



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 10:10 AM UTC

PDB ID : 7K7A / pdb_00007k7a
BMRB ID : 30799
Title : Transmembrane structure of TNFR1
Authors : Zhao, L.; Chou, J.
Deposited on : 2020-09-22

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

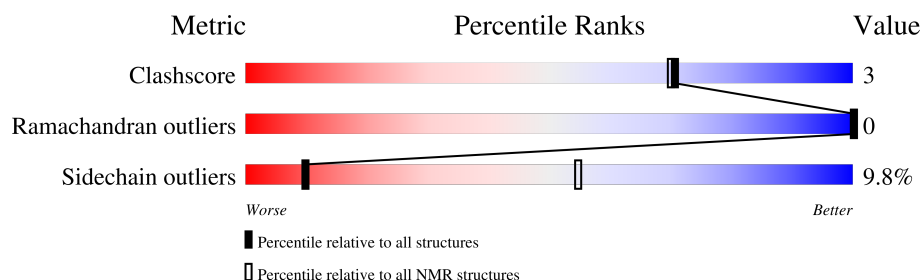
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 9%.

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	30	70% 10% 20%
1	B	30	63% 30%
1	C	30	70% 10% 20%

2 Ensemble composition and analysis

This entry contains 15 models. Model 2 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:211-A:234, B:212-B:232, C:213-C:236 (69)	0.71	2

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

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

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

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 15
2	5, 14

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1515 atoms, of which 795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor necrosis factor receptor superfamily member 1A.

Mol	Chain	Residues	Atoms					Trace
1	A	30	Total	C	H	N	O	0
			505	166	265	37	37	
1	B	30	Total	C	H	N	O	0
			505	166	265	37	37	
1	C	30	Total	C	H	N	O	0
			505	166	265	37	37	

There are 6 discrepancies between the modelled and reference sequences:

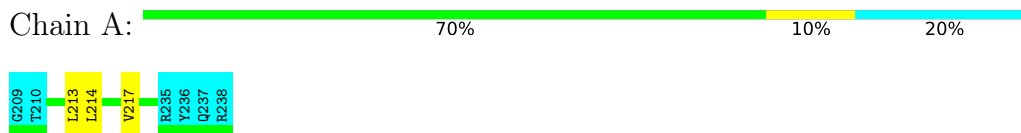
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	CYS	engineered mutation	UNP P19438
A	233	ALA	MET	engineered mutation	UNP P19438
B	223	ALA	CYS	engineered mutation	UNP P19438
B	233	ALA	MET	engineered mutation	UNP P19438
C	223	ALA	CYS	engineered mutation	UNP P19438
C	233	ALA	MET	engineered mutation	UNP P19438

4 Residue-property plots [i](#)

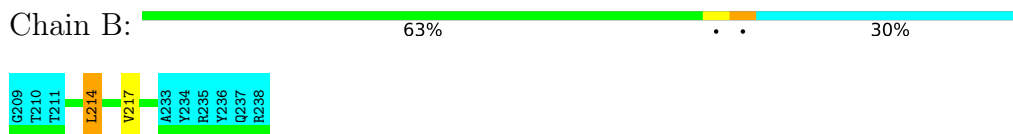
4.1 Average score per residue in the NMR ensemble

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

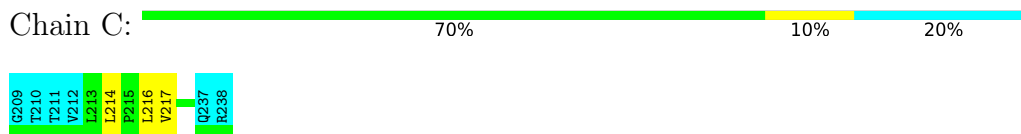
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



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- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

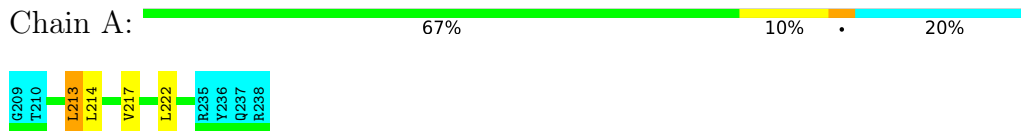


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

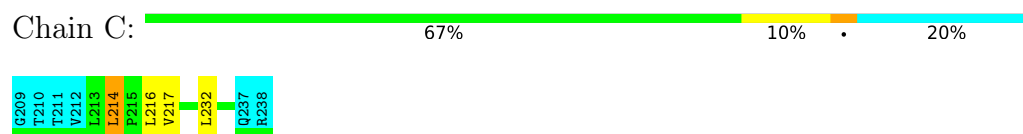
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

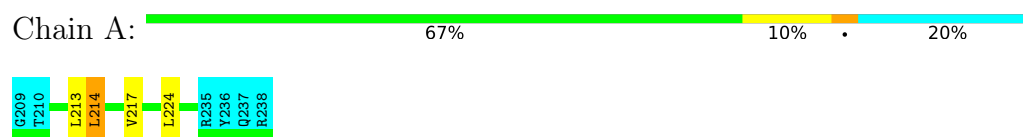


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.2 Score per residue for model 2 (medoid)

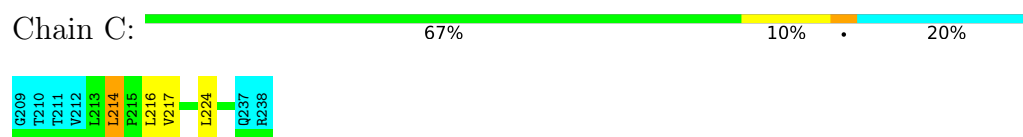
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

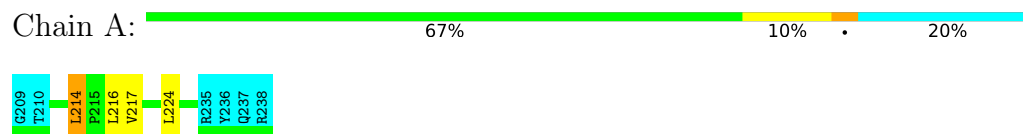


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.3 Score per residue for model 3

- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

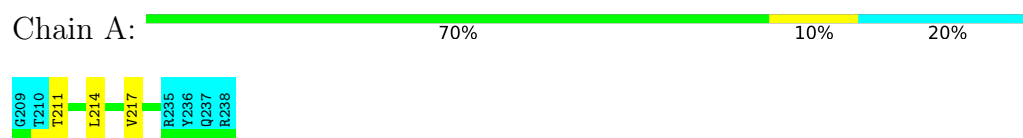


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.4 Score per residue for model 4

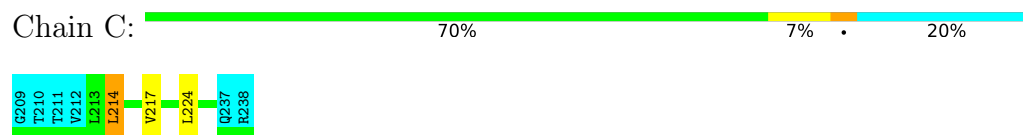
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

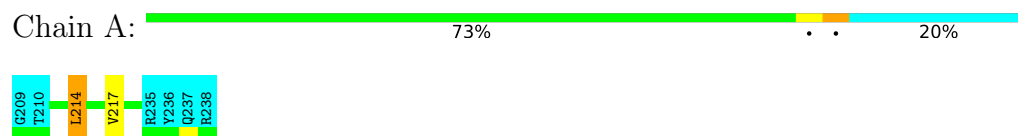


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.5 Score per residue for model 5

- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A





- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.6 Score per residue for model 6

- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

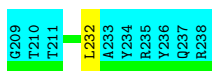


4.2.7 Score per residue for model 7

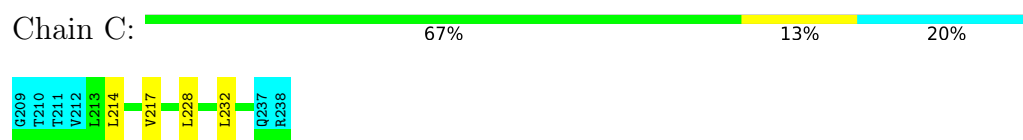
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

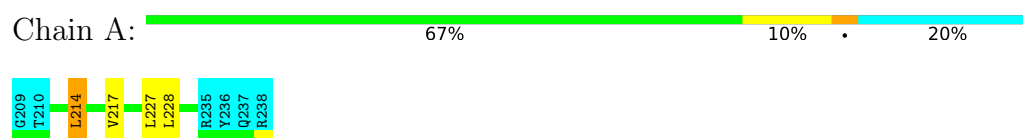


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.8 Score per residue for model 8

- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

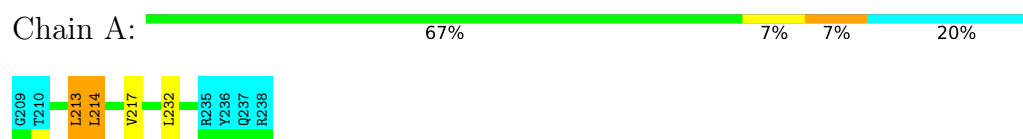


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.9 Score per residue for model 9

- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

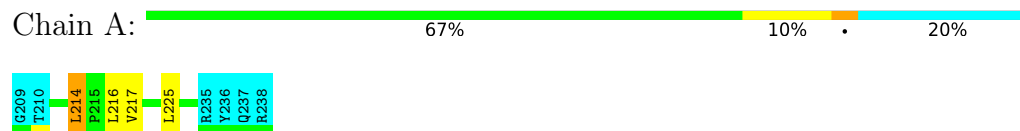


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.10 Score per residue for model 10

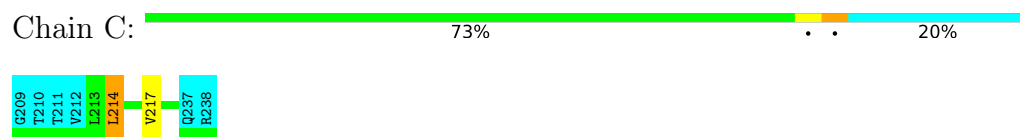
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

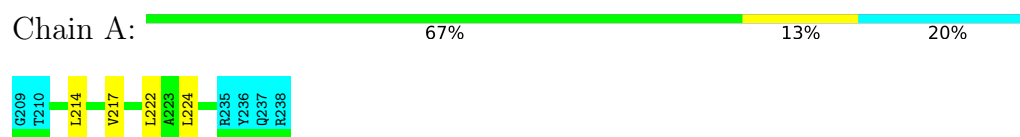


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.11 Score per residue for model 11

- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

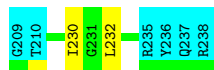




4.2.12 Score per residue for model 12

- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

Chain A: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

Chain B: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

Chain C: 



4.2.13 Score per residue for model 13

- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

Chain A: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

Chain B: 



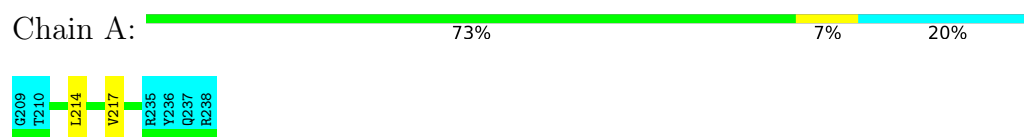
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

Chain C: 



4.2.14 Score per residue for model 14

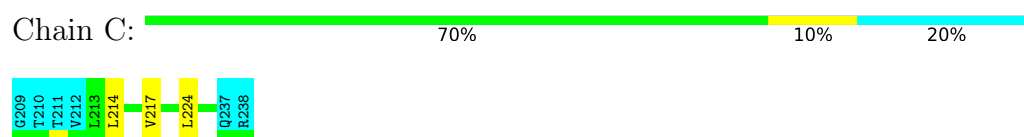
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A

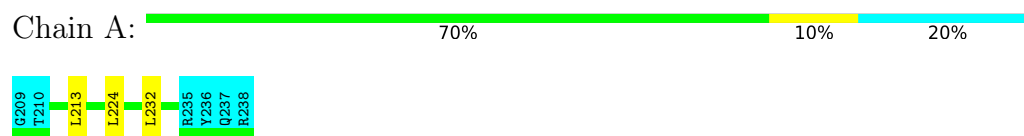


- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



4.2.15 Score per residue for model 15

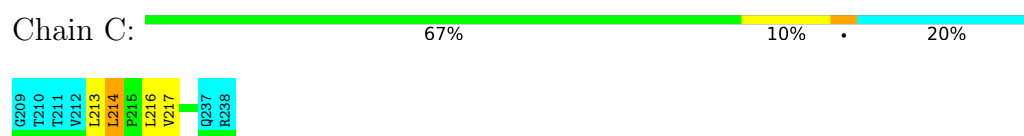
- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



- Molecule 1: Tumor necrosis factor receptor superfamily member 1A



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	106
Number of shifts mapped to atoms	106
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	185	210	210	1±0
1	B	161	189	189	1±1
1	C	194	216	216	2±1
All	All	8100	9225	9225	60

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:227:LEU:O	1:B:230:ILE:HG22	0.57	1.98	6	1
1:A:213:LEU:O	1:A:213:LEU:HD13	0.50	2.06	6	3
1:C:214:LEU:O	1:C:217:VAL:HG12	0.50	2.06	15	15
1:A:232:LEU:HD13	1:A:232:LEU:C	0.49	2.32	15	1
1:C:232:LEU:C	1:C:232:LEU:HD13	0.48	2.32	3	1
1:A:214:LEU:O	1:A:217:VAL:HG12	0.48	2.08	11	13
1:C:214:LEU:CD2	1:C:218:ILE:HD11	0.48	2.39	3	1
1:B:214:LEU:O	1:B:217:VAL:HG12	0.47	2.09	10	12
1:B:232:LEU:HD13	1:B:232:LEU:C	0.46	2.34	13	1
1:B:232:LEU:C	1:B:232:LEU:HD23	0.46	2.35	6	2
1:A:225:LEU:HD11	1:C:228:LEU:HD12	0.46	1.87	7	1
1:C:213:LEU:O	1:C:213:LEU:HD23	0.45	2.12	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:232:LEU:HD23	1:C:232:LEU:C	0.45	2.36	7	3
1:A:232:LEU:C	1:A:232:LEU:HD23	0.44	2.38	12	1
1:C:213:LEU:HD13	1:C:213:LEU:O	0.43	2.14	13	1
1:C:216:LEU:O	1:C:216:LEU:HD13	0.43	2.14	3	1
1:B:216:LEU:HD13	1:B:216:LEU:O	0.42	2.15	3	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	24/30 (80%)	23±0 (98±2%)	1±0 (2±2%)	0±0 (0±0%)	100	100
1	B	21/30 (70%)	21±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	C	24/30 (80%)	24±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1035/1350 (77%)	1026 (99%)	9 (1%)	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	20/25 (80%)	18±1 (90±5%)	2±1 (10±5%)	10	55
1	B	18/25 (72%)	16±1 (89±3%)	2±1 (11±3%)	8	50
1	C	20/25 (80%)	18±1 (92±5%)	2±1 (8±5%)	12	59
All	All	870/1125 (77%)	785 (90%)	85 (10%)	10	55

All 28 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	B	214	LEU	11
1	C	216	LEU	9
1	A	214	LEU	8
1	C	214	LEU	6
1	B	216	LEU	6
1	A	213	LEU	5
1	A	224	LEU	4
1	C	224	LEU	4
1	A	222	LEU	3
1	B	222	LEU	3
1	A	216	LEU	3
1	B	224	LEU	3
1	B	220	PHE	2
1	B	226	SER	2
1	C	213	LEU	2
1	C	222	LEU	2
1	C	232	LEU	1
1	A	220	PHE	1
1	B	232	LEU	1
1	A	227	LEU	1
1	A	228	LEU	1
1	B	227	LEU	1
1	A	232	LEU	1
1	A	225	LEU	1
1	B	225	LEU	1
1	A	230	ILE	1
1	C	228	LEU	1
1	B	228	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *bmrbl.txt*

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	106
Number of shifts mapped to atoms	106
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	28	0.20 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	26	-2.01 ± 0.09	Should be applied
^{15}N	26	0.55 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 9%, i.e. 91 atoms were assigned a chemical shift out of a possible 1057. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	91/345 (26%)	22/141 (16%)	47/138 (34%)	22/66 (33%)
Sidechain	0/595 (0%)	0/410 (0%)	0/182 (0%)	0/3 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/117 (0%)	0/57 (0%)	0/60 (0%)	0/0 (—%)
Overall	91/1057 (9%)	22/608 (4%)	47/380 (12%)	22/69 (32%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 106 atoms were assigned a chemical shift out of a possible 1365. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	106/453 (23%)	26/186 (14%)	54/180 (30%)	26/87 (30%)
Sidechain	0/768 (0%)	0/519 (0%)	0/228 (0%)	0/21 (0%)
Aromatic	0/144 (0%)	0/69 (0%)	0/75 (0%)	0/0 (—%)
Overall	106/1365 (8%)	26/774 (3%)	54/483 (11%)	26/108 (24%)

