Full wwPDB NMR Structure Validation Report (i)

Mar 12, 2026 – 04:32 PM UTC

PDB ID	:	6E8W / pdb_00006e8w
BMRB ID	:	30503
Title	:	MPER-TM Domain of HIV-1 envelope glycoprotein (Env)
Authors	:	Fu, Q.; Shaik, M.M.; Cai, Y.; Ghantous, F.; Piai, A.; Peng, H.; Rits-Volloch, S.; Liu, Z.; Harrison, S.C.; Seaman, M.S.; Chen, B.; Chou, J.J.
Deposited on	:	2018-07-31

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 (i) 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 (i)) were used in the production of this report:

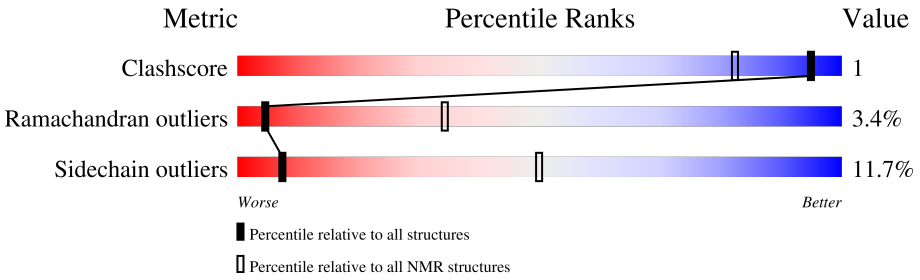
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 8%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	51	12% 80% 8%
1	B	51	12% 84% .
1	C	51	10% 86% .

2 Ensemble composition and analysis

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:660-A:710, B:660-B:710, C:660-C:710 (153)	1.33	1

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2712 atoms, of which 1389 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					Trace
1	A	51	Total	C	H	N	O	0
			904	301	463	73	67	
1	B	51	Total	C	H	N	O	0
			904	301	463	73	67	
1	C	51	Total	C	H	N	O	0
			904	301	463	73	67	

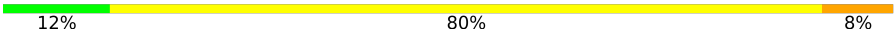
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

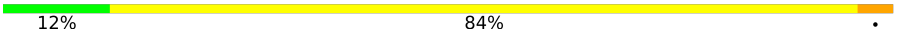
• Molecule 1: Envelope glycoprotein gp160

Chain A:



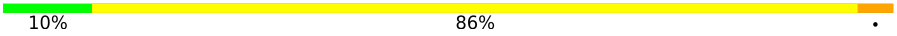
• Molecule 1: Envelope glycoprotein gp160

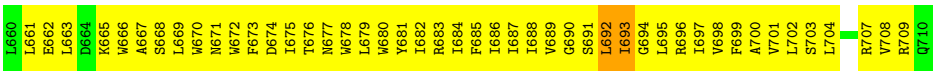
Chain B:



• Molecule 1: Envelope glycoprotein gp160

Chain C:





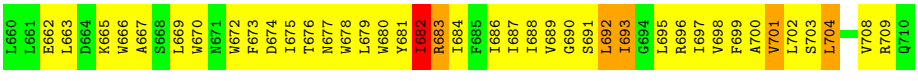
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

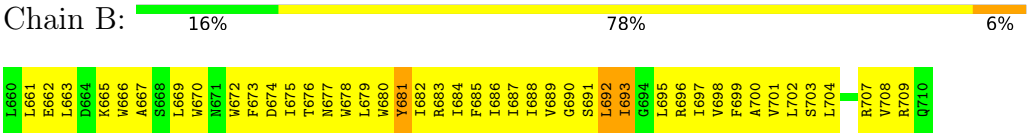
• Molecule 1: Envelope glycoprotein gp160

Chain A:



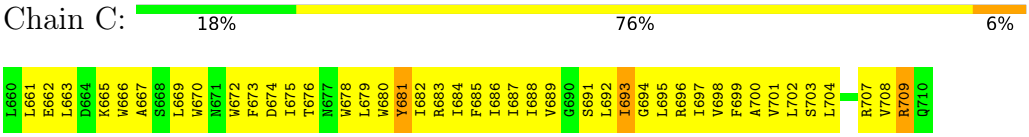
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

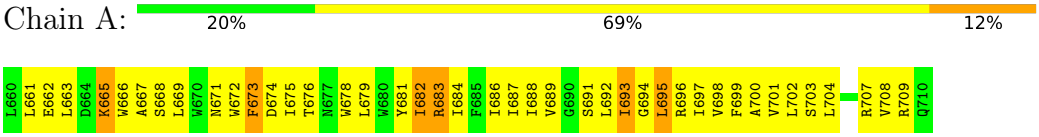
Chain C:



4.2.2 Score per residue for model 2

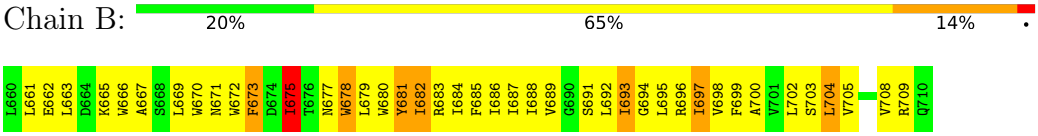
• Molecule 1: Envelope glycoprotein gp160

Chain A:



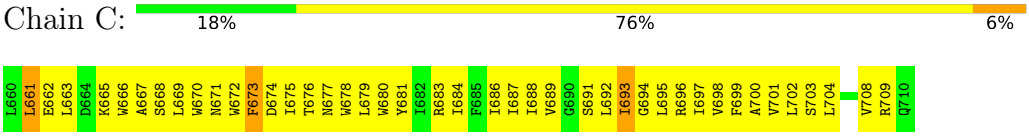
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

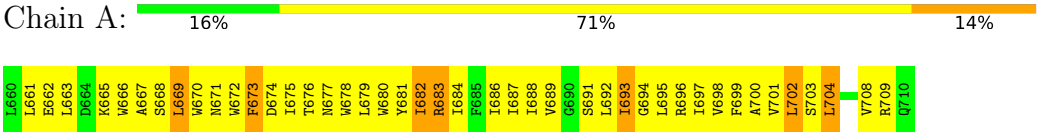
Chain C:



4.2.3 Score per residue for model 3

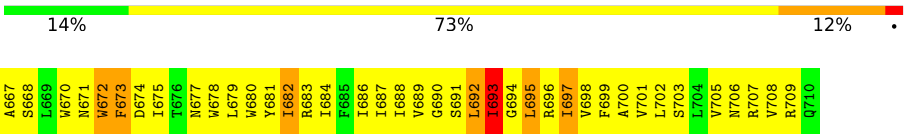
• Molecule 1: Envelope glycoprotein gp160

Chain A:



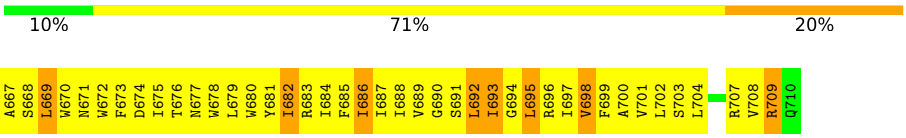
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

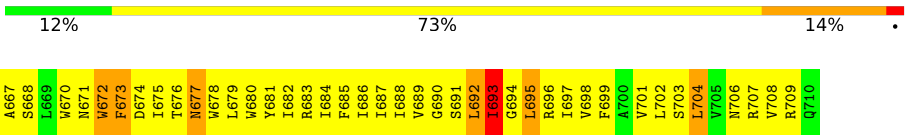
Chain C:



4.2.4 Score per residue for model 4

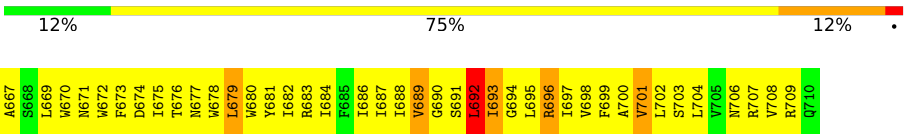
• Molecule 1: Envelope glycoprotein gp160

Chain A:



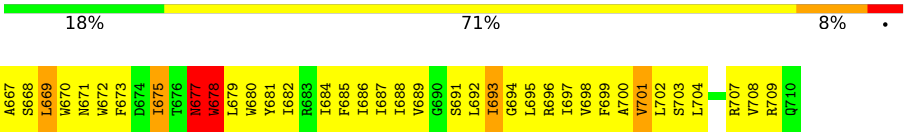
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

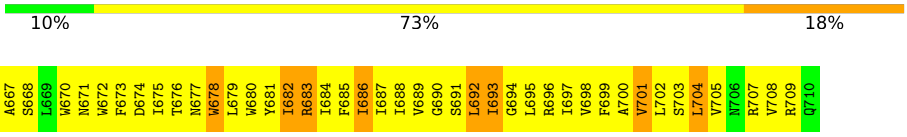
Chain C:



4.2.5 Score per residue for model 5

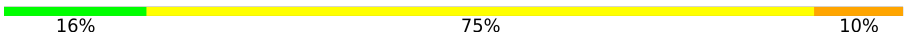
• Molecule 1: Envelope glycoprotein gp160

Chain A:



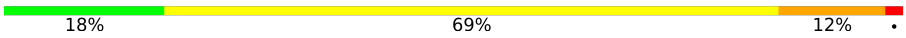
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

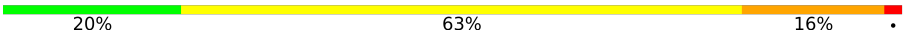
Chain C:



4.2.6 Score per residue for model 6

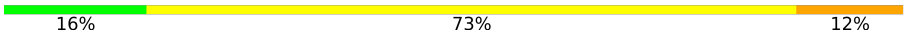
• Molecule 1: Envelope glycoprotein gp160

Chain A:



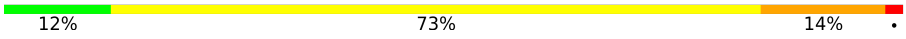
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

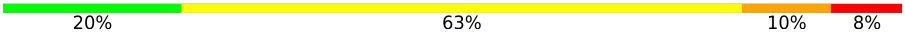
Chain C:



4.2.7 Score per residue for model 7

• Molecule 1: Envelope glycoprotein gp160

Chain A:

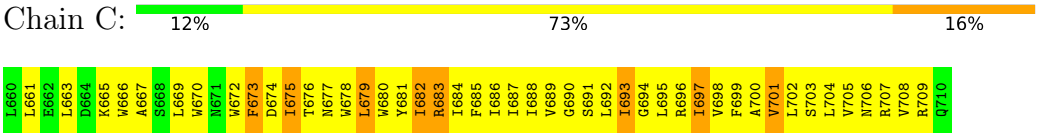


• Molecule 1: Envelope glycoprotein gp160

Chain B:

• Molecule 1: Envelope glycoprotein gp160

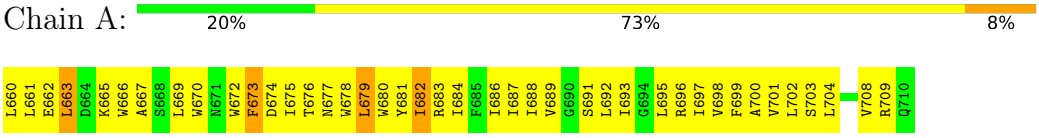
Chain C:



4.2.8 Score per residue for model 8

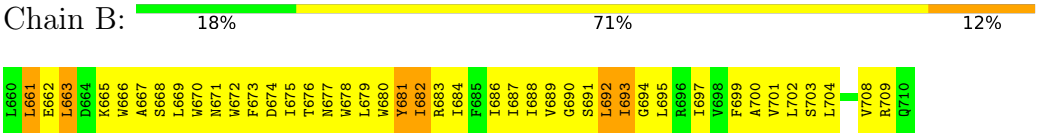
• Molecule 1: Envelope glycoprotein gp160

Chain A:



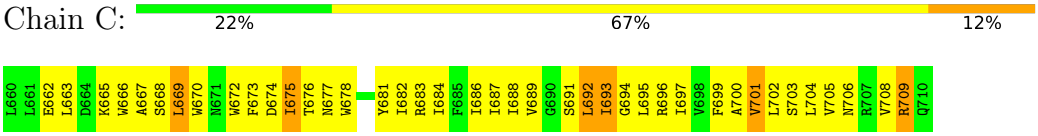
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

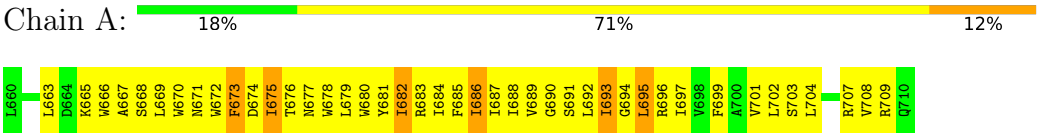
Chain C:



4.2.9 Score per residue for model 9

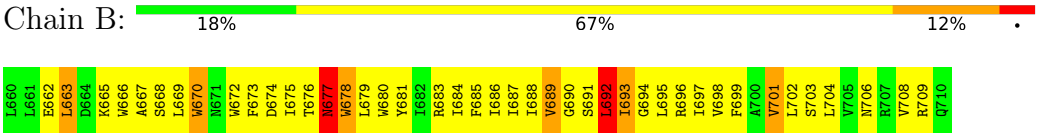
• Molecule 1: Envelope glycoprotein gp160

Chain A:



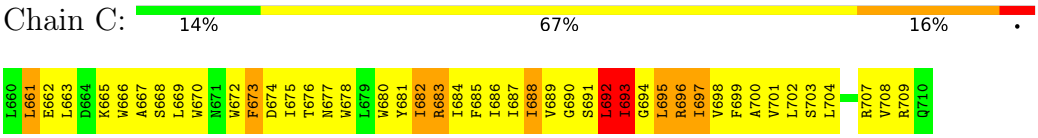
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

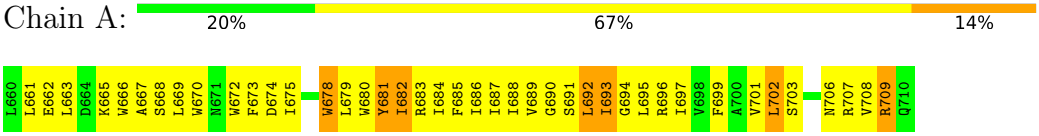
Chain C:



4.2.10 Score per residue for model 10

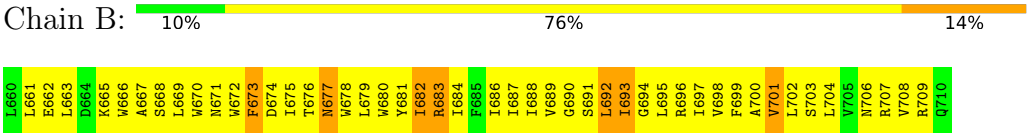
• Molecule 1: Envelope glycoprotein gp160

Chain A:



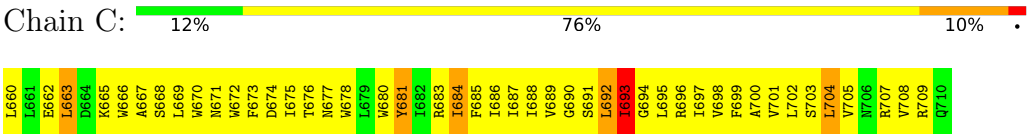
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

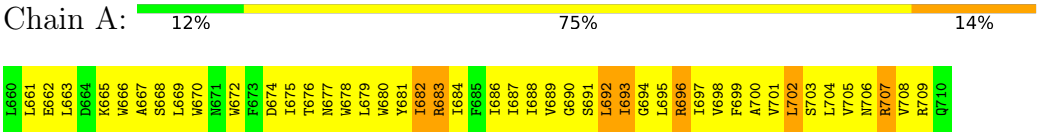
Chain C:



4.2.11 Score per residue for model 11

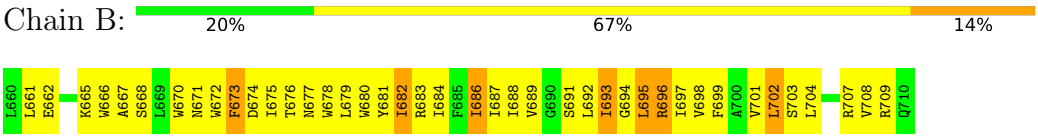
• Molecule 1: Envelope glycoprotein gp160

Chain A:



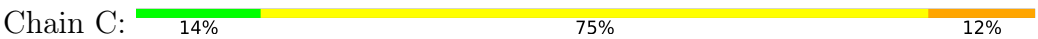
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

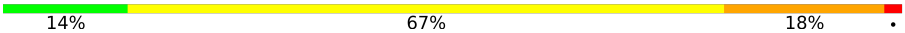
Chain C:



4.2.12 Score per residue for model 12

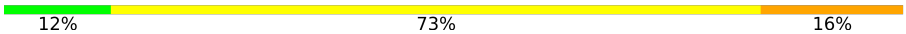
• Molecule 1: Envelope glycoprotein gp160

Chain A:



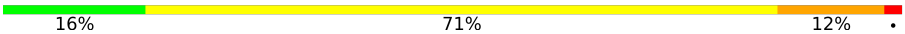
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

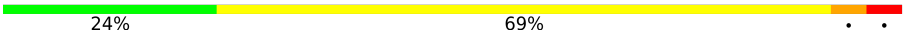
Chain C:

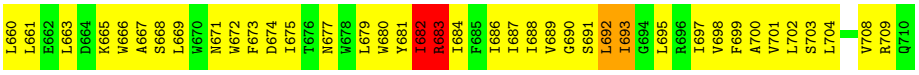


4.2.13 Score per residue for model 13

• Molecule 1: Envelope glycoprotein gp160

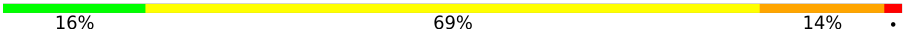
Chain A:





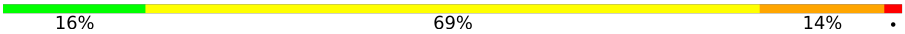
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

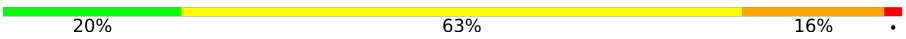
Chain C:

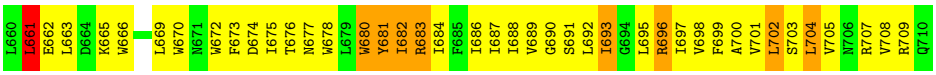


4.2.14 Score per residue for model 14

• Molecule 1: Envelope glycoprotein gp160

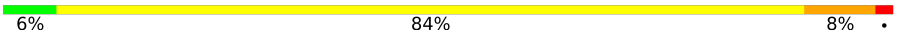
Chain A:

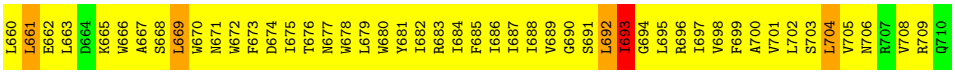




• Molecule 1: Envelope glycoprotein gp160

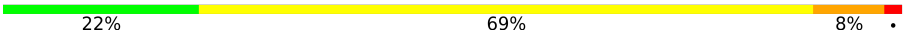
Chain B:





• Molecule 1: Envelope glycoprotein gp160

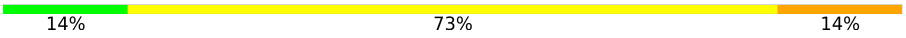
Chain C:



4.2.15 Score per residue for model 15

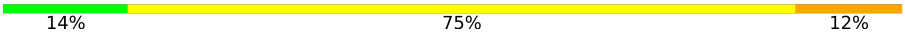
• Molecule 1: Envelope glycoprotein gp160

Chain A:



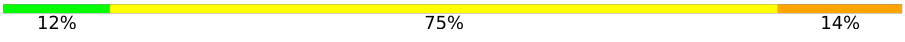
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

Chain C:



5 Refinement protocol and experimental data overview

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

Of the 150 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	2.48
X-PLOR NIH	structure calculation	2.48

