0.34
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	3	0.34
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	3	0.34
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	3	0.34
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	3	0.34
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	3	0.34
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	3	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	2	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	2	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	2	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	3	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	3	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	3	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	4	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	4	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	4	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	6	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	6	0.34
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	6	0.34
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	5	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	5	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	5	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	5	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	5	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	5	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	9	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	9	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	9	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	9	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	9	0.33
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	9	0.33
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	9	0.33
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	9	0.33
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	9	0.33
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	9	0.33
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	9	0.33
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	9	0.33
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	9	0.33
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	9	0.33
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	6	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	9	0.33
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	9	0.33
(3,140)	1:32:A:GLN:H	1:33:A:ILE:H	5	0.33
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	10	0.33
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	10	0.33
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	10	0.33
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	10	0.33
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	10	0.33
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	10	0.33
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	1	0.33
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	1	0.33
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	1	0.33
(1,22)	1:38:A:ILE:O	1:41:A:PHE:N	10	0.33
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	3	0.33
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	4	0.33
(3,270)	1:64:A:GLY:HA2	1:121:A:ASP:H	4	0.32
(3,270)	1:64:A:GLY:HA3	1:121:A:ASP:H	4	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	1	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	1	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	1	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	1	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	1	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	2	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	2	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	2	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	2	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	2	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	2	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	3	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	3	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	3	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	3	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	3	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	3	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	4	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	4	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	4	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	4	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	4	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	4	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	6	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	6	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	6	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	6	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	6	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	6	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG11	10	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG12	10	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG13	10	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG21	10	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG22	10	0.32