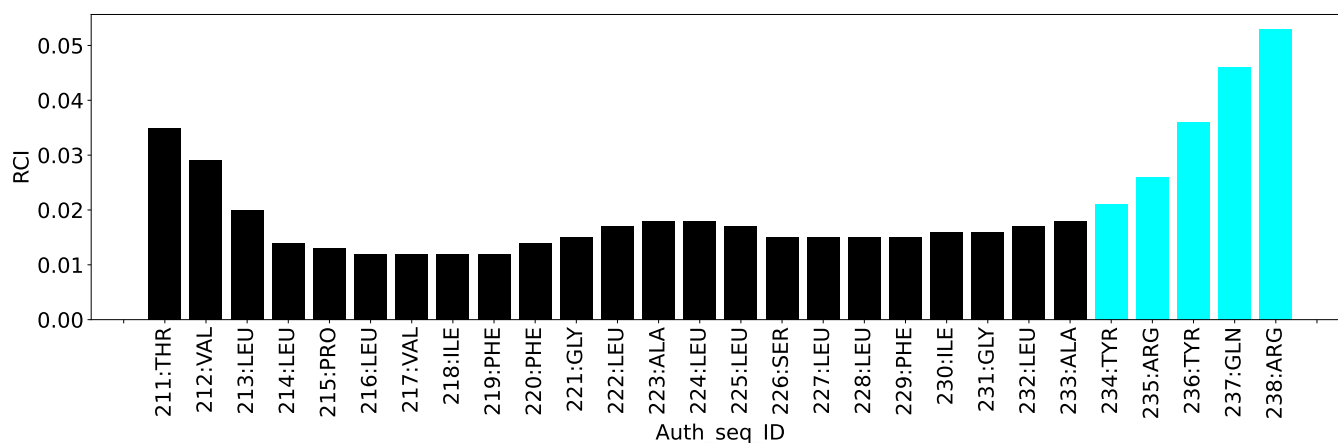
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	540
Intra-residue ($ i-j =0$)	180
Sequential ($ i-j =1$)	219
Medium range ($ i-j >1$ and $ i-j <5$)	138
Long range ($ i-j \geq 5$)	3
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	6.0
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	22.4	0.2
0.2-0.5 (Medium)	16.2	0.5
>0.5 (Large)	27.2	5.91

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

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

9 Distance violation analysis ⓘ

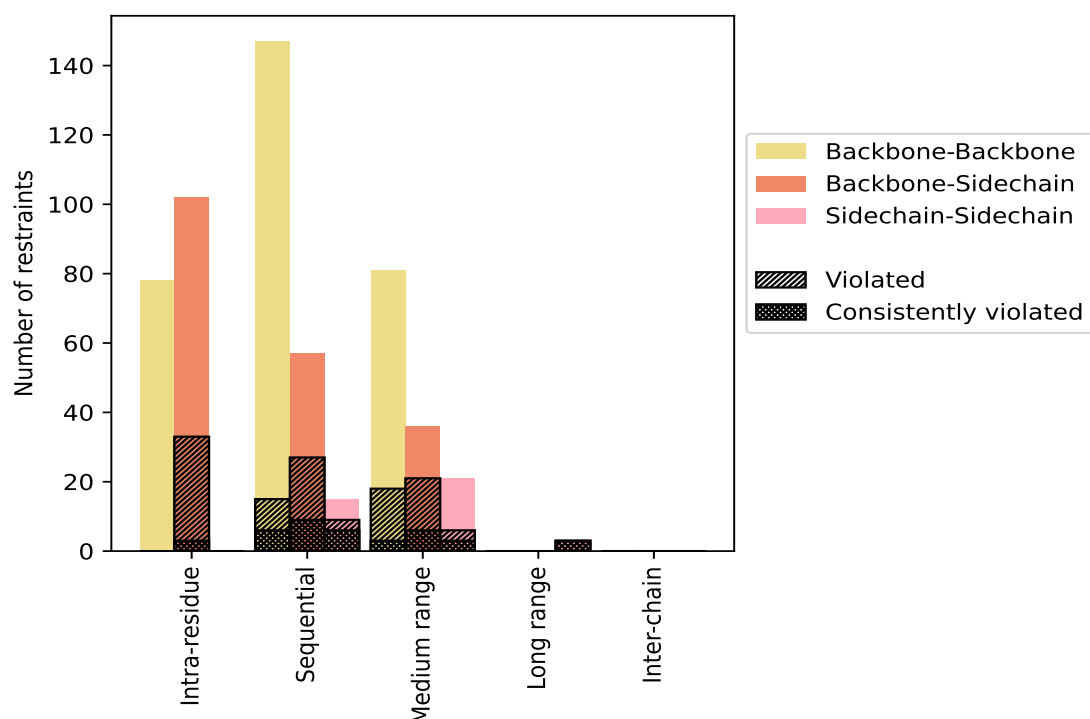
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	180	33.3	33	18.3	6.1	3	1.7	0.6
Backbone-Backbone	78	14.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	102	18.9	33	32.4	6.1	3	2.9	0.6
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	219	40.6	51	23.3	9.4	21	9.6	3.9
Backbone-Backbone	147	27.2	15	10.2	2.8	6	4.1	1.1
Backbone-Sidechain	57	10.6	27	47.4	5.0	9	15.8	1.7
Sidechain-Sidechain	15	2.8	9	60.0	1.7	6	40.0	1.1
Medium range (i-j >1 & i-j <5)	138	25.6	45	32.6	8.3	12	8.7	2.2
Backbone-Backbone	81	15.0	18	22.2	3.3	3	3.7	0.6
Backbone-Sidechain	36	6.7	21	58.3	3.9	6	16.7	1.1
Sidechain-Sidechain	21	3.9	6	28.6	1.1	3	14.3	0.6
Long range (i-j ≥5)	3	0.6	3	100.0	0.6	3	100.0	0.6
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	3	0.6	3	100.0	0.6	3	100.0	0.6
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	540	100.0	132	24.4	24.4	39	7.2	7.2
Backbone-Backbone	306	56.7	33	10.8	6.1	9	2.9	1.7
Backbone-Sidechain	195	36.1	81	41.5	15.0	18	9.2	3.3
Sidechain-Sidechain	39	7.2	18	46.2	3.3	12	30.8	2.2

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	15	36	27	3	0	81	0.97	5.14	1.3	0.31
2	15	36	24	3	0	78	0.94	5.54	1.36	0.22
3	9	30	27	3	0	69	1.09	5.86	1.49	0.27
4	12	27	18	3	0	60	1.24	5.91	1.55	0.36
5	21	27	30	3	0	81	0.97	5.74	1.34	0.25
6	12	27	21	3	0	63	1.18	5.18	1.4	0.38
7	6	33	18	3	0	60	1.32	5.28	1.53	0.38
8	12	27	18	3	0	60	1.15	5.75	1.54	0.28
9	12	27	21	3	0	63	1.13	4.97	1.4	0.25
10	18	27	24	3	0	72	1.04	5.08	1.34	0.32

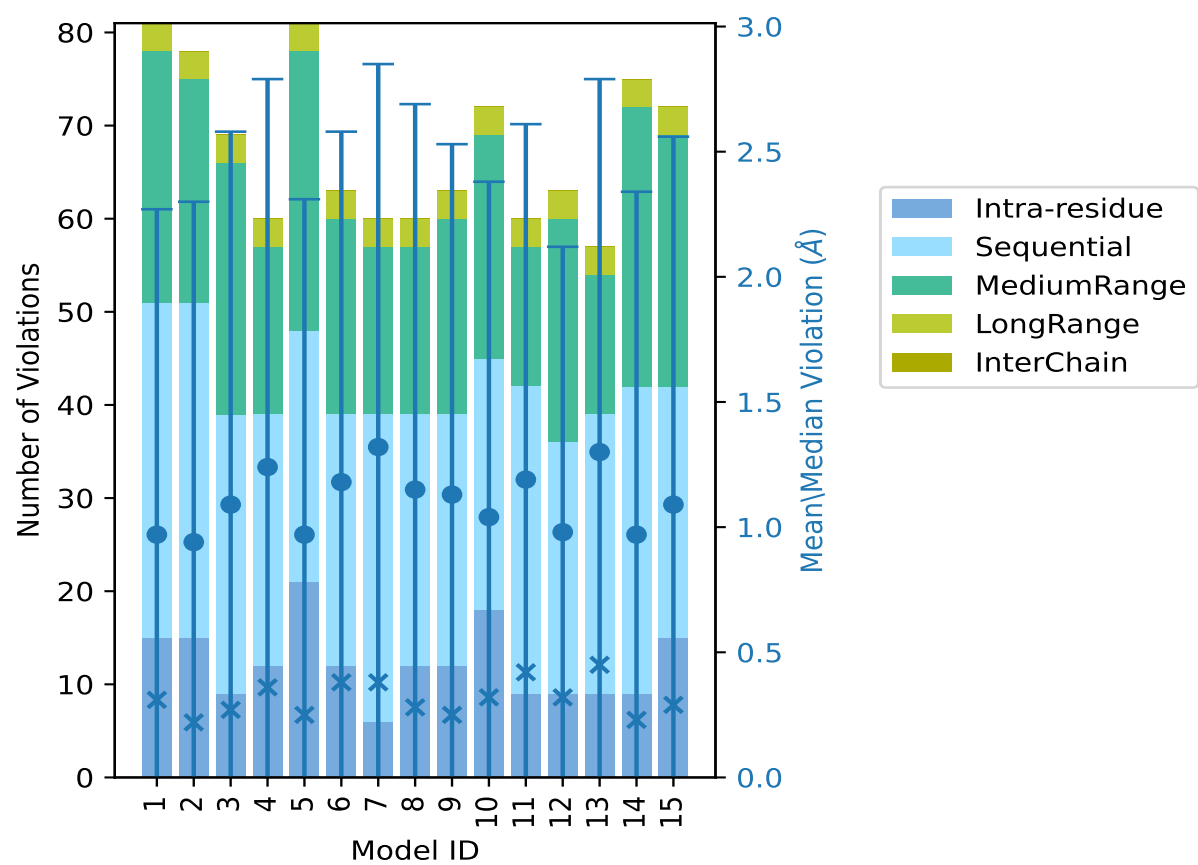
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	9	33	15	3	0	60	1.19	5.04	1.42	0.42
12	9	27	24	3	0	63	0.98	4.26	1.14	0.32
13	9	30	15	3	0	57	1.3	5.03	1.49	0.45
14	9	33	30	3	0	75	0.97	5.27	1.37	0.23
15	15	27	27	3	0	72	1.09	5.76	1.47	0.29

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

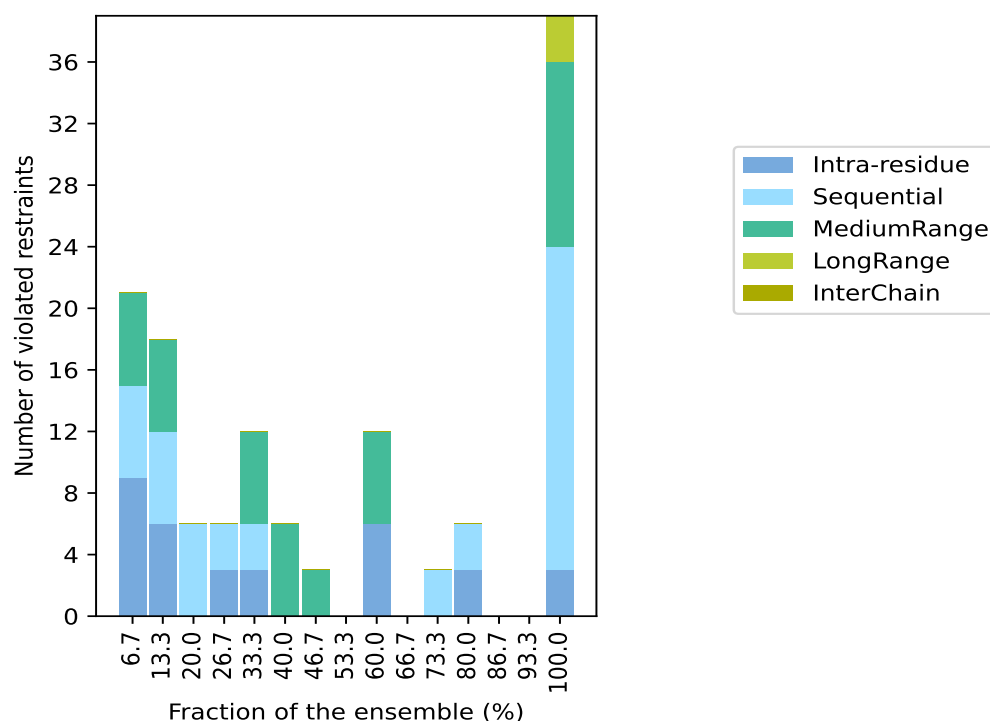
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 408(IR:147, SQ:168, MR:93, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
9	6	6	0	0	21	1	6.7
6	6	6	0	0	18	2	13.3
0	6	0	0	0	6	3	20.0
3	3	0	0	0	6	4	26.7
3	3	6	0	0	12	5	33.3
0	0	6	0	0	6	6	40.0
0	0	3	0	0	3	7	46.7
0	0	0	0	0	0	8	53.3
6	0	6	0	0	12	9	60.0
0	0	0	0	0	0	10	66.7
0	3	0	0	0	3	11	73.3
3	3	0	0	0	6	12	80.0
0	0	0	0	0	0	13	86.7
0	0	0	0	0	0	14	93.3
3	21	12	3	0	39	15	100.0