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	188
Number of shifts mapped to atoms	188
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	3.12±0.03	57±3/454 (12.5± 0.8%)	1.32±0.04	0±1/619 (0.0± 0.1%)
1	B	3.10±0.04	57±3/454 (12.5± 0.6%)	1.32±0.04	0±1/619 (0.0± 0.1%)
1	C	3.11±0.03	57±3/454 (12.6± 0.6%)	1.32±0.04	0±1/619 (0.0± 0.1%)
All	All	3.11	2564/20430 (12.6%)	1.32	11/27855 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.5
1	B	0.0±0.0	0.1±0.2
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	681	TYR	CA-CB	12.18	1.62	1.53	2	1
1	C	693	ILE	CA-CB	10.37	1.66	1.54	11	13
1	B	693	ILE	CA-CB	10.22	1.66	1.54	14	15
1	C	684	ILE	CA-CB	9.89	1.66	1.54	10	15
1	A	686	ILE	CA-CB	9.40	1.65	1.54	4	13
1	C	708	VAL	N-CA	9.14	1.56	1.46	5	14
1	A	693	ILE	CA-CB	9.10	1.64	1.54	13	15
1	C	686	ILE	CA-CB	8.97	1.64	1.54	13	11
1	A	684	ILE	CA-CB	8.79	1.65	1.54	14	15
1	B	686	ILE	CA-CB	8.71	1.64	1.54	7	13
1	C	680	TRP	N-CA	8.62	1.55	1.46	7	13
1	B	707	ARG	N-CA	8.52	1.57	1.46	11	9
1	B	684	ILE	CA-CB	8.52	1.64	1.54	5	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	701	VAL	CA-CB	8.49	1.65	1.54	8	13
1	A	682	ILE	CA-CB	8.38	1.65	1.54	13	15
1	A	708	VAL	N-CA	8.36	1.54	1.46	10	15
1	A	697	ILE	N-CA	8.36	1.56	1.46	9	14
1	C	697	ILE	N-CA	8.33	1.56	1.46	8	15
1	A	681	TYR	CA-CB	8.30	1.61	1.53	14	1
1	A	672	TRP	N-CA	8.24	1.56	1.46	4	15
1	A	695	LEU	N-CA	8.24	1.56	1.46	7	15
1	B	701	VAL	N-CA	8.22	1.56	1.46	13	13
1	A	686	ILE	N-CA	8.22	1.56	1.46	13	14
1	A	684	ILE	N-CA	8.21	1.56	1.46	14	13
1	B	681	TYR	N-CA	8.05	1.54	1.46	14	13
1	B	693	ILE	N-CA	7.95	1.55	1.46	14	15
1	C	673	PHE	N-CA	7.92	1.56	1.46	4	4
1	B	675	ILE	CA-CB	7.91	1.66	1.54	2	8
1	A	701	VAL	CA-CB	7.90	1.63	1.54	12	11
1	B	682	ILE	CA-CB	7.82	1.64	1.54	13	9
1	A	693	ILE	N-CA	7.80	1.55	1.46	13	14
1	C	670	TRP	N-CA	7.71	1.56	1.46	4	15
1	A	701	VAL	N-CA	7.70	1.55	1.46	15	14
1	A	675	ILE	CA-CB	7.65	1.65	1.54	7	9
1	B	672	TRP	N-CA	7.65	1.56	1.46	3	15
1	C	701	VAL	N-CA	7.64	1.55	1.46	5	15
1	A	688	ILE	N-CA	7.63	1.55	1.46	8	15
1	C	675	ILE	CA-CB	7.63	1.64	1.54	12	8
1	C	696	ARG	N-CA	7.63	1.55	1.46	9	15
1	A	696	ARG	N-CA	7.63	1.56	1.46	14	13
1	A	680	TRP	N-CA	7.62	1.56	1.46	8	13
1	B	686	ILE	N-CA	7.62	1.55	1.46	9	15
1	C	708	VAL	CA-CB	7.61	1.62	1.54	5	11
1	B	675	ILE	N-CA	7.61	1.56	1.46	2	15
1	A	682	ILE	N-CA	7.60	1.55	1.46	8	15
1	B	697	ILE	N-CA	7.59	1.55	1.46	8	15
1	C	686	ILE	N-CA	7.58	1.55	1.46	6	15
1	B	698	VAL	N-CA	7.57	1.56	1.46	2	13
1	C	688	ILE	N-CA	7.56	1.55	1.46	4	15
1	C	688	ILE	CA-CB	7.52	1.63	1.54	13	15
1	B	701	VAL	CA-CB	7.51	1.64	1.54	4	9
1	A	679	LEU	N-CA	7.51	1.55	1.46	7	14
1	C	698	VAL	N-CA	7.51	1.55	1.46	2	14
1	A	683	ARG	N-CA	7.50	1.55	1.46	6	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	688	ILE	CA-CB	7.47	1.64	1.54	14	15
1	C	693	ILE	N-CA	7.46	1.55	1.46	11	13
1	A	681	TYR	N-CA	7.45	1.55	1.46	4	14
1	A	678	TRP	CA-CB	7.42	1.65	1.53	10	6
1	B	688	ILE	N-CA	7.41	1.55	1.46	6	15
1	A	687	ILE	N-CA	7.40	1.55	1.46	12	15
1	B	680	TRP	N-CA	7.39	1.55	1.46	14	14
1	C	689	VAL	N-CA	7.38	1.55	1.46	9	15
1	C	681	TYR	N-CA	7.36	1.55	1.46	7	13
1	B	708	VAL	N-CA	7.35	1.54	1.45	14	15
1	B	699	PHE	N-CA	7.34	1.55	1.46	5	15
1	C	695	LEU	N-CA	7.33	1.55	1.46	5	15
1	B	682	ILE	N-CA	7.31	1.55	1.46	11	10
1	B	696	ARG	N-CA	7.31	1.55	1.46	11	11
1	A	688	ILE	CA-CB	7.27	1.63	1.54	5	15
1	C	662	GLU	N-CA	7.24	1.55	1.46	13	12
1	A	709	ARG	N-CA	7.18	1.55	1.46	13	14
1	C	678	TRP	CA-CB	7.17	1.64	1.53	4	8
1	B	665	LYS	N-CA	7.16	1.55	1.46	11	15
1	C	661	LEU	N-CA	7.15	1.54	1.45	9	9
1	C	675	ILE	N-CA	7.15	1.55	1.46	12	15
1	A	698	VAL	N-CA	7.14	1.55	1.46	3	12
1	B	678	TRP	CA-CB	7.13	1.64	1.53	2	4
1	C	682	ILE	CA-CB	7.12	1.63	1.54	12	8
1	C	687	ILE	CA-CB	7.12	1.62	1.54	11	15
1	C	699	PHE	N-CA	7.10	1.54	1.46	13	15
1	C	682	ILE	N-CA	7.07	1.54	1.46	12	12
1	B	702	LEU	N-CA	7.06	1.55	1.46	15	14
1	B	679	LEU	N-CA	7.04	1.55	1.46	7	15
1	B	662	GLU	N-CA	7.03	1.54	1.45	14	14
1	A	697	ILE	CA-CB	7.01	1.63	1.54	10	13
1	A	699	PHE	N-CA	7.00	1.54	1.46	7	15
1	B	663	LEU	N-CA	7.00	1.54	1.46	4	13
1	A	661	LEU	N-CA	7.00	1.54	1.45	12	10
1	C	697	ILE	CA-CB	6.98	1.63	1.54	14	15
1	A	707	ARG	N-CA	6.96	1.54	1.46	10	9
1	A	675	ILE	N-CA	6.92	1.54	1.46	6	15
1	B	684	ILE	N-CA	6.92	1.54	1.46	5	10
1	A	662	GLU	N-CA	6.91	1.54	1.46	11	12
1	A	689	VAL	CA-CB	6.91	1.63	1.54	7	10
1	C	687	ILE	N-CA	6.88	1.54	1.46	3	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	695	LEU	N-CA	6.86	1.54	1.46	15	15
1	C	679	LEU	N-CA	6.86	1.55	1.46	11	10
1	C	691	SER	N-CA	6.86	1.54	1.46	14	15
1	C	700	ALA	N-CA	6.84	1.54	1.46	13	14
1	A	702	LEU	N-CA	6.82	1.55	1.46	7	15
1	C	667	ALA	N-CA	6.81	1.54	1.46	2	14
1	C	669	LEU	CA-CB	6.81	1.64	1.53	4	3
1	B	697	ILE	CA-CB	6.78	1.62	1.54	8	15
1	A	663	LEU	N-CA	6.73	1.54	1.46	7	14
1	C	669	LEU	N-CA	6.73	1.55	1.46	9	14
1	C	707	ARG	N-CA	6.73	1.54	1.46	15	12
1	A	689	VAL	N-CA	6.71	1.54	1.46	14	15
1	A	674	ASP	N-CA	6.70	1.54	1.46	13	15
1	A	663	LEU	CA-CB	6.69	1.64	1.53	7	3
1	B	689	VAL	CA-CB	6.67	1.63	1.54	3	9
1	B	689	VAL	N-CA	6.66	1.54	1.46	1	15
1	C	709	ARG	N-CA	6.65	1.54	1.46	9	13
1	A	687	ILE	CA-CB	6.65	1.62	1.54	12	15
1	A	671	ASN	N-CA	6.65	1.54	1.46	13	8
1	C	671	ASN	N-CA	6.64	1.54	1.46	15	10
1	A	665	LYS	N-CA	6.63	1.54	1.46	9	15
1	B	691	SER	N-CA	6.62	1.54	1.46	14	15
1	A	666	TRP	N-CA	6.62	1.54	1.46	6	15
1	B	674	ASP	N-CA	6.61	1.54	1.46	3	14
1	C	676	THR	N-CA	6.60	1.54	1.46	2	14
1	B	687	ILE	CA-CB	6.58	1.62	1.54	8	15
1	C	702	LEU	N-CA	6.57	1.54	1.46	15	15
1	C	665	LYS	N-CA	6.56	1.54	1.46	5	15
1	A	691	SER	N-CA	6.56	1.54	1.46	10	15
1	B	687	ILE	N-CA	6.53	1.54	1.46	2	15
1	C	692	LEU	CA-CB	6.52	1.63	1.53	2	9
1	B	666	TRP	N-CA	6.50	1.54	1.46	10	15
1	C	683	ARG	N-CA	6.50	1.54	1.46	6	14
1	B	690	GLY	N-CA	6.49	1.53	1.45	4	11
1	B	700	ALA	N-CA	6.47	1.54	1.46	8	13
1	B	683	ARG	N-CA	6.47	1.54	1.46	11	14
1	C	709	ARG	CA-CB	6.47	1.62	1.53	9	1
1	C	689	VAL	CA-CB	6.46	1.63	1.54	10	10
1	C	678	TRP	N-CA	6.46	1.54	1.46	14	15
1	C	694	GLY	N-CA	6.46	1.53	1.45	9	14
1	B	709	ARG	N-CA	6.45	1.53	1.46	2	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	684	ILE	N-CA	6.43	1.54	1.46	10	12
1	C	666	TRP	N-CA	6.42	1.53	1.46	11	14
1	A	667	ALA	N-CA	6.42	1.54	1.46	10	13
1	A	700	ALA	N-CA	6.42	1.54	1.46	6	12
1	A	692	LEU	CA-CB	6.41	1.63	1.53	3	10
1	B	692	LEU	CA-CB	6.40	1.63	1.53	15	12
1	B	676	THR	N-CA	6.38	1.54	1.46	12	13
1	A	703	SER	N-CA	6.37	1.54	1.46	3	15
1	A	679	LEU	CA-CB	6.34	1.63	1.53	7	4
1	B	661	LEU	N-CA	6.33	1.53	1.45	12	11
1	C	685	PHE	N-CA	6.33	1.54	1.46	7	10
1	B	686	ILE	CB-CG1	6.32	1.66	1.53	11	3
1	A	678	TRP	N-CA	6.30	1.53	1.46	5	14
1	B	665	LYS	CA-CB	6.30	1.63	1.53	11	2
1	A	692	LEU	N-CA	6.28	1.53	1.46	3	11
1	B	694	GLY	N-CA	6.27	1.53	1.45	4	14
1	B	703	SER	N-CA	6.26	1.53	1.46	12	15
1	A	694	GLY	N-CA	6.26	1.53	1.45	5	9
1	C	692	LEU	N-CA	6.25	1.53	1.46	2	13
1	C	677	ASN	N-CA	6.24	1.53	1.46	9	11
1	B	670	TRP	N-CA	6.23	1.54	1.46	6	14
1	C	674	ASP	N-CA	6.21	1.53	1.46	13	12
1	C	690	GLY	N-CA	6.21	1.53	1.45	13	9
1	C	698	VAL	CA-CB	6.20	1.63	1.54	3	2
1	B	692	LEU	N-CA	6.20	1.54	1.46	3	14
1	B	692	LEU	CB-CG	6.19	1.65	1.53	13	3
1	B	678	TRP	N-CA	6.17	1.53	1.46	14	14
1	A	670	TRP	N-CA	6.16	1.54	1.46	11	12
1	B	667	ALA	N-CA	6.15	1.53	1.46	5	15
1	C	680	TRP	CA-CB	6.14	1.59	1.53	10	3
1	A	704	LEU	N-CA	6.12	1.53	1.46	14	13
1	B	677	ASN	N-CA	6.11	1.53	1.46	3	15
1	A	708	VAL	CA-CB	6.08	1.61	1.54	15	13
1	B	708	VAL	CA-CB	6.07	1.61	1.54	5	14
1	A	661	LEU	CA-CB	6.07	1.62	1.53	6	2
1	C	703	SER	N-CA	6.06	1.53	1.46	8	15
1	B	672	TRP	CA-CB	6.06	1.63	1.53	3	1
1	A	662	GLU	CA-CB	6.05	1.63	1.53	6	1
1	A	676	THR	N-CA	6.03	1.53	1.46	14	13
1	C	663	LEU	N-CA	6.01	1.53	1.46	13	14
1	A	665	LYS	CA-CB	5.99	1.62	1.53	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	669	LEU	N-CA	5.99	1.54	1.46	1	11
1	B	704	LEU	N-CA	5.98	1.53	1.46	2	13
1	A	663	LEU	CB-CG	5.98	1.65	1.53	10	8
1	A	669	LEU	N-CA	5.98	1.54	1.46	8	12
1	B	702	LEU	CB-CG	5.95	1.65	1.53	11	12
1	B	671	ASN	N-CA	5.95	1.53	1.46	4	12
1	C	704	LEU	N-CA	5.93	1.53	1.46	9	12
1	A	698	VAL	CA-CB	5.93	1.63	1.54	12	2
1	B	704	LEU	CB-CG	5.92	1.65	1.53	10	4
1	C	687	ILE	CB-CG1	5.92	1.65	1.53	13	4
1	B	663	LEU	CB-CG	5.92	1.65	1.53	12	4
1	C	692	LEU	CB-CG	5.91	1.65	1.53	12	4
1	C	702	LEU	CB-CG	5.89	1.65	1.53	13	13
1	C	685	PHE	CA-CB	5.89	1.62	1.53	4	1
1	C	663	LEU	CB-CG	5.88	1.65	1.53	4	9
1	A	702	LEU	CB-CG	5.87	1.65	1.53	11	10
1	A	702	LEU	CA-CB	5.87	1.63	1.53	14	5
1	A	706	ASN	N-CA	5.86	1.53	1.46	10	5
1	A	695	LEU	CA-CB	5.86	1.62	1.53	2	8
1	B	673	PHE	N-CA	5.85	1.53	1.46	2	6
1	B	668	SER	N-CA	5.84	1.53	1.46	14	11
1	A	677	ASN	N-CA	5.83	1.53	1.46	12	12
1	C	672	TRP	N-CA	5.83	1.53	1.46	15	14
1	A	675	ILE	CB-CG1	5.81	1.65	1.53	5	3
1	B	706	ASN	N-CA	5.81	1.53	1.46	3	5
1	C	706	ASN	N-CA	5.81	1.53	1.46	15	3
1	A	685	PHE	N-CA	5.80	1.53	1.46	4	4
1	A	690	GLY	N-CA	5.79	1.53	1.45	6	11
1	C	673	PHE	CA-CB	5.78	1.63	1.53	4	1
1	B	705	VAL	N-CA	5.77	1.53	1.46	15	6
1	B	702	LEU	CA-CB	5.77	1.63	1.53	15	2
1	C	661	LEU	CA-CB	5.75	1.63	1.53	13	3
1	A	668	SER	N-CA	5.74	1.53	1.46	15	10
1	A	683	ARG	CA-CB	5.72	1.63	1.53	14	2
1	B	695	LEU	CA-CB	5.68	1.62	1.53	2	3
1	C	668	SER	N-CA	5.66	1.53	1.46	4	12
1	B	679	LEU	CA-CB	5.65	1.62	1.53	4	4
1	B	698	VAL	CA-CB	5.65	1.63	1.54	3	1
1	C	695	LEU	CA-CB	5.64	1.62	1.53	1	9
1	B	669	LEU	CA-CB	5.64	1.62	1.53	6	2
1	A	669	LEU	CA-CB	5.64	1.62	1.53	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	685	PHE	CA-CB	5.62	1.62	1.53	2	2
1	C	686	ILE	CB-CG1	5.60	1.64	1.53	9	2
1	B	662	GLU	CA-CB	5.59	1.62	1.53	15	1
1	B	661	LEU	CA-CB	5.59	1.61	1.53	3	1
1	C	683	ARG	CA-CB	5.56	1.61	1.53	15	1
1	A	693	ILE	CB-CG1	5.52	1.64	1.53	6	6
1	C	705	VAL	N-CA	5.51	1.53	1.46	6	4
1	C	679	LEU	CA-CB	5.48	1.62	1.53	7	2
1	B	693	ILE	CB-CG1	5.47	1.64	1.53	8	5
1	C	681	TYR	CA-CB	5.45	1.61	1.53	5	1
1	C	693	ILE	CB-CG1	5.45	1.64	1.53	14	4
1	C	673	PHE	CA-C	5.45	1.58	1.52	14	2
1	C	683	ARG	CD-NE	5.45	1.53	1.46	8	3
1	B	675	ILE	CB-CG1	5.43	1.64	1.53	10	7
1	A	687	ILE	CB-CG1	5.43	1.64	1.53	8	6
1	A	686	ILE	CB-CG1	5.42	1.64	1.53	12	2
1	A	705	VAL	N-CA	5.42	1.53	1.46	5	5
1	C	705	VAL	CA-CB	5.41	1.61	1.54	11	4
1	C	675	ILE	CB-CG1	5.40	1.64	1.53	11	8
1	A	682	ILE	CB-CG1	5.39	1.64	1.53	4	2
1	B	709	ARG	CA-CB	5.39	1.59	1.52	1	1
1	A	709	ARG	CA-CB	5.38	1.62	1.53	3	2
1	B	663	LEU	CA-CB	5.38	1.61	1.53	4	1
1	B	705	VAL	CA-CB	5.37	1.61	1.54	5	5
1	A	673	PHE	N-CA	5.34	1.53	1.46	9	5
1	C	696	ARG	CD-NE	5.30	1.53	1.46	4	3
1	A	664	ASP	N-CA	5.30	1.52	1.46	7	1
1	C	682	ILE	CB-CG1	5.29	1.64	1.53	8	2
1	A	704	LEU	CB-CG	5.28	1.64	1.53	7	4
1	A	697	ILE	CB-CG1	5.26	1.64	1.53	10	4
1	C	697	ILE	CA-C	5.26	1.59	1.52	2	1
1	C	697	ILE	CB-CG1	5.25	1.64	1.53	8	1
1	C	669	LEU	CB-CG	5.25	1.64	1.53	10	1
1	C	662	GLU	CA-CB	5.24	1.60	1.53	9	1
1	A	683	ARG	CD-NE	5.23	1.53	1.46	14	2
1	B	697	ILE	CB-CG1	5.23	1.64	1.53	8	2
1	A	669	LEU	CB-CG	5.22	1.63	1.53	3	3
1	B	685	PHE	N-CA	5.22	1.52	1.46	1	4
1	A	692	LEU	CB-CG	5.17	1.63	1.53	5	3
1	B	669	LEU	CB-CG	5.16	1.63	1.53	13	1
1	B	696	ARG	CD-NE	5.16	1.53	1.46	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	683	ARG	CD-NE	5.15	1.53	1.46	9	3
1	C	665	LYS	CA-CB	5.14	1.61	1.53	5	1
1	B	697	ILE	CA-C	5.14	1.59	1.52	2	1
1	B	707	ARG	CD-NE	5.12	1.53	1.46	5	1
1	B	679	LEU	CB-CG	5.12	1.63	1.53	13	2
1	C	679	LEU	CB-CG	5.11	1.63	1.53	7	2
1	C	663	LEU	CA-CB	5.10	1.61	1.53	4	1
1	C	678	TRP	CA-C	5.10	1.59	1.52	4	1
1	B	687	ILE	CB-CG1	5.10	1.63	1.53	8	1
1	B	682	ILE	CB-CG1	5.09	1.63	1.53	5	2
1	A	679	LEU	CB-CG	5.07	1.63	1.53	8	1
1	C	688	ILE	CB-CG1	5.05	1.63	1.53	14	1
1	C	704	LEU	CB-CG	5.05	1.63	1.53	10	1
1	C	661	LEU	CA-C	5.04	1.57	1.53	5	1
1	A	672	TRP	CA-CB	5.03	1.61	1.53	4	1
1	A	705	VAL	CA-CB	5.03	1.61	1.54	11	1
1	B	701	VAL	C-N	5.01	1.40	1.33	15	1
1	A	704	LEU	CA-CB	5.01	1.61	1.53	1	1
1	B	660	LEU	CB-CG	5.01	1.63	1.53	7	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	681	TYR	N-CA-C	-6.53	105.44	113.41	12	1
1	A	682	ILE	CA-C-N	5.69	128.69	120.38	14	1
1	A	682	ILE	C-N-CA	5.69	128.69	120.38	14	1
1	B	695	LEU	CA-C-N	5.46	128.35	120.38	8	1
1	B	695	LEU	C-N-CA	5.46	128.35	120.38	8	1
1	C	673	PHE	CA-C-N	5.24	128.28	120.31	4	1
1	C	673	PHE	C-N-CA	5.24	128.28	120.31	4	1
1	A	695	LEU	N-CA-C	5.21	116.77	111.14	14	1
1	B	670	TRP	CB-CG-CD2	5.18	134.05	126.80	9	1
1	C	694	GLY	CA-C-N	5.06	127.32	120.44	13	1
1	C	694	GLY	C-N-CA	5.06	127.32	120.44	13	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	696	ARG	Sidechain	1
1	A	683	ARG	Sidechain	1
1	A	696	ARG	Sidechain	1