(3,260)	1:59:A:VAL:HA	1:59:A:VAL:HG23	10	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	5	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	5	0.32
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE1	10	0.32
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE2	10	0.32
(3,213)	1:41:A:PHE:HD1	1:170:A:MET:HE3	10	0.32
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE1	10	0.32
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE2	10	0.32
(3,213)	1:41:A:PHE:HD2	1:170:A:MET:HE3	10	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	5	0.32
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	5	0.32
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	10	0.32
(1,22)	1:38:A:ILE:O	1:41:A:PHE:N	8	0.32
(1,18)	1:34:A:LEU:O	1:45:A:GLU:N	4	0.32
(1,10)	1:38:A:ILE:N	1:41:A:PHE:O	8	0.32
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	10	0.31
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	10	0.31
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	10	0.31
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD21	9	0.31
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD22	9	0.31
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD23	9	0.31
(1,22)	1:38:A:ILE:O	1:41:A:PHE:N	1	0.31
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	5	0.31
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	1	0.31
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	8	0.31
(3,266)	1:61:A:ASN:HA	1:62:A:LEU:H	6	0.3
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	7	0.3
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	7	0.3
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	7	0.3
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	7	0.3
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	7	0.3
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	7	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD21	1	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD22	1	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD23	1	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD21	3	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD22	3	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD23	3	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD21	6	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD22	6	0.3
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD23	6	0.3
(1,22)	1:38:A:ILE:O	1:41:A:PHE:N	7	0.3
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	9	0.3
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	1	0.29
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	1	0.29
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	1	0.29
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	1	0.29
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	2	0.29
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	6	0.29
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	8	0.29
(1,10)	1:38:A:ILE:N	1:41:A:PHE:O	1	0.29
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	7	0.28
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	7	0.28
(3,169)	1:34:A:LEU:HD11	1:45:A:GLU:H	4	0.28
(3,169)	1:34:A:LEU:HD12	1:45:A:GLU:H	4	0.28
(3,169)	1:34:A:LEU:HD13	1:45:A:GLU:H	4	0.28
(3,169)	1:34:A:LEU:HD21	1:45:A:GLU:H	4	0.28
(3,169)	1:34:A:LEU:HD22	1:45:A:GLU:H	4	0.28
(3,169)	1:34:A:LEU:HD23	1:45:A:GLU:H	4	0.28
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	7	0.28
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	2	0.27
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	2	0.27
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	2	0.27
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	8	0.27
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	8	0.27
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	8	0.27
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	8	0.27
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	8	0.27
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	8	0.27
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD21	2	0.27
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD22	2	0.27
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD23	2	0.27
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD21	10	0.27
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD22	10	0.27
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD23	10	0.27
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	4	0.27
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	6	0.26
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	6	0.26
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	6	0.26
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	6	0.26
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	6	0.26
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	6	0.26
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	6	0.26