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

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

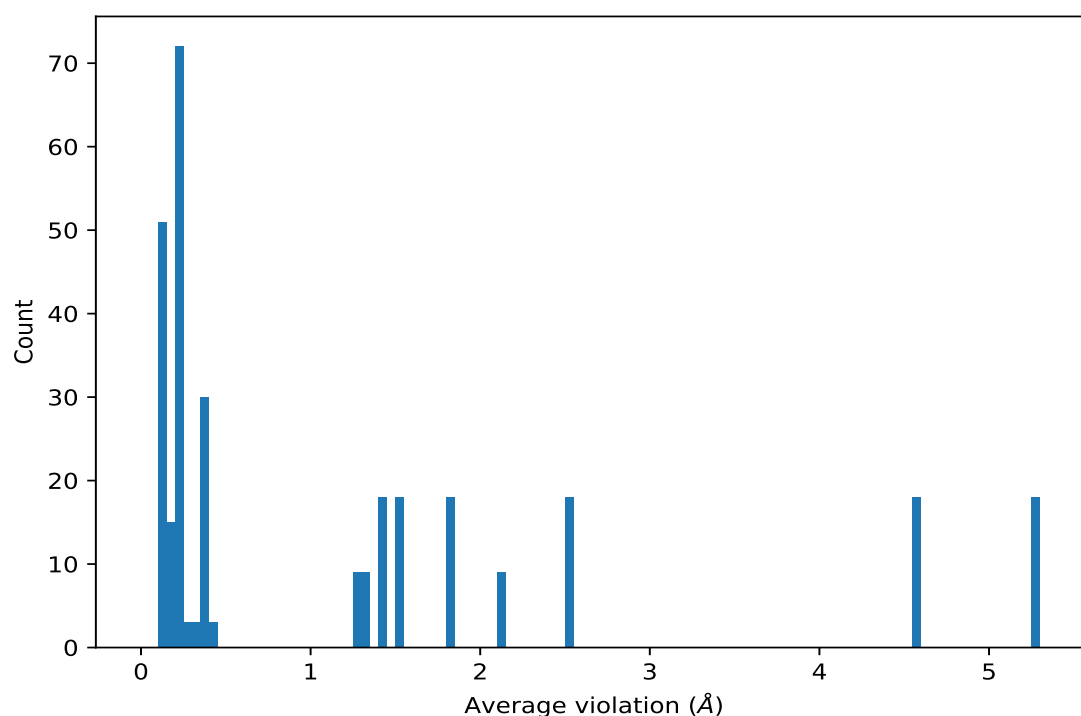
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	15	5.26	0.61	5.27
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	15	5.26	0.61	5.27
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	15	5.26	0.61	5.27
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	15	5.26	0.61	5.27
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	15	5.26	0.61	5.27
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	15	5.26	0.61	5.27
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	15	5.26	0.61	5.27
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	15	5.26	0.61	5.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	15	5.26	0.61	5.27
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	15	5.26	0.61	5.27
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	15	4.55	0.16	4.57
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	15	4.55	0.16	4.57
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	15	2.5	0.24	2.44
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	15	2.5	0.24	2.44
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	15	2.1	0.05	2.08
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	15	2.1	0.05	2.08
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	15	2.1	0.05	2.08
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	15	2.1	0.05	2.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	15	2.1	0.05	2.08
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	15	2.1	0.05	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	15	2.1	0.05	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	15	2.1	0.05	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	15	2.1	0.05	2.08
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	15	1.8	0.44	1.68
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	15	1.8	0.44	1.68
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	15	1.52	0.1	1.56
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	15	1.52	0.1	1.56
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	15	1.41	0.57	1.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	15	1.41	0.57	1.36
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	15	1.41	0.57	1.36
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	15	1.41	0.57	1.36
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	15	1.41	0.57	1.36
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	15	1.41	0.57	1.36
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	15	1.41	0.57	1.36
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	15	1.41	0.57	1.36
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	15	1.41	0.57	1.36
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	15	1.41	0.57	1.36
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	15	1.31	0.02	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	15	1.31	0.02	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	15	1.31	0.02	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	15	1.31	0.02	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	15	1.31	0.02	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	15	1.31	0.02	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	15	1.31	0.02	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	15	1.31	0.02	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	15	1.31	0.02	1.3
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	15	1.27	0.25	1.3
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	15	1.27	0.25	1.3
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	15	1.27	0.25	1.3
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	15	1.27	0.25	1.3
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	15	1.27	0.25	1.3
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	15	1.27	0.25	1.3
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	15	1.27	0.25	1.3
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	15	1.27	0.25	1.3
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	15	1.27	0.25	1.3
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	15	0.32	0.01	0.32
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	15	0.32	0.01	0.32
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	15	0.32	0.01	0.32
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	15	0.21	0.01	0.21
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	15	0.21	0.01	0.21
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	15	0.21	0.01	0.21
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	15	0.21	0.04	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	15	0.21	0.04	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	15	0.21	0.04	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	15	0.21	0.04	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	15	0.21	0.04	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	15	0.21	0.04	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	15	0.21	0.04	0.2
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	15	0.21	0.04	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	15	0.21	0.04	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	15	0.21	0.04	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	15	0.21	0.04	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	15	0.21	0.04	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	15	0.21	0.04	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	15	0.21	0.04	0.2
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	15	0.21	0.04	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	15	0.21	0.04	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	15	0.21	0.04	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	15	0.21	0.04	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	15	0.21	0.04	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	15	0.21	0.04	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	15	0.21	0.04	0.2
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	12	0.26	0.1	0.23
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	12	0.26	0.1	0.23
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	12	0.26	0.1	0.23
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	12	0.2	0.1	0.16
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	12	0.2	0.1	0.16
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	12	0.2	0.1	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	12	0.2	0.1	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	12	0.2	0.1	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	12	0.2	0.1	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	12	0.2	0.1	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	12	0.2	0.1	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	12	0.2	0.1	0.16
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	11	0.14	0.02	0.13
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	11	0.14	0.02	0.13
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	11	0.14	0.02	0.13
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	9	0.43	0.08	0.45
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	9	0.43	0.08	0.45
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	9	0.43	0.08	0.45
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	9	0.24	0.11	0.2
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	9	0.24	0.11	0.2
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	9	0.24	0.11	0.2
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	9	0.24	0.11	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	9	0.24	0.11	0.2
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	9	0.24	0.11	0.2
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	9	0.24	0.11	0.2
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	9	0.24	0.11	0.2
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	9	0.24	0.11	0.2
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	9	0.13	0.01	0.13
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	9	0.11	0.01	0.11
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	9	0.11	0.01	0.11
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	9	0.11	0.01	0.11
(2,39)	1:219:C:PHE:H	1:216:C:LEU:HA	7	0.13	0.02	0.12
(2,207)	1:219:C:PHE:H	1:216:C:LEU:HA	7	0.13	0.02	0.12
(2,375)	1:219:C:PHE:H	1:216:C:LEU:HA	7	0.13	0.02	0.12
(2,51)	1:221:C:GLY:H	1:218:C:ILE:HA	6	0.13	0.03	0.12
(2,219)	1:221:C:GLY:H	1:218:C:ILE:HA	6	0.13	0.03	0.12
(2,387)	1:221:C:GLY:H	1:218:C:ILE:HA	6	0.13	0.03	0.12
(2,29)	1:217:C:VAL:HG11	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,29)	1:217:C:VAL:HG12	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,29)	1:217:C:VAL:HG13	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,197)	1:217:C:VAL:HG11	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,197)	1:217:C:VAL:HG12	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,197)	1:217:C:VAL:HG13	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,365)	1:217:C:VAL:HG11	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,365)	1:217:C:VAL:HG12	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,365)	1:217:C:VAL:HG13	1:213:C:LEU:HA	6	0.13	0.02	0.12
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	5	0.35	0.07	0.34
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	5	0.35	0.07	0.34
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	5	0.35	0.07	0.34
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	5	0.35	0.07	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	5	0.35	0.07	0.34
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	5	0.35	0.07	0.34
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	5	0.35	0.07	0.34
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	5	0.35	0.07	0.34
(2,96)	1:227:C:LEU:H	1:227:C:LEU:HG	5	0.22	0.13	0.13
(2,264)	1:227:C:LEU:H	1:227:C:LEU:HG	5	0.22	0.13	0.13
(2,432)	1:227:C:LEU:H	1:227:C:LEU:HG	5	0.22	0.13	0.13
(2,8)	1:214:C:LEU:H	1:211:C:THR:HA	5	0.17	0.08	0.13
(2,176)	1:214:C:LEU:H	1:211:C:THR:HA	5	0.17	0.08	0.13
(2,344)	1:214:C:LEU:H	1:211:C:THR:HA	5	0.17	0.08	0.13
(2,109)	1:229:C:PHE:H	1:228:C:LEU:HB2	5	0.13	0.02	0.14
(2,277)	1:229:C:PHE:H	1:228:C:LEU:HB2	5	0.13	0.02	0.14
(2,445)	1:229:C:PHE:H	1:228:C:LEU:HB2	5	0.13	0.02	0.14
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	4	0.23	0.11	0.18
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	4	0.23	0.11	0.18
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	4	0.23	0.11	0.18
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	4	0.23	0.11	0.18
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	4	0.23	0.11	0.18
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	4	0.23	0.11	0.18
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	4	0.23	0.11	0.18
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	4	0.23	0.11	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	4	0.23	0.11	0.18
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	4	0.23	0.11	0.18
(2,12)	1:214:C:LEU:H	1:214:C:LEU:HB3	4	0.15	0.05	0.13
(2,180)	1:214:C:LEU:H	1:214:C:LEU:HB3	4	0.15	0.05	0.13
(2,348)	1:214:C:LEU:H	1:214:C:LEU:HB3	4	0.15	0.05	0.13
(2,167)	1:238:C:ARG:H	1:237:C:GLN:HA	3	0.2	0.0	0.2
(2,335)	1:238:C:ARG:H	1:237:C:GLN:HA	3	0.2	0.0	0.2
(2,503)	1:238:C:ARG:H	1:237:C:GLN:HA	3	0.2	0.0	0.2
(2,66)	1:222:C:LEU:HD21	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,66)	1:222:C:LEU:HD22	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,66)	1:222:C:LEU:HD23	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,234)	1:222:C:LEU:HD21	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,234)	1:222:C:LEU:HD22	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,234)	1:222:C:LEU:HD23	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,402)	1:222:C:LEU:HD21	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,402)	1:222:C:LEU:HD22	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,402)	1:222:C:LEU:HD23	1:223:C:ALA:HA	3	0.11	0.01	0.11
(2,5)	1:213:C:LEU:H	1:213:C:LEU:HB3	2	0.35	0.11	0.35
(2,173)	1:213:C:LEU:H	1:213:C:LEU:HB3	2	0.35	0.11	0.35
(2,341)	1:213:C:LEU:H	1:213:C:LEU:HB3	2	0.35	0.11	0.35
(2,152)	1:235:C:ARG:H	1:235:C:ARG:HD2	2	0.22	0.07	0.22
(2,152)	1:235:C:ARG:H	1:235:C:ARG:HD3	2	0.22	0.07	0.22
(2,320)	1:235:C:ARG:H	1:235:C:ARG:HD2	2	0.22	0.07	0.22
(2,320)	1:235:C:ARG:H	1:235:C:ARG:HD3	2	0.22	0.07	0.22
(2,488)	1:235:C:ARG:H	1:235:C:ARG:HD2	2	0.22	0.07	0.22
(2,488)	1:235:C:ARG:H	1:235:C:ARG:HD3	2	0.22	0.07	0.22
(2,166)	1:237:C:GLN:H	1:238:C:ARG:H	2	0.18	0.04	0.18
(2,334)	1:237:C:GLN:H	1:238:C:ARG:H	2	0.18	0.04	0.18
(2,502)	1:237:C:GLN:H	1:238:C:ARG:H	2	0.18	0.04	0.18
(2,108)	1:229:C:PHE:H	1:228:C:LEU:HB3	2	0.18	0.0	0.18
(2,276)	1:229:C:PHE:H	1:228:C:LEU:HB3	2	0.18	0.0	0.18
(2,444)	1:229:C:PHE:H	1:228:C:LEU:HB3	2	0.18	0.0	0.18
(2,162)	1:237:C:GLN:H	1:235:C:ARG:HA	2	0.16	0.05	0.16
(2,330)	1:237:C:GLN:H	1:235:C:ARG:HA	2	0.16	0.05	0.16
(2,498)	1:237:C:GLN:H	1:235:C:ARG:HA	2	0.16	0.05	0.16
(2,113)	1:230:C:ILE:HG21	1:227:C:LEU:HA	2	0.12	0.0	0.12
(2,113)	1:230:C:ILE:HG22	1:227:C:LEU:HA	2	0.12	0.0	0.12
(2,113)	1:230:C:ILE:HG23	1:227:C:LEU:HA	2	0.12	0.0	0.12
(2,281)	1:230:C:ILE:HG21	1:227:C:LEU:HA	2	0.12	0.0	0.12
(2,281)	1:230:C:ILE:HG22	1:227:C:LEU:HA	2	0.12	0.0	0.12
(2,281)	1:230:C:ILE:HG23	1:227:C:LEU:HA	2	0.12	0.0	0.12
(2,449)	1:230:C:ILE:HG21	1:227:C:LEU:HA	2	0.12	0.0	0.12