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	441	463	460	1±1
1	B	441	463	460	1±1
1	C	441	463	460	1±1
All	All	19845	20835	20700	45

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:682:ILE:HD12	1:A:683:ARG:N	0.62	2.10	15	3
1:C:692:LEU:HD13	1:C:693:ILE:N	0.61	2.10	9	1
1:C:682:ILE:HD12	1:C:683:ARG:N	0.59	2.11	9	3
1:B:682:ILE:HD12	1:B:683:ARG:N	0.58	2.13	10	1
1:C:679:LEU:HD13	1:C:679:LEU:O	0.56	2.01	5	1
1:A:702:LEU:O	1:A:702:LEU:HD22	0.52	2.04	7	1
1:A:693:ILE:HD12	1:A:693:ILE:O	0.51	2.05	7	3
1:B:680:TRP:CD1	1:B:681:TYR:H	0.51	2.23	8	1
1:A:680:TRP:O	1:A:681:TYR:CD2	0.51	2.64	14	1
1:A:683:ARG:NH1	1:B:678:TRP:HE1	0.50	2.03	12	1
1:B:693:ILE:HD12	1:B:693:ILE:O	0.49	2.07	3	1
1:A:679:LEU:H	1:A:679:LEU:HD13	0.48	1.67	7	1
1:C:693:ILE:O	1:C:693:ILE:HD13	0.48	2.09	9	2
1:A:679:LEU:HD13	1:A:679:LEU:N	0.46	2.24	7	1
1:A:682:ILE:HD12	1:A:683:ARG:H	0.45	1.71	1	3
1:C:693:ILE:HD12	1:C:694:GLY:N	0.44	2.26	14	1
1:A:683:ARG:HH22	1:B:682:ILE:HD12	0.44	1.73	12	1
1:B:693:ILE:C	1:B:693:ILE:HD12	0.43	2.38	14	1
1:B:660:LEU:N	1:B:665:LYS:HZ3	0.43	2.11	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:663:LEU:HD13	1:A:664:ASP:N	0.43	2.28	7	1
1:A:696:ARG:NE	1:C:693:ILE:HD11	0.42	2.29	6	1
1:B:677:ASN:HD22	1:B:678:TRP:N	0.42	2.12	9	1
1:A:683:ARG:HH12	1:B:678:TRP:CD1	0.42	2.33	5	1
1:C:677:ASN:HD22	1:C:677:ASN:H	0.42	1.56	5	1
1:B:689:VAL:O	1:B:692:LEU:HD11	0.42	2.15	9	2
1:A:693:ILE:HD11	1:B:696:ARG:HE	0.42	1.75	4	1
1:B:707:ARG:HE	1:C:707:ARG:HH11	0.42	1.56	13	1
1:B:682:ILE:HD12	1:B:683:ARG:H	0.42	1.75	13	1
1:A:696:ARG:HE	1:C:693:ILE:HD11	0.41	1.75	6	1
1:B:675:ILE:O	1:B:675:ILE:HD12	0.41	2.16	2	1
1:A:693:ILE:HD11	1:B:696:ARG:NE	0.41	2.31	4	1
1:C:677:ASN:ND2	1:C:678:TRP:H	0.41	2.13	4	1
1:C:677:ASN:HD22	1:C:677:ASN:N	0.40	2.13	5	1
1:C:693:ILE:HD12	1:C:693:ILE:C	0.40	2.41	10	1
1:B:695:LEU:HD23	1:B:695:LEU:C	0.40	2.42	11	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	49/51 (96%)	46±1 (94±3%)	2±1 (3±2%)	1±1 (3±2%)	5	38
1	B	49/51 (96%)	45±2 (92±3%)	2±2 (5±4%)	2±1 (3±1%)	5	37
1	C	49/51 (96%)	45±1 (93±2%)	2±1 (3±2%)	2±1 (4±2%)	4	30
All	All	2205/2295 (96%)	2047 (93%)	84 (4%)	74 (3%)	4	34

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	673	PHE	15
1	A	673	PHE	14
1	C	673	PHE	13

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Mol	Chain	Res	Type	Models (Total)
1	C	709	ARG	7
1	C	661	LEU	5
1	A	661	LEU	4
1	B	661	LEU	3
1	B	681	TYR	2
1	C	681	TYR	2
1	C	662	GLU	2
1	B	709	ARG	2
1	A	662	GLU	1
1	A	681	TYR	1
1	A	709	ARG	1
1	B	662	GLU	1
1	A	680	TRP	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	47/47 (100%)	41±2 (87±4%)	6±2 (13±4%)	6 47
1	B	47/47 (100%)	42±1 (90±3%)	5±1 (10±3%)	9 52
1	C	47/47 (100%)	42±2 (88±5%)	5±2 (12±5%)	7 50
All	All	2115/2115 (100%)	1867 (88%)	248 (12%)	7 50

All 71 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	693	ILE	15
1	C	693	ILE	15
1	A	693	ILE	14
1	B	692	LEU	12
1	A	682	ILE	10
1	A	692	LEU	10
1	C	692	LEU	8
1	B	682	ILE	7
1	A	704	LEU	6
1	A	695	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	C	695	LEU	6
1	C	675	ILE	6
1	C	701	VAL	6
1	A	702	LEU	5
1	A	663	LEU	5
1	A	701	VAL	4
1	B	704	LEU	4
1	C	686	ILE	4
1	B	663	LEU	4
1	B	701	VAL	4
1	A	679	LEU	4
1	C	697	ILE	4
1	A	669	LEU	3
1	C	661	LEU	3
1	C	663	LEU	3
1	C	669	LEU	3
1	C	682	ILE	3
1	B	660	LEU	3
1	B	679	LEU	3
1	A	661	LEU	3
1	A	675	ILE	3
1	A	707	ARG	3
1	B	669	LEU	3
1	B	677	ASN	3
1	B	702	LEU	3
1	C	702	LEU	3
1	B	675	ILE	2
1	B	697	ILE	2
1	C	677	ASN	2
1	C	678	TRP	2
1	A	678	TRP	2
1	A	686	ILE	2
1	A	660	LEU	2
1	C	696	ARG	2
1	C	660	LEU	2
1	C	704	LEU	2
1	C	710	GLN	2
1	A	683	ARG	2
1	A	665	LYS	1
1	B	678	TRP	1
1	B	681	TYR	1
1	B	672	TRP	1

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Mol	Chain	Res	Type	Models (Total)
1	B	695	LEU	1
1	C	698	VAL	1
1	A	672	TRP	1
1	A	677	ASN	1
1	C	681	TYR	1
1	B	661	LEU	1
1	B	665	LYS	1
1	A	662	GLU	1
1	A	697	ILE	1
1	C	679	LEU	1
1	B	670	TRP	1
1	C	688	ILE	1
1	A	681	TYR	1
1	C	684	ILE	1
1	B	686	ILE	1
1	B	696	ARG	1
1	A	696	ARG	1
1	A	710	GLN	1
1	C	671	ASN	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 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *bmrb.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	188
Number of shifts mapped to atoms	188
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	47	-0.43 ± 0.34	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	43	-0.06 ± 0.16	None needed (< 0.5 ppm)
^{15}N	49	0.78 ± 0.43	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 188 atoms were assigned a chemical shift out of a possible 2424. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	188/771 (24%)	49/312 (16%)	90/306 (29%)	49/153 (32%)
Sidechain	0/1356 (0%)	0/900 (0%)	0/405 (0%)	0/51 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/297 (0%)	0/147 (0%)	0/135 (0%)	0/15 (0%)
Overall	188/2424 (8%)	49/1359 (4%)	90/846 (11%)	49/219 (22%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 188 atoms were assigned a chemical shift out of a possible 2424. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	188/771 (24%)	49/312 (16%)	90/306 (29%)	49/153 (32%)
Sidechain	0/1356 (0%)	0/900 (0%)	0/405 (0%)	0/51 (0%)
Aromatic	0/297 (0%)	0/147 (0%)	0/135 (0%)	0/15 (0%)
Overall	188/2424 (8%)	49/1359 (4%)	90/846 (11%)	49/219 (22%)

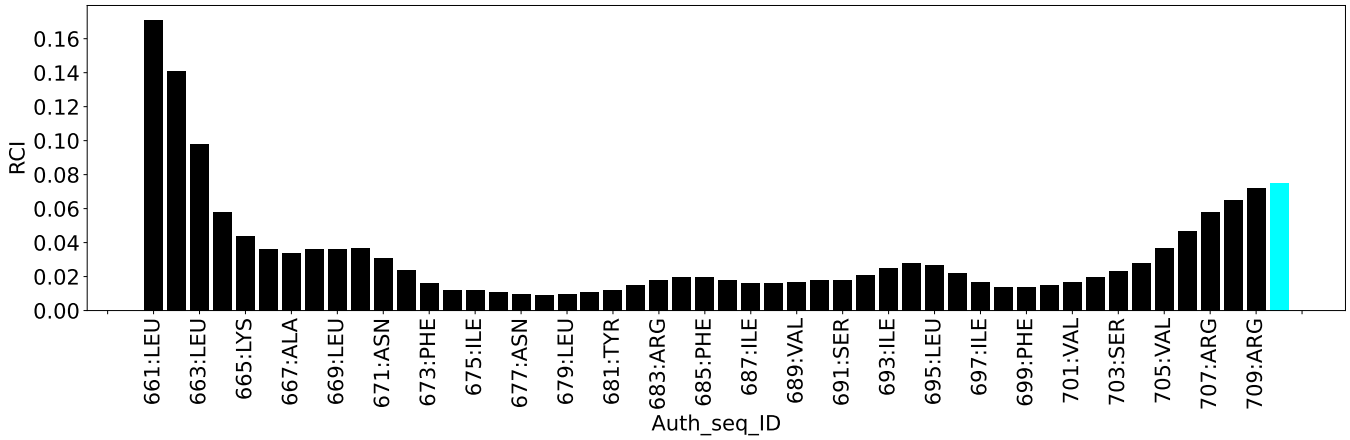
7.1.4 Statistically unusual chemical shifts (i)

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	708
Intra-residue (|i-j|=0)	96
Sequential (|i-j|=1)	294
Medium range (|i-j|>1 and |i-j|<5)	285
Long range (|i-j|≥5)	33
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	78
Number of unmapped restraints	0
Number of restraints per residue	5.1
Number of long range restraints per residue[1]	0.2

[1]Long 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)	60.6	0.2
0.2-0.5 (Medium)	74.8	0.5
>0.5 (Large)	46.8	10.69

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	21.1	9.88
10.0-20.0 (Medium)	6.6	19.83
>20.0 (Large)	2.6	42.15

9 Distance violation analysis (i)

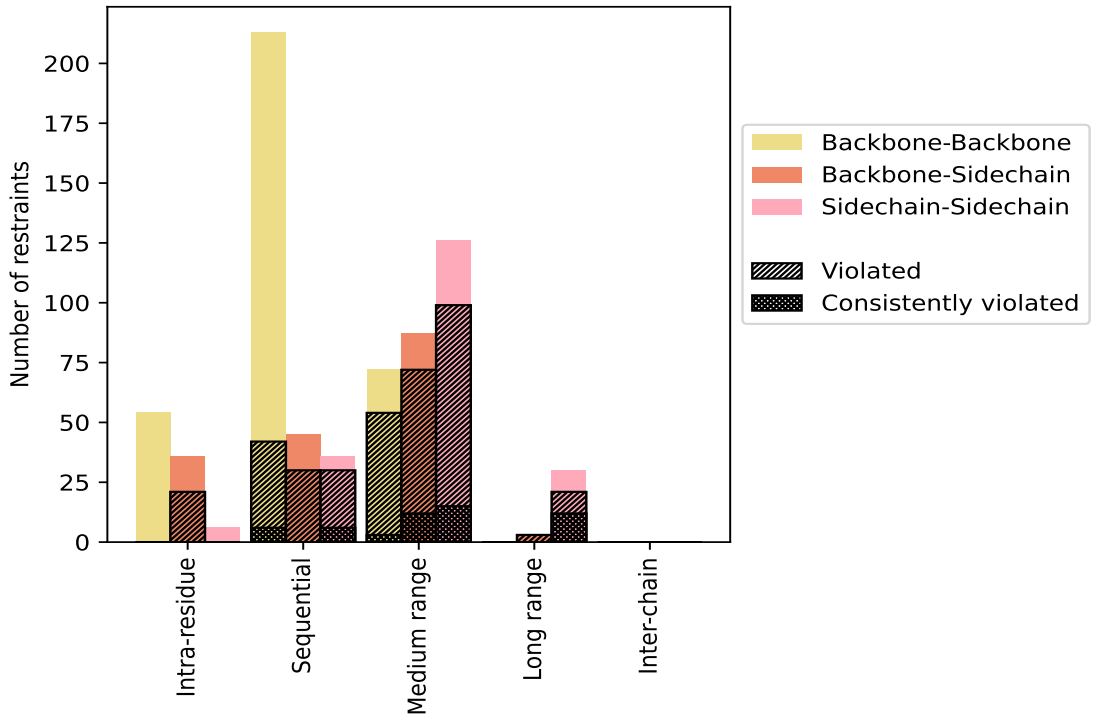
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	96	13.6	21	21.9	3.0	0	0.0	0.0
Backbone-Backbone	54	7.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	36	5.1	21	58.3	3.0	0	0.0	0.0
Sidechain-Sidechain	6	0.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	294	41.5	102	34.7	14.4	12	4.1	1.7
Backbone-Backbone	213	30.1	42	19.7	5.9	6	2.8	0.8
Backbone-Sidechain	45	6.4	30	66.7	4.2	0	0.0	0.0
Sidechain-Sidechain	36	5.1	30	83.3	4.2	6	16.7	0.8
Medium range (|i-j|>1 & |i-j|<5)	285	40.3	225	78.9	31.8	30	10.5	4.2
Backbone-Backbone	72	10.2	54	75.0	7.6	3	4.2	0.4
Backbone-Sidechain	87	12.3	72	82.8	10.2	12	13.8	1.7
Sidechain-Sidechain	126	17.8	99	78.6	14.0	15	11.9	2.1
Long range (|i-j|≥5)	33	4.7	24	72.7	3.4	12	36.4	1.7
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	0.4	3	100.0	0.4	0	0.0	0.0
Sidechain-Sidechain	30	4.2	21	70.0	3.0	12	40.0	1.7
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	708	100.0	372	52.5	52.5	54	7.6	7.6
Backbone-Backbone	339	47.9	96	28.3	13.6	9	2.7	1.3
Backbone-Sidechain	171	24.2	126	73.7	17.8	12	7.0	1.7
Sidechain-Sidechain	198	28.0	150	75.8	21.2	33	16.7	4.7

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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	12	36	120	15	0	183	1.09	9.49	2.12	0.23
2	3	45	126	24	0	198	1.07	9.93	2.18	0.23
3	6	39	123	18	0	186	1.04	9.38	2.1	0.25
4	6	36	123	18	0	183	1.1	9.65	2.16	0.25
5	3	45	120	21	0	189	1.09	9.79	2.16	0.29
6	6	30	108	18	0	162	1.1	10.02	2.14	0.27
7	3	48	111	18	0	180	1.02	9.96	2.04	0.26
8	9	39	93	18	0	159	1.1	8.49	1.94	0.27
9	6	39	129	18	0	192	1.01	9.41	2.04	0.26
10	12	48	111	18	0	189	0.96	8.17	1.85	0.28

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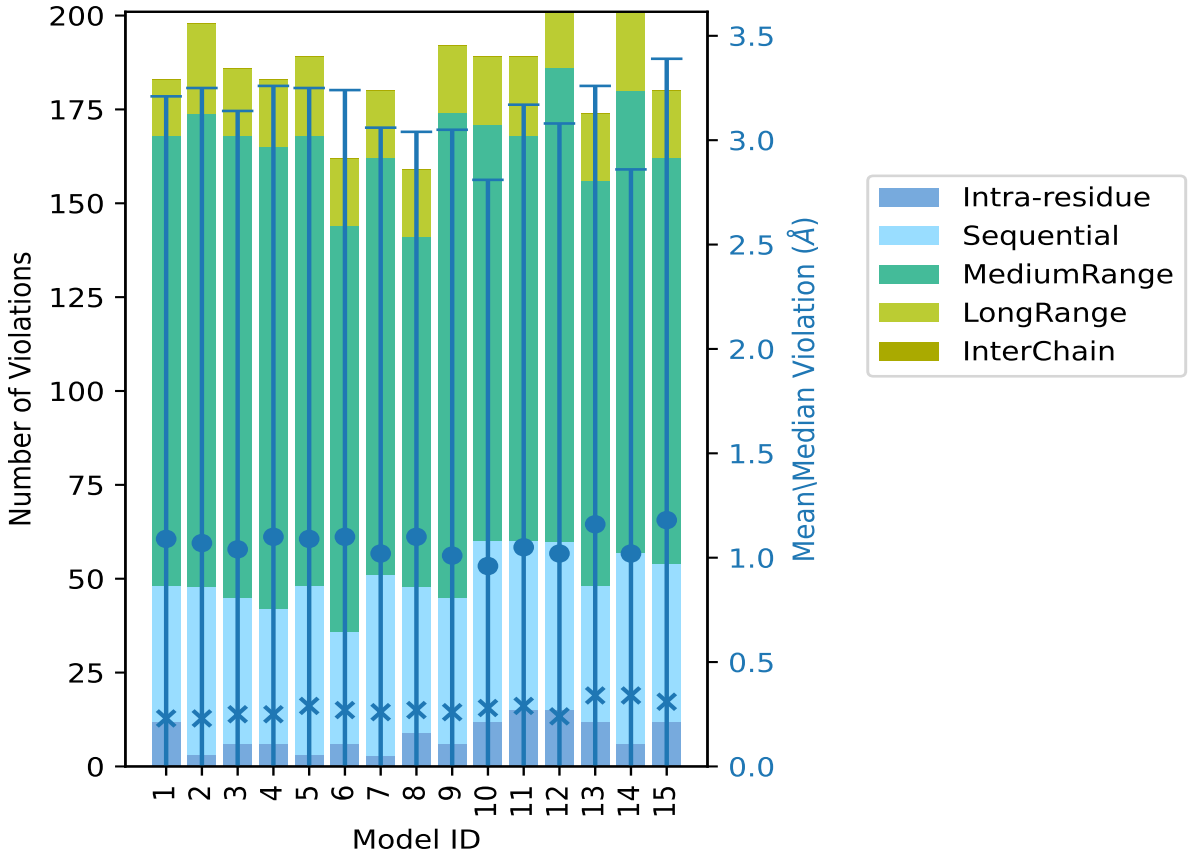
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	15	45	108	21	0	189	1.05	10.14	2.12	0.29
12	15	45	126	15	0	201	1.02	9.56	2.06	0.24
13	12	36	108	18	0	174	1.16	9.36	2.1	0.34
14	6	51	123	21	0	201	1.02	9.16	1.84	0.34
15	12	42	108	18	0	180	1.18	10.69	2.21	0.31