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	6	0.26
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	6	0.26
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD11	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD12	9	0.26
(3,217)	1:43:A:ILE:HG21	1:43:A:ILE:HD13	9	0.26
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD11	9	0.26
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD12	9	0.26
(3,217)	1:43:A:ILE:HG22	1:43:A:ILE:HD13	9	0.26
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD11	9	0.26
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD12	9	0.26
(3,217)	1:43:A:ILE:HG23	1:43:A:ILE:HD13	9	0.26
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD21	7	0.26
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD22	7	0.26
(3,162)	1:34:A:LEU:HA	1:34:A:LEU:HD23	7	0.26
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD21	8	0.26
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD22	8	0.26
(3,26)	1:34:A:LEU:H	1:34:A:LEU:HD23	8	0.26
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD11	10	0.26
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD12	10	0.26
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD13	10	0.26
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	3	0.26
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	4	0.26
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG11	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG12	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG13	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG21	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG22	1	0.25
(3,176)	1:37:A:VAL:H	1:37:A:VAL:HG23	1	0.25
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	7	0.25
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	7	0.25
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	7	0.25
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD11	3	0.25
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD12	3	0.25
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD13	3	0.25
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG21	1	0.25
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG22	1	0.25
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG23	1	0.25
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG21	10	0.25
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG22	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG23	10	0.25
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	7	0.25
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD11	2	0.24
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD12	2	0.24
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD13	2	0.24
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD11	8	0.24
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD12	8	0.24
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD13	8	0.24
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	6	0.24
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	9	0.24
(1,1)	1:34:A:LEU:H	1:45:A:GLU:O	5	0.24
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	3	0.23
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	3	0.23
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	3	0.23
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	3	0.23
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	3	0.23
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	3	0.23
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	3	0.23
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	3	0.23
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	3	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	8	0.23
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	8	0.23
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	6	0.23
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	6	0.23
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	6	0.23
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	9	0.22
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	9	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	7	0.22
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	7	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD11	1	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD12	1	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD13	1	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD11	6	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD12	6	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD13	6	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD11	9	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD12	9	0.22
(3,24)	1:34:A:LEU:H	1:34:A:LEU:HD13	9	0.22
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	2	0.22
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	3	0.21
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	3	0.21
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	3	0.21
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	7	0.21
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	7	0.21