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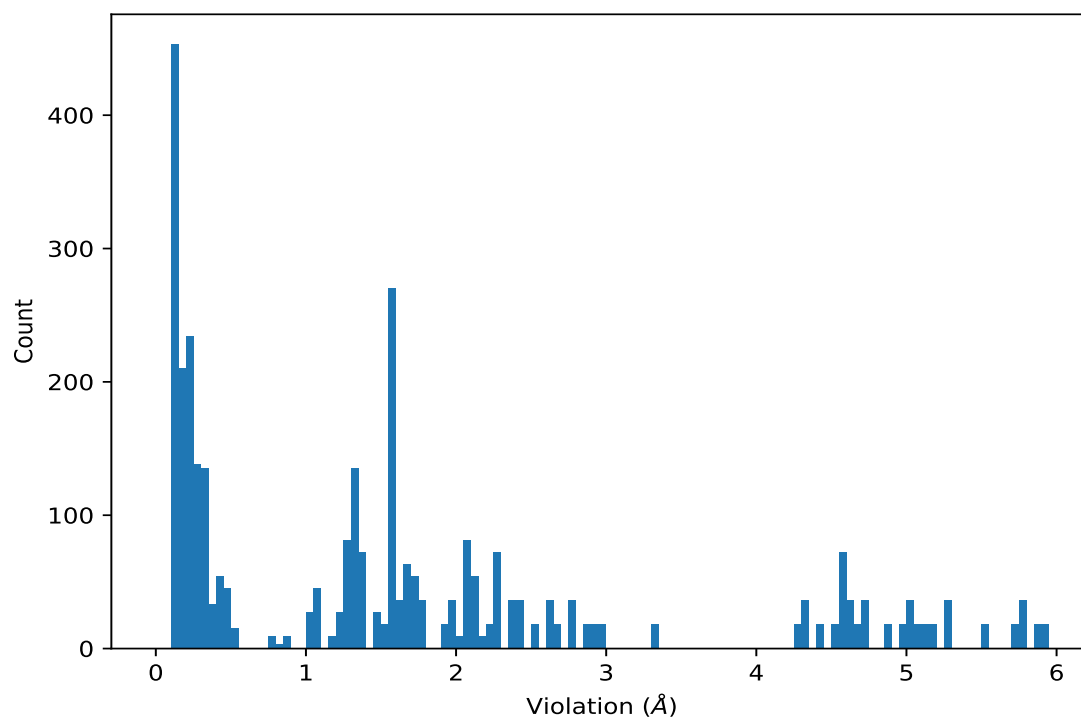
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,449)	1:230:C:ILE:HG22	1:227:C:LEU:HA	2	0.12	0.0	0.12
(2,449)	1:230:C:ILE:HG23	1:227:C:LEU:HA	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	4	5.91
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	4	5.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	4	5.91
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	4	5.91
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	4	5.91
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	4	5.91
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	4	5.91
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	4	5.91
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	4	5.91
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	4	5.91
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	4	5.91
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	4	5.91
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	4	5.91
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	4	5.91
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	4	5.91
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	4	5.91
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	4	5.91
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	4	5.91
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	3	5.86
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	3	5.86
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	3	5.86
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	3	5.86
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	3	5.86
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	3	5.86
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	3	5.86
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	3	5.86
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	3	5.86
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	3	5.86
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	3	5.86
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	3	5.86
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	3	5.86
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	3	5.86
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	3	5.86
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	3	5.86
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	3	5.86
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	3	5.86
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	15	5.76
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	15	5.76
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	15	5.76
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	15	5.76
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	15	5.76
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	15	5.76
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	15	5.76
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	15	5.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	15	5.76
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	15	5.76
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	15	5.76
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	15	5.76
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	15	5.76
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	15	5.76
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	15	5.76
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	15	5.76
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	15	5.76
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	15	5.76
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	8	5.75
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	8	5.75
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	8	5.75
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	8	5.75
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	8	5.75
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	8	5.75
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	8	5.75
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	8	5.75
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	8	5.75
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	8	5.75
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	8	5.75
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	8	5.75
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	8	5.75
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	8	5.75
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	8	5.75
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	8	5.75
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	8	5.75
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	8	5.75
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	5	5.74
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	5	5.74
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	5	5.74
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	5	5.74
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	5	5.74
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	5	5.74
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	5	5.74
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	5	5.74
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	5	5.74
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	5	5.74
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	5	5.74
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	5	5.74
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	5	5.74
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	5	5.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	5	5.74
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	5	5.74
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	5	5.74
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	5	5.74
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	2	5.54
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	2	5.54
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	2	5.54
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	2	5.54
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	2	5.54
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	2	5.54
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	2	5.54
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	2	5.54
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	2	5.54
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	2	5.54
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	2	5.54
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	2	5.54
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	2	5.54
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	2	5.54
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	2	5.54
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	2	5.54
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	2	5.54
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	2	5.54
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	7	5.28
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	7	5.28
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	7	5.28
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	7	5.28
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	7	5.28
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	7	5.28
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	7	5.28
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	7	5.28
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	7	5.28
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	7	5.28
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	7	5.28
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	7	5.28
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	7	5.28
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	7	5.28
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	7	5.28
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	7	5.28
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	7	5.28
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	7	5.28
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	14	5.27
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	14	5.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	14	5.27
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	14	5.27
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	14	5.27
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	14	5.27
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	14	5.27
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	14	5.27
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	14	5.27
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	14	5.27
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	14	5.27
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	14	5.27
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	14	5.27
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	14	5.27
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	14	5.27
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	14	5.27
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	14	5.27
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	14	5.27
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	6	5.18
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	6	5.18
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	6	5.18
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	6	5.18
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	6	5.18
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	6	5.18
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	6	5.18
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	6	5.18
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	6	5.18
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	6	5.18
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	6	5.18
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	6	5.18
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	6	5.18
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	6	5.18
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	6	5.18
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	6	5.18
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	6	5.18
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	6	5.18
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	1	5.14
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	1	5.14
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	1	5.14
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	1	5.14
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	1	5.14
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	1	5.14
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	1	5.14
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	1	5.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	1	5.14
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	1	5.14
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	1	5.14
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	1	5.14
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	1	5.14
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	1	5.14
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	1	5.14
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	1	5.14
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	1	5.14
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	1	5.14
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	10	5.08
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	10	5.08
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	10	5.08
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	10	5.08
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	10	5.08
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	10	5.08
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	10	5.08
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	10	5.08
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	10	5.08
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	10	5.08
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	10	5.08
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	10	5.08
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	10	5.08
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	10	5.08
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	10	5.08
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	10	5.08
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	10	5.08
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	10	5.08
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	11	5.04
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	11	5.04
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	11	5.04
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	11	5.04
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	11	5.04
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	11	5.04
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	11	5.04
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	11	5.04
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	11	5.04
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	11	5.04
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	11	5.04
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	11	5.04
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	11	5.04
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	11	5.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	11	5.04
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	11	5.04
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	11	5.04
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	11	5.04
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	13	5.03
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	13	5.03
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	13	5.03
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	13	5.03
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	13	5.03
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	13	5.03
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	13	5.03
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	13	5.03
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	13	5.03
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	13	5.03
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	13	5.03
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	13	5.03
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	13	5.03
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	13	5.03
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	13	5.03
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	13	5.03
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	13	5.03
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	13	5.03
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	9	4.97
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	9	4.97
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	9	4.97
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	9	4.97
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	9	4.97
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	9	4.97
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	9	4.97
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	9	4.97
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	9	4.97
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	9	4.97
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	9	4.97
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	9	4.97
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	9	4.97
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	9	4.97
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	9	4.97
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	9	4.97
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	9	4.97
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	9	4.97
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	15	4.86
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	15	4.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	15	4.86
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	15	4.86
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	15	4.86
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	15	4.86
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	15	4.86
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	15	4.86
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	15	4.86
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	15	4.86
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	15	4.86
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	15	4.86
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	15	4.86
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	15	4.86
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	15	4.86
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	15	4.86
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	15	4.86
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	15	4.86
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	3	4.71
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	3	4.71
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	3	4.71
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	3	4.71
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	3	4.71
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	3	4.71
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	3	4.71
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	3	4.71
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	3	4.71
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	3	4.71
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	3	4.71
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	3	4.71
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	3	4.71
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	3	4.71
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	3	4.71
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	3	4.71
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	3	4.71
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	3	4.71
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	4	4.7
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	4	4.7
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	4	4.7
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	4	4.7
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	4	4.7
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	4	4.7
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	4	4.7
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	4	4.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	4	4.7
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	4	4.7
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	4	4.7
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	4	4.7
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	4	4.7
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	4	4.7
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	4	4.7
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	4	4.7
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	4	4.7
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	4	4.7
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	7	4.68
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	7	4.68
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	7	4.68
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	7	4.68
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	7	4.68
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	7	4.68
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	7	4.68
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	7	4.68
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	7	4.68
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	7	4.68
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	7	4.68
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	7	4.68
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	7	4.68
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	7	4.68
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	7	4.68
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	7	4.68
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	7	4.68
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	7	4.68
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	13	4.63
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	13	4.63
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	13	4.63
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	13	4.63
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	13	4.63
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	13	4.63
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	13	4.63
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	13	4.63
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	13	4.63
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	13	4.63
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	13	4.63
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	13	4.63
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	13	4.63
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	13	4.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	13	4.63
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	13	4.63
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	13	4.63
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	13	4.63
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	8	4.62
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	8	4.62
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	8	4.62
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	8	4.62
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	8	4.62
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	8	4.62
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	8	4.62
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	8	4.62
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	8	4.62
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	8	4.62
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	8	4.62
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	8	4.62
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	8	4.62
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	8	4.62
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	8	4.62
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	8	4.62
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	8	4.62
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	8	4.62
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	1	4.57
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	1	4.57
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	1	4.57
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	1	4.57
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	1	4.57
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	1	4.57
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	14	4.57
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	14	4.57
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	14	4.57
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	14	4.57
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	14	4.57
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	14	4.57
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	1	4.57
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	1	4.57
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	1	4.57
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	1	4.57
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	1	4.57
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	1	4.57
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	14	4.57
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	14	4.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	14	4.57
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	14	4.57
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	14	4.57
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	14	4.57
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	1	4.57
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	1	4.57
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	1	4.57
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	1	4.57
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	1	4.57
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	1	4.57
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	14	4.57
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	14	4.57
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	14	4.57
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	14	4.57
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	14	4.57
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	14	4.57
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	6	4.56
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	6	4.56
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	6	4.56
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	6	4.56
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	6	4.56
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	6	4.56
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	6	4.56
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	6	4.56
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	6	4.56
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	6	4.56
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	6	4.56
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	6	4.56
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	6	4.56
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	6	4.56
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	6	4.56
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	6	4.56
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	6	4.56
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	6	4.56
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	10	4.55
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	10	4.55
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	10	4.55
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	10	4.55
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	10	4.55
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	10	4.55
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	10	4.55
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	10	4.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	10	4.55
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	10	4.55
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	10	4.55
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	10	4.55
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	10	4.55
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	10	4.55
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	10	4.55
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	10	4.55
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	10	4.55
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	10	4.55
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	11	4.52
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	11	4.52
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	11	4.52
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	11	4.52
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	11	4.52
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	11	4.52
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	11	4.52
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	11	4.52
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	11	4.52
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	11	4.52
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	11	4.52
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	11	4.52
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	11	4.52
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	11	4.52
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	11	4.52
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	11	4.52
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	11	4.52
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	11	4.52
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	2	4.4
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	2	4.4
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	2	4.4
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	2	4.4
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	2	4.4
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	2	4.4
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	2	4.4
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	2	4.4
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	2	4.4
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	2	4.4
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	2	4.4
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	2	4.4
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	2	4.4
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	2	4.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	2	4.4
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	2	4.4
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	2	4.4
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	2	4.4
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	5	4.35
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	5	4.35
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	5	4.35
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	5	4.35
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	5	4.35
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	5	4.35
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	5	4.35
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	5	4.35
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	5	4.35
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	5	4.35
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	5	4.35
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	5	4.35
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	5	4.35
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	5	4.35
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	5	4.35
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	5	4.35
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	5	4.35
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	5	4.35
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	9	4.32
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	9	4.32
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	9	4.32
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	9	4.32
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	9	4.32
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	9	4.32
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	9	4.32
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	9	4.32
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	9	4.32
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	9	4.32
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	9	4.32
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	9	4.32
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	9	4.32
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	9	4.32
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	9	4.32
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	9	4.32
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	9	4.32
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	9	4.32
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	12	4.26
(1,30)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	12	4.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	12	4.26
(1,30)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	12	4.26
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	12	4.26
(1,30)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	12	4.26
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	12	4.26
(1,29)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	12	4.26
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	12	4.26
(1,29)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	12	4.26
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	12	4.26
(1,29)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	12	4.26
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE1	12	4.26
(1,28)	1:228:B:LEU:HD11	1:229:B:PHE:HE2	12	4.26
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE1	12	4.26
(1,28)	1:228:B:LEU:HD12	1:229:B:PHE:HE2	12	4.26
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE1	12	4.26
(1,28)	1:228:B:LEU:HD13	1:229:B:PHE:HE2	12	4.26
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	12	3.33
(1,21)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	12	3.33
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	12	3.33
(1,21)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	12	3.33
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	12	3.33
(1,21)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	12	3.33
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	12	3.33
(1,20)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	12	3.33
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	12	3.33
(1,20)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	12	3.33
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	12	3.33
(1,20)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	12	3.33
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD1	12	3.33
(1,19)	1:224:B:LEU:HD21	1:229:B:PHE:HD2	12	3.33
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD1	12	3.33
(1,19)	1:224:B:LEU:HD22	1:229:B:PHE:HD2	12	3.33
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD1	12	3.33
(1,19)	1:224:B:LEU:HD23	1:229:B:PHE:HD2	12	3.33
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	9	2.98
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	9	2.98
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	9	2.98
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	9	2.98
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	9	2.98
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	9	2.98
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	9	2.98
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	9	2.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	9	2.98
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	9	2.98
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	9	2.98
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	9	2.98
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	9	2.98
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	9	2.98
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	9	2.98
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	9	2.98
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	9	2.98
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	9	2.98
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	7	2.92
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	7	2.92
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	7	2.92
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	7	2.92
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	7	2.92
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	7	2.92
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	7	2.92
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	7	2.92
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	7	2.92
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	7	2.92
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	7	2.92
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	7	2.92
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	7	2.92
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	7	2.92
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	7	2.92
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	7	2.92
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	7	2.92
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	7	2.92
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	13	2.88
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	13	2.88
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	13	2.88
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	13	2.88
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	13	2.88
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	13	2.88
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	13	2.88
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	13	2.88
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	13	2.88
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	13	2.88
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	13	2.88
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	13	2.88
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	13	2.88
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	13	2.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	13	2.88
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	13	2.88
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	13	2.88
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	13	2.88
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	4	2.8
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	4	2.8
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	4	2.8
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	4	2.8
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	4	2.8
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	4	2.8
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	4	2.8
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	4	2.8
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	4	2.8
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	4	2.8
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	4	2.8
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	4	2.8
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	4	2.8
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	4	2.8
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	4	2.8
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	4	2.8
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	4	2.8
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	4	2.8
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	11	2.79
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	11	2.79
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	11	2.79
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	11	2.79
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	11	2.79
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	11	2.79
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	11	2.79
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	11	2.79
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	11	2.79
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	11	2.79
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	11	2.79
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	11	2.79
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	11	2.79
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	11	2.79
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	11	2.79
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	11	2.79
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	11	2.79
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	11	2.79
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	14	2.68
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	14	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	14	2.68
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	14	2.68