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

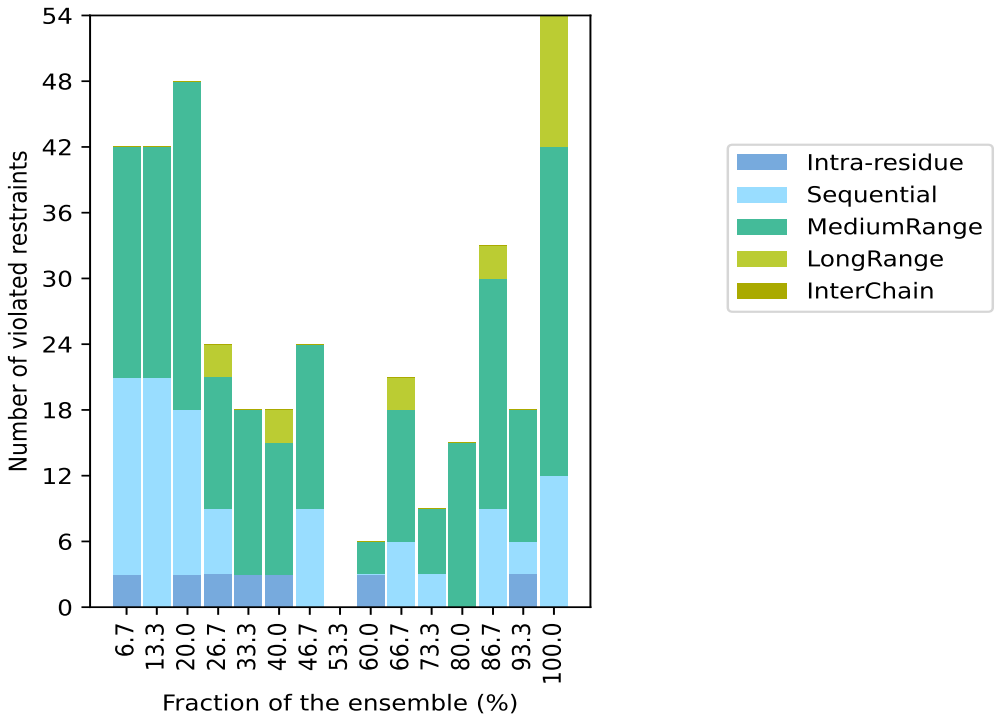
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 336(IR:75, SQ:192, MR:60, LR:9, 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]	%
3	18	21	0	0	42	1	6.7
0	21	21	0	0	42	2	13.3
3	15	30	0	0	48	3	20.0
3	6	12	3	0	24	4	26.7
3	0	15	0	0	18	5	33.3
3	0	12	3	0	18	6	40.0
0	9	15	0	0	24	7	46.7
0	0	0	0	0	0	8	53.3
3	0	3	0	0	6	9	60.0
0	6	12	3	0	21	10	66.7
0	3	6	0	0	9	11	73.3
0	0	15	0	0	15	12	80.0
0	9	21	3	0	33	13	86.7
3	3	12	0	0	18	14	93.3
0	12	30	12	0	54	15	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

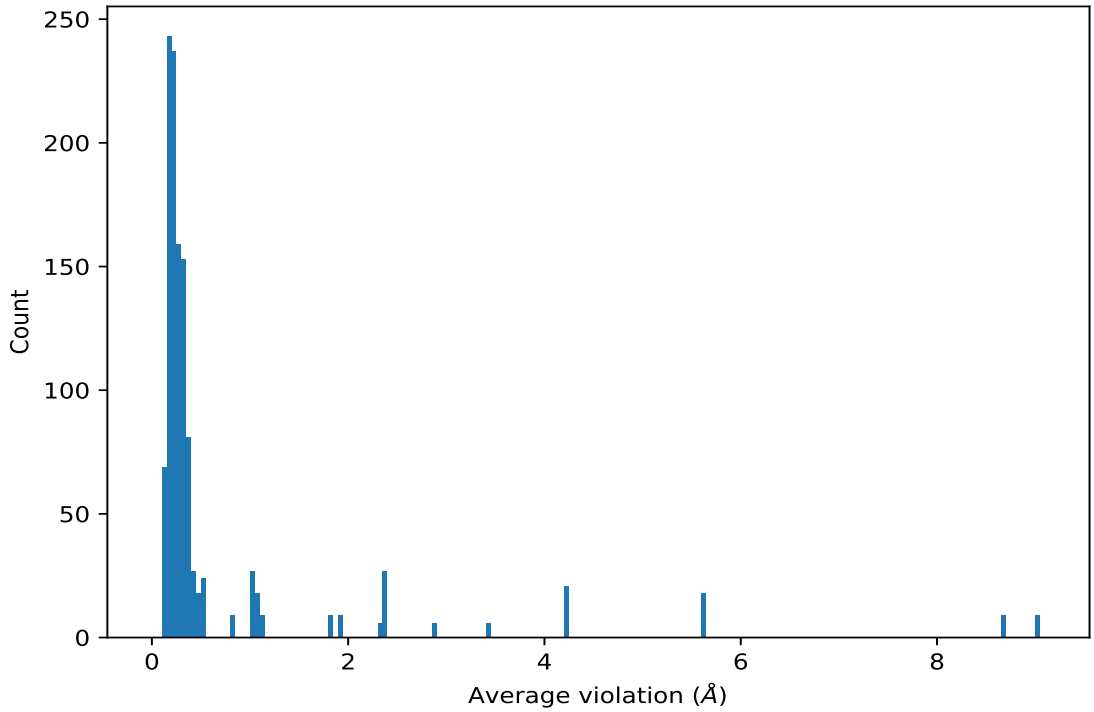
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation 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)
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	9.04	0.91	9.28
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	9.04	0.91	9.28
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	9.04	0.91	9.28
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	9.04	0.91	9.28
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	9.04	0.91	9.28
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	9.04	0.91	9.28
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	9.04	0.91	9.28
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	9.04	0.91	9.28
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	9.04	0.91	9.28
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.67	1.24	9.34
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.67	1.24	9.34
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	8.67	1.24	9.34
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	8.67	0.74	8.6
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	8.67	0.74	8.6
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	8.67	0.74	8.6
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	8.67	0.74	8.6

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	8.67	0.74	8.6
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	8.67	0.74	8.6
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	5.6	0.58	5.57
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,694)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,694)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,694)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,694)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	4.2	1.48	4.47
(1,694)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,695)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,695)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,695)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,695)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	4.2	1.48	4.47
(1,695)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,696)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,696)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,696)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	15	4.2	1.48	4.47
(1,696)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	15	4.2	1.48	4.47
(1,696)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	4.2	1.48	4.47
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.42	0.58	3.33

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.42	0.58	3.33
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.42	0.58	3.33
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.42	0.58	3.33
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.42	0.58	3.33
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.42	0.58	3.33
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.39	0.48	2.53
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.39	0.48	2.53
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	2.31	0.59	2.27
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	2.31	0.59	2.27
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	2.31	0.59	2.27
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	2.31	0.59	2.27
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	2.31	0.59	2.27
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	2.31	0.59	2.27
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.92	0.82	2.2
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.92	0.82	2.2
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.92	0.82	2.2
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.92	0.82	2.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.92	0.82	2.2
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.92	0.82	2.2
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	1.92	0.82	2.2
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	1.92	0.82	2.2
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	1.92	0.82	2.2
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	1.03	0.13	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	1.03	0.13	1.04
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	15	0.38	0.03	0.38
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	15	0.37	0.11	0.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	15	0.37	0.11	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	15	0.37	0.11	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	15	0.37	0.11	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	15	0.37	0.11	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	15	0.37	0.11	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	15	0.37	0.11	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	15	0.37	0.11	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	15	0.37	0.11	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	15	0.37	0.11	0.41
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.33	0.05	0.35
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.33	0.05	0.35
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	15	0.31	0.06	0.28
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	15	0.31	0.06	0.28
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	15	0.31	0.06	0.28
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	15	0.31	0.06	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	15	0.31	0.06	0.28
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	15	0.31	0.06	0.28
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	15	0.31	0.06	0.28
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	15	0.31	0.06	0.28
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	15	0.31	0.06	0.28
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	15	0.31	0.06	0.28
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.29	0.06	0.29
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.29	0.06	0.29
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.29	0.06	0.29
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.24	0.03	0.24
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.24	0.03	0.24
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.24	0.03	0.24
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.23	0.07	0.23
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.23	0.07	0.23
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.2	0.02	0.2
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.2	0.02	0.2
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.2	0.02	0.2
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	14	2.85	1.57	2.62
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	14	2.85	1.57	2.62
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	14	2.85	1.57	2.62
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	14	2.85	1.57	2.62

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	14	2.85	1.57	2.62
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	14	2.85	1.57	2.62
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.43	0.13	0.43
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.43	0.13	0.43
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.43	0.13	0.43
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.43	0.13	0.43
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.43	0.13	0.43
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.43	0.13	0.43
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.43	0.13	0.43
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.43	0.13	0.43
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.43	0.13	0.43
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.37	0.21	0.32
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.37	0.21	0.32
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.37	0.21	0.32
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.37	0.11	0.36
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.37	0.11	0.36
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.37	0.11	0.36
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.27	0.11	0.26
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.27	0.11	0.26
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.27	0.11	0.26
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.27	0.09	0.26
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.27	0.09	0.26
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.27	0.09	0.26
(1,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,389)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,389)	1:692:A:LEU:HD13	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,389)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,389)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,389)	1:692:A:LEU:HD11	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,389)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,603)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,603)	1:692:A:LEU:HD13	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,603)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,603)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,603)	1:692:A:LEU:HD11	1:696:A:ARG:HH21	13	1.07	0.3	1.01
(1,603)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	13	1.07	0.3	1.01
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.34	0.17	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.34	0.17	0.27
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.34	0.17	0.27
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.31	0.16	0.28
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.28	0.13	0.25
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.28	0.13	0.25
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.26	0.12	0.23
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.26	0.12	0.23
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.26	0.12	0.23
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.25	0.18	0.21
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.25	0.18	0.21
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.25	0.18	0.21
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.25	0.18	0.21
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.25	0.18	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.25	0.18	0.21
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.25	0.18	0.21
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.25	0.18	0.21
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.25	0.18	0.21
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.25	0.18	0.21
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.21	0.09	0.21
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.21	0.09	0.21
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.21	0.09	0.21
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	13	0.2	0.06	0.2
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	13	0.19	0.04	0.21
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	13	0.19	0.04	0.21
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	13	0.19	0.04	0.21
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	13	0.17	0.04	0.16
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	13	0.17	0.04	0.16
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	13	0.17	0.04	0.16
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.17	0.02	0.17
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.17	0.02	0.17
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.17	0.02	0.17
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.82	0.2	1.83
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.82	0.2	1.83
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.82	0.2	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.82	0.2	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.82	0.2	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.82	0.2	1.83
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.82	0.2	1.83
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.82	0.2	1.83
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.82	0.2	1.83
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	12	0.22	0.09	0.2
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	12	0.22	0.09	0.2
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	12	0.22	0.09	0.2
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	12	0.2	0.08	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	12	0.2	0.08	0.17
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	12	0.2	0.08	0.17
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	12	0.2	0.08	0.2
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	12	0.2	0.08	0.2
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	12	0.2	0.08	0.2
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	12	0.2	0.08	0.2
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	12	0.2	0.08	0.2
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	12	0.2	0.08	0.2
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	12	0.2	0.08	0.2
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	12	0.2	0.08	0.2
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	12	0.2	0.08	0.2
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	12	0.2	0.06	0.18
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	12	0.2	0.06	0.18
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	12	0.2	0.06	0.18
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	12	0.2	0.06	0.18
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	12	0.2	0.06	0.18
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	12	0.2	0.06	0.18
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	12	0.2	0.06	0.18
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	12	0.2	0.06	0.18
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	12	0.2	0.06	0.18
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	11	0.39	0.21	0.33
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	11	0.29	0.24	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	11	0.29	0.24	0.16
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	11	0.21	0.07	0.24
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	11	0.21	0.07	0.24
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	11	0.21	0.07	0.24
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	10	0.47	0.34	0.34
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	10	0.47	0.34	0.34
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	10	0.47	0.34	0.34
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	10	0.47	0.34	0.34
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	10	0.47	0.34	0.34
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	10	0.47	0.34	0.34
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	10	0.47	0.34	0.34
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	10	0.47	0.34	0.34
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	10	0.47	0.34	0.34
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	10	0.32	0.27	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	10	0.32	0.27	0.24
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	10	0.32	0.27	0.24
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.25	0.08	0.24
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.25	0.08	0.24
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.25	0.08	0.24
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	10	0.23	0.08	0.22
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	10	0.22	0.04	0.22
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	10	0.22	0.04	0.22
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	10	0.21	0.1	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	10	0.21	0.1	0.18
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	10	0.21	0.1	0.18
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	10	0.21	0.1	0.18
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	10	0.21	0.1	0.18
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	10	0.21	0.1	0.18
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	10	0.21	0.1	0.18
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	10	0.21	0.1	0.18
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	10	0.21	0.1	0.18
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.19	0.06	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.19	0.06	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.19	0.06	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.19	0.06	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.19	0.06	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.19	0.06	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.19	0.06	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.19	0.06	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.19	0.06	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.19	0.06	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.19	0.06	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.19	0.06	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.19	0.06	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.19	0.06	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.19	0.06	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.19	0.06	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.19	0.06	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.19	0.06	0.2
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	9	0.33	0.15	0.33
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	9	0.33	0.15	0.33
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	9	0.33	0.15	0.33
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	9	0.33	0.15	0.33
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	9	0.33	0.15	0.33
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	9	0.33	0.15	0.33
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.29	0.17	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.29	0.17	0.23
(1,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,427)	1:701:A:VAL:HG11	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,427)	1:701:A:VAL:HG12	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,427)	1:701:A:VAL:HG13	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	7	0.37	0.21	0.46
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.32	0.09	0.35
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.32	0.09	0.35
(1,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.31	0.03	0.31
(1,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.31	0.03	0.31
(1,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.31	0.03	0.31
(1,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.31	0.03	0.31
(1,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.31	0.03	0.31
(1,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.31	0.03	0.31
(1,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.31	0.03	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.31	0.03	0.31
(1,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.31	0.03	0.31
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	7	0.29	0.16	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	7	0.29	0.16	0.17
(1,15)	1:665:A:LYS:H	1:662:A:GLU:HA	7	0.19	0.11	0.15
(1,229)	1:665:A:LYS:H	1:662:A:GLU:HA	7	0.19	0.11	0.15
(1,443)	1:665:A:LYS:H	1:662:A:GLU:HA	7	0.19	0.11	0.15
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	7	0.19	0.06	0.18
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	7	0.19	0.06	0.18
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	7	0.19	0.06	0.18
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	7	0.19	0.06	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	7	0.19	0.06	0.18
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	7	0.19	0.06	0.18
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	7	0.19	0.06	0.18
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	7	0.19	0.06	0.18
(1,21)	1:666:A:TRP:H	1:663:A:LEU:HA	7	0.17	0.03	0.16
(1,235)	1:666:A:TRP:H	1:663:A:LEU:HA	7	0.17	0.03	0.16
(1,449)	1:666:A:TRP:H	1:663:A:LEU:HA	7	0.17	0.03	0.16
(1,60)	1:675:A:ILE:H	1:674:A:ASP:H	7	0.15	0.03	0.15
(1,274)	1:675:A:ILE:H	1:674:A:ASP:H	7	0.15	0.03	0.15
(1,488)	1:675:A:ILE:H	1:674:A:ASP:H	7	0.15	0.03	0.15
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.51	0.2	0.55
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.51	0.2	0.55
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.51	0.2	0.55
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.51	0.2	0.55
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.51	0.2	0.55
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.51	0.2	0.55
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB2	6	0.49	0.15	0.44
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB3	6	0.49	0.15	0.44
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB2	6	0.49	0.15	0.44
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB3	6	0.49	0.15	0.44
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB2	6	0.49	0.15	0.44
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB3	6	0.49	0.15	0.44
(1,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	6	0.23	0.05	0.24
(1,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	6	0.23	0.05	0.24
(1,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	6	0.23	0.05	0.24
(1,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	6	0.23	0.05	0.24
(1,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	6	0.23	0.05	0.24
(1,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	6	0.23	0.05	0.24
(1,615)	1:695:A:LEU:HD21	1:698:A:VAL:HB	6	0.23	0.05	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,615)	1:695:A:LEU:HD22	1:698:A:VAL:HB	6	0.23	0.05	0.24
(1,615)	1:695:A:LEU:HD23	1:698:A:VAL:HB	6	0.23	0.05	0.24
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	6	0.21	0.1	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	6	0.21	0.1	0.2
(1,172)	1:692:A:LEU:HD11	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,172)	1:692:A:LEU:HD12	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,172)	1:692:A:LEU:HD13	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,386)	1:692:A:LEU:HD11	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,386)	1:692:A:LEU:HD12	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,386)	1:692:A:LEU:HD13	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	6	0.19	0.04	0.2
(1,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	6	0.19	0.08	0.18
(1,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	6	0.19	0.08	0.18
(1,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	6	0.19	0.08	0.18
(1,278)	1:676:A:THR:HG21	1:669:A:LEU:HA	6	0.19	0.08	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,278)	1:676:A:THR:HG22	1:669:A:LEU:HA	6	0.19	0.08	0.18
(1,278)	1:676:A:THR:HG23	1:669:A:LEU:HA	6	0.19	0.08	0.18
(1,492)	1:676:A:THR:HG21	1:669:A:LEU:HA	6	0.19	0.08	0.18
(1,492)	1:676:A:THR:HG22	1:669:A:LEU:HA	6	0.19	0.08	0.18
(1,492)	1:676:A:THR:HG23	1:669:A:LEU:HA	6	0.19	0.08	0.18
(1,176)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	5	0.8	0.29	0.83
(1,176)	1:692:A:LEU:HD23	1:696:A:ARG:HH11	5	0.8	0.29	0.83
(1,176)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	5	0.8	0.29	0.83
(1,390)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	5	0.8	0.29	0.83
(1,390)	1:692:A:LEU:HD23	1:696:A:ARG:HH11	5	0.8	0.29	0.83
(1,390)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	5	0.8	0.29	0.83
(1,604)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	5	0.8	0.29	0.83
(1,604)	1:692:A:LEU:HD23	1:696:A:ARG:HH11	5	0.8	0.29	0.83
(1,604)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	5	0.8	0.29	0.83
(1,28)	1:666:A:TRP:HE1	1:662:A:GLU:H	5	0.23	0.12	0.17
(1,242)	1:666:A:TRP:HE1	1:662:A:GLU:H	5	0.23	0.12	0.17
(1,456)	1:666:A:TRP:HE1	1:662:A:GLU:H	5	0.23	0.12	0.17
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.19	0.06	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.19	0.06	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.19	0.06	0.18
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	5	0.18	0.08	0.15
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	5	0.18	0.08	0.15
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	5	0.18	0.08	0.15
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	5	0.18	0.08	0.15
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	5	0.18	0.08	0.15
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	5	0.18	0.08	0.15
(1,34)	1:667:A:ALA:HB1	1:664:A:ASP:HA	5	0.17	0.04	0.15
(1,34)	1:667:A:ALA:HB2	1:664:A:ASP:HA	5	0.17	0.04	0.15
(1,34)	1:667:A:ALA:HB3	1:664:A:ASP:HA	5	0.17	0.04	0.15
(1,248)	1:667:A:ALA:HB1	1:664:A:ASP:HA	5	0.17	0.04	0.15
(1,248)	1:667:A:ALA:HB2	1:664:A:ASP:HA	5	0.17	0.04	0.15
(1,248)	1:667:A:ALA:HB3	1:664:A:ASP:HA	5	0.17	0.04	0.15
(1,462)	1:667:A:ALA:HB1	1:664:A:ASP:HA	5	0.17	0.04	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,462)	1:667:A:ALA:HB2	1:664:A:ASP:HA	5	0.17	0.04	0.15
(1,462)	1:667:A:ALA:HB3	1:664:A:ASP:HA	5	0.17	0.04	0.15
(1,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	5	0.15	0.05	0.13
(1,122)	1:704:A:LEU:H	1:704:A:LEU:HB3	4	0.49	0.32	0.5
(1,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	4	0.49	0.32	0.5
(1,550)	1:704:A:LEU:H	1:704:A:LEU:HB3	4	0.49	0.32	0.5
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	4	0.25	0.11	0.23
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	4	0.25	0.11	0.23
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	4	0.25	0.11	0.23
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	4	0.25	0.11	0.23
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	4	0.25	0.11	0.23
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	4	0.25	0.11	0.23
(1,74)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,74)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,74)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	4	0.25	0.11	0.23
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	4	0.25	0.11	0.23
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	4	0.25	0.11	0.23
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	4	0.25	0.11	0.23
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	4	0.25	0.11	0.23
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	4	0.25	0.11	0.23
(1,288)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,288)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,288)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	4	0.25	0.11	0.23
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	4	0.25	0.11	0.23
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	4	0.25	0.11	0.23
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	4	0.25	0.11	0.23
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	4	0.25	0.11	0.23
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	4	0.25	0.11	0.23
(1,502)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,502)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,502)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	4	0.25	0.1	0.24
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	4	0.24	0.07	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	4	0.24	0.07	0.24
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	4	0.24	0.07	0.24
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	4	0.24	0.07	0.24
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	4	0.24	0.07	0.24
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	4	0.24	0.07	0.24
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	4	0.24	0.07	0.24
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	4	0.24	0.07	0.24
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	4	0.24	0.07	0.24
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	4	0.24	0.07	0.24
(1,160)	1:686:A:ILE:HD11	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,160)	1:686:A:ILE:HD12	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,160)	1:686:A:ILE:HD13	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,374)	1:686:A:ILE:HD11	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,374)	1:686:A:ILE:HD12	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,374)	1:686:A:ILE:HD13	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,588)	1:686:A:ILE:HD11	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,588)	1:686:A:ILE:HD12	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,588)	1:686:A:ILE:HD13	1:685:A:PHE:H	4	0.22	0.08	0.2
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	4	0.18	0.02	0.17
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	4	0.18	0.02	0.17
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	4	0.18	0.02	0.17
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	4	0.18	0.02	0.17
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	4	0.18	0.02	0.17
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	4	0.18	0.02	0.17
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	4	0.18	0.02	0.17
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	4	0.18	0.02	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	4	0.18	0.02	0.17
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	4	0.18	0.02	0.17
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	4	0.13	0.01	0.13
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	4	0.13	0.01	0.13
(1,190)	1:696:A:ARG:H	1:693:A:ILE:HA	4	0.12	0.01	0.12
(1,404)	1:696:A:ARG:H	1:693:A:ILE:HA	4	0.12	0.01	0.12
(1,618)	1:696:A:ARG:H	1:693:A:ILE:HA	4	0.12	0.01	0.12
(1,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	1.11	0.03	1.1
(1,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	3	0.42	0.08	0.44
(1,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	3	0.42	0.08	0.44
(1,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	3	0.42	0.08	0.44
(1,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	3	0.42	0.08	0.44
(1,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	3	0.42	0.08	0.44