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	7	0.21
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	9	0.21
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	9	0.21
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	9	0.21
(3,117)	1:57:A:LEU:HA	1:58:A:LEU:H	3	0.21
(3,97)	1:43:A:ILE:HG21	1:165:A:ARG:H	1	0.21
(3,97)	1:43:A:ILE:HG22	1:165:A:ARG:H	1	0.21
(3,97)	1:43:A:ILE:HG23	1:165:A:ARG:H	1	0.21
(3,97)	1:43:A:ILE:HG21	1:165:A:ARG:H	8	0.21
(3,97)	1:43:A:ILE:HG22	1:165:A:ARG:H	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,97)	1:43:A:ILE:HG23	1:165:A:ARG:H	8	0.21
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	9	0.21
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	9	0.21
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	9	0.21
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	2	0.21
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	4	0.21
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	3	0.21
(1,10)	1:38:A:ILE:N	1:41:A:PHE:O	10	0.21
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	9	0.2
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	9	0.2
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	9	0.2
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	9	0.2
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	9	0.2
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	9	0.2
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	9	0.2
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	9	0.2
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	9	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG11	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG12	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG13	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG21	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG22	1	0.2
(3,214)	1:42:A:VAL:H	1:42:A:VAL:HG23	1	0.2
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	10	0.2
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	10	0.2
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	10	0.2
(3,121)	1:58:A:LEU:HA	1:59:A:VAL:H	3	0.2
(1,20)	1:36:A:HIS:O	1:43:A:ILE:N	10	0.2
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	5	0.19
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	5	0.19
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	5	0.19
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	5	0.19
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	5	0.19
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	5	0.19
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	5	0.19
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	5	0.19
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	3	0.19
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	3	0.19
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	3	0.19
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	3	0.19
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	3	0.19
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	3	0.19
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	3	0.19
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	3	0.19
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	3	0.19
(3,74)	1:40:A:GLY:H	1:41:A:PHE:HD1	7	0.19
(3,74)	1:40:A:GLY:H	1:41:A:PHE:HD2	7	0.19
(1,21)	1:38:A:ILE:N	1:41:A:PHE:O	5	0.19
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	1	0.19
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	6	0.18
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	6	0.18
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	6	0.18
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	6	0.18
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	6	0.18
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	6	0.18
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	6	0.18
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	6	0.18
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	6	0.18
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	2	0.18
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	2	0.18
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	2	0.18
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	2	0.18
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	2	0.18
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	2	0.18
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	2	0.18
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	2	0.18
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	2	0.18
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	5	0.18
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	5	0.18
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	5	0.18
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	5	0.18
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	5	0.18
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	5	0.18
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	5	0.18
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	5	0.18
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	5	0.18