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	14	2.68
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	14	2.68
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	14	2.68
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	14	2.68
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	14	2.68
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	14	2.68
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	14	2.68
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	14	2.68
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	14	2.68
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	14	2.68
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	14	2.68
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	14	2.68
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	14	2.68
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	14	2.68
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	2	2.65
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	2	2.65
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	2	2.65
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	2	2.65
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	2	2.65
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	2	2.65
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	8	2.65
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	8	2.65
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	8	2.65
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	8	2.65
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	8	2.65
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	8	2.65
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	2	2.65
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	2	2.65
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	2	2.65
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	2	2.65
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	2	2.65
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	2	2.65
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	8	2.65
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	8	2.65
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	8	2.65
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	8	2.65
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	8	2.65
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	8	2.65
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	2	2.65
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	2	2.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	2	2.65
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	2	2.65
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	2	2.65
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	2	2.65
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	8	2.65
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	8	2.65
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	8	2.65
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	8	2.65
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	8	2.65
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	8	2.65
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	7	2.5
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	7	2.5
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	7	2.5
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	7	2.5
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	7	2.5
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	7	2.5
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	7	2.5
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	7	2.5
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	7	2.5
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	7	2.5
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	7	2.5
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	7	2.5
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	7	2.5
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	7	2.5
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	7	2.5
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	7	2.5
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	7	2.5
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	7	2.5
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	10	2.44
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	10	2.44
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	10	2.44
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	10	2.44
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	10	2.44
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	10	2.44
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	10	2.44
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	10	2.44
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	10	2.44
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	10	2.44
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	10	2.44
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	10	2.44
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	10	2.44
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	10	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	10	2.44
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	10	2.44
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	10	2.44
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	10	2.44
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	15	2.41
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	15	2.41
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	15	2.41
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	15	2.41
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	15	2.41
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	15	2.41
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	15	2.41
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	15	2.41
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	15	2.41
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	15	2.41
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	15	2.41
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	15	2.41
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	15	2.41
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	15	2.41
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	15	2.41
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	15	2.41
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	15	2.41
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	15	2.41
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	3	2.38
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	3	2.38
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	3	2.38
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	3	2.38
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	3	2.38
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	3	2.38
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	13	2.38
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	13	2.38
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	13	2.38
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	13	2.38
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	13	2.38
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	13	2.38
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	3	2.38
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	3	2.38
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	3	2.38
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	3	2.38
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	3	2.38
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	3	2.38
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	13	2.38
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	13	2.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	13	2.38
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	13	2.38
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	13	2.38
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	13	2.38
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	3	2.38
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	3	2.38
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	3	2.38
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	3	2.38
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	3	2.38
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	3	2.38
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	13	2.38
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	13	2.38
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	13	2.38
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	13	2.38
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	13	2.38
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	13	2.38
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	7	2.29
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	7	2.29
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	7	2.29
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	7	2.29
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	7	2.29
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	7	2.29
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	7	2.29
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	7	2.29
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	7	2.29
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	7	2.29
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	7	2.29
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	7	2.29
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	7	2.29
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	7	2.29
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	7	2.29
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	7	2.29
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	7	2.29
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	7	2.29
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	1	2.29
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	1	2.29
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	1	2.29
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	1	2.29
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	1	2.29
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	1	2.29
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	5	2.29
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	5	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	5	2.29
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	5	2.29
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	5	2.29
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	5	2.29
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	1	2.29
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	1	2.29
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	1	2.29
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	1	2.29
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	1	2.29
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	1	2.29
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	5	2.29
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	5	2.29
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	5	2.29
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	5	2.29
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	5	2.29
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	5	2.29
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	1	2.29
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	1	2.29
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	1	2.29
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	1	2.29
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	1	2.29
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	1	2.29
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	5	2.29
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	5	2.29
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	5	2.29
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	5	2.29
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	5	2.29
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	5	2.29
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	6	2.27
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	6	2.27
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	6	2.27
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	6	2.27
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	6	2.27
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	6	2.27
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	6	2.27
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	6	2.27
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	6	2.27
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	6	2.27
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	6	2.27
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	6	2.27
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	6	2.27
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	6	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	6	2.27
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	6	2.27
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	6	2.27
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	6	2.27
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	9	2.21
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	9	2.21
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	9	2.21
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	9	2.21
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	9	2.21
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	9	2.21
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	9	2.21
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	9	2.21
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	9	2.21
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	14	2.2
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	14	2.2
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	14	2.2
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	14	2.2
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	14	2.2
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	14	2.2
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	14	2.2
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	14	2.2
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	14	2.2
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	7	2.15
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	7	2.15
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	7	2.15
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	7	2.15
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	7	2.15
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	7	2.15
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	7	2.15
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	7	2.15
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	7	2.15
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	15	2.14
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	15	2.14
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	15	2.14
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	15	2.14
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	15	2.14
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	15	2.14
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	15	2.14
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	15	2.14
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	15	2.14
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	3	2.13
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	3	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	3	2.13
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	4	2.13
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	4	2.13
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	4	2.13
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	3	2.13
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	3	2.13
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	3	2.13
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	4	2.13
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	4	2.13
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	4	2.13
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	3	2.13
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	3	2.13
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	3	2.13
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	4	2.13
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	4	2.13
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	4	2.13
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	6	2.11
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	6	2.11
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	6	2.11
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	6	2.11
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	6	2.11
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	6	2.11
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	6	2.11
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	6	2.11
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	6	2.11
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	15	2.1
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	15	2.1
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	15	2.1
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	15	2.1
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	15	2.1
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	15	2.1
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	15	2.1
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	15	2.1
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	15	2.1
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	15	2.1
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	15	2.1
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	15	2.1
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	15	2.1
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	15	2.1
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	15	2.1
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	15	2.1
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	15	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	15	2.1
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	5	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	5	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	5	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	10	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	10	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	10	2.08
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	5	2.08
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	5	2.08
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	5	2.08
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	10	2.08
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	10	2.08
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	10	2.08
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	5	2.08
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	5	2.08
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	5	2.08
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	10	2.08
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	10	2.08
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	10	2.08
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	1	2.07
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	1	2.07
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	1	2.07
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	2	2.07
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	2	2.07
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	2	2.07
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	12	2.07
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	12	2.07
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	12	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	1	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	1	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	1	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	2	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	2	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	2	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	12	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	12	2.07
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	12	2.07
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	1	2.07
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	1	2.07
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	1	2.07
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	2	2.07
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	2	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	2	2.07
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	12	2.07
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	12	2.07
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	12	2.07
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	12	2.06
(1,27)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	12	2.06
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	12	2.06
(1,27)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	12	2.06
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	12	2.06
(1,27)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	12	2.06
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	12	2.06
(1,26)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	12	2.06
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	12	2.06
(1,26)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	12	2.06
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	12	2.06
(1,26)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	12	2.06
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA2	12	2.06
(1,25)	1:225:B:LEU:HD21	1:221:B:GLY:HA3	12	2.06
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA2	12	2.06
(1,25)	1:225:B:LEU:HD22	1:221:B:GLY:HA3	12	2.06
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA2	12	2.06
(1,25)	1:225:B:LEU:HD23	1:221:B:GLY:HA3	12	2.06
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	8	2.06
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	8	2.06
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	8	2.06
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	11	2.06
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	11	2.06
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	11	2.06
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	8	2.06
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	8	2.06
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	8	2.06
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	11	2.06
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	11	2.06
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	11	2.06
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	8	2.06
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	8	2.06
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	8	2.06
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	11	2.06
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	11	2.06
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	11	2.06
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD11	13	2.0
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD12	13	2.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:221:B:GLY:H	1:222:B:LEU:HD13	13	2.0
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD11	13	2.0
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD12	13	2.0
(1,8)	1:221:B:GLY:H	1:222:B:LEU:HD13	13	2.0
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD11	13	2.0
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD12	13	2.0
(1,7)	1:221:B:GLY:H	1:222:B:LEU:HD13	13	2.0
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	13	1.97
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	13	1.97
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	13	1.97
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	13	1.97
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	13	1.97
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	13	1.97
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	13	1.97
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	13	1.97
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	13	1.97
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	13	1.97
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	13	1.97
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	13	1.97
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	13	1.97
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	13	1.97
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	13	1.97
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	13	1.97
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	13	1.97
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	13	1.97
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	1	1.96
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	1	1.96
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	1	1.96
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	1	1.96
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	1	1.96
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	1	1.96
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	1	1.96
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	1	1.96
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	1	1.96
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	1	1.96
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	1	1.96
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	1	1.96
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	1	1.96
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	1	1.96
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	1	1.96
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	1	1.96
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	1	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	1	1.96
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	6	1.94
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	6	1.94
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	6	1.94
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	6	1.94
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	6	1.94
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	6	1.94
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	6	1.94
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	6	1.94
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	6	1.94
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	6	1.94
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	6	1.94
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	6	1.94
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	6	1.94
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	6	1.94
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	6	1.94
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	6	1.94
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	6	1.94
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	6	1.94
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	3	1.79
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	3	1.79
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	3	1.79
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	3	1.79
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	3	1.79
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	3	1.79
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	3	1.79
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	3	1.79
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	3	1.79
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	3	1.79
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	3	1.79
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	3	1.79
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	3	1.79
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	3	1.79
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	3	1.79
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	3	1.79
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	3	1.79
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	3	1.79
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	1	1.76
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	1	1.76
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	1	1.76
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	1	1.76
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	1	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	1	1.76
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	1	1.76
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	1	1.76
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	1	1.76
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	1	1.76
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	1	1.76
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	1	1.76
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	1	1.76
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	1	1.76
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	1	1.76
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	1	1.76
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	1	1.76
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	1	1.76
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	12	1.74
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	12	1.74
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	12	1.74
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	12	1.74
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	12	1.74
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	12	1.74
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	12	1.74
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	12	1.74
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	12	1.74
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	12	1.74
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	12	1.74
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	12	1.74
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	12	1.74
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	12	1.74
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	12	1.74
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	12	1.74
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	12	1.74
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	12	1.74
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	10	1.71
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	10	1.71
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	10	1.71
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	10	1.71
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	10	1.71
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	10	1.71
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	11	1.71
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	11	1.71
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	11	1.71
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	11	1.71
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	11	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	11	1.71
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	10	1.71
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	10	1.71
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	10	1.71
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	10	1.71
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	10	1.71
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	10	1.71
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	11	1.71
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	11	1.71
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	11	1.71
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	11	1.71
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	11	1.71
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	11	1.71
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	10	1.71
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	10	1.71
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	10	1.71
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	10	1.71
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	10	1.71
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	10	1.71
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	11	1.71
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	11	1.71
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	11	1.71
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	11	1.71
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	11	1.71
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	11	1.71
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	5	1.69
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	5	1.69
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	5	1.69
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	5	1.69
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	5	1.69
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	5	1.69
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	5	1.69
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	5	1.69
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	5	1.69
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	10	1.68
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	10	1.68
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	10	1.68
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	10	1.68
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	10	1.68
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	10	1.68
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	10	1.68
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	10	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	10	1.68
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	10	1.68
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	10	1.68
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	10	1.68
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	10	1.68
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	10	1.68
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	10	1.68
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	10	1.68
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	10	1.68
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	10	1.68
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	9	1.68
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	9	1.68
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	9	1.68
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	9	1.68
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	9	1.68
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	9	1.68
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	9	1.68
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	9	1.68
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	9	1.68
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	9	1.68
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	9	1.68
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	9	1.68
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	9	1.68
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	9	1.68
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	9	1.68
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	9	1.68
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	9	1.68
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	9	1.68
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	2	1.66
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	2	1.66
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	2	1.66
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	2	1.66
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	2	1.66
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	2	1.66
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	2	1.66
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	2	1.66
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	2	1.66
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	2	1.66
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	2	1.66
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	2	1.66
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	2	1.66
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	2	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	2	1.66
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	2	1.66
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	2	1.66
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	2	1.66
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	5	1.61
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	5	1.61
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	5	1.61
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	5	1.61
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	5	1.61
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	5	1.61
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	8	1.61
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	8	1.61
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	8	1.61
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	8	1.61
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	8	1.61
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	8	1.61
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	5	1.61
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	5	1.61
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	5	1.61
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	5	1.61
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	5	1.61
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	5	1.61
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	8	1.61
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	8	1.61
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	8	1.61
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	8	1.61
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	8	1.61
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	8	1.61
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	5	1.61
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	5	1.61
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	5	1.61
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	5	1.61
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	5	1.61
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	5	1.61
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	8	1.61
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	8	1.61
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	8	1.61
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	8	1.61
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	8	1.61
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	8	1.61
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	10	1.58
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	10	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	10	1.58
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	10	1.58
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	10	1.58
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	10	1.58
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	11	1.58
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	11	1.58
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	11	1.58
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	11	1.58
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	11	1.58
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	11	1.58
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	10	1.58