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	3	0.42	0.08	0.44
(1,610)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,610)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	3	0.42	0.08	0.44
(1,610)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,610)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	3	0.42	0.08	0.44
(1,610)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	3	0.42	0.08	0.44
(1,610)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	3	0.42	0.08	0.44
(1,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.34	0.17	0.22
(1,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,400)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,400)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,400)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,400)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,400)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,400)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,614)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,614)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,614)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,614)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,614)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	3	0.32	0.07	0.33
(1,614)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	3	0.32	0.07	0.33
(1,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	3	0.3	0.24	0.15
(1,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	3	0.3	0.24	0.15
(1,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	3	0.3	0.24	0.15
(1,294)	1:682:A:ILE:HG21	1:679:A:LEU:H	3	0.3	0.24	0.15
(1,294)	1:682:A:ILE:HG22	1:679:A:LEU:H	3	0.3	0.24	0.15
(1,294)	1:682:A:ILE:HG23	1:679:A:LEU:H	3	0.3	0.24	0.15
(1,508)	1:682:A:ILE:HG21	1:679:A:LEU:H	3	0.3	0.24	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,508)	1:682:A:ILE:HG22	1:679:A:LEU:H	3	0.3	0.24	0.15
(1,508)	1:682:A:ILE:HG23	1:679:A:LEU:H	3	0.3	0.24	0.15
(1,137)	1:705:A:VAL:HG21	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,137)	1:705:A:VAL:HG22	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,137)	1:705:A:VAL:HG23	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,565)	1:705:A:VAL:HG21	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,565)	1:705:A:VAL:HG22	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,565)	1:705:A:VAL:HG23	1:702:A:LEU:HG	3	0.26	0.1	0.28
(1,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,407)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,407)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,407)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,407)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,407)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,407)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	3	0.23	0.07	0.24
(1,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	3	0.23	0.07	0.24
(1,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	3	0.21	0.12	0.15
(1,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	3	0.21	0.12	0.15
(1,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	3	0.21	0.12	0.15
(1,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,412)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	3	0.21	0.12	0.15
(1,412)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,412)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	3	0.21	0.12	0.15
(1,412)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,412)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	3	0.21	0.12	0.15
(1,412)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,626)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	3	0.21	0.12	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,626)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,626)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	3	0.21	0.12	0.15
(1,626)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,626)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	3	0.21	0.12	0.15
(1,626)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	3	0.21	0.12	0.15
(1,94)	1:684:A:ILE:HG21	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,94)	1:684:A:ILE:HG22	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,94)	1:684:A:ILE:HG23	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,308)	1:684:A:ILE:HG21	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,308)	1:684:A:ILE:HG22	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,308)	1:684:A:ILE:HG23	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,522)	1:684:A:ILE:HG21	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,522)	1:684:A:ILE:HG22	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,522)	1:684:A:ILE:HG23	1:688:A:ILE:H	3	0.2	0.06	0.22
(1,188)	1:695:A:LEU:HD21	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,188)	1:695:A:LEU:HD22	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,188)	1:695:A:LEU:HD23	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,402)	1:695:A:LEU:HD21	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,402)	1:695:A:LEU:HD22	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,402)	1:695:A:LEU:HD23	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,616)	1:695:A:LEU:HD21	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,616)	1:695:A:LEU:HD22	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,616)	1:695:A:LEU:HD23	1:698:A:VAL:H	3	0.19	0.05	0.22
(1,197)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,197)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,197)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,411)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,411)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,411)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,625)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,625)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,625)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.18	0.04	0.17
(1,25)	1:666:A:TRP:H	1:666:A:TRP:HE1	3	0.17	0.02	0.18
(1,239)	1:666:A:TRP:H	1:666:A:TRP:HE1	3	0.17	0.02	0.18
(1,453)	1:666:A:TRP:H	1:666:A:TRP:HE1	3	0.17	0.02	0.18
(1,135)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	3	0.14	0.02	0.13
(1,135)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,135)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	3	0.14	0.02	0.13
(1,135)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,135)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	3	0.14	0.02	0.13
(1,135)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,349)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	3	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,349)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,349)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	3	0.14	0.02	0.13
(1,349)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,349)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	3	0.14	0.02	0.13
(1,349)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,563)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	3	0.14	0.02	0.13
(1,563)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,563)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	3	0.14	0.02	0.13
(1,563)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,563)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	3	0.14	0.02	0.13
(1,563)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	3	0.14	0.02	0.13
(1,66)	1:676:A:THR:HG21	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,66)	1:676:A:THR:HG22	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,66)	1:676:A:THR:HG23	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,280)	1:676:A:THR:HG21	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,280)	1:676:A:THR:HG22	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,280)	1:676:A:THR:HG23	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,494)	1:676:A:THR:HG21	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,494)	1:676:A:THR:HG22	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,494)	1:676:A:THR:HG23	1:679:A:LEU:H	3	0.14	0.03	0.12
(1,164)	1:687:A:ILE:HG21	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,164)	1:687:A:ILE:HG22	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,164)	1:687:A:ILE:HG23	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	3	0.13	0.01	0.13
(1,22)	1:666:A:TRP:H	1:665:A:LYS:HA	3	0.12	0.02	0.11
(1,236)	1:666:A:TRP:H	1:665:A:LYS:HA	3	0.12	0.02	0.11
(1,450)	1:666:A:TRP:H	1:665:A:LYS:HA	3	0.12	0.02	0.11
(1,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	2	0.52	0.11	0.52
(1,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	2	0.52	0.11	0.52
(1,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	2	0.52	0.11	0.52
(1,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	2	0.52	0.11	0.52
(1,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	2	0.52	0.11	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	2	0.52	0.11	0.52
(1,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	2	0.52	0.11	0.52
(1,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	2	0.52	0.11	0.52
(1,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	2	0.52	0.11	0.52
(1,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	2	0.52	0.11	0.52
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.37	0.15	0.37
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.37	0.15	0.37
(1,183)	1:695:A:LEU:H	1:691:A:SER:HA	2	0.36	0.01	0.36
(1,397)	1:695:A:LEU:H	1:691:A:SER:HA	2	0.36	0.01	0.36
(1,611)	1:695:A:LEU:H	1:691:A:SER:HA	2	0.36	0.01	0.36
(1,126)	1:704:A:LEU:HD11	1:707:A:ARG:HE	2	0.26	0.07	0.26
(1,126)	1:704:A:LEU:HD12	1:707:A:ARG:HE	2	0.26	0.07	0.26
(1,126)	1:704:A:LEU:HD13	1:707:A:ARG:HE	2	0.26	0.07	0.26
(1,340)	1:704:A:LEU:HD11	1:707:A:ARG:HE	2	0.26	0.07	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,340)	1:704:A:LEU:HD12	1:707:A:ARG:HE	2	0.26	0.07	0.26
(1,340)	1:704:A:LEU:HD13	1:707:A:ARG:HE	2	0.26	0.07	0.26
(1,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	2	0.26	0.07	0.26
(1,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	2	0.26	0.07	0.26
(1,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	2	0.26	0.07	0.26
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	2	0.2	0.06	0.2
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	2	0.2	0.06	0.2
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	2	0.17	0.06	0.17
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	2	0.17	0.06	0.17
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	2	0.17	0.06	0.17
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	2	0.17	0.06	0.17
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	2	0.17	0.06	0.17
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	2	0.17	0.06	0.17
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	2	0.17	0.06	0.17
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	2	0.17	0.06	0.17
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	2	0.17	0.06	0.17
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	2	0.17	0.06	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	2	0.17	0.06	0.17
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	2	0.17	0.06	0.17
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	2	0.17	0.06	0.17
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	2	0.17	0.06	0.17
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	2	0.17	0.06	0.17
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	2	0.17	0.06	0.17
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	2	0.17	0.06	0.17
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	2	0.17	0.06	0.17
(1,214)	1:701:A:VAL:HG21	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,214)	1:701:A:VAL:HG22	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,214)	1:701:A:VAL:HG23	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,428)	1:701:A:VAL:HG21	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,428)	1:701:A:VAL:HG22	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,428)	1:701:A:VAL:HG23	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	2	0.16	0.04	0.16
(1,159)	1:686:A:ILE:HD11	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,159)	1:686:A:ILE:HD12	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,159)	1:686:A:ILE:HD13	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,373)	1:686:A:ILE:HD11	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,373)	1:686:A:ILE:HD12	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,373)	1:686:A:ILE:HD13	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,587)	1:686:A:ILE:HD11	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,587)	1:686:A:ILE:HD12	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,587)	1:686:A:ILE:HD13	1:683:A:ARG:HA	2	0.15	0.0	0.15
(1,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	2	0.15	0.03	0.15
(1,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	2	0.15	0.03	0.15
(1,184)	1:695:A:LEU:H	1:694:A:GLY:H	2	0.15	0.0	0.15
(1,267)	1:671:A:ASN:H	1:672:A:TRP:HE1	2	0.15	0.03	0.15
(1,271)	1:672:A:TRP:HE1	1:671:A:ASN:H	2	0.15	0.03	0.15
(1,398)	1:695:A:LEU:H	1:694:A:GLY:H	2	0.15	0.0	0.15
(1,481)	1:671:A:ASN:H	1:672:A:TRP:HE1	2	0.15	0.03	0.15
(1,485)	1:672:A:TRP:HE1	1:671:A:ASN:H	2	0.15	0.03	0.15
(1,612)	1:695:A:LEU:H	1:694:A:GLY:H	2	0.15	0.0	0.15
(1,79)	1:681:A:TYR:H	1:682:A:ILE:H	2	0.12	0.0	0.12
(1,96)	1:685:A:PHE:H	1:686:A:ILE:H	2	0.12	0.0	0.12
(1,293)	1:681:A:TYR:H	1:682:A:ILE:H	2	0.12	0.0	0.12
(1,310)	1:685:A:PHE:H	1:686:A:ILE:H	2	0.12	0.0	0.12
(1,507)	1:681:A:TYR:H	1:682:A:ILE:H	2	0.12	0.0	0.12
(1,524)	1:685:A:PHE:H	1:686:A:ILE:H	2	0.12	0.0	0.12
(1,41)	1:669:A:LEU:H	1:668:A:SER:HA	2	0.1	0.0	0.1

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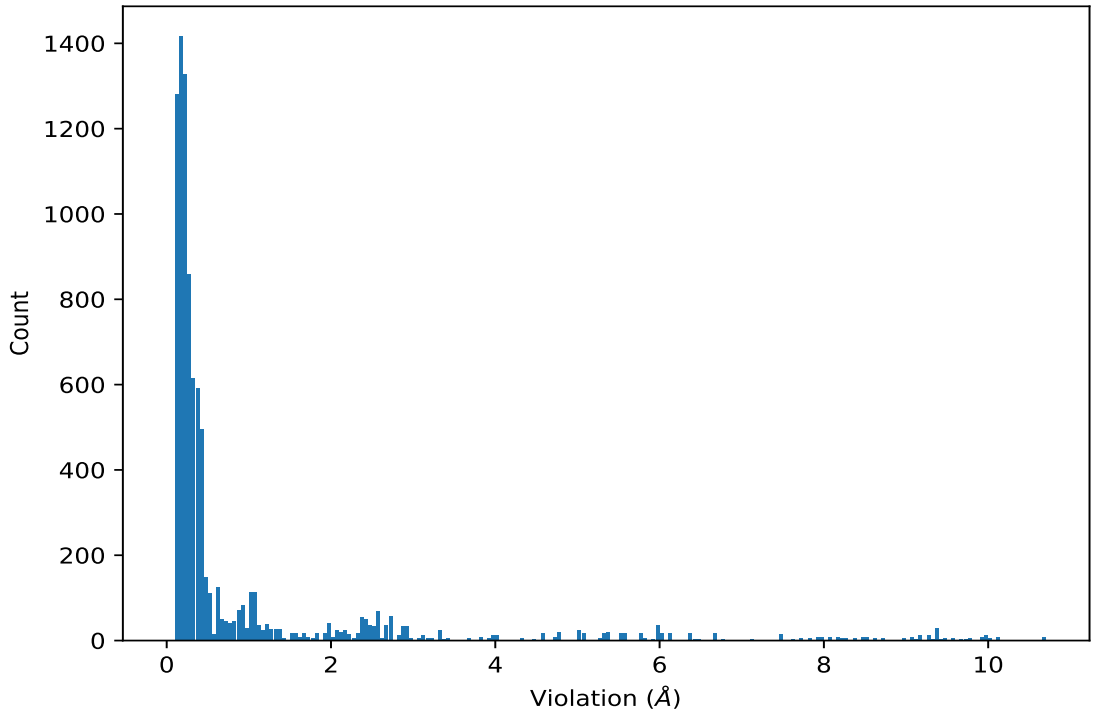
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,255)	1:669:A:LEU:H	1:668:A:SER:HA	2	0.1	0.0	0.1
(1,469)	1:669:A:LEU:H	1:668:A:SER:HA	2	0.1	0.0	0.1