(3,119)	1:58:A:LEU:H	1:58:A:LEU:HB2	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,119)	1:58:A:LEU:H	1:58:A:LEU:HB3	7	0.18
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	4	0.18
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	4	0.18
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	4	0.18
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	8	0.18
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	8	0.18
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	8	0.18
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	6	0.18
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	6	0.18
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	6	0.18
(3,74)	1:40:A:GLY:H	1:41:A:PHE:HD1	1	0.18
(3,74)	1:40:A:GLY:H	1:41:A:PHE:HD2	1	0.18
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	2	0.17
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	2	0.17
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	2	0.17
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	2	0.17
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	2	0.17
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	2	0.17
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	2	0.17
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	2	0.17
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	2	0.17
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	4	0.17
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	4	0.17
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	4	0.17
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	4	0.17
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	4	0.17
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	4	0.17
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	4	0.17
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	4	0.17
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	4	0.17
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE1	7	0.17
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE2	7	0.17
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE3	7	0.17
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE1	7	0.17
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE2	7	0.17
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE3	7	0.17
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE1	7	0.17
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE2	7	0.17
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE3	7	0.17
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	2	0.17
(1,18)	1:34:A:LEU:O	1:45:A:GLU:N	5	0.17
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:36:A:HIS:O	1:43:A:ILE:H	9	0.17
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG11	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG12	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG13	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG21	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG22	10	0.16
(3,249)	1:52:A:VAL:H	1:52:A:VAL:HG23	10	0.16
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	3	0.16
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	3	0.16
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	3	0.16
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	3	0.16
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	3	0.16
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	3	0.16
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	3	0.16
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	3	0.16
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	3	0.16
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE1	4	0.16
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE2	4	0.16
(3,235)	1:43:A:ILE:HG21	1:170:A:MET:HE3	4	0.16
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE1	4	0.16
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE2	4	0.16
(3,235)	1:43:A:ILE:HG22	1:170:A:MET:HE3	4	0.16
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE1	4	0.16
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE2	4	0.16
(3,235)	1:43:A:ILE:HG23	1:170:A:MET:HE3	4	0.16
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	1	0.16
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	1	0.16
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	1	0.16
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	2	0.16
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	2	0.16
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	2	0.16
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	5	0.16
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	5	0.16
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	5	0.16
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE1	10	0.16
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE2	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE3	10	0.16
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE1	10	0.16
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE2	10	0.16
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE3	10	0.16