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	10	1.58
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	10	1.58
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	10	1.58
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	10	1.58
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	10	1.58
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	11	1.58
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	11	1.58
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	11	1.58
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	11	1.58
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	11	1.58
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	11	1.58
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	10	1.58
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	10	1.58
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	10	1.58
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	10	1.58
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	10	1.58
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	10	1.58
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	11	1.58
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	11	1.58
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	11	1.58
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	11	1.58
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	11	1.58
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	11	1.58
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	7	1.58
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	7	1.58
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	7	1.58
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	7	1.58
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	7	1.58
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	7	1.58
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	7	1.58
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	7	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	7	1.58
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	6	1.58
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	6	1.58
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	6	1.58
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	6	1.58
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	6	1.58
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	6	1.58
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	6	1.58
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	6	1.58
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	6	1.58
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	6	1.58
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	6	1.58
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	6	1.58
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	6	1.58
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	6	1.58
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	6	1.58
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	6	1.58
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	6	1.58
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	6	1.58
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	7	1.57
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	7	1.57
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	7	1.57
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	7	1.57
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	7	1.57
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	7	1.57
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	9	1.57
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	9	1.57
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	9	1.57
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	9	1.57
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	9	1.57
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	9	1.57
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	13	1.57
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	13	1.57
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	13	1.57
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	13	1.57
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	13	1.57
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	13	1.57
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	15	1.57
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	15	1.57
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	15	1.57
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	15	1.57
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	15	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	15	1.57
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	7	1.57
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	7	1.57
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	7	1.57
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	7	1.57
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	7	1.57
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	7	1.57
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	9	1.57
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	9	1.57
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	9	1.57
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	9	1.57
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	9	1.57
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	9	1.57
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	13	1.57
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	13	1.57
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	13	1.57
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	13	1.57
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	13	1.57
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	13	1.57
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	15	1.57
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	15	1.57
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	15	1.57
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	15	1.57
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	15	1.57
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	15	1.57
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	7	1.57
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	7	1.57
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	7	1.57
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	7	1.57
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	7	1.57
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	7	1.57
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	9	1.57
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	9	1.57
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	9	1.57
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	9	1.57
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	9	1.57
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	9	1.57
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	13	1.57
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	13	1.57
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	13	1.57
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	13	1.57
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	13	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	13	1.57
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	15	1.57
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	15	1.57
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	15	1.57
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	15	1.57
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	15	1.57
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	15	1.57
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	2	1.56
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	2	1.56
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	2	1.56
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	2	1.56
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	2	1.56
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	2	1.56
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	5	1.56
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	5	1.56
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	5	1.56
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	5	1.56
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	5	1.56
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	5	1.56
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	8	1.56
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	8	1.56
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	8	1.56
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	8	1.56
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	8	1.56
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	8	1.56
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	2	1.56
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	2	1.56
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	2	1.56
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	2	1.56
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	2	1.56
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	2	1.56
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	5	1.56
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	5	1.56
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	5	1.56
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	5	1.56
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	5	1.56
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	5	1.56
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	8	1.56
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	8	1.56
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	8	1.56
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	8	1.56
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	8	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	8	1.56
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	2	1.56
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	2	1.56
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	2	1.56
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	2	1.56
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	2	1.56
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	2	1.56
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	5	1.56
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	5	1.56
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	5	1.56
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	5	1.56
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	5	1.56
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	5	1.56
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	8	1.56
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	8	1.56
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	8	1.56
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	8	1.56
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	8	1.56
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	8	1.56
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	1	1.56
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	1	1.56
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	1	1.56
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	1	1.56
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	1	1.56
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	1	1.56
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	1	1.56
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	1	1.56
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	1	1.56
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	14	1.56
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	14	1.56
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	14	1.56
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	14	1.56
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	14	1.56
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	14	1.56
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	14	1.56
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	14	1.56
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	14	1.56
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	14	1.56
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	14	1.56
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	14	1.56
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	14	1.56
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	14	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	14	1.56
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	14	1.56
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	14	1.56
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	14	1.56
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	3	1.55
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	3	1.55
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	3	1.55
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	3	1.55
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	3	1.55
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	3	1.55
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	6	1.55
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	6	1.55
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	6	1.55
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	6	1.55
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	6	1.55
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	6	1.55
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	12	1.55
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	12	1.55
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	12	1.55
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	12	1.55
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	12	1.55
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	12	1.55
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	3	1.55
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	3	1.55
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	3	1.55
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	3	1.55
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	3	1.55
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	3	1.55
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	6	1.55
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	6	1.55
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	6	1.55
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	6	1.55
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	6	1.55
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	6	1.55
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	12	1.55
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	12	1.55
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	12	1.55
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	12	1.55
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	12	1.55
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	12	1.55
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	3	1.55
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	3	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	3	1.55
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	3	1.55
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	3	1.55
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	3	1.55
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	6	1.55
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	6	1.55
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	6	1.55
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	6	1.55
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	6	1.55
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	6	1.55
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	12	1.55
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	12	1.55
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	12	1.55
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	12	1.55
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	12	1.55
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	12	1.55
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	14	1.54
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	14	1.54
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	14	1.54
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	14	1.54
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	14	1.54
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	14	1.54
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	14	1.54
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	14	1.54
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	14	1.54
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	14	1.54
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	14	1.54
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	14	1.54
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	14	1.54
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	14	1.54
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	14	1.54
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	14	1.54
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	14	1.54
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	14	1.54
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	3	1.48
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	3	1.48
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	3	1.48
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	3	1.48
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	3	1.48
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	3	1.48
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	3	1.48
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	3	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	3	1.48
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	4	1.46
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	4	1.46
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	4	1.46
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	4	1.46
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	4	1.46
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	4	1.46
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	4	1.46
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	4	1.46
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	4	1.46
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	4	1.46
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	4	1.46
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	4	1.46
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	4	1.46
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	4	1.46
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	4	1.46
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	4	1.46
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	4	1.46
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	4	1.46
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	1	1.4
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	1	1.4
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	1	1.4
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	1	1.4
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	1	1.4
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	1	1.4
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	1	1.4
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	1	1.4
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	1	1.4
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	1	1.4
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	1	1.4
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	1	1.4
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	1	1.4
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	1	1.4
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	1	1.4
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	1	1.4
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	1	1.4
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	1	1.4
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	15	1.38
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	15	1.38
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	15	1.38
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	15	1.38
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	15	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	15	1.38
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	15	1.38
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	15	1.38
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	15	1.38
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	11	1.37
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	11	1.37
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	11	1.37
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	11	1.37
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	11	1.37
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	11	1.37
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	11	1.37
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	11	1.37
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	11	1.37
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	15	1.37
(1,3)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	15	1.37
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	15	1.37
(1,3)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	15	1.37
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	15	1.37
(1,3)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	15	1.37
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	15	1.37
(1,2)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	15	1.37
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	15	1.37
(1,2)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	15	1.37
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	15	1.37
(1,2)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	15	1.37
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD1	15	1.37
(1,1)	1:218:B:ILE:HG21	1:219:B:PHE:HD2	15	1.37
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD1	15	1.37
(1,1)	1:218:B:ILE:HG22	1:219:B:PHE:HD2	15	1.37
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD1	15	1.37
(1,1)	1:218:B:ILE:HG23	1:219:B:PHE:HD2	15	1.37
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	4	1.36
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	4	1.36
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	4	1.36
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	4	1.36
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	4	1.36
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	4	1.36
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	4	1.36
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	4	1.36
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	4	1.36
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	4	1.36
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	4	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	4	1.36
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	4	1.36
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	4	1.36
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	4	1.36
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	4	1.36
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	4	1.36
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	4	1.36
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	7	1.32
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	7	1.32
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	7	1.32
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	7	1.32
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	7	1.32
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	7	1.32
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	7	1.32
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	7	1.32
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	7	1.32
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	9	1.32
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	9	1.32
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	9	1.32
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	9	1.32
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	9	1.32
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	9	1.32
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	9	1.32
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	9	1.32
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	9	1.32
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	3	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	3	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	3	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	5	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	5	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	5	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	6	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	6	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	6	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	13	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	13	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	13	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	14	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	14	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	14	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	3	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	3	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	3	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	5	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	5	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	5	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	6	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	6	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	6	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	13	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	13	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	13	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	14	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	14	1.31
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	14	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	3	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	3	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	3	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	5	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	5	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	5	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	6	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	6	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	6	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	13	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	13	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	13	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	14	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	14	1.31
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	14	1.31
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	4	1.31
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	4	1.31
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	4	1.31
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	4	1.31
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	4	1.31
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	4	1.31
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	4	1.31
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	4	1.31
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	4	1.31
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	1	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	1	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	1	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	2	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	2	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	2	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	4	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	4	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	4	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	8	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	8	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	8	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	9	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	9	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	9	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	10	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	10	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	10	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	1	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	1	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	1	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	2	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	2	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	2	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	4	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	4	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	4	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	8	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	8	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	8	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	9	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	9	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	9	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	10	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	10	1.3
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	10	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	1	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	1	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	1	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	2	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	2	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	2	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	4	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	4	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	4	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	8	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	8	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	8	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	9	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	9	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	9	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	10	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	10	1.3
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	10	1.3
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	6	1.3
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	6	1.3
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	6	1.3
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	6	1.3
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	6	1.3
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	6	1.3
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	6	1.3
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	6	1.3
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	6	1.3
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	12	1.29
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	12	1.29
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	12	1.29
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	12	1.29
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	12	1.29
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	12	1.29
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	12	1.29
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	12	1.29
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	12	1.29
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	4	1.29
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	4	1.29
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	4	1.29
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	4	1.29
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	4	1.29
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	4	1.29
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	14	1.29
(1,18)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	14	1.29
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	14	1.29
(1,18)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	14	1.29
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	14	1.29
(1,18)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	14	1.29
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	4	1.29
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	4	1.29
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	4	1.29
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	4	1.29
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	4	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	4	1.29
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	14	1.29
(1,17)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	14	1.29
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	14	1.29
(1,17)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	14	1.29
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	14	1.29
(1,17)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	14	1.29
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	4	1.29
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	4	1.29
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	4	1.29
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	4	1.29
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	4	1.29
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	4	1.29
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA2	14	1.29
(1,16)	1:222:B:LEU:HD21	1:221:B:GLY:HA3	14	1.29
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA2	14	1.29
(1,16)	1:222:B:LEU:HD22	1:221:B:GLY:HA3	14	1.29
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA2	14	1.29
(1,16)	1:222:B:LEU:HD23	1:221:B:GLY:HA3	14	1.29
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	3	1.28
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	3	1.28
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	3	1.28
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	3	1.28
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	3	1.28
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	3	1.28
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	3	1.28
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	3	1.28
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	3	1.28
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	3	1.28
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	3	1.28
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	3	1.28
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	3	1.28
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	3	1.28
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	3	1.28
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	3	1.28
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	3	1.28
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	3	1.28
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD21	15	1.27
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD22	15	1.27
(1,24)	1:225:B:LEU:H	1:225:B:LEU:HD23	15	1.27
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD21	15	1.27
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD22	15	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:225:B:LEU:H	1:225:B:LEU:HD23	15	1.27
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD21	15	1.27
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD22	15	1.27
(1,22)	1:225:B:LEU:H	1:225:B:LEU:HD23	15	1.27
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	11	1.25
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	11	1.25
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	11	1.25
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	11	1.25
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	11	1.25
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	11	1.25
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	11	1.25
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	11	1.25
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	11	1.25
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	12	1.24
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	12	1.24
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	12	1.24
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	12	1.24
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	12	1.24
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	12	1.24
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	12	1.24
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	12	1.24
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	12	1.24
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	9	1.23
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	9	1.23
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	9	1.23
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	9	1.23
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	9	1.23
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	9	1.23
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	9	1.23
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	9	1.23
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	9	1.23
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	9	1.23
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	9	1.23
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	9	1.23
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	9	1.23
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	9	1.23
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	9	1.23
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	9	1.23
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	9	1.23
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	9	1.23
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	2	1.18
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	2	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	2	1.18
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	2	1.18
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	2	1.18
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	2	1.18
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	2	1.18
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	2	1.18
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	2	1.18
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	5	1.07
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	5	1.07
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	5	1.07
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	5	1.07
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	5	1.07
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	5	1.07
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	11	1.07
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	11	1.07
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	11	1.07
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	11	1.07
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	11	1.07
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	11	1.07
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	5	1.07
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	5	1.07
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	5	1.07
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	5	1.07
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	5	1.07
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	5	1.07
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	11	1.07
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	11	1.07