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	10.69
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	10.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	10.69
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	10.69
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	10.69
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	10.69
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	15	10.69
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	15	10.69
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	15	10.69
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	10.14
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	10.14
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	10.14
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	10.14
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	10.14
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	10.14
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	10.14
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	10.14
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	10.14
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	10.02
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	10.02
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	10.02
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	10.02
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	10.02
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	10.02
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	9.96
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	9.96
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	9.96
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	9.96
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	9.96
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	9.96
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	9.96
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	9.96
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	9.96
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	9.95
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	9.95
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	15	9.95
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	9.93
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	9.93
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	9.93
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	9.93
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	9.93
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	9.93
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	9.93
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	9.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	9.93
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	9.79
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	9.79
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	9.79
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	9.79
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	9.79
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	9.79
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	9.71
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	9.71
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	9.71
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	9.65
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	9.65
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	9.65
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	9.56
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	9.56
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	9.56
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	9.56
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	9.56
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	9.56
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	9.49
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	9.49
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	9.49
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	9.46
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	9.46
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	9.46
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	9.41
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	9.41
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	9.41
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.38
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.38
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.38
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.38
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.38
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.38
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.38
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.38
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.38
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	9.37
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	9.37
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	9.37
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	9.37
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	9.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	9.37
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	9.37
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	9.37
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	9.37
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.36
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.36
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.36
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	9.35
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	9.35
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	9.35
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	9.35
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	9.35
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	9.35
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	9.35
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	9.35
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	9.35
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	9.34
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	9.34
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	9.34
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	9.28
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	9.28
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	9.28
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	9.28
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	9.28
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	9.28
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	9.28
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	9.28
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	9.28
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	9.27
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	9.27
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	9.27
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	9.16
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	9.16
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	9.16
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	9.16
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	9.16
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	9.16
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	9.15
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	9.15
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	9.15
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	9.15
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	9.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	9.15
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	9.13
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	9.13
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	9.13
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.07
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.07
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.07
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.07
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.07
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.07
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.07
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.07
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.07
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	8.95
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	8.95
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	8.95
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	8.95
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	8.95
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	8.95
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	8.74
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	8.74
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	8.74
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	8.74
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	8.74
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	8.74
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	8.6
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	8.6
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	8.6
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	8.6
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	8.6
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	8.6
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	8.53
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	8.53
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	8.53
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	8.53
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	8.53
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	8.53
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	8.53
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	8.53
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	8.53
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	8.49
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	8.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	8.49
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	8.49
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	8.49
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	8.49
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	8.49
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	8.49
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	8.49
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	8.35
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	8.35
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	8.35
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	8.35
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	8.35
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	8.35
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	8.27
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	8.27
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	8.27
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	8.27
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	8.27
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	8.27
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	8.23
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	8.23
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	8.23
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	8.23
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	15	8.23
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	15	8.23
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	8.17
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	8.17
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	8.17
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	8.16
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	8.16
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	8.16
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	8.16
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	8.16
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	8.16
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	8.06
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	8.06
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	8.06
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	8.06
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	8.06
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	8.06
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	8.06
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	8.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	8.06
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	7.95
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	7.95
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	7.95
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	7.95
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	7.95
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	7.95
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	7.95
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	7.95
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	7.95
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	7.92
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	7.92
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	7.92
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	7.92
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	7.92
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	7.92
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	7.92
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	7.92
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	7.92
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	7.8
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	7.8
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	7.8
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	7.8
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	7.8
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	7.8
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.72
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.72
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.72
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.72
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.72
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.72
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	7.6
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	7.6
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	7.6
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	7.48
(1,660)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	7.48
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	7.48
(1,659)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	7.48
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	7.48
(1,658)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	7.48
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	7.46
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	7.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	7.46
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	7.46
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	7.46
(1,665)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	7.46
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	7.46
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	7.46
(1,664)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	7.46
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	7.14
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	7.14
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	7.14
(1,696)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	13	6.75
(1,695)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	13	6.75
(1,694)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	13	6.75
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	6.69
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	6.69
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	6.69
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	6.69
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	6.69
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	6.69
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	6.69
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	6.69
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	6.69
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	6.69
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	6.69
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	6.69
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	6.69
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	6.69
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	6.69
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	6.69
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	6.69
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	6.69
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	6.45
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	6.45
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	6.45
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	1	6.41
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	1	6.41
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	1	6.41
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	6.35
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	6.35
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	6.35
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	6.35
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	6.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	6.35
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	6.35
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	6.35
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	6.35
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	6.35
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	6.35
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	6.35
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	6.35
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	6.35
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	6.35
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	6.35
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	6.35
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	6.35
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	6.13
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	6.13
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	6.13
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	6.13
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	6.13
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	6.13
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	6.13
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	6.13
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	6.13
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	6.13
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	6.13
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	6.13
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	6.13
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	6.13
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	6.13
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	6.13
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	6.13
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	6.13
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	6.0
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	6.0
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	6.0
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	6.0
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	6.0
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	6.0
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	6.0
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	6.0
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	6.0
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	6.0
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	6.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	6.0
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	6.0
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	6.0
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	6.0
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	6.0
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	6.0
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	6.0
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	5.99
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	5.99
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	5.99
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	5.99
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	5.99
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	5.99
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	5.99
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	5.99
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	5.99
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	5.99
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	5.99
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	5.99
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	5.99
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	5.99
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	5.99
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	5.99
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	5.99
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	5.99
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	5.99
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	5.99
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	5.99
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	5.99
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	5.99
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	5.99
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	5.99
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	5.99
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	5.99
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	5.99
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	5.99
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	5.99
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	5.99
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	5.99
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	5.99
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	5.99
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	5.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	5.99
(1,663)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	5.93
(1,662)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	5.93
(1,661)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	5.93
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	14	5.8
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	14	5.8
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	14	5.8
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	14	5.8
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	14	5.8
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	14	5.8
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	5.75
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	5.75
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	5.75
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	5.75
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	5.75
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	5.75
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	5.75
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	5.75
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	5.75
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	5.75
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	5.75
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	5.75
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	5.75
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	5.75
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	5.75
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	5.75
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	5.75
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	5.75
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	5.57
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	5.57
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	5.57
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	5.57
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	5.57
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	5.57
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	5.57
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	5.57
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	5.57
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	5.57
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	5.57
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	5.57
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	5.57
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	5.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	5.57
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	5.57
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	5.57
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	5.57
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	5.52
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	5.52
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	5.52
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	5.52
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	5.52
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	5.52
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	5.52
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	5.52
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	5.52
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	5.52
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	5.52
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	5.52
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	5.52
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	5.52
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	5.52
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	5.52
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	5.52
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	5.52
(1,696)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	5	5.38
(1,695)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	5	5.38
(1,694)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	5	5.38
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	5.36
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	5.36
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	5.36
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	5.36
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	5.36
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	5.36
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	5.36
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	5.36
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	5.36
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	5.36
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	5.36
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	5.36
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	5.36
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	5.36
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	5.36
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	5.36
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	5.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	5.36
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	5.31
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	5.31
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	5.31
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	5.31
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	5.31
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	5.31
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	5.31
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	5.31
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	5.31
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	5.31
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	5.31
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	5.31
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	5.31
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	5.31
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	5.31
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	5.31
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	5.31
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	5.31
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	12	5.29
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	12	5.29
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	12	5.29
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	12	5.29
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	12	5.29
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	12	5.29
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	5.06
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	5.06
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	5.06
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	5.06
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	5.06
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	5.06
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	5.06
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	5.06
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	5.06
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	5.06
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	5.06
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	5.06
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	5.06
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	5.06
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	5.06
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	5.06
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	5.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	5.06
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	3	5.04
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	12	5.04
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	3	5.04
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	12	5.04
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	3	5.04
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	12	5.04
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	5.02
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	5.02
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	5.02
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	5.02
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	5.02
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	5.02
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	5.02
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	5.02
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	5.02
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	5.02
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	5.02
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	5.02
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	5.02
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	5.02
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	5.02
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	5.02
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	5.02
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	5.02
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	2	4.78
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	2	4.78
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	2	4.78
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	4.76
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	4.76
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	4.76
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	4.76
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	4.76
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	4.76
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	4.76
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	4.76
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	4.76
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	4.76
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	4.76
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	4.76
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	15	4.76
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	15	4.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	15	4.76
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	15	4.76
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	15	4.76
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	15	4.76
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	9	4.7
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	9	4.7
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	9	4.7
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	10	4.7
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	10	4.7
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	10	4.7
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	10	4.7
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	10	4.7
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	10	4.7
(1,645)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	4.56
(1,645)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	4.56
(1,645)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	4.56
(1,645)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	4.56
(1,645)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	4.56
(1,645)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	4.56
(1,644)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	4.56
(1,644)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	4.56
(1,644)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	4.56
(1,644)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	4.56
(1,644)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	4.56
(1,644)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	4.56
(1,643)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	4.56
(1,643)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	4.56
(1,643)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	4.56
(1,643)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	4.56
(1,643)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	4.56
(1,643)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	4.56
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	8	4.47
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	8	4.47
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	8	4.47
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	4.32
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	4.32
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	4.32
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	4.32
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	4.32
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	4.32
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	4.03
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	4.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	4.03
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	4.03
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	4.03
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	4.03
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	4.01
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	4.01
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	4.01
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	4.01
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	4.01
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	4.01
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	3.99
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	3.99
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	3.99
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	3.99
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	3.99
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	3.99
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.96
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.96
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.96
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.96
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	15	3.96
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	15	3.96
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	2	3.91
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	2	3.91
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	2	3.91
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	2	3.91
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	2	3.91
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	2	3.91
(1,696)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	4	3.83
(1,696)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	10	3.83
(1,695)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	4	3.83
(1,695)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	10	3.83
(1,694)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	4	3.83
(1,694)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	10	3.83
(1,696)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	7	3.81
(1,695)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	7	3.81
(1,694)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	7	3.81
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	3.68
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	3.68
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	3.68
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	3.68
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	3.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	3.68
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	3.41
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	3.41
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	3.41
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	3.41
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	3.41
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	3.41
(1,696)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	3.36
(1,695)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	3.36
(1,694)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	15	3.36
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	15	3.34
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	15	3.34
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	15	3.34
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	15	3.34
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	15	3.34
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	15	3.34
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	3.33
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	3.33
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	3.33
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	3.33
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	3.33
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	3.33
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	3.32
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	3.32
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	3.32
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	3.32
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	3.32
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	3.32
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.3
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.3
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.3
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.3
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.3
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.3
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	3.21
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	3.21
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	3.21
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	3.21
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	3.21
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	3.21
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	3.17
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	3.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	3.17
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	3.17
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	15	3.17
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	15	3.17
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	3.11
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	3.11
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	3.11
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	3.11
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	3.11
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	3.11
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	4	3.1
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	4	3.1
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	4	3.1
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	4	3.1
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	4	3.1
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	4	3.1
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	3.05
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	3.05
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	3.05
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	3.05
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	3.05
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	3.05
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	2.99
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	2.99
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	2.99
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	2.99
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	2.99
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	2.99
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	2.94
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	2.94
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	2.94
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	2.94
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	2.94
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	2.94
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	2.94
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	2.94
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	2.94
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	2.94
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	2.94
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	2.94
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	2.94
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	2.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	2.94
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	2.94
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	2.94
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	2.94
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	2.94
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	2.94
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	2.94
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	2.94
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	2.94
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	2.94
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	2.94
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	2.94
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	2.94
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	2.94
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	2.94
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	2.94
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	2.94
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	2.94
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	2.94
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	2.88
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	2.88
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	2.88
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	2.88
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	2.88
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	2.88
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.87
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.87
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.87
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.87
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.87
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.87
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.87
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.87
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.87
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.87
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.87
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.87
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.87
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.87
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.87
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.87
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.87
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.87
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.87
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.87
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.87
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.87
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.87
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.87
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.87
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.87
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	2.84
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	2.84
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	2.84
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	2.84
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	2.84
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	2.84
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	1	2.83
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	1	2.83
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	1	2.83
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	1	2.83
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	1	2.83
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	1	2.83
(1,696)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	6	2.73
(1,695)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	6	2.73
(1,694)	1:693:A:ILE:HD11	1:696:A:ARG:HH11	6	2.73
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.72
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.72
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.72
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.72
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.72
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.72
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.72
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.72
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.72
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.72
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.72
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.72
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.72
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.72
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.72
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.72
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.72
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.72
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.72
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.72
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.72
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.72
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.72
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.72
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.72
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.72
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.72
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.72
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.72
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.72
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.72
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.72
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.72
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.72
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.72
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.72
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.72
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.72
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.72
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.72
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.72
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.72
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.72
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.72
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	15	2.72
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	15	2.72
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	15	2.72
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	15	2.72
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	15	2.72
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	15	2.72
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	15	2.72
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	15	2.72
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	15	2.72
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.69
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.69
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.69
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.69
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.69
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.69
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.69
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.69
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.69
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.69
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.69
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.69
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.69
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.69
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.69
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.69
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.69
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.69
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.69
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.69
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.69
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.69
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.69
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.69
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.69
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.69
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	2.68
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	2.68
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	2.68
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	2.68
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	2.68
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	2.68
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	2.68
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	2.68
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	2.68
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	2.61
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	2.61
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	2.61
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	2.61
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	2.61
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	2.61
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	2.59
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	2.59
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	2.59
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	2.59
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	2.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	2.59
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	2.59
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	2.59
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	2.59
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	2.59
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	2.59
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	2.59
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	2.59
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	2.59
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	2.59
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	2.59
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	2.59
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	2.59
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	2.59
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	2.59
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	2.59
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	2.59
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	2.59
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	2.59
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	2.59
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	2.59
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	2.59
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	2.58
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	2.58
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	2.58
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	2.58
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	2.58
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	2.58
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	2.58
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	2.58
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	2.58
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	2.58
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	2.58
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	2.58
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	2.58
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	2.58
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	2.58
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.56
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.56
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.56
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.56
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.56
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.56
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.56
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.56
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.56
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.56
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.56
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.56
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.56
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.56
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.56
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.56
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.56
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.56
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.56
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.56
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.56
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.56
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.56
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.56
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.56
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.56
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.53
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.53
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.53
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.53
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.53
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.53
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	2.53
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	2.53
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	2.53
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	2.53
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	2.53
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	2.53
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	2.53
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	2.53
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	2.53
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	2.53
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	2.53
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	2.53
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	2.53
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	2.53
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	2.53
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	2.53
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	2.53
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	2.53
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	2.53
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	2.53
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	2.53
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	2.53
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	2.53
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	2.53
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	2.53
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	2.53
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.46
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.46
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.46
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.46
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.46
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.46
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.46
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.46
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.46
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.46
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.46
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.46
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.46
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.46
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.46
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.46
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.46
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.46
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.46
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.46
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.46
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.46
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.46
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.46
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.46
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.46
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.46
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	2.45
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	2.45
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	2.45
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	2.45
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	2.45
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	2.45
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	2.45
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	2.45
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	2.44
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	2.44
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	2.44
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	2.44
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	2.44
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	2.44
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	2.44
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	2.44
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	2.44
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	5	2.42
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	5	2.42
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	5	2.42
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	5	2.42
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	5	2.42
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	5	2.42
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	2.4
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	2.4
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	2.4
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	2.4
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	2.4
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	2.4
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	2.4
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	2.4
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	2.4
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	2.4
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	2.4
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	2.4
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	2.4
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	2.4
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	2.4
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	2.4
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	2.4
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	2.4
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	2.4
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	2.4
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	2.4
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	2.4
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	2.4
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	2.4
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	2.4
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	2.4
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	2.4
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	2.4
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	2.4
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	2.4
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	2.4
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	2.4
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	2.4
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	2.4
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	2.4
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	2.37
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	2.37
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	2.37
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	2.37
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	2.37
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	2.37
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	2.37
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	2.37
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	2.37
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	2.37
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	2.37
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	2.37
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	2.37
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	2.37
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	2.37
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	2.37
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	2.37
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	2.37
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	2.37
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	2.37
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	2.37
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	2.37
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	2.37
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	2.37
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	2.37
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	2.37
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	2.36
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	2.36
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	2.36
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	2.36
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	2.36
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	2.36
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	2.36
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	2.36
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	2.36
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	2.36
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	2.36
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	2.36
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	2.36
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	2.36
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	2.36
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	2.36
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	2.36
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	2.36
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	2.36
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	2.36
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	2.36
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	2.36
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	2.36
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	2.36
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	2.36
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	2.36
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	2.36
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	2.33
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	2.33
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	2.33
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	2.33
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	2.33
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	2.33
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	2.33
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	2.33
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	2.33
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	2.33
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	2.33
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	2.33
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	2.33
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	2.33
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	2.33
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	2.33
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	2.33
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.27
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.27
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.27
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.27
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.27
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.27
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	11	2.22
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	11	2.22
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	11	2.22
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	11	2.22
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	11	2.22
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	11	2.22
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	2.2
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	2.2
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	2.2
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	2.2
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	2.2
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	2.2
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	2.2
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	2.2
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	2.2
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	2.18
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	2.18
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	2.18
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	2.18
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	2.18
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	2.18
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	2.18
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	2.18
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	2.18
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	2.18
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	2.18
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	2.18
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	2.18
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	2.18
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	2.18
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	2.18
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	2.18
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	6	2.18
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	6	2.18
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	6	2.18
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	6	2.18
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	6	2.18
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	6	2.18
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	2.13
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	2.13
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	2.13
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	2.13
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	2.13
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	2.13
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	15	2.13
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	15	2.13
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	15	2.13
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	2.1
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	2.1
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	2.1
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	2.1
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	2.1
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	2.1
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	2.1
(1,651)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	2.1
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	2.1
(1,650)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	2.1
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	2.1
(1,649)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	2.1
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	2.08
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	2.08
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	2.08
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	2.08
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	2.08
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	2.08
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	2.08
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	2.08
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	2.08
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	2.08
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	2.08