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE1	10	0.16
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE2	10	0.16
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE3	10	0.16
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	3	0.16
(3,7)	1:32:A:GLN:HA	1:33:A:ILE:H	5	0.16
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG21	7	0.16
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG22	7	0.16
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG23	7	0.16
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	10	0.16
(1,15)	1:46:A:GLY:H	1:163:A:TYR:O	2	0.16
(1,13)	1:46:A:GLY:H	1:163:A:TYR:O	2	0.16
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	2	0.15
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	2	0.15
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	2	0.15
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	2	0.15
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	2	0.15
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	2	0.15
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	2	0.15
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	2	0.15
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	2	0.15
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	7	0.15
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	7	0.15
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	7	0.15
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	7	0.15
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	7	0.15
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	7	0.15
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	7	0.15
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	7	0.15
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	7	0.15
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	10	0.15
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	10	0.15
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	10	0.15
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	10	0.15
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	10	0.15
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	10	0.15
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	10	0.15
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	10	0.15
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD11	4	0.15
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD12	4	0.15
(3,159)	1:34:A:LEU:H	1:34:A:LEU:HD13	4	0.15
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD11	4	0.15
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD12	4	0.15
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD13	4	0.15
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD21	4	0.15
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD22	4	0.15
(3,157)	1:34:A:LEU:H	1:34:A:LEU:HD23	4	0.15
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	5	0.15
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	5	0.15
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	5	0.15
(3,74)	1:40:A:GLY:H	1:41:A:PHE:HD1	8	0.15
(3,74)	1:40:A:GLY:H	1:41:A:PHE:HD2	8	0.15
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	5	0.15
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG21	8	0.15
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG22	8	0.15
(3,4)	1:32:A:GLN:HA	1:33:A:ILE:HG23	8	0.15
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	9	0.15
(1,15)	1:46:A:GLY:H	1:163:A:TYR:O	10	0.15
(1,13)	1:46:A:GLY:H	1:163:A:TYR:O	10	0.15
(1,7)	1:36:A:HIS:O	1:43:A:ILE:H	6	0.15
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	5	0.14
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	5	0.14
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	5	0.14
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	5	0.14
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	5	0.14
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	5	0.14
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	5	0.14
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	5	0.14
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	5	0.14
(3,126)	1:59:A:VAL:H	1:59:A:VAL:HB	7	0.14
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	3	0.14
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	3	0.14
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	3	0.14
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	8	0.14
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	8	0.14
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	8	0.14
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	8	0.14
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	8	0.14
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	8	0.14
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	6	0.14
(1,7)	1:36:A:HIS:O	1:43:A:ILE:H	8	0.14
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE1	4	0.13
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE2	4	0.13
(3,233)	1:43:A:ILE:HD11	1:170:A:MET:HE3	4	0.13
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE1	4	0.13
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE2	4	0.13