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	11	1.07
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	11	1.07
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	11	1.07
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	11	1.07
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	5	1.07
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	5	1.07
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	5	1.07
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	5	1.07
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	5	1.07
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	5	1.07
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	11	1.07
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	11	1.07
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	11	1.07
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	11	1.07
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	11	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	11	1.07
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	10	1.07
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	10	1.07
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	10	1.07
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	10	1.07
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	10	1.07
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	10	1.07
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	10	1.07
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	10	1.07
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	10	1.07
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	8	1.04
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	8	1.04
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	8	1.04
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	8	1.04
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	8	1.04
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	8	1.04
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	8	1.04
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	8	1.04
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	8	1.04
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	2	1.02
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	2	1.02
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	2	1.02
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	2	1.02
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	2	1.02
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	2	1.02
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	2	1.02
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	2	1.02
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	2	1.02
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	2	1.02
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	2	1.02
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	2	1.02
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	2	1.02
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	2	1.02
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	2	1.02
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	2	1.02
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	2	1.02
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	2	1.02
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	14	0.87
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	14	0.87
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	14	0.87
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	14	0.87
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	14	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	14	0.87
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	14	0.87
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	14	0.87
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	14	0.87
(2,448)	1:230:C:ILE:H	1:230:C:ILE:HB	5	0.82
(2,280)	1:230:C:ILE:H	1:230:C:ILE:HB	5	0.82
(2,112)	1:230:C:ILE:H	1:230:C:ILE:HB	5	0.82
(1,15)	1:222:B:LEU:HD11	1:218:B:ILE:HA	13	0.76
(1,15)	1:222:B:LEU:HD12	1:218:B:ILE:HA	13	0.76
(1,15)	1:222:B:LEU:HD13	1:218:B:ILE:HA	13	0.76
(1,14)	1:222:B:LEU:HD11	1:218:B:ILE:HA	13	0.76
(1,14)	1:222:B:LEU:HD12	1:218:B:ILE:HA	13	0.76
(1,14)	1:222:B:LEU:HD13	1:218:B:ILE:HA	13	0.76
(1,13)	1:222:B:LEU:HD11	1:218:B:ILE:HA	13	0.76
(1,13)	1:222:B:LEU:HD12	1:218:B:ILE:HA	13	0.76
(1,13)	1:222:B:LEU:HD13	1:218:B:ILE:HA	13	0.76
(2,342)	1:213:C:LEU:H	1:213:C:LEU:HB2	1	0.52
(2,174)	1:213:C:LEU:H	1:213:C:LEU:HB2	1	0.52
(2,6)	1:213:C:LEU:H	1:213:C:LEU:HB2	1	0.52
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	15	0.51
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	15	0.51
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	15	0.51
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	1	0.5
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	1	0.5
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	1	0.5
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	1	0.5
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	1	0.5
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	1	0.5
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	1	0.5
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	1	0.5
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	1	0.5
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	12	0.49
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	12	0.49
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	12	0.49
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	6	0.48
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	6	0.48
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	6	0.48
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	1	0.47
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	1	0.47
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	1	0.47
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	1	0.47
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	1	0.47
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	1	0.47
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	1	0.47
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	1	0.47
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	1	0.47
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	1	0.47
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	1	0.47
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	1	0.47
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	1	0.47
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	1	0.47
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	1	0.47
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	1	0.47
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	1	0.47
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	1	0.47
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	1	0.47
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	1	0.47
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	1	0.47
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	1	0.47
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	1	0.47
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	1	0.47
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	1	0.47
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	1	0.47
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	5	0.46
(2,341)	1:213:C:LEU:H	1:213:C:LEU:HB3	10	0.46
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	5	0.46
(2,173)	1:213:C:LEU:H	1:213:C:LEU:HB3	10	0.46
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	5	0.46
(2,5)	1:213:C:LEU:H	1:213:C:LEU:HB3	10	0.46
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	10	0.45
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	13	0.45
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	10	0.45
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	13	0.45
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	10	0.45
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	13	0.45
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	11	0.44
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	7	0.44
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	11	0.44
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	7	0.44
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	11	0.44
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	7	0.44
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	14	0.44
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	14	0.44
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	14	0.44
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	14	0.44
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	14	0.44
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	14	0.44
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	14	0.44
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	14	0.44
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	12	0.43
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	12	0.43
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	12	0.43
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	12	0.43
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	12	0.43
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	12	0.43
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	12	0.43
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	12	0.43
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	12	0.43
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	12	0.43
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	12	0.43
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	12	0.43
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	12	0.43
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	12	0.43
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	12	0.43
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	12	0.43
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	12	0.43
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	12	0.43
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	5	0.42
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	5	0.42
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	5	0.42
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	5	0.42
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	5	0.42
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	5	0.42
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	5	0.42
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	5	0.42
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	5	0.42
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	5	0.42
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	5	0.42
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	5	0.42
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	5	0.42
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	5	0.42
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	5	0.42
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	5	0.42
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	5	0.42
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	11	0.4
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	11	0.4
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	11	0.4
(2,432)	1:227:C:LEU:H	1:227:C:LEU:HG	6	0.38
(2,264)	1:227:C:LEU:H	1:227:C:LEU:HG	6	0.38
(2,96)	1:227:C:LEU:H	1:227:C:LEU:HG	6	0.38
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	15	0.37
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	15	0.37
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	15	0.37
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	15	0.37
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	15	0.37
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	15	0.37
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	15	0.37
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	15	0.37
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	15	0.37
(2,432)	1:227:C:LEU:H	1:227:C:LEU:HG	4	0.37
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	15	0.37
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	15	0.37
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	15	0.37
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	15	0.37
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	15	0.37
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	15	0.37
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	15	0.37
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	15	0.37
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	15	0.37
(2,264)	1:227:C:LEU:H	1:227:C:LEU:HG	4	0.37
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	15	0.37
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	15	0.37
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	15	0.37
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	15	0.37
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	15	0.37
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	15	0.37
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	15	0.37
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	15	0.37
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	15	0.37
(2,96)	1:227:C:LEU:H	1:227:C:LEU:HG	4	0.37
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	4	0.35
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	4	0.35
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	4	0.35
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	3	0.34
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	3	0.34
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	3	0.34
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	3	0.34
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	3	0.34
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	3	0.34
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	3	0.34
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	3	0.34
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	2	0.34
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	6	0.34
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	3	0.34
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	3	0.34
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	3	0.34
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	3	0.34
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	3	0.34
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	3	0.34
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	3	0.34
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	3	0.34
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	3	0.34
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	2	0.34
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	6	0.34
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	3	0.34
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	3	0.34
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	3	0.34
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	3	0.34
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	3	0.34
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	3	0.34
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	3	0.34
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	3	0.34
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	3	0.34
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	2	0.34
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	6	0.34
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	2	0.33
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	8	0.33
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	9	0.33
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	14	0.33
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	2	0.33
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	8	0.33
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	9	0.33
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	14	0.33
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	2	0.33
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	8	0.33
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	14	0.33
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	1	0.33
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	1	0.33
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	1	0.33
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	1	0.33
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	1	0.33
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	1	0.33
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	1	0.33
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	1	0.33
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	1	0.33
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	4	0.32
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	6	0.32
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	7	0.32
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	10	0.32
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	13	0.32
(2,344)	1:214:C:LEU:H	1:211:C:THR:HA	12	0.32
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	4	0.32
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	6	0.32
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	7	0.32
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	10	0.32
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	13	0.32
(2,176)	1:214:C:LEU:H	1:211:C:THR:HA	12	0.32
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	4	0.32
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	6	0.32
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	7	0.32
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	10	0.32
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	13	0.32
(2,8)	1:214:C:LEU:H	1:211:C:THR:HA	12	0.32
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	1	0.31
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	3	0.31
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	5	0.31
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	11	0.31
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	15	0.31
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	10	0.31
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	10	0.31
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	10	0.31
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	10	0.31
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	10	0.31
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	10	0.31
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	10	0.31
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	10	0.31
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	6	0.31
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	6	0.31
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	6	0.31
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	6	0.31
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	6	0.31
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	6	0.31
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	1	0.31
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	3	0.31
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	5	0.31
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	11	0.31
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	15	0.31
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	10	0.31
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	10	0.31
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	10	0.31
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	10	0.31
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	10	0.31
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	10	0.31
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	10	0.31
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	10	0.31
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	10	0.31
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	6	0.31
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	6	0.31
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	6	0.31
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	6	0.31
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	6	0.31
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	6	0.31
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	1	0.31
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	3	0.31
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	5	0.31
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	11	0.31
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	15	0.31
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	10	0.31
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	10	0.31
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	10	0.31
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	10	0.31
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	10	0.31
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	10	0.31
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	10	0.31
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	10	0.31
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	10	0.31
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	6	0.31
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	6	0.31
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	6	0.31
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	6	0.31
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	6	0.31
(2,468)	1:233:C:ALA:H	1:232:C:LEU:HA	12	0.3
(2,300)	1:233:C:ALA:H	1:232:C:LEU:HA	12	0.3
(2,132)	1:233:C:ALA:H	1:232:C:LEU:HA	12	0.3
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	4	0.3
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	4	0.3
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	4	0.3
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	4	0.3
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	4	0.3
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	4	0.3
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	4	0.3
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	4	0.3
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	4	0.3
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	10	0.29
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	10	0.29
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	10	0.29
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	11	0.29
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	10	0.29
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	10	0.29
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	10	0.29
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	11	0.29
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	10	0.29
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	10	0.29
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	10	0.29
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	11	0.29
(2,488)	1:235:C:ARG:H	1:235:C:ARG:HD2	8	0.28
(2,488)	1:235:C:ARG:H	1:235:C:ARG:HD3	8	0.28
(2,320)	1:235:C:ARG:H	1:235:C:ARG:HD2	8	0.28
(2,320)	1:235:C:ARG:H	1:235:C:ARG:HD3	8	0.28
(2,152)	1:235:C:ARG:H	1:235:C:ARG:HD2	8	0.28
(2,152)	1:235:C:ARG:H	1:235:C:ARG:HD3	8	0.28
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	3	0.27
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	3	0.27
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	3	0.27
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	15	0.27
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	3	0.27
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	3	0.27
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	3	0.27
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	3	0.27
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	3	0.27
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	3	0.27
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	15	0.27
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	8	0.27
(1,33)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	8	0.27
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	8	0.27
(1,33)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	8	0.27
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	8	0.27
(1,33)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	8	0.27
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	8	0.27
(1,32)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	8	0.27
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	8	0.27
(1,32)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	8	0.27
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	8	0.27
(1,32)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	8	0.27
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB2	8	0.27
(1,31)	1:228:B:LEU:HD21	1:232:B:LEU:HB3	8	0.27
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB2	8	0.27
(1,31)	1:228:B:LEU:HD22	1:232:B:LEU:HB3	8	0.27
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB2	8	0.27
(1,31)	1:228:B:LEU:HD23	1:232:B:LEU:HB3	8	0.27
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	3	0.26
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	3	0.26
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	3	0.26
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	3	0.26
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	3	0.26
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	3	0.26
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	3	0.26
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	3	0.26
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	3	0.26
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	3	0.26
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	3	0.26
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	3	0.26
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	3	0.26
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	3	0.26
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	3	0.26
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	3	0.26
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	3	0.26
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	3	0.26
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	15	0.25
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	15	0.25
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	5	0.25
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	5	0.25
(2,451)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	5	0.25
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	5	0.25
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	5	0.25
(2,451)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	5	0.25
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	5	0.25
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	5	0.25
(2,451)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	5	0.25
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	13	0.25
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	13	0.25
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	13	0.25
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	13	0.25
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	13	0.25
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	13	0.25
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	6	0.25
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	9	0.25
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	15	0.25
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	15	0.25
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	15	0.25
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	5	0.25
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	5	0.25
(2,283)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	5	0.25
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	5	0.25
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	5	0.25
(2,283)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	5	0.25
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	5	0.25
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	5	0.25
(2,283)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	5	0.25
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	13	0.25
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	13	0.25
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	13	0.25
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	13	0.25
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	13	0.25
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	13	0.25
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	6	0.25
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	9	0.25
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	15	0.25
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	15	0.25
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	15	0.25
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB1	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB2	5	0.25
(2,115)	1:230:C:ILE:HD11	1:233:C:ALA:HB3	5	0.25
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB1	5	0.25
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB2	5	0.25
(2,115)	1:230:C:ILE:HD12	1:233:C:ALA:HB3	5	0.25
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB1	5	0.25
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB2	5	0.25
(2,115)	1:230:C:ILE:HD13	1:233:C:ALA:HB3	5	0.25
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	13	0.25
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	13	0.25
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	13	0.25
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	13	0.25
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	13	0.25
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	13	0.25
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	6	0.25
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	9	0.25
(2,414)	1:224:C:LEU:H	1:224:C:LEU:HB3	9	0.24
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	4	0.24
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	4	0.24
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	4	0.24
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	4	0.24
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	4	0.24
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	4	0.24
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	4	0.24
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	12	0.24
(2,341)	1:213:C:LEU:H	1:213:C:LEU:HB3	5	0.24
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	14	0.24
(2,246)	1:224:C:LEU:H	1:224:C:LEU:HB3	9	0.24
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	4	0.24
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	4	0.24
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	4	0.24
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	4	0.24
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	4	0.24
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	4	0.24
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	4	0.24
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	12	0.24
(2,173)	1:213:C:LEU:H	1:213:C:LEU:HB3	5	0.24
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	14	0.24
(2,78)	1:224:C:LEU:H	1:224:C:LEU:HB3	9	0.24
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	4	0.24
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	4	0.24
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	4	0.24
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	4	0.24
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	4	0.24
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	4	0.24
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	12	0.24
(2,5)	1:213:C:LEU:H	1:213:C:LEU:HB3	5	0.24
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	14	0.24
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	14	0.23
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	1	0.23
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	1	0.23
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	1	0.23
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	1	0.23
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	1	0.23
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	1	0.23
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	8	0.23
(2,348)	1:214:C:LEU:H	1:214:C:LEU:HB3	15	0.23
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	14	0.23
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	1	0.23
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	1	0.23
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	1	0.23
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	1	0.23
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	1	0.23
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	1	0.23
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	8	0.23
(2,180)	1:214:C:LEU:H	1:214:C:LEU:HB3	15	0.23
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	14	0.23
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	1	0.23
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	1	0.23
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	1	0.23
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	1	0.23
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	1	0.23
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	1	0.23
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	8	0.23
(2,12)	1:214:C:LEU:H	1:214:C:LEU:HB3	15	0.23
(2,502)	1:237:C:GLN:H	1:238:C:ARG:H	2	0.22
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	1	0.22
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	2	0.22
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	4	0.22
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	8	0.22
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	9	0.22
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	12	0.22
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	8	0.22
(2,334)	1:237:C:GLN:H	1:238:C:ARG:H	2	0.22
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	1	0.22
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	2	0.22
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	4	0.22
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	8	0.22
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	9	0.22
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	12	0.22
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	7	0.22
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	8	0.22
(2,166)	1:237:C:GLN:H	1:238:C:ARG:H	2	0.22
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	1	0.22
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	2	0.22
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	4	0.22
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	8	0.22
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	9	0.22
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	12	0.22
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	7	0.22
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	8	0.22
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	9	0.22
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	9	0.22
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	9	0.22
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	9	0.22
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	9	0.22
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	9	0.22
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	9	0.22
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	9	0.22
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	9	0.22
(2,498)	1:237:C:GLN:H	1:235:C:ARG:HA	2	0.21
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	3	0.21
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	6	0.21
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	10	0.21
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	15	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	8	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	8	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	8	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	8	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	8	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	8	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	12	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	12	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	12	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	12	0.21
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	12	0.21
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	15	0.21
(2,330)	1:237:C:GLN:H	1:235:C:ARG:HA	2	0.21
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	3	0.21
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	6	0.21
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	10	0.21
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	15	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	8	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	8	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	8	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	8	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	8	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	8	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	12	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	12	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	12	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	12	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	12	0.21
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	12	0.21
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	15	0.21
(2,162)	1:237:C:GLN:H	1:235:C:ARG:HA	2	0.21
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	3	0.21
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	6	0.21
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	10	0.21
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	15	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	8	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	8	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	8	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	8	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	8	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	8	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	12	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	12	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	12	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	12	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	12	0.21
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	12	0.21
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	15	0.21
(2,503)	1:238:C:ARG:H	1:237:C:GLN:HA	2	0.2
(2,503)	1:238:C:ARG:H	1:237:C:GLN:HA	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,503)	1:238:C:ARG:H	1:237:C:GLN:HA	13	0.2
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	5	0.2
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	5	0.2
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	5	0.2
(2,458)	1:232:C:LEU:H	1:229:C:PHE:HA	5	0.2
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	5	0.2
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	7	0.2
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	11	0.2
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	11	0.2
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	11	0.2
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	11	0.2
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	11	0.2
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	11	0.2
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	11	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	2	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	2	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	2	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	2	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	2	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	2	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	7	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	7	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	7	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	7	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	7	0.2