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	2.08
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	2.08
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	2.08
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	2.06
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	2.06
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	2.06
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	2.06
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	2.06
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	2.06
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	2.06
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	2.06
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	2.06
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	2.02
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	2.02
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	2.02
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	2.02
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	2.02
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	2.02
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	2.02
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	2.02
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	2.02
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	1.96
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	1.96
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	1.96
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	1.96
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	1.96
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	1.96
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	1.96
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	1.96
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	1.96
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	1.96
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	1.96
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	1.96
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	1.96
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	1.96
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	1.96
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	1.96
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	1.96
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	1.96
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	1.96
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	1.96
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	1.96
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	1.96
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	1.96
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	1.96
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	1.96
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	1.96
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	1.96
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	1.96
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	1.96
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	1.96
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	1.96
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	1.96
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.95
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.95
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.95
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.95
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.95
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.95
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.95
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.95
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.95
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.94
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.94
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.94
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.94
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.94
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.94
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.94
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.94
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.94
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.9
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.9
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.9
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.9
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.9
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.9
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.9
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.9
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.9
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.83
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.83
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.83
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.83
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.83
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.83
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.83
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.83
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.83
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.83
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.83
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.83
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	1.75
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	1.75
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	1.75
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	1.75
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	1.75
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	1.75
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.7
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.7
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.7
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.7
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.7
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.7
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.7
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.7
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.7
(1,603)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	14	1.69
(1,389)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	14	1.69
(1,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	14	1.69
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.68
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.68
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.68
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.68
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.68
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.68
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.68
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.68
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.68
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.65
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.65
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.65
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.65
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.65
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.63
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.63
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.63
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.63
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.63
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.63
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	15	1.63
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	15	1.63
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	15	1.63
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	1.56
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	1.56
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	1.56
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	1.56
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	1.56
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	1.56
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.56
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.56
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.56
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.56
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.56
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.56
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.56
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.56
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.56
(1,603)	1:692:A:LEU:HD11	1:696:A:ARG:HH21	7	1.56
(1,389)	1:692:A:LEU:HD11	1:696:A:ARG:HH21	7	1.56
(1,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH21	7	1.56
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	8	1.54
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	8	1.54
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	8	1.54
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	8	1.54
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	8	1.54
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	8	1.54
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	1.52
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	1.52
(1,699)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	1.52
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	1.52
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,698)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	1.52
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	1.52
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	1.52
(1,697)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	1.52
(1,696)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	1.5
(1,695)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	1.5
(1,694)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	1.5
(1,696)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.44
(1,695)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.44
(1,694)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.44
(1,603)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	10	1.4
(1,389)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	10	1.4
(1,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	10	1.4
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	1.39
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	1.39
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	1.39
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	1.39
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	1.39
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	1.39
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	1.39
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	1.39
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	1.39
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	1.39
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	1.39
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	1.39
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	1.39
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	1.39
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	1.39
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	1.39
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	1.39
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	1.39
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	1.39
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	1.39
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	1.39
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	1.39
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	1.39
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	1.39
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	1.39
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	1.39
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	1.39
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	7	1.32
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	7	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	7	1.32
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	7	1.32
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	7	1.32
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	7	1.32
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	7	1.32
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	7	1.32
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	7	1.32
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	7	1.32
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	7	1.32
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	7	1.32
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	7	1.32
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	7	1.32
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	7	1.32
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	7	1.32
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	7	1.32
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	7	1.32
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	7	1.32
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	7	1.32
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	7	1.32
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	7	1.32
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	7	1.32
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	7	1.32
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	7	1.32
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	7	1.32
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	7	1.32
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	1.26
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	1.26
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	1.26
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	1.26
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	1.26
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	1.26
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	1.26
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	1.26
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	1.26
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	1.26
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	1.26
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	1.26
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	1.26
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	1.26
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	1.26
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	1.26
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	1.26
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	15	1.26
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	15	1.26
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	15	1.26
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	15	1.26
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	15	1.26
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	15	1.26
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	15	1.26
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	15	1.26
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	15	1.26
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	9	1.23
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	9	1.23
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	9	1.23
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	9	1.23
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	9	1.23
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	9	1.23
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.22
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.22
(1,669)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.22
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.22
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.22
(1,669)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.22
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.22
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.22
(1,669)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.22
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.22
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.22
(1,668)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.22
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.22
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.22
(1,668)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.22
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.22
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.22
(1,668)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.22
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.22
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.22
(1,667)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.22
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.22
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.22
(1,667)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.22
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.22
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.22
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.21
(1,705)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.21
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.21
(1,704)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.21
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.21
(1,703)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.21
(1,604)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	15	1.19
(1,390)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	15	1.19
(1,176)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	15	1.19
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	14	1.16
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	14	1.16
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	14	1.16
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	14	1.16
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	14	1.16
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	14	1.16
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	14	1.16
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	14	1.16
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	14	1.16
(1,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	6	1.16
(1,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	6	1.16
(1,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	6	1.16
(1,603)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	6	1.16
(1,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	6	1.16
(1,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	6	1.16
(1,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	6	1.16
(1,389)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	6	1.16
(1,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	6	1.16
(1,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	6	1.16
(1,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	6	1.16
(1,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	6	1.16
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	1.13
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	1.13
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	1.13
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	1.13
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	1.13
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	1.13
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	1.13
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	1.13
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	1.13
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	1.13
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	1.13
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	1.13
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	1.13
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	1.13
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	1.13
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	1.13
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	1.13
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	1.13
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	1.13
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	1.13
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	1.13
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	1.13
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	1.13
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	1.13
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	1.13
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	1.13
(1,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	1.1
(1,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	1.1
(1,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	1.1
(1,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	1.1
(1,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	1.1
(1,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	1.1
(1,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	1.1
(1,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	1.1
(1,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	1.1
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	1.09
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	1.09
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	1.09
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	1.09
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	1.09
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	1.09
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	1.09
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	1.09
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	1.09
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	1.09
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	1.09
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	1.09
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	1.09
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	1.09
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	1.09
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	1.09
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	1.09
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	1.09
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	1.09
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	1.09
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	1.09
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	1.09
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	1.09
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	1.09
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	1.09
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	1.09
(1,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	9	1.08
(1,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	9	1.08
(1,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	9	1.08
(1,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	9	1.08
(1,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	9	1.08
(1,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	9	1.08
(1,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	9	1.08
(1,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	9	1.08
(1,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	9	1.08
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	1.07
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	1.07
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	1.07
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	1.07
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	1.07
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	1.07
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	1.07
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	1.07
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	1.07
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	1.07
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	1.07
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	1.07
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	1.07
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	1.07
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	1.07
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	1.07
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	1.07
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	1.07
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	1.07
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	1.07
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	1.07
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	1.07
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	1.07
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	1.07
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	1.07
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	1.07
(1,562)	1:705:A:VAL:HG11	1:706:A:ASN:HA	5	1.07
(1,562)	1:705:A:VAL:HG12	1:706:A:ASN:HA	5	1.07
(1,562)	1:705:A:VAL:HG13	1:706:A:ASN:HA	5	1.07
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	7	1.07
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	7	1.07
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	7	1.07
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	7	1.07
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	7	1.07
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	7	1.07
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	7	1.07
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	7	1.07
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	7	1.07
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	7	1.07
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	7	1.07
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	7	1.07
(1,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	5	1.07
(1,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	5	1.07
(1,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	5	1.07
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	7	1.07
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	7	1.07
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	7	1.07
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	7	1.07
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	7	1.07
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	7	1.07
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	7	1.07
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	7	1.07
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	7	1.07
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	7	1.07
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	7	1.07
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	7	1.07
(1,134)	1:705:A:VAL:HG11	1:706:A:ASN:HA	5	1.07
(1,134)	1:705:A:VAL:HG12	1:706:A:ASN:HA	5	1.07
(1,134)	1:705:A:VAL:HG13	1:706:A:ASN:HA	5	1.07
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	7	1.07
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	7	1.07
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	7	1.07
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	7	1.07
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	7	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	7	1.07
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	7	1.07
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	7	1.07
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	7	1.07
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	7	1.07
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	7	1.07
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	7	1.07
(1,603)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	9	1.06
(1,603)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	15	1.06
(1,389)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	9	1.06
(1,389)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	15	1.06
(1,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	9	1.06
(1,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	15	1.06
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	1.04
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	1.04
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	1.04
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	1.04
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	1.04
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	1.04
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	1.04
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	1.04
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	1.04
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	1.04
(1,604)	1:692:A:LEU:HD23	1:696:A:ARG:HH11	11	1.03
(1,390)	1:692:A:LEU:HD23	1:696:A:ARG:HH11	11	1.03
(1,176)	1:692:A:LEU:HD23	1:696:A:ARG:HH11	11	1.03
(1,603)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	4	1.01
(1,389)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	4	1.01
(1,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	4	1.01
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	1.0
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	1.0
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	1.0
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	1.0
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	1.0
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	1.0
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	1.0
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	1.0
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	1.0
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	1.0
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	1.0
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	1.0
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	1.0
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	1.0
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	1.0
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	1.0
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	1.0
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	1.0
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	1.0
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	1.0
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	1.0
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	1.0
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	1.0
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	1.0
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	1.0
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	1.0
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.99
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.99
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.99
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.99
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.99
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.99
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.99
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.99
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.99
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.99
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.99
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.99
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.99
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.99
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.99
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.99
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.99
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.99
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.99
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.99
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.99
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.99
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.99
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.99
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.99
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.99
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.99
(1,603)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	13	0.97
(1,389)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	13	0.97
(1,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	13	0.97
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.94
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.94
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.94
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.94
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.94
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.94
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.94
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.94
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.94
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.94
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.94
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.94
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.94
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.94
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.94
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.94
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.94
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.94
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.94
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.94
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.94
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.94
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.94
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.94
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.94
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.94
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.92
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.92
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.92
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.92
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.92
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.92
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.92
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.92
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.92
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.92
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.92
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.92
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.92
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.92
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.92
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.92
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.92
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.92
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.92
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.92
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.92
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.92
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.92
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.92
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.92
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.92
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.92
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.92
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.92
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.92
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.92
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.92
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.92
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.92
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.92
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.92
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.92
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.92
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.92
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.92
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.92
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.92
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.92
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.92
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.92
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.92
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.92
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.92
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.92
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.92
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.92
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.92
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.92
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	7	0.92
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	7	0.92
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	7	0.92
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	13	0.89
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	13	0.89
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	13	0.89
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	13	0.89
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	13	0.89
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	13	0.89
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	13	0.89
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	13	0.89
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	13	0.89
(1,603)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	3	0.89
(1,389)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	3	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	3	0.89
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.88
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.88
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.88
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.88
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.88
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.88
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.88
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.88
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.88
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.88
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.88
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.88
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.88
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.88
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.88
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.88
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.88
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.88
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.88
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.88
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.88
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.88
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.88
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.88
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.88
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.88
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.88
(1,603)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	12	0.88
(1,389)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	12	0.88
(1,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	12	0.88
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.85
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.85
(1,681)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.85
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.85
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.85
(1,681)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.85
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.85
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.85
(1,681)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.85
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.85
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.85
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.85
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.85
(1,680)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.85
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.85
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.85
(1,680)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.85
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.85
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.85
(1,679)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.85
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.85
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.85
(1,679)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.85
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.85
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.85
(1,679)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.85
(1,550)	1:704:A:LEU:H	1:704:A:LEU:HB3	15	0.85
(1,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	15	0.85
(1,122)	1:704:A:LEU:H	1:704:A:LEU:HB3	15	0.85
(1,604)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	14	0.83
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	13	0.83
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	13	0.83
(1,390)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	14	0.83
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	13	0.83
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	13	0.83
(1,176)	1:692:A:LEU:HD22	1:696:A:ARG:HH21	14	0.83
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	13	0.83
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	13	0.83
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	3	0.82
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	3	0.82
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	3	0.82
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	3	0.82
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	3	0.82
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	3	0.82
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	15	0.82
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	15	0.82
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	15	0.82
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	15	0.82
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	15	0.82
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	15	0.82
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	3	0.82
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	3	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	3	0.82
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	3	0.82
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	3	0.82
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	3	0.82
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	15	0.82
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	15	0.82
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	15	0.82
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	15	0.82
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	15	0.82
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	15	0.82
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	3	0.82
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	3	0.82
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	3	0.82
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	3	0.82
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	3	0.82
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	3	0.82
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	15	0.82
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	15	0.82
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	15	0.82
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	15	0.82
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	15	0.82
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	15	0.82
(1,603)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	8	0.79
(1,389)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	8	0.79
(1,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH11	8	0.79
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.78
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.78
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.78
(1,603)	1:692:A:LEU:HD13	1:696:A:ARG:HH21	2	0.77
(1,389)	1:692:A:LEU:HD13	1:696:A:ARG:HH21	2	0.77
(1,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH21	2	0.77
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.76
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.76
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.76
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.76
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB2	14	0.76
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB3	14	0.76
(1,550)	1:704:A:LEU:H	1:704:A:LEU:HB3	10	0.76
(1,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	10	0.76
(1,122)	1:704:A:LEU:H	1:704:A:LEU:HB3	10	0.76
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG12	1	0.75
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG13	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG12	1	0.75
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG13	1	0.75
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG12	1	0.75
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG13	1	0.75
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	2	0.75
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	2	0.75
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	2	0.75
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	2	0.75
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	2	0.75
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	2	0.75
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	2	0.75
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	2	0.75
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	2	0.75
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	2	0.75
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	2	0.75
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	2	0.75
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	2	0.75
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	2	0.75
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	2	0.75
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	2	0.75
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	2	0.75
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	2	0.75
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	1	0.72
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	1	0.72
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	1	0.72
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	1	0.72
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	1	0.72
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	1	0.72
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	1	0.72
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	1	0.72
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	1	0.72
(1,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	7	0.72
(1,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	7	0.72
(1,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	7	0.72
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	5	0.72
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	5	0.72
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	5	0.72
(1,427)	1:701:A:VAL:HG11	1:698:A:VAL:HA	7	0.72
(1,427)	1:701:A:VAL:HG12	1:698:A:VAL:HA	7	0.72
(1,427)	1:701:A:VAL:HG13	1:698:A:VAL:HA	7	0.72
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	5	0.72
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	5	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	5	0.72
(1,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	7	0.72
(1,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	7	0.72
(1,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	7	0.72
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	5	0.72
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	5	0.72
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	5	0.72
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	14	0.71
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	14	0.71
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	14	0.71
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	14	0.71
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	14	0.71
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	14	0.71
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	14	0.71
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	14	0.71
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	14	0.71
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	15	0.7
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	15	0.7
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	15	0.7
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	15	0.7
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	15	0.7
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	15	0.7
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	15	0.7
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	15	0.7
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	15	0.7
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG12	11	0.67
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG13	11	0.67
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG12	11	0.67
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG13	11	0.67
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG12	11	0.67
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG13	11	0.67
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	11	0.66
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	11	0.66
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	11	0.66
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	10	0.66
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	10	0.66
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	10	0.66
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	10	0.66
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	10	0.66
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	10	0.66
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	11	0.66
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	11	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	11	0.66
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	10	0.66
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	10	0.66
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	10	0.66
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	10	0.66
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	10	0.66
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	10	0.66
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	11	0.66
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	11	0.66
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	11	0.66
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	10	0.66
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	10	0.66
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	10	0.66
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	10	0.66
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	10	0.66
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	10	0.66
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG12	15	0.65
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG13	15	0.65
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG12	15	0.65
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG13	15	0.65
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG12	15	0.65
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG13	15	0.65
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	5	0.65
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.65
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.65
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.65
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	5	0.65
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.65
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.65
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.65
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	5	0.65
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	14	0.65
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	14	0.65
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	14	0.65
(1,508)	1:682:A:ILE:HG21	1:679:A:LEU:H	14	0.64
(1,508)	1:682:A:ILE:HG22	1:679:A:LEU:H	14	0.64
(1,508)	1:682:A:ILE:HG23	1:679:A:LEU:H	14	0.64
(1,294)	1:682:A:ILE:HG21	1:679:A:LEU:H	14	0.64
(1,294)	1:682:A:ILE:HG22	1:679:A:LEU:H	14	0.64
(1,294)	1:682:A:ILE:HG23	1:679:A:LEU:H	14	0.64
(1,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	14	0.64
(1,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	14	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	14	0.64
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	15	0.63
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	15	0.63
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	15	0.63
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	15	0.63
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	15	0.63
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	15	0.63
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	15	0.63
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	15	0.63
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	15	0.63
(1,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	8	0.63
(1,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	8	0.63
(1,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	8	0.63
(1,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	8	0.63
(1,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	8	0.63
(1,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	8	0.63
(1,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	8	0.63
(1,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	8	0.63
(1,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	8	0.63
(1,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	8	0.63
(1,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	8	0.63
(1,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	8	0.63
(1,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	8	0.63
(1,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	8	0.63
(1,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	8	0.63
(1,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	8	0.63
(1,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	8	0.63
(1,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	8	0.63
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB2	2	0.62
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB3	2	0.62
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB2	2	0.62
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB3	2	0.62
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB2	2	0.62
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB3	2	0.62
(1,603)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	1	0.62
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.62
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.62
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.62
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.62
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.62
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.62
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.62
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.62
(1,389)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	1	0.62
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.62
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.62
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.62
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.62
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.62
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.62
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.62
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.62
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.62
(1,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	1	0.62
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.62
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.62
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.62
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.62
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.62
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.62
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.62
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.62
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.62
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.61
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.61
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.61
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.61
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.61
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.61
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.61
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.61
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.61
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.61
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.61
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.61
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.61
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.61
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.61
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.61
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.61
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.61
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.61
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.61
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.6
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.6
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.6
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.6
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.6
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.6
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.6
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.6
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.6
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.6
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.6
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.6
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.6
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.6
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.6
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.6
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.6
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.6
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.6
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.6
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.6
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.6
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.6
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.6
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.6
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.6
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.6
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.6
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.6
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.6
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.6
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.6
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.6
(1,604)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	2	0.59
(1,390)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	2	0.59
(1,176)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	2	0.59
(1,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.58
(1,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.58
(1,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.58
(1,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.58
(1,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.58
(1,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.58
(1,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.58
(1,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.58
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	2	0.55
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	2	0.55
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	2	0.55
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.53
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.53
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.53
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.53
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.53
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.53
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.53
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.53
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.53
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	8	0.52
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	8	0.52
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	8	0.52
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	6	0.52
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	6	0.52
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	6	0.52
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	6	0.52
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	6	0.52
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	6	0.52
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	6	0.52
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	6	0.52
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	6	0.52
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	8	0.52
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	8	0.52
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	8	0.52
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	6	0.52
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	6	0.52
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	6	0.52
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	6	0.52
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	6	0.52
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	6	0.52
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	6	0.52
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	6	0.52
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	6	0.52
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	8	0.52
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	8	0.52
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	6	0.52
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	6	0.52
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	6	0.52
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	6	0.52
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	6	0.52
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	6	0.52
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	6	0.52
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	6	0.52
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	6	0.52
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	13	0.51
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	15	0.51
(1,610)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	11	0.51
(1,610)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	11	0.51
(1,610)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	11	0.51
(1,610)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	11	0.51
(1,610)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	11	0.51
(1,610)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	11	0.51
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	13	0.51
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	15	0.51
(1,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	11	0.51
(1,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	11	0.51
(1,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	11	0.51
(1,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	11	0.51
(1,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	11	0.51
(1,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	11	0.51
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	13	0.51
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	15	0.51
(1,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	11	0.51
(1,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	11	0.51
(1,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	11	0.51
(1,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	11	0.51
(1,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	11	0.51
(1,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	11	0.51
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB2	10	0.5
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB3	10	0.5
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB2	10	0.5
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB3	10	0.5
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB2	10	0.5
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB3	10	0.5
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	9	0.5
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	9	0.5
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	14	0.5
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	14	0.5
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	14	0.5
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	3	0.5
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	3	0.5
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	3	0.5
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	3	0.5
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	3	0.5
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	3	0.5
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	9	0.5
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	9	0.5
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	9	0.5
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	14	0.5
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	14	0.5
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	14	0.5
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	3	0.5
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	3	0.5
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	3	0.5
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	3	0.5
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	3	0.5
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	3	0.5
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	9	0.5
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	9	0.5
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	9	0.5
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	14	0.5
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	14	0.5
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	14	0.5
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	3	0.5
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	3	0.5
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	3	0.5
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	3	0.5
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	3	0.5
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	3	0.5
(1,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	13	0.49
(1,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	13	0.49
(1,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	13	0.49
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.49
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.49
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.49
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.49
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.49
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	3	0.49
(1,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	3	0.49
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.49
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.49
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.49
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.49
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.49
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.49
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	13	0.49
(1,427)	1:701:A:VAL:HG11	1:698:A:VAL:HA	13	0.49
(1,427)	1:701:A:VAL:HG12	1:698:A:VAL:HA	13	0.49
(1,427)	1:701:A:VAL:HG13	1:698:A:VAL:HA	13	0.49
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.49
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.49
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.49
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.49
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.49
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.49
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	3	0.49
(1,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	3	0.49
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.49
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.49
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.49
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.49
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.49
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.49
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	13	0.49
(1,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	13	0.49
(1,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	13	0.49
(1,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	13	0.49
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.49
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.49
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.49
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.49
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.49
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.49
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	3	0.49
(1,76)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	3	0.49
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.49
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.49
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.49
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.49
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.49
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	13	0.49
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	7	0.48
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	12	0.48
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	12	0.48
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	12	0.48
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	12	0.48
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	12	0.48
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	12	0.48
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	7	0.48
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	12	0.48
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	12	0.48
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	12	0.48
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	12	0.48
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	12	0.48
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	12	0.48
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	7	0.48
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	12	0.48
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	12	0.48
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	12	0.48
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	12	0.48
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	12	0.48
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	12	0.48
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	0.47
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	0.47
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	0.47
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	0.47
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	0.47