(3,233)	1:43:A:ILE:HD12	1:170:A:MET:HE3	4	0.13
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE1	4	0.13
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE2	4	0.13
(3,233)	1:43:A:ILE:HD13	1:170:A:MET:HE3	4	0.13
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD11	1	0.13
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD12	1	0.13
(3,145)	1:33:A:ILE:HA	1:33:A:ILE:HD13	1	0.13
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	1	0.13
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	1	0.13
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	1	0.13
(3,97)	1:43:A:ILE:HG21	1:165:A:ARG:H	7	0.13
(3,97)	1:43:A:ILE:HG22	1:165:A:ARG:H	7	0.13
(3,97)	1:43:A:ILE:HG23	1:165:A:ARG:H	7	0.13
(3,97)	1:43:A:ILE:HG21	1:165:A:ARG:H	10	0.13
(3,97)	1:43:A:ILE:HG22	1:165:A:ARG:H	10	0.13
(3,97)	1:43:A:ILE:HG23	1:165:A:ARG:H	10	0.13
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	2	0.13
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	2	0.13
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	2	0.13
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	3	0.13
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	3	0.13
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	3	0.13
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE1	4	0.13
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE2	4	0.13
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE3	4	0.13
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE1	4	0.13
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE2	4	0.13
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE3	4	0.13
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE1	4	0.13
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE2	4	0.13
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE3	4	0.13
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	1	0.13
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	1	0.13
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	1	0.13
(3,48)	1:37:A:VAL:HA	1:41:A:PHE:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:38:A:ILE:H	1:41:A:PHE:O	3	0.13
(1,7)	1:36:A:HIS:O	1:43:A:ILE:H	1	0.13
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG11	7	0.12
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG12	7	0.12
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG13	7	0.12
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG21	7	0.12
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG22	7	0.12
(3,262)	1:59:A:VAL:H	1:59:A:VAL:HG23	7	0.12
(3,230)	1:43:A:ILE:HD11	1:164:A:LEU:HD21	10	0.12
(3,230)	1:43:A:ILE:HD11	1:164:A:LEU:HD22	10	0.12
(3,230)	1:43:A:ILE:HD11	1:164:A:LEU:HD23	10	0.12
(3,230)	1:43:A:ILE:HD12	1:164:A:LEU:HD21	10	0.12
(3,230)	1:43:A:ILE:HD12	1:164:A:LEU:HD22	10	0.12
(3,230)	1:43:A:ILE:HD12	1:164:A:LEU:HD23	10	0.12
(3,230)	1:43:A:ILE:HD13	1:164:A:LEU:HD21	10	0.12
(3,230)	1:43:A:ILE:HD13	1:164:A:LEU:HD22	10	0.12
(3,230)	1:43:A:ILE:HD13	1:164:A:LEU:HD23	10	0.12
(3,224)	1:43:A:ILE:HD11	1:164:A:LEU:HD21	10	0.12
(3,224)	1:43:A:ILE:HD11	1:164:A:LEU:HD22	10	0.12
(3,224)	1:43:A:ILE:HD11	1:164:A:LEU:HD23	10	0.12
(3,224)	1:43:A:ILE:HD12	1:164:A:LEU:HD21	10	0.12
(3,224)	1:43:A:ILE:HD12	1:164:A:LEU:HD22	10	0.12
(3,224)	1:43:A:ILE:HD12	1:164:A:LEU:HD23	10	0.12
(3,224)	1:43:A:ILE:HD13	1:164:A:LEU:HD21	10	0.12
(3,224)	1:43:A:ILE:HD13	1:164:A:LEU:HD22	10	0.12
(3,224)	1:43:A:ILE:HD13	1:164:A:LEU:HD23	10	0.12
(3,131)	1:61:A:ASN:HA	1:62:A:LEU:H	8	0.12
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE1	8	0.12
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE2	8	0.12
(3,101)	1:43:A:ILE:HA	1:170:A:MET:HE3	8	0.12
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	7	0.12
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	7	0.12
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	7	0.12
(3,96)	1:43:A:ILE:HD11	1:165:A:ARG:H	10	0.12
(3,96)	1:43:A:ILE:HD12	1:165:A:ARG:H	10	0.12
(3,96)	1:43:A:ILE:HD13	1:165:A:ARG:H	10	0.12
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD21	4	0.12
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD22	4	0.12
(3,94)	1:43:A:ILE:HA	1:164:A:LEU:HD23	4	0.12
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE1	2	0.12
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE2	2	0.12
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE1	2	0.12
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE2	2	0.12
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE3	2	0.12
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE1	2	0.12
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE2	2	0.12
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE3	2	0.12
(3,58)	1:38:A:ILE:HD11	1:41:A:PHE:H	8	0.12
(3,58)	1:38:A:ILE:HD12	1:41:A:PHE:H	8	0.12
(3,58)	1:38:A:ILE:HD13	1:41:A:PHE:H	8	0.12
(3,7)	1:32:A:GLN:HA	1:33:A:ILE:H	4	0.12
(3,3)	1:32:A:GLN:HA	1:33:A:ILE:HD11	5	0.12
(3,3)	1:32:A:GLN:HA	1:33:A:ILE:HD12	5	0.12
(3,3)	1:32:A:GLN:HA	1:33:A:ILE:HD13	5	0.12
(1,17)	1:34:A:LEU:N	1:45:A:GLU:O	8	0.12
(1,16)	1:46:A:GLY:N	1:163:A:TYR:O	2	0.12