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	7	0.2
(2,335)	1:238:C:ARG:H	1:237:C:GLN:HA	2	0.2
(2,335)	1:238:C:ARG:H	1:237:C:GLN:HA	5	0.2
(2,335)	1:238:C:ARG:H	1:237:C:GLN:HA	13	0.2
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	5	0.2
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	5	0.2
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	5	0.2
(2,290)	1:232:C:LEU:H	1:229:C:PHE:HA	5	0.2
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	5	0.2
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	7	0.2
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	11	0.2
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	11	0.2
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	11	0.2
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	11	0.2
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	11	0.2
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	11	0.2
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	2	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	2	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	2	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	2	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	2	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	2	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	7	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	7	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	7	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	7	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	7	0.2
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	7	0.2
(2,167)	1:238:C:ARG:H	1:237:C:GLN:HA	2	0.2
(2,167)	1:238:C:ARG:H	1:237:C:GLN:HA	5	0.2
(2,167)	1:238:C:ARG:H	1:237:C:GLN:HA	13	0.2
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	5	0.2
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	5	0.2
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	5	0.2
(2,122)	1:232:C:LEU:H	1:229:C:PHE:HA	5	0.2
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	5	0.2
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	7	0.2
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	11	0.2
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	11	0.2
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	11	0.2
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	11	0.2
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	11	0.2
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	11	0.2
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	11	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	2	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	2	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	2	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	2	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	2	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	2	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	7	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	7	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	7	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	7	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	7	0.2
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	7	0.2
(2,453)	1:231:C:GLY:H	1:230:C:ILE:HA	13	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	5	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	5	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	5	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	5	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	5	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	11	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	11	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	11	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	11	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	11	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	11	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	14	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	14	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	14	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	14	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	14	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	14	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	15	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	15	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	15	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	15	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	15	0.19
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	15	0.19
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	10	0.19
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	13	0.19
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	14	0.19
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	1	0.19
(2,285)	1:231:C:GLY:H	1:230:C:ILE:HA	13	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	5	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	5	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	5	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	5	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	5	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	5	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	11	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	11	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	11	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	11	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	11	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	11	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	14	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	14	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	14	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	14	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	14	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	15	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	15	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	15	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	15	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	15	0.19
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	15	0.19
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	10	0.19
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	13	0.19
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	14	0.19
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	1	0.19
(2,117)	1:231:C:GLY:H	1:230:C:ILE:HA	13	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	5	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	5	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	5	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	5	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	5	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	5	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	11	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	11	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	11	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	11	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	11	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	11	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	14	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	14	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	14	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	14	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	14	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	14	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	15	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	15	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	15	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	15	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	15	0.19
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	15	0.19
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	10	0.19
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	13	0.19
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	1	0.19
(2,492)	1:236:C:TYR:H	1:235:C:ARG:HB2	4	0.18
(2,492)	1:236:C:TYR:H	1:235:C:ARG:HB3	4	0.18
(2,444)	1:229:C:PHE:H	1:228:C:LEU:HB3	3	0.18
(2,387)	1:221:C:GLY:H	1:218:C:ILE:HA	9	0.18
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	5	0.18
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	3	0.18
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	10	0.18
(2,324)	1:236:C:TYR:H	1:235:C:ARG:HB2	4	0.18
(2,324)	1:236:C:TYR:H	1:235:C:ARG:HB3	4	0.18
(2,276)	1:229:C:PHE:H	1:228:C:LEU:HB3	3	0.18
(2,219)	1:221:C:GLY:H	1:218:C:ILE:HA	9	0.18
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	5	0.18
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	3	0.18
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	10	0.18
(2,156)	1:236:C:TYR:H	1:235:C:ARG:HB2	4	0.18
(2,156)	1:236:C:TYR:H	1:235:C:ARG:HB3	4	0.18
(2,108)	1:229:C:PHE:H	1:228:C:LEU:HB3	3	0.18
(2,51)	1:221:C:GLY:H	1:218:C:ILE:HA	9	0.18
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	5	0.18
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	3	0.18
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	10	0.18
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	8	0.17
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	8	0.17
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	8	0.17
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	13	0.17
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	13	0.17
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	13	0.17
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	13	0.17
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	13	0.17
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	13	0.17
(2,444)	1:229:C:PHE:H	1:228:C:LEU:HB3	14	0.17
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	10	0.17
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	10	0.17
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	10	0.17
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	10	0.17
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	10	0.17
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	10	0.17
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	3	0.17
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	12	0.17
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	2	0.17
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	8	0.17
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	8	0.17
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	8	0.17
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	13	0.17
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	13	0.17
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	13	0.17
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	13	0.17
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	13	0.17
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	13	0.17
(2,276)	1:229:C:PHE:H	1:228:C:LEU:HB3	14	0.17
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	10	0.17
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	10	0.17
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	10	0.17
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	10	0.17
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	10	0.17
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	10	0.17
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	3	0.17
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	12	0.17
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	2	0.17
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	3	0.17
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	8	0.17
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	8	0.17
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	8	0.17
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	13	0.17
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	13	0.17
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	13	0.17
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	13	0.17
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	13	0.17
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	13	0.17
(2,108)	1:229:C:PHE:H	1:228:C:LEU:HB3	14	0.17
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	10	0.17
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	10	0.17
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	10	0.17
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	10	0.17
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	10	0.17
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	10	0.17
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	3	0.17
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	12	0.17
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	2	0.17
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	3	0.17
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	14	0.16
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	14	0.16
(2,387)	1:221:C:GLY:H	1:218:C:ILE:HA	6	0.16
(2,369)	1:218:C:ILE:H	1:215:C:PRO:HA	1	0.16
(2,365)	1:217:C:VAL:HG11	1:213:C:LEU:HA	10	0.16
(2,365)	1:217:C:VAL:HG12	1:213:C:LEU:HA	10	0.16
(2,365)	1:217:C:VAL:HG13	1:213:C:LEU:HA	10	0.16
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	14	0.16
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	14	0.16
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	14	0.16
(2,219)	1:221:C:GLY:H	1:218:C:ILE:HA	6	0.16
(2,201)	1:218:C:ILE:H	1:215:C:PRO:HA	1	0.16
(2,197)	1:217:C:VAL:HG11	1:213:C:LEU:HA	10	0.16
(2,197)	1:217:C:VAL:HG12	1:213:C:LEU:HA	10	0.16
(2,197)	1:217:C:VAL:HG13	1:213:C:LEU:HA	10	0.16
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	14	0.16
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	14	0.16
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	14	0.16
(2,51)	1:221:C:GLY:H	1:218:C:ILE:HA	6	0.16
(2,33)	1:218:C:ILE:H	1:215:C:PRO:HA	1	0.16
(2,29)	1:217:C:VAL:HG11	1:213:C:LEU:HA	10	0.16
(2,29)	1:217:C:VAL:HG12	1:213:C:LEU:HA	10	0.16
(2,29)	1:217:C:VAL:HG13	1:213:C:LEU:HA	10	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	3	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	3	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	3	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	7	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	7	0.16
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	7	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	3	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	3	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	3	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	7	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	7	0.16
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	7	0.16
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	3	0.16
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	3	0.16
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	3	0.16
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	7	0.16
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	7	0.16
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	7	0.16
(2,502)	1:237:C:GLN:H	1:238:C:ARG:H	1	0.15
(2,488)	1:235:C:ARG:H	1:235:C:ARG:HD2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,488)	1:235:C:ARG:H	1:235:C:ARG:HD3	10	0.15
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	12	0.15
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	12	0.15
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	12	0.15
(2,445)	1:229:C:PHE:H	1:228:C:LEU:HB2	10	0.15
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	1	0.15
(2,375)	1:219:C:PHE:H	1:216:C:LEU:HA	2	0.15
(2,375)	1:219:C:PHE:H	1:216:C:LEU:HA	4	0.15
(2,365)	1:217:C:VAL:HG11	1:213:C:LEU:HA	15	0.15
(2,365)	1:217:C:VAL:HG12	1:213:C:LEU:HA	15	0.15
(2,365)	1:217:C:VAL:HG13	1:213:C:LEU:HA	15	0.15
(2,344)	1:214:C:LEU:H	1:211:C:THR:HA	5	0.15
(2,334)	1:237:C:GLN:H	1:238:C:ARG:H	1	0.15
(2,320)	1:235:C:ARG:H	1:235:C:ARG:HD2	10	0.15
(2,320)	1:235:C:ARG:H	1:235:C:ARG:HD3	10	0.15
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	12	0.15
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	12	0.15
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	12	0.15
(2,277)	1:229:C:PHE:H	1:228:C:LEU:HB2	10	0.15
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	1	0.15
(2,207)	1:219:C:PHE:H	1:216:C:LEU:HA	2	0.15
(2,207)	1:219:C:PHE:H	1:216:C:LEU:HA	4	0.15
(2,197)	1:217:C:VAL:HG11	1:213:C:LEU:HA	15	0.15
(2,197)	1:217:C:VAL:HG12	1:213:C:LEU:HA	15	0.15
(2,197)	1:217:C:VAL:HG13	1:213:C:LEU:HA	15	0.15
(2,176)	1:214:C:LEU:H	1:211:C:THR:HA	5	0.15
(2,166)	1:237:C:GLN:H	1:238:C:ARG:H	1	0.15
(2,152)	1:235:C:ARG:H	1:235:C:ARG:HD2	10	0.15
(2,152)	1:235:C:ARG:H	1:235:C:ARG:HD3	10	0.15
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	12	0.15
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	12	0.15
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	12	0.15
(2,109)	1:229:C:PHE:H	1:228:C:LEU:HB2	10	0.15
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	1	0.15
(2,39)	1:219:C:PHE:H	1:216:C:LEU:HA	2	0.15
(2,39)	1:219:C:PHE:H	1:216:C:LEU:HA	4	0.15
(2,29)	1:217:C:VAL:HG11	1:213:C:LEU:HA	15	0.15
(2,29)	1:217:C:VAL:HG12	1:213:C:LEU:HA	15	0.15
(2,29)	1:217:C:VAL:HG13	1:213:C:LEU:HA	15	0.15
(2,8)	1:214:C:LEU:H	1:211:C:THR:HA	5	0.15
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	10	0.15
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	10	0.15
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	10	0.15
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	10	0.15
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	10	0.15
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	10	0.15
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	10	0.15
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	10	0.15
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	7	0.14
(2,450)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	7	0.14
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	7	0.14
(2,450)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	7	0.14
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	7	0.14
(2,450)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	7	0.14
(2,445)	1:229:C:PHE:H	1:228:C:LEU:HB2	1	0.14
(2,445)	1:229:C:PHE:H	1:228:C:LEU:HB2	12	0.14
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD11	9	0.14
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD12	9	0.14
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD13	9	0.14
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD21	9	0.14
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD22	9	0.14
(2,393)	1:221:C:GLY:H	1:222:C:LEU:HD23	9	0.14
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	9	0.14
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	14	0.14
(2,375)	1:219:C:PHE:H	1:216:C:LEU:HA	9	0.14
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	6	0.14
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	6	0.14
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	6	0.14
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	7	0.14
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	7	0.14
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	7	0.14
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	14	0.14
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	14	0.14
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	14	0.14
(2,365)	1:217:C:VAL:HG11	1:213:C:LEU:HA	5	0.14
(2,365)	1:217:C:VAL:HG12	1:213:C:LEU:HA	5	0.14
(2,365)	1:217:C:VAL:HG13	1:213:C:LEU:HA	5	0.14
(2,361)	1:217:C:VAL:H	1:216:C:LEU:HB2	14	0.14
(2,348)	1:214:C:LEU:H	1:214:C:LEU:HB3	2	0.14
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	7	0.14
(2,282)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	7	0.14
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	7	0.14
(2,282)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	7	0.14
(2,282)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	7	0.14
(2,277)	1:229:C:PHE:H	1:228:C:LEU:HB2	1	0.14
(2,277)	1:229:C:PHE:H	1:228:C:LEU:HB2	12	0.14
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD11	9	0.14
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD12	9	0.14
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD13	9	0.14
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD21	9	0.14
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD22	9	0.14
(2,225)	1:221:C:GLY:H	1:222:C:LEU:HD23	9	0.14
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	9	0.14
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	14	0.14
(2,207)	1:219:C:PHE:H	1:216:C:LEU:HA	9	0.14
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	6	0.14
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	6	0.14
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	6	0.14
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	7	0.14
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	7	0.14
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	7	0.14
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	14	0.14
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	14	0.14
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	14	0.14
(2,197)	1:217:C:VAL:HG11	1:213:C:LEU:HA	5	0.14
(2,197)	1:217:C:VAL:HG12	1:213:C:LEU:HA	5	0.14
(2,197)	1:217:C:VAL:HG13	1:213:C:LEU:HA	5	0.14
(2,193)	1:217:C:VAL:H	1:216:C:LEU:HB2	14	0.14
(2,180)	1:214:C:LEU:H	1:214:C:LEU:HB3	2	0.14
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB2	7	0.14
(2,114)	1:230:C:ILE:HD11	1:229:C:PHE:HB3	7	0.14
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB2	7	0.14
(2,114)	1:230:C:ILE:HD12	1:229:C:PHE:HB3	7	0.14
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB2	7	0.14
(2,114)	1:230:C:ILE:HD13	1:229:C:PHE:HB3	7	0.14
(2,109)	1:229:C:PHE:H	1:228:C:LEU:HB2	1	0.14
(2,109)	1:229:C:PHE:H	1:228:C:LEU:HB2	12	0.14
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD11	9	0.14
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD12	9	0.14
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD13	9	0.14
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD21	9	0.14
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD22	9	0.14
(2,57)	1:221:C:GLY:H	1:222:C:LEU:HD23	9	0.14
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	14	0.14
(2,39)	1:219:C:PHE:H	1:216:C:LEU:HA	9	0.14
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	6	0.14
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	6	0.14
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	6	0.14
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	7	0.14
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	7	0.14
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	7	0.14
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	14	0.14
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	14	0.14
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	14	0.14
(2,29)	1:217:C:VAL:HG11	1:213:C:LEU:HA	5	0.14
(2,29)	1:217:C:VAL:HG12	1:213:C:LEU:HA	5	0.14
(2,29)	1:217:C:VAL:HG13	1:213:C:LEU:HA	5	0.14
(2,25)	1:217:C:VAL:H	1:216:C:LEU:HB2	14	0.14
(2,12)	1:214:C:LEU:H	1:214:C:LEU:HB3	2	0.14
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	6	0.14
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	6	0.14
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	6	0.14
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	8	0.14
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	8	0.14
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	8	0.14
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	6	0.14
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	6	0.14
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	6	0.14
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	8	0.14
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	8	0.14
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	8	0.14
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	6	0.14
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	6	0.14
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	6	0.14
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	8	0.14
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	8	0.14
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	8	0.14
(2,473)	1:233:C:ALA:HB1	1:230:C:ILE:HA	2	0.13
(2,473)	1:233:C:ALA:HB2	1:230:C:ILE:HA	2	0.13
(2,473)	1:233:C:ALA:HB3	1:230:C:ILE:HA	2	0.13
(2,432)	1:227:C:LEU:H	1:227:C:LEU:HG	14	0.13
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	2	0.13
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	6	0.13
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	7	0.13
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	13	0.13
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	5	0.13
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	5	0.13
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	5	0.13
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	8	0.13
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	8	0.13
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	8	0.13
(2,344)	1:214:C:LEU:H	1:211:C:THR:HA	1	0.13
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	2	0.13
(2,337)	1:212:C:VAL:H	1:211:C:THR:HA	9	0.13
(2,305)	1:233:C:ALA:HB1	1:230:C:ILE:HA	2	0.13
(2,305)	1:233:C:ALA:HB2	1:230:C:ILE:HA	2	0.13
(2,305)	1:233:C:ALA:HB3	1:230:C:ILE:HA	2	0.13
(2,264)	1:227:C:LEU:H	1:227:C:LEU:HG	14	0.13
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	2	0.13
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	6	0.13
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	7	0.13
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	8	0.13
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	13	0.13
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	5	0.13
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	5	0.13
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	5	0.13
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	8	0.13
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	8	0.13
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	8	0.13
(2,176)	1:214:C:LEU:H	1:211:C:THR:HA	1	0.13
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	2	0.13
(2,169)	1:212:C:VAL:H	1:211:C:THR:HA	9	0.13
(2,137)	1:233:C:ALA:HB1	1:230:C:ILE:HA	2	0.13
(2,137)	1:233:C:ALA:HB2	1:230:C:ILE:HA	2	0.13
(2,137)	1:233:C:ALA:HB3	1:230:C:ILE:HA	2	0.13
(2,96)	1:227:C:LEU:H	1:227:C:LEU:HG	14	0.13
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	2	0.13
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	6	0.13
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	7	0.13
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	8	0.13
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	13	0.13
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	5	0.13
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	5	0.13
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	5	0.13
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	8	0.13
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	8	0.13
(2,8)	1:214:C:LEU:H	1:211:C:THR:HA	1	0.13
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	2	0.13
(2,1)	1:212:C:VAL:H	1:211:C:THR:HA	9	0.13
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	5	0.13
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	5	0.13
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	5	0.13
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	5	0.13
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	5	0.13
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	5	0.13
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	5	0.13
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	5	0.13
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	5	0.13
(2,449)	1:230:C:ILE:HG21	1:227:C:LEU:HA	14	0.12
(2,449)	1:230:C:ILE:HG22	1:227:C:LEU:HA	14	0.12
(2,449)	1:230:C:ILE:HG23	1:227:C:LEU:HA	14	0.12
(2,445)	1:229:C:PHE:H	1:228:C:LEU:HB2	15	0.12
(2,402)	1:222:C:LEU:HD21	1:223:C:ALA:HA	1	0.12
(2,402)	1:222:C:LEU:HD22	1:223:C:ALA:HA	1	0.12
(2,402)	1:222:C:LEU:HD23	1:223:C:ALA:HA	1	0.12
(2,390)	1:221:C:GLY:H	1:220:C:PHE:HB2	11	0.12
(2,387)	1:221:C:GLY:H	1:218:C:ILE:HA	2	0.12
(2,387)	1:221:C:GLY:H	1:218:C:ILE:HA	4	0.12
(2,387)	1:221:C:GLY:H	1:218:C:ILE:HA	14	0.12
(2,375)	1:219:C:PHE:H	1:216:C:LEU:HA	1	0.12
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	12	0.12
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	12	0.12
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	12	0.12
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	1	0.12
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	5	0.12
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	10	0.12
(2,348)	1:214:C:LEU:H	1:214:C:LEU:HB3	4	0.12
(2,344)	1:214:C:LEU:H	1:211:C:THR:HA	14	0.12
(2,344)	1:214:C:LEU:H	1:211:C:THR:HA	15	0.12
(2,281)	1:230:C:ILE:HG21	1:227:C:LEU:HA	14	0.12
(2,281)	1:230:C:ILE:HG22	1:227:C:LEU:HA	14	0.12
(2,281)	1:230:C:ILE:HG23	1:227:C:LEU:HA	14	0.12
(2,277)	1:229:C:PHE:H	1:228:C:LEU:HB2	15	0.12
(2,234)	1:222:C:LEU:HD21	1:223:C:ALA:HA	1	0.12
(2,234)	1:222:C:LEU:HD22	1:223:C:ALA:HA	1	0.12
(2,234)	1:222:C:LEU:HD23	1:223:C:ALA:HA	1	0.12
(2,222)	1:221:C:GLY:H	1:220:C:PHE:HB2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,219)	1:221:C:GLY:H	1:218:C:ILE:HA	2	0.12
(2,219)	1:221:C:GLY:H	1:218:C:ILE:HA	4	0.12
(2,219)	1:221:C:GLY:H	1:218:C:ILE:HA	14	0.12
(2,207)	1:219:C:PHE:H	1:216:C:LEU:HA	1	0.12
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	12	0.12
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	12	0.12
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	12	0.12
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	1	0.12
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	5	0.12
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	10	0.12
(2,180)	1:214:C:LEU:H	1:214:C:LEU:HB3	4	0.12
(2,176)	1:214:C:LEU:H	1:211:C:THR:HA	14	0.12
(2,176)	1:214:C:LEU:H	1:211:C:THR:HA	15	0.12
(2,113)	1:230:C:ILE:HG21	1:227:C:LEU:HA	14	0.12
(2,113)	1:230:C:ILE:HG22	1:227:C:LEU:HA	14	0.12
(2,113)	1:230:C:ILE:HG23	1:227:C:LEU:HA	14	0.12
(2,109)	1:229:C:PHE:H	1:228:C:LEU:HB2	15	0.12
(2,66)	1:222:C:LEU:HD21	1:223:C:ALA:HA	1	0.12
(2,66)	1:222:C:LEU:HD22	1:223:C:ALA:HA	1	0.12
(2,66)	1:222:C:LEU:HD23	1:223:C:ALA:HA	1	0.12
(2,54)	1:221:C:GLY:H	1:220:C:PHE:HB2	11	0.12
(2,51)	1:221:C:GLY:H	1:218:C:ILE:HA	2	0.12
(2,51)	1:221:C:GLY:H	1:218:C:ILE:HA	4	0.12
(2,51)	1:221:C:GLY:H	1:218:C:ILE:HA	14	0.12
(2,39)	1:219:C:PHE:H	1:216:C:LEU:HA	1	0.12
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	12	0.12
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	12	0.12
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	12	0.12
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	1	0.12
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	5	0.12
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	10	0.12
(2,12)	1:214:C:LEU:H	1:214:C:LEU:HB3	4	0.12
(2,8)	1:214:C:LEU:H	1:211:C:THR:HA	14	0.12
(2,8)	1:214:C:LEU:H	1:211:C:THR:HA	15	0.12
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	15	0.12
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	15	0.12
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	15	0.12
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	15	0.12
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	15	0.12
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	15	0.12
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	15	0.12
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	15	0.12
(2,498)	1:237:C:GLN:H	1:235:C:ARG:HA	3	0.11
(2,449)	1:230:C:ILE:HG21	1:227:C:LEU:HA	15	0.11
(2,449)	1:230:C:ILE:HG22	1:227:C:LEU:HA	15	0.11
(2,449)	1:230:C:ILE:HG23	1:227:C:LEU:HA	15	0.11
(2,432)	1:227:C:LEU:H	1:227:C:LEU:HG	2	0.11
(2,432)	1:227:C:LEU:H	1:227:C:LEU:HG	5	0.11
(2,417)	1:224:C:LEU:HD11	1:221:C:GLY:HA2	7	0.11
(2,417)	1:224:C:LEU:HD11	1:221:C:GLY:HA3	7	0.11
(2,417)	1:224:C:LEU:HD12	1:221:C:GLY:HA2	7	0.11
(2,417)	1:224:C:LEU:HD12	1:221:C:GLY:HA3	7	0.11
(2,417)	1:224:C:LEU:HD13	1:221:C:GLY:HA2	7	0.11
(2,417)	1:224:C:LEU:HD13	1:221:C:GLY:HA3	7	0.11
(2,402)	1:222:C:LEU:HD21	1:223:C:ALA:HA	11	0.11
(2,402)	1:222:C:LEU:HD22	1:223:C:ALA:HA	11	0.11
(2,402)	1:222:C:LEU:HD23	1:223:C:ALA:HA	11	0.11
(2,375)	1:219:C:PHE:H	1:216:C:LEU:HA	6	0.11
(2,375)	1:219:C:PHE:H	1:216:C:LEU:HA	10	0.11
(2,375)	1:219:C:PHE:H	1:216:C:LEU:HA	14	0.11
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	3	0.11
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	3	0.11
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	3	0.11
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	11	0.11
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	11	0.11
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	11	0.11
(2,366)	1:217:C:VAL:HG11	1:214:C:LEU:HA	13	0.11
(2,366)	1:217:C:VAL:HG12	1:214:C:LEU:HA	13	0.11
(2,366)	1:217:C:VAL:HG13	1:214:C:LEU:HA	13	0.11
(2,365)	1:217:C:VAL:HG11	1:213:C:LEU:HA	1	0.11
(2,365)	1:217:C:VAL:HG12	1:213:C:LEU:HA	1	0.11
(2,365)	1:217:C:VAL:HG13	1:213:C:LEU:HA	1	0.11
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	3	0.11
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	12	0.11
(2,353)	1:216:C:LEU:H	1:216:C:LEU:HB3	15	0.11
(2,348)	1:214:C:LEU:H	1:214:C:LEU:HB3	1	0.11
(2,330)	1:237:C:GLN:H	1:235:C:ARG:HA	3	0.11
(2,281)	1:230:C:ILE:HG21	1:227:C:LEU:HA	15	0.11
(2,281)	1:230:C:ILE:HG22	1:227:C:LEU:HA	15	0.11
(2,281)	1:230:C:ILE:HG23	1:227:C:LEU:HA	15	0.11
(2,264)	1:227:C:LEU:H	1:227:C:LEU:HG	2	0.11
(2,264)	1:227:C:LEU:H	1:227:C:LEU:HG	5	0.11
(2,249)	1:224:C:LEU:HD11	1:221:C:GLY:HA2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,249)	1:224:C:LEU:HD11	1:221:C:GLY:HA3	7	0.11
(2,249)	1:224:C:LEU:HD12	1:221:C:GLY:HA2	7	0.11
(2,249)	1:224:C:LEU:HD12	1:221:C:GLY:HA3	7	0.11
(2,249)	1:224:C:LEU:HD13	1:221:C:GLY:HA2	7	0.11
(2,249)	1:224:C:LEU:HD13	1:221:C:GLY:HA3	7	0.11
(2,234)	1:222:C:LEU:HD21	1:223:C:ALA:HA	11	0.11
(2,234)	1:222:C:LEU:HD22	1:223:C:ALA:HA	11	0.11
(2,234)	1:222:C:LEU:HD23	1:223:C:ALA:HA	11	0.11
(2,207)	1:219:C:PHE:H	1:216:C:LEU:HA	6	0.11
(2,207)	1:219:C:PHE:H	1:216:C:LEU:HA	10	0.11
(2,207)	1:219:C:PHE:H	1:216:C:LEU:HA	14	0.11
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	3	0.11
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	3	0.11
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	3	0.11
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	11	0.11
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	11	0.11
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	11	0.11
(2,198)	1:217:C:VAL:HG11	1:214:C:LEU:HA	13	0.11
(2,198)	1:217:C:VAL:HG12	1:214:C:LEU:HA	13	0.11
(2,198)	1:217:C:VAL:HG13	1:214:C:LEU:HA	13	0.11
(2,197)	1:217:C:VAL:HG11	1:213:C:LEU:HA	1	0.11
(2,197)	1:217:C:VAL:HG12	1:213:C:LEU:HA	1	0.11
(2,197)	1:217:C:VAL:HG13	1:213:C:LEU:HA	1	0.11
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	3	0.11
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	12	0.11
(2,185)	1:216:C:LEU:H	1:216:C:LEU:HB3	15	0.11
(2,180)	1:214:C:LEU:H	1:214:C:LEU:HB3	1	0.11
(2,162)	1:237:C:GLN:H	1:235:C:ARG:HA	3	0.11
(2,113)	1:230:C:ILE:HG21	1:227:C:LEU:HA	15	0.11
(2,113)	1:230:C:ILE:HG22	1:227:C:LEU:HA	15	0.11
(2,113)	1:230:C:ILE:HG23	1:227:C:LEU:HA	15	0.11
(2,96)	1:227:C:LEU:H	1:227:C:LEU:HG	2	0.11
(2,96)	1:227:C:LEU:H	1:227:C:LEU:HG	5	0.11
(2,81)	1:224:C:LEU:HD11	1:221:C:GLY:HA2	7	0.11
(2,81)	1:224:C:LEU:HD11	1:221:C:GLY:HA3	7	0.11
(2,81)	1:224:C:LEU:HD12	1:221:C:GLY:HA2	7	0.11
(2,81)	1:224:C:LEU:HD12	1:221:C:GLY:HA3	7	0.11
(2,81)	1:224:C:LEU:HD13	1:221:C:GLY:HA2	7	0.11
(2,81)	1:224:C:LEU:HD13	1:221:C:GLY:HA3	7	0.11
(2,66)	1:222:C:LEU:HD21	1:223:C:ALA:HA	11	0.11
(2,66)	1:222:C:LEU:HD22	1:223:C:ALA:HA	11	0.11
(2,66)	1:222:C:LEU:HD23	1:223:C:ALA:HA	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:219:C:PHE:H	1:216:C:LEU:HA	6	0.11
(2,39)	1:219:C:PHE:H	1:216:C:LEU:HA	10	0.11
(2,39)	1:219:C:PHE:H	1:216:C:LEU:HA	14	0.11
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	3	0.11
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	3	0.11
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	3	0.11
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	11	0.11
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	11	0.11
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	11	0.11
(2,30)	1:217:C:VAL:HG11	1:214:C:LEU:HA	13	0.11
(2,30)	1:217:C:VAL:HG12	1:214:C:LEU:HA	13	0.11
(2,30)	1:217:C:VAL:HG13	1:214:C:LEU:HA	13	0.11
(2,29)	1:217:C:VAL:HG11	1:213:C:LEU:HA	1	0.11
(2,29)	1:217:C:VAL:HG12	1:213:C:LEU:HA	1	0.11
(2,29)	1:217:C:VAL:HG13	1:213:C:LEU:HA	1	0.11
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	3	0.11
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	12	0.11
(2,17)	1:216:C:LEU:H	1:216:C:LEU:HB3	15	0.11
(2,12)	1:214:C:LEU:H	1:214:C:LEU:HB3	1	0.11
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD11	11	0.11
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD12	11	0.11
(1,12)	1:222:B:LEU:H	1:222:B:LEU:HD13	11	0.11
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD11	11	0.11
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD12	11	0.11
(1,11)	1:222:B:LEU:H	1:222:B:LEU:HD13	11	0.11
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD11	11	0.11
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD12	11	0.11
(1,10)	1:222:B:LEU:H	1:222:B:LEU:HD13	11	0.11
(2,445)	1:229:C:PHE:H	1:228:C:LEU:HB2	2	0.1
(2,402)	1:222:C:LEU:HD21	1:223:C:ALA:HA	7	0.1
(2,402)	1:222:C:LEU:HD22	1:223:C:ALA:HA	7	0.1
(2,402)	1:222:C:LEU:HD23	1:223:C:ALA:HA	7	0.1
(2,387)	1:221:C:GLY:H	1:218:C:ILE:HA	12	0.1
(2,365)	1:217:C:VAL:HG11	1:213:C:LEU:HA	3	0.1
(2,365)	1:217:C:VAL:HG12	1:213:C:LEU:HA	3	0.1
(2,365)	1:217:C:VAL:HG13	1:213:C:LEU:HA	3	0.1
(2,365)	1:217:C:VAL:HG11	1:213:C:LEU:HA	9	0.1
(2,365)	1:217:C:VAL:HG12	1:213:C:LEU:HA	9	0.1
(2,365)	1:217:C:VAL:HG13	1:213:C:LEU:HA	9	0.1
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	2	0.1
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	8	0.1
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,364)	1:217:C:VAL:H	1:217:C:VAL:HB	13	0.1
(2,277)	1:229:C:PHE:H	1:228:C:LEU:HB2	2	0.1
(2,234)	1:222:C:LEU:HD21	1:223:C:ALA:HA	7	0.1
(2,234)	1:222:C:LEU:HD22	1:223:C:ALA:HA	7	0.1
(2,234)	1:222:C:LEU:HD23	1:223:C:ALA:HA	7	0.1
(2,219)	1:221:C:GLY:H	1:218:C:ILE:HA	12	0.1
(2,197)	1:217:C:VAL:HG11	1:213:C:LEU:HA	3	0.1
(2,197)	1:217:C:VAL:HG12	1:213:C:LEU:HA	3	0.1
(2,197)	1:217:C:VAL:HG13	1:213:C:LEU:HA	3	0.1
(2,197)	1:217:C:VAL:HG11	1:213:C:LEU:HA	9	0.1
(2,197)	1:217:C:VAL:HG12	1:213:C:LEU:HA	9	0.1
(2,197)	1:217:C:VAL:HG13	1:213:C:LEU:HA	9	0.1
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	2	0.1
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	8	0.1
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	9	0.1
(2,196)	1:217:C:VAL:H	1:217:C:VAL:HB	13	0.1
(2,109)	1:229:C:PHE:H	1:228:C:LEU:HB2	2	0.1
(2,66)	1:222:C:LEU:HD21	1:223:C:ALA:HA	7	0.1
(2,66)	1:222:C:LEU:HD22	1:223:C:ALA:HA	7	0.1
(2,66)	1:222:C:LEU:HD23	1:223:C:ALA:HA	7	0.1
(2,51)	1:221:C:GLY:H	1:218:C:ILE:HA	12	0.1
(2,29)	1:217:C:VAL:HG11	1:213:C:LEU:HA	3	0.1
(2,29)	1:217:C:VAL:HG12	1:213:C:LEU:HA	3	0.1
(2,29)	1:217:C:VAL:HG13	1:213:C:LEU:HA	3	0.1
(2,29)	1:217:C:VAL:HG11	1:213:C:LEU:HA	9	0.1
(2,29)	1:217:C:VAL:HG12	1:213:C:LEU:HA	9	0.1
(2,29)	1:217:C:VAL:HG13	1:213:C:LEU:HA	9	0.1
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	2	0.1
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	8	0.1
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	9	0.1
(2,28)	1:217:C:VAL:H	1:217:C:VAL:HB	13	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found