(1,14)	1:46:A:GLY:N	1:163:A:TYR:O	2	0.12
(1,11)	1:38:A:ILE:O	1:41:A:PHE:H	10	0.12
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	6	0.11
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	6	0.11
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	6	0.11
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	6	0.11
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	6	0.11
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	6	0.11
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	6	0.11
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	6	0.11
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	6	0.11
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD11	9	0.11
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD12	9	0.11
(3,195)	1:38:A:ILE:HD11	1:43:A:ILE:HD13	9	0.11
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD11	9	0.11
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD12	9	0.11
(3,195)	1:38:A:ILE:HD12	1:43:A:ILE:HD13	9	0.11
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD11	9	0.11
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD12	9	0.11
(3,195)	1:38:A:ILE:HD13	1:43:A:ILE:HD13	9	0.11
(3,124)	1:58:A:LEU:HB2	1:60:A:GLY:H	7	0.11
(3,124)	1:58:A:LEU:HB3	1:60:A:GLY:H	7	0.11
(3,65)	1:38:A:ILE:HG21	1:174:A:HIS:H	2	0.11
(3,65)	1:38:A:ILE:HG22	1:174:A:HIS:H	2	0.11
(3,65)	1:38:A:ILE:HG23	1:174:A:HIS:H	2	0.11
(3,65)	1:38:A:ILE:HG21	1:174:A:HIS:H	3	0.11
(3,65)	1:38:A:ILE:HG22	1:174:A:HIS:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,65)	1:38:A:ILE:HG23	1:174:A:HIS:H	3	0.11
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE1	3	0.11
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE2	3	0.11
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE3	3	0.11
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE1	3	0.11
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE2	3	0.11
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE3	3	0.11
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE1	3	0.11
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE2	3	0.11
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE3	3	0.11
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE1	5	0.11
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE2	5	0.11
(3,63)	1:38:A:ILE:HG21	1:170:A:MET:HE3	5	0.11
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE1	5	0.11
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE2	5	0.11
(3,63)	1:38:A:ILE:HG22	1:170:A:MET:HE3	5	0.11
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE1	5	0.11
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE2	5	0.11
(3,63)	1:38:A:ILE:HG23	1:170:A:MET:HE3	5	0.11
(1,19)	1:36:A:HIS:N	1:43:A:ILE:O	5	0.11
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG12	9	0.1
(3,197)	1:38:A:ILE:HG21	1:43:A:ILE:HG13	9	0.1
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG12	9	0.1
(3,197)	1:38:A:ILE:HG22	1:43:A:ILE:HG13	9	0.1
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG12	9	0.1
(3,197)	1:38:A:ILE:HG23	1:43:A:ILE:HG13	9	0.1
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB2	1	0.1
(3,64)	1:38:A:ILE:HG21	1:170:A:MET:HB3	1	0.1
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB2	1	0.1
(3,64)	1:38:A:ILE:HG22	1:170:A:MET:HB3	1	0.1
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB2	1	0.1
(3,64)	1:38:A:ILE:HG23	1:170:A:MET:HB3	1	0.1
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG21	9	0.1
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG22	9	0.1
(3,38)	1:36:A:HIS:H	1:38:A:ILE:HG23	9	0.1
(1,16)	1:46:A:GLY:N	1:163:A:TYR:O	10	0.1
(1,14)	1:46:A:GLY:N	1:163:A:TYR:O	10	0.1

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

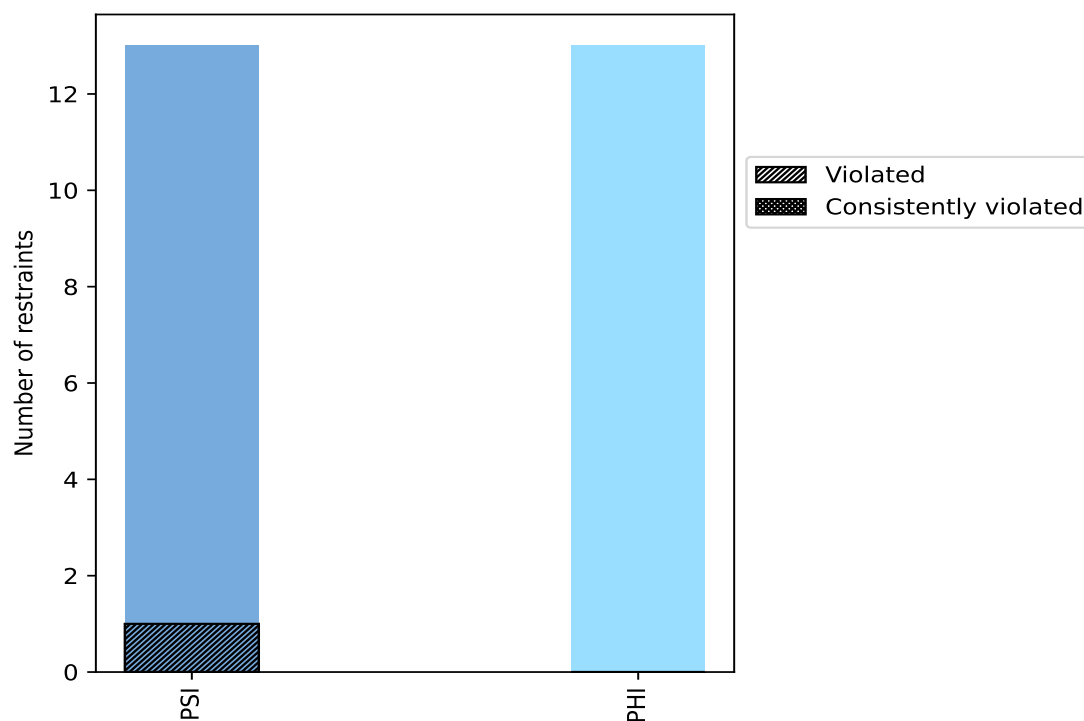
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	13	50.0	1	7.7	3.8	0	0.0	0.0
PHI	13	50.0	0	0.0	0.0	0	0.0	0.0
Total	26	100.0	1	3.8	3.8	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](#)



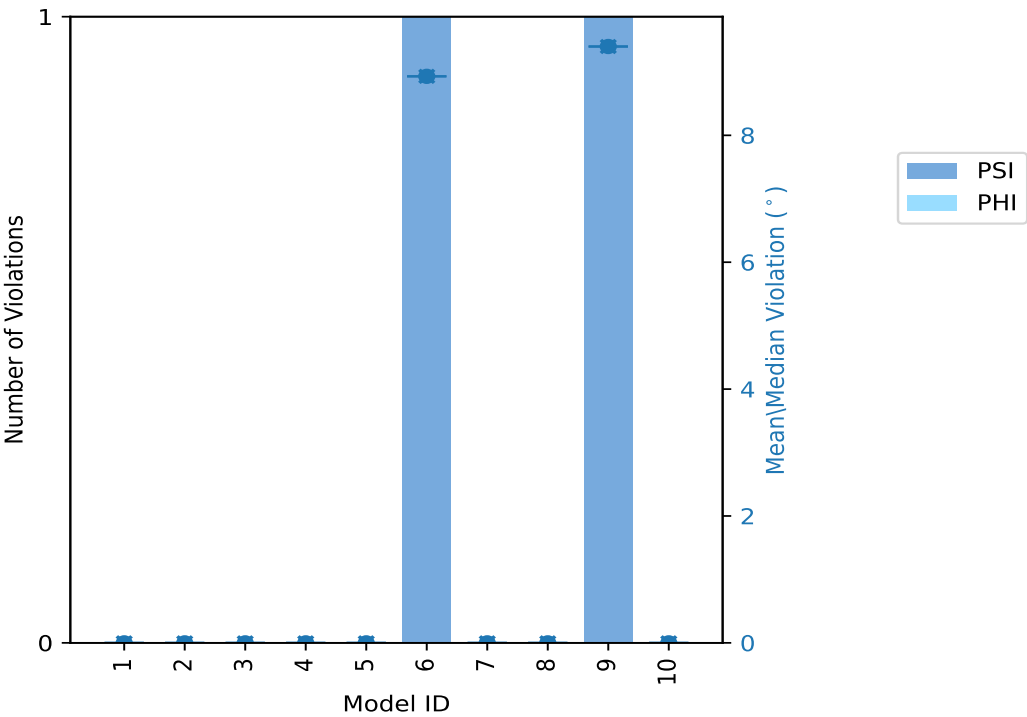
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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 (°)
	PSI	PHI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	1	0	1	8.93	8.93	0.0	8.93
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	1	0	1	9.4	9.4	0.0	9.4
10	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

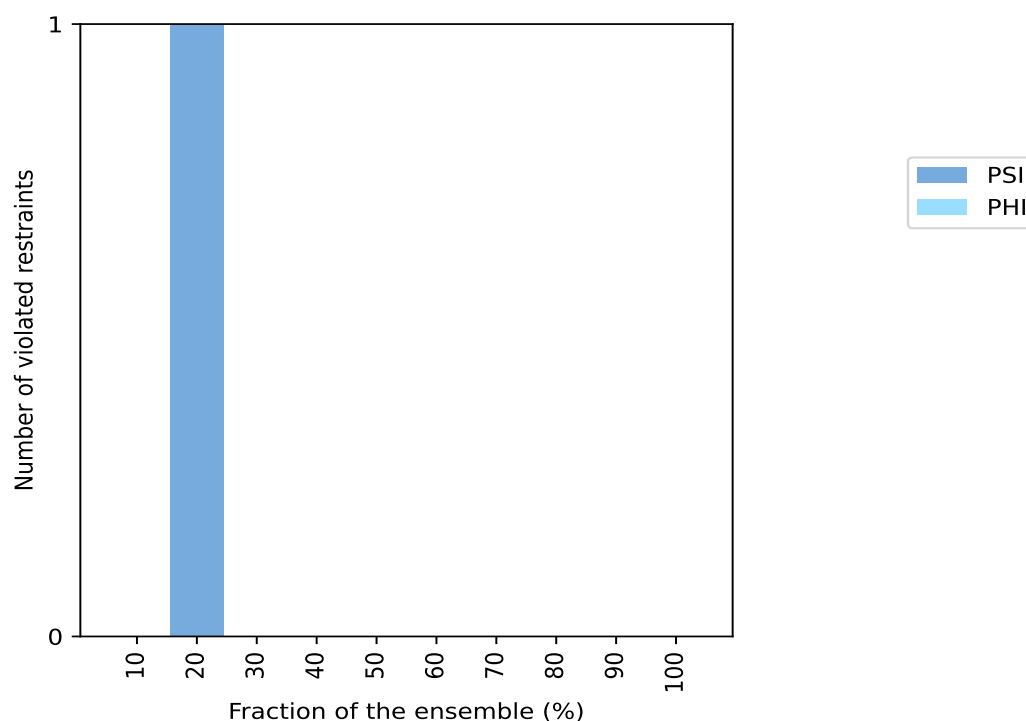
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PSI	PHI	Total	Count ¹	%
0	0	0	1	10.0
1	0	1	2	20.0
0	0	0	3	30.0
0	0	0	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
0	0	0	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

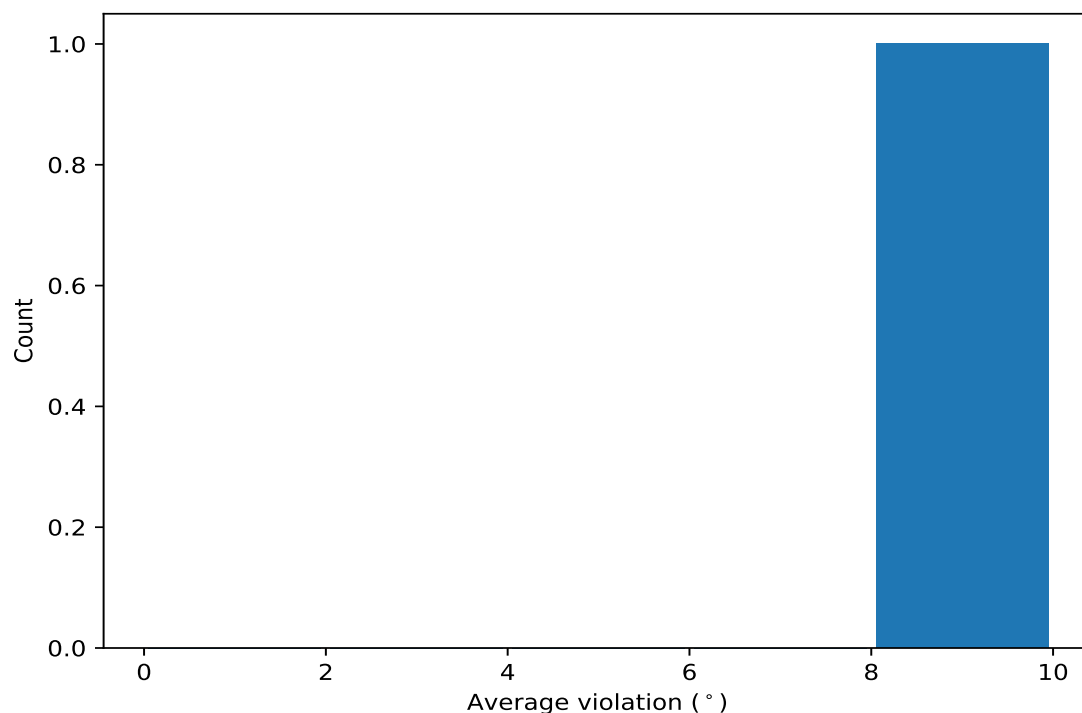
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,12)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:GLU:N	2	9.16	0.24	9.16

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.

Data insufficient to plot histogram

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 (°)
(1,12)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:GLU:N	9	9.4
(1,12)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:GLU:N	6	8.93