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	0.47
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	0.47
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	0.47
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	0.47
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	4	0.47
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.47
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	4	0.47
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.47
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	4	0.47
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	13	0.47
(1,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	6	0.46
(1,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	6	0.46
(1,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	11	0.46
(1,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	11	0.46
(1,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	11	0.46
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	15	0.46
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	14	0.46
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	14	0.46
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	14	0.46
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	11	0.46
(1,427)	1:701:A:VAL:HG11	1:698:A:VAL:HA	6	0.46
(1,427)	1:701:A:VAL:HG12	1:698:A:VAL:HA	6	0.46
(1,427)	1:701:A:VAL:HG13	1:698:A:VAL:HA	6	0.46
(1,427)	1:701:A:VAL:HG11	1:698:A:VAL:HA	11	0.46
(1,427)	1:701:A:VAL:HG12	1:698:A:VAL:HA	11	0.46
(1,427)	1:701:A:VAL:HG13	1:698:A:VAL:HA	11	0.46
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	15	0.46
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	14	0.46
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	14	0.46
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	14	0.46
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	11	0.46
(1,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	6	0.46
(1,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	6	0.46
(1,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	6	0.46
(1,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	11	0.46
(1,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	11	0.46
(1,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	11	0.46
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	15	0.46
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	14	0.46
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	14	0.46
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	14	0.46
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	11	0.46
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	13	0.45
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	13	0.45
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	13	0.45
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	1	0.45
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	1	0.45
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	10	0.45
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	3	0.45
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	3	0.45
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	3	0.45
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	13	0.45
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	13	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	13	0.45
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	1	0.45
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	1	0.45
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	10	0.45
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	3	0.45
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	3	0.45
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	3	0.45
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	13	0.45
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	13	0.45
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	13	0.45
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	1	0.45
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	1	0.45
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	10	0.45
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	3	0.45
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	3	0.45
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	3	0.45
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	0.44
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	0.44
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	0.44
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	0.44
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	0.44
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	0.44
(1,610)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	14	0.44
(1,610)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	14	0.44
(1,610)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	14	0.44
(1,610)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	14	0.44
(1,610)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	14	0.44
(1,610)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	14	0.44
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.44
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.44
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.44
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.44
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.44
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.44
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	11	0.44
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	11	0.44
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	11	0.44
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	11	0.44
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	11	0.44
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	11	0.44
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	10	0.44
(1,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	14	0.44
(1,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	14	0.44
(1,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	14	0.44
(1,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	14	0.44
(1,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	14	0.44
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.44
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.44
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.44
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.44
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.44
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.44
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	11	0.44
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	11	0.44
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	11	0.44
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	11	0.44
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	11	0.44
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	11	0.44
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	10	0.44
(1,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	14	0.44
(1,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	14	0.44
(1,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	14	0.44
(1,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	14	0.44
(1,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	14	0.44
(1,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	14	0.44
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	13	0.44
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	13	0.44
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	13	0.44
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	13	0.44
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	13	0.44
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	13	0.44
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	11	0.44
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	11	0.44
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	11	0.44
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	11	0.44
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	11	0.44
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	11	0.44
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	10	0.44
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	11	0.43
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	11	0.43
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	11	0.43
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	11	0.43
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	11	0.43
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	1	0.43
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	1	0.43
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	1	0.43
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	3	0.43
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	3	0.43
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.43
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.43
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.43
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	5	0.43
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.43
(1,456)	1:666:A:TRP:HE1	1:662:A:GLU:H	11	0.43
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	11	0.43
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	11	0.43
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	11	0.43
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	11	0.43
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	11	0.43
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	11	0.43
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	1	0.43
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	1	0.43
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	1	0.43
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	3	0.43
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	3	0.43
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.43
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.43
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.43
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	5	0.43
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.43
(1,242)	1:666:A:TRP:HE1	1:662:A:GLU:H	11	0.43
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	11	0.43
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	11	0.43
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	11	0.43
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	11	0.43
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	11	0.43
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	11	0.43
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	1	0.43
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	1	0.43
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	1	0.43
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	3	0.43
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	3	0.43
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.43
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.43
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	5	0.43
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.43
(1,28)	1:666:A:TRP:HE1	1:662:A:GLU:H	11	0.43
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.42
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	10	0.42
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	10	0.42
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	10	0.42
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	10	0.42
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	10	0.42
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	10	0.42
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	10	0.42
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	10	0.42
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	10	0.42
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	10	0.42
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	7	0.42
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	7	0.42
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	7	0.42
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	8	0.42
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	8	0.42
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	8	0.42
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	8	0.42
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	8	0.42
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	8	0.42
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.42
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	10	0.42
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	10	0.42
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	10	0.42
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	10	0.42
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	10	0.42
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	10	0.42
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	10	0.42
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	10	0.42
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	10	0.42
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	10	0.42
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	7	0.42
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	7	0.42
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	7	0.42
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	8	0.42
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	8	0.42
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	8	0.42
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	8	0.42
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	8	0.42
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.42
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	10	0.42
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	10	0.42
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	10	0.42
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	10	0.42
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	10	0.42
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	10	0.42
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	10	0.42
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	10	0.42
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	10	0.42
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	10	0.42
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	7	0.42
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	7	0.42
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	7	0.42
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	8	0.42
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	8	0.42
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	8	0.42
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	8	0.42
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	8	0.42
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	8	0.42
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	13	0.41
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	13	0.41
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	13	0.41
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	13	0.41
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	13	0.41
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	13	0.41
(1,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	4	0.41
(1,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	4	0.41
(1,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	4	0.41
(1,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	4	0.41
(1,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	4	0.41
(1,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	4	0.41
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	12	0.41
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	12	0.41
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	12	0.41
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.41
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.41
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.41
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	3	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	6	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	6	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	6	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	6	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	6	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	6	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	9	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	9	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	9	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	9	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	9	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	9	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	13	0.41
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	13	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	13	0.41
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	13	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	13	0.41
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	13	0.41
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	2	0.41
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	2	0.41
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	2	0.41
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	2	0.41
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	2	0.41
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	2	0.41
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.41
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.41
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.41
(1,443)	1:665:A:LYS:H	1:662:A:GLU:HA	9	0.41
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	6	0.41
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	6	0.41
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	6	0.41
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	6	0.41
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	6	0.41
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	6	0.41
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	6	0.41
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	6	0.41
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	6	0.41
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	6	0.41
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	6	0.41
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	13	0.41
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	13	0.41
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	13	0.41
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	13	0.41
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	13	0.41
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	13	0.41
(1,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	4	0.41
(1,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	4	0.41
(1,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	4	0.41
(1,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	4	0.41
(1,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	4	0.41
(1,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	4	0.41
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	12	0.41
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	12	0.41
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	12	0.41
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.41
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.41
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.41
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	3	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	6	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	6	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	6	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	6	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	6	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	6	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	9	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	9	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	9	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	9	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	9	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	9	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	13	0.41
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	13	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	13	0.41
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	13	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	13	0.41
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	13	0.41
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	2	0.41
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	2	0.41
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	2	0.41
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	2	0.41
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	2	0.41
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	2	0.41
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.41
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.41
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.41
(1,229)	1:665:A:LYS:H	1:662:A:GLU:HA	9	0.41
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	6	0.41
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	6	0.41
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	6	0.41
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	6	0.41
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	6	0.41
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	6	0.41
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	6	0.41
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	6	0.41
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	6	0.41
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	6	0.41
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	6	0.41
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	6	0.41
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	13	0.41
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	13	0.41
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	13	0.41
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	13	0.41
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	13	0.41
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	13	0.41
(1,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	4	0.41
(1,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	4	0.41
(1,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	4	0.41
(1,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	4	0.41
(1,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	4	0.41
(1,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	4	0.41
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	12	0.41
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	12	0.41
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	12	0.41
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.41
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.41
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	3	0.41
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.41
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.41
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	6	0.41
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	6	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	6	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	6	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	6	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	6	0.41
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	9	0.41
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	9	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	9	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	9	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	9	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	9	0.41
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	13	0.41
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	13	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	13	0.41
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	13	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	13	0.41
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	13	0.41
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	2	0.41
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	2	0.41
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	2	0.41
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	2	0.41
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	2	0.41
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	2	0.41
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.41
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.41
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.41
(1,15)	1:665:A:LYS:H	1:662:A:GLU:HA	9	0.41
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	6	0.41
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	6	0.41
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	6	0.41
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	6	0.41
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	6	0.41
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	6	0.41
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	6	0.41
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	6	0.41
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	6	0.41
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	6	0.41
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	6	0.41
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	7	0.4
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	7	0.4
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	7	0.4
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	7	0.4
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	7	0.4
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	7	0.4
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	7	0.4
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	7	0.4
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	7	0.4
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	2	0.4
(1,614)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	11	0.4
(1,614)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	11	0.4
(1,614)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	11	0.4
(1,614)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	11	0.4
(1,614)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	11	0.4
(1,614)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	11	0.4
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	0.4
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	0.4
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	0.4
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	0.4
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	0.4
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	0.4
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	0.4
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	0.4
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	0.4
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.4
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.4
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.4
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.4
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.4
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.4
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.4
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.4
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.4
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.4
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.4
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.4
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	6	0.4
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	6	0.4
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	6	0.4
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	10	0.4
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	10	0.4
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	10	0.4
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.4
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	12	0.4
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	12	0.4
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	12	0.4
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	2	0.4
(1,400)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	11	0.4
(1,400)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	11	0.4
(1,400)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	11	0.4
(1,400)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	11	0.4
(1,400)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	11	0.4
(1,400)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	11	0.4
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	0.4
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	0.4
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	0.4
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	0.4
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	0.4
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	0.4
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	0.4
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	0.4
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	0.4
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.4
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.4
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.4
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.4
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.4
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.4
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.4
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.4
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.4
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	5	0.4
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.4
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.4
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	6	0.4
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	6	0.4
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	6	0.4
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	10	0.4
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	10	0.4
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	10	0.4
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.4
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	12	0.4
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	12	0.4
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	12	0.4
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	2	0.4
(1,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	11	0.4
(1,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	11	0.4
(1,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	11	0.4
(1,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	11	0.4
(1,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	11	0.4
(1,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	11	0.4
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	0.4
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	0.4
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	0.4
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	0.4
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	0.4
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	0.4
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	0.4
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	0.4
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	0.4
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.4
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.4
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.4
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.4
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.4
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.4
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.4
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.4
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.4
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	5	0.4
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.4
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.4
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.4
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	6	0.4
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	6	0.4
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	10	0.4
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	10	0.4
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	10	0.4
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	13	0.4
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	12	0.4
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	12	0.4
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	12	0.4
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.39
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.39
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.39
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.39
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.39
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.39
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB2	15	0.39
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB3	15	0.39
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB2	15	0.39
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB3	15	0.39
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB2	15	0.39
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB3	15	0.39
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.39
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.39
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.39
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.39
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.39
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.39
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	15	0.39
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	15	0.39
(1,556)	1:705:A:VAL:H	1:702:A:LEU:HA	5	0.39
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	14	0.39
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	3	0.39
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	3	0.39
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	3	0.39
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	3	0.39
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	3	0.39
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	3	0.39
(1,506)	1:681:A:TYR:H	1:680:A:TRP:H	14	0.39
(1,502)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	5	0.39
(1,502)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	5	0.39
(1,502)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	5	0.39
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.39
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.39
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.39
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.39
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.39
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	15	0.39
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	15	0.39
(1,342)	1:705:A:VAL:H	1:702:A:LEU:HA	5	0.39
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	14	0.39
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	3	0.39
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	3	0.39
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	3	0.39
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	3	0.39
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	3	0.39
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	3	0.39
(1,292)	1:681:A:TYR:H	1:680:A:TRP:H	14	0.39
(1,288)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	5	0.39
(1,288)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	5	0.39
(1,288)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	5	0.39
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.39
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.39
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.39
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.39
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.39
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.39
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	15	0.39
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	15	0.39
(1,128)	1:705:A:VAL:H	1:702:A:LEU:HA	5	0.39
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	14	0.39
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	3	0.39
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	3	0.39
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	3	0.39
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	3	0.39
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	3	0.39
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	3	0.39
(1,78)	1:681:A:TYR:H	1:680:A:TRP:H	14	0.39
(1,74)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	5	0.39
(1,74)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	5	0.39
(1,74)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	5	0.39
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	5	0.38
(1,626)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	3	0.38
(1,626)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	3	0.38
(1,626)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	3	0.38
(1,626)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	3	0.38
(1,626)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	3	0.38
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	15	0.38
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	15	0.38
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	15	0.38
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	15	0.38
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	15	0.38
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	15	0.38
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	2	0.38
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	11	0.38
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	12	0.38
(1,565)	1:705:A:VAL:HG21	1:702:A:LEU:HG	5	0.38
(1,565)	1:705:A:VAL:HG22	1:702:A:LEU:HG	5	0.38
(1,565)	1:705:A:VAL:HG23	1:702:A:LEU:HG	5	0.38
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	2	0.38
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	2	0.38
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	2	0.38
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.38
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.38
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.38
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	6	0.38
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	6	0.38
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	6	0.38
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	6	0.38
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	6	0.38
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	6	0.38
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.38
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.38
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.38
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.38
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.38
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.38
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	1	0.38
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	1	0.38
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	1	0.38
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	1	0.38
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	1	0.38
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	1	0.38
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	5	0.38
(1,412)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	3	0.38
(1,412)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	3	0.38
(1,412)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	3	0.38
(1,412)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	3	0.38
(1,412)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	3	0.38
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	15	0.38
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	15	0.38
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	15	0.38
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	15	0.38
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	15	0.38
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	15	0.38
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	2	0.38
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	11	0.38
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	12	0.38
(1,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	5	0.38
(1,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	5	0.38
(1,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	5	0.38
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	2	0.38
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	2	0.38
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	2	0.38
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.38
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.38
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.38
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	6	0.38
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	6	0.38
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	6	0.38
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	6	0.38
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	6	0.38
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	6	0.38
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.38
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.38
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.38
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.38
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.38
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.38
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	1	0.38
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	1	0.38
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	1	0.38
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	1	0.38
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	1	0.38
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	1	0.38
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	5	0.38
(1,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	3	0.38
(1,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	3	0.38
(1,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	3	0.38
(1,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	3	0.38
(1,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	3	0.38
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	15	0.38
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	15	0.38
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	15	0.38
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	15	0.38
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	15	0.38
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	15	0.38
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	2	0.38
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	11	0.38
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	12	0.38
(1,137)	1:705:A:VAL:HG21	1:702:A:LEU:HG	5	0.38
(1,137)	1:705:A:VAL:HG22	1:702:A:LEU:HG	5	0.38
(1,137)	1:705:A:VAL:HG23	1:702:A:LEU:HG	5	0.38
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	2	0.38
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	2	0.38
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	2	0.38
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.38
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.38
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.38
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	6	0.38
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	6	0.38
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	6	0.38
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	6	0.38
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	6	0.38
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	6	0.38
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	15	0.38
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	15	0.38
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	15	0.38
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	15	0.38
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	15	0.38
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	15	0.38
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	1	0.38
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	1	0.38
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	1	0.38
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	1	0.38
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	1	0.38
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	1	0.38
(1,611)	1:695:A:LEU:H	1:691:A:SER:HA	6	0.37
(1,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.37
(1,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.37
(1,604)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	4	0.37
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.37
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.37
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.37
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.37
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.37
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.37
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	8	0.37
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	8	0.37
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	8	0.37
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	11	0.37
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	11	0.37
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	11	0.37
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	14	0.37
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	14	0.37
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	14	0.37
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	15	0.37
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	15	0.37
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	15	0.37
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.37
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.37
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.37
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.37
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.37
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.37
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.37
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.37
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.37
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.37
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.37
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.37
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.37
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.37
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.37
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.37
(1,397)	1:695:A:LEU:H	1:691:A:SER:HA	6	0.37
(1,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.37
(1,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.37
(1,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.37
(1,390)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.37
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.37
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.37
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.37
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.37
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.37
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	8	0.37
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	8	0.37
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	8	0.37
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	11	0.37
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	11	0.37
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	11	0.37
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	14	0.37
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	14	0.37
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	14	0.37
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	15	0.37
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	15	0.37
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	15	0.37
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.37
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.37
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.37
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.37
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.37
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.37
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.37
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.37
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.37
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.37
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.37
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.37
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.37
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.37
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.37
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.37
(1,183)	1:695:A:LEU:H	1:691:A:SER:HA	6	0.37
(1,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.37
(1,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.37
(1,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.37
(1,176)	1:692:A:LEU:HD21	1:696:A:ARG:HH21	4	0.37
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.37
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.37
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.37
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.37
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.37
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	8	0.37
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	8	0.37
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	8	0.37
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	11	0.37
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	11	0.37
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	11	0.37
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	14	0.37
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	14	0.37
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	14	0.37
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	15	0.37
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	15	0.37
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	15	0.37
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.37
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.37
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.37
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.37
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.37
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.37
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.37
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.37
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.37
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.37
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.37
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.37
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.37
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.37
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.37
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.37
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	9	0.36
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	7	0.36
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	7	0.36
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	7	0.36
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	7	0.36
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	7	0.36
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	7	0.36
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	10	0.36
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	10	0.36
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	10	0.36
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	10	0.36
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	10	0.36
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.36
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.36
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.36
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.36
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.36
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.36
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	1	0.36
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.36
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.36
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.36
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	12	0.36
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	12	0.36
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	12	0.36
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	8	0.36
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	1	0.36
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	1	0.36
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	1	0.36
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	1	0.36
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	1	0.36
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	1	0.36
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.36
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.36
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.36
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.36
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.36
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.36
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	10	0.36
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	10	0.36
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	10	0.36
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	10	0.36
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	10	0.36
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	10	0.36
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	14	0.36
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	9	0.36
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	7	0.36
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	7	0.36
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	7	0.36
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	7	0.36
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	7	0.36
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	10	0.36
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	10	0.36
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	10	0.36
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	10	0.36
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	10	0.36
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	10	0.36
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.36
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.36
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.36
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.36
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.36
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.36
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	1	0.36
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.36
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.36
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.36
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	12	0.36
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	12	0.36
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	12	0.36
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	8	0.36
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	1	0.36
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	1	0.36
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	1	0.36
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	1	0.36
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	1	0.36
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	1	0.36
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.36
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.36
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.36
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.36
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.36
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.36
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	10	0.36
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	10	0.36
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	10	0.36
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	10	0.36
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	10	0.36
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	10	0.36
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	14	0.36
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	9	0.36
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	7	0.36
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	7	0.36
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	7	0.36
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	7	0.36
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	7	0.36
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	10	0.36
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	10	0.36
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	10	0.36
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	10	0.36
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	10	0.36
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	10	0.36
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	7	0.36
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	7	0.36
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	7	0.36
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	7	0.36
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	7	0.36
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	7	0.36
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	1	0.36
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.36
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.36
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.36
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	12	0.36
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	12	0.36
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	12	0.36
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	8	0.36
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	1	0.36
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	1	0.36
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	1	0.36
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	1	0.36
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	1	0.36
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	1	0.36
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.36
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.36
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.36
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.36
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.36
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.36
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	10	0.36
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	10	0.36
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	10	0.36
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	10	0.36
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	10	0.36
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	14	0.36
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	0.35
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	0.35
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	0.35
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	0.35
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	0.35
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	0.35
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	0.35
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	0.35
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	0.35
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB2	1	0.35
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB3	1	0.35
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB2	1	0.35
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB3	1	0.35
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB2	1	0.35
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB3	1	0.35
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	15	0.35
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	15	0.35
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	15	0.35
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	15	0.35
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	15	0.35
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	15	0.35
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.35
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	4	0.35
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	9	0.35
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	7	0.35
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	7	0.35
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	7	0.35
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	7	0.35
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	7	0.35
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	7	0.35
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	8	0.35
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	8	0.35
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	8	0.35
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	8	0.35
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	8	0.35
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	8	0.35
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	3	0.35
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	3	0.35
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	3	0.35
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	3	0.35
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	3	0.35
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	10	0.35
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	13	0.35
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	13	0.35
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	13	0.35
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	13	0.35
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	13	0.35
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	13	0.35
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	13	0.35
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	13	0.35
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	13	0.35
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	13	0.35
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	13	0.35
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	13	0.35
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	15	0.35
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	15	0.35
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	15	0.35
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	15	0.35
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	15	0.35
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	15	0.35
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.35
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	4	0.35
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	9	0.35
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	7	0.35
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	7	0.35
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	7	0.35
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	7	0.35
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	7	0.35
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	7	0.35
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	8	0.35
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	8	0.35
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	8	0.35
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	8	0.35
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	8	0.35
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	8	0.35
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	3	0.35
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	3	0.35
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	3	0.35
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	3	0.35
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	3	0.35
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	3	0.35
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	13	0.35
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	13	0.35
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	13	0.35
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	13	0.35
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	13	0.35
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	13	0.35
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	13	0.35
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	13	0.35
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	13	0.35
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	13	0.35
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	13	0.35
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	13	0.35
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	15	0.35
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	15	0.35
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	15	0.35
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	15	0.35
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	15	0.35
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	15	0.35
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.35
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	4	0.35
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	9	0.35
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	7	0.35
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	7	0.35
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	7	0.35
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	7	0.35
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	7	0.35
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	7	0.35
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	8	0.35
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	8	0.35
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	8	0.35
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	8	0.35
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	8	0.35
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	8	0.35
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	3	0.35
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	3	0.35
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	3	0.35
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	3	0.35
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	3	0.35
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	3	0.35
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	10	0.35
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	13	0.35
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	13	0.35
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	13	0.35
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	13	0.35
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	13	0.35
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	13	0.35
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	13	0.35
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	13	0.35
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	13	0.35
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	13	0.35
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	13	0.35
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB2	8	0.34
(1,648)	1:663:A:LEU:H	1:661:A:LEU:HB3	8	0.34
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB2	8	0.34
(1,647)	1:663:A:LEU:H	1:661:A:LEU:HB3	8	0.34
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB2	8	0.34
(1,646)	1:663:A:LEU:H	1:661:A:LEU:HB3	8	0.34
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.34
(1,611)	1:695:A:LEU:H	1:691:A:SER:HA	7	0.34
(1,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.34
(1,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.34
(1,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.34
(1,588)	1:686:A:ILE:HD11	1:685:A:PHE:H	12	0.34
(1,588)	1:686:A:ILE:HD12	1:685:A:PHE:H	12	0.34
(1,588)	1:686:A:ILE:HD13	1:685:A:PHE:H	12	0.34
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	10	0.34
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	10	0.34
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	7	0.34
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.34
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	11	0.34
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	11	0.34
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	11	0.34
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	11	0.34
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	11	0.34
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	11	0.34
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	14	0.34
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	14	0.34
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	14	0.34
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	14	0.34
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	14	0.34
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	14	0.34
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	10	0.34
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	10	0.34
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.34
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.34
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.34
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.34
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.34
(1,397)	1:695:A:LEU:H	1:691:A:SER:HA	7	0.34
(1,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.34
(1,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.34
(1,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.34
(1,374)	1:686:A:ILE:HD11	1:685:A:PHE:H	12	0.34
(1,374)	1:686:A:ILE:HD12	1:685:A:PHE:H	12	0.34
(1,374)	1:686:A:ILE:HD13	1:685:A:PHE:H	12	0.34
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	10	0.34
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	10	0.34
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	7	0.34
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.34
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	11	0.34
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	11	0.34
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	11	0.34
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	11	0.34
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	11	0.34
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	11	0.34
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	14	0.34
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	14	0.34
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	14	0.34
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	14	0.34
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	14	0.34
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	14	0.34
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	10	0.34
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	10	0.34
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	10	0.34
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.34
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.34
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.34
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.34
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.34
(1,183)	1:695:A:LEU:H	1:691:A:SER:HA	7	0.34
(1,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.34
(1,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.34
(1,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.34
(1,160)	1:686:A:ILE:HD11	1:685:A:PHE:H	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:686:A:ILE:HD12	1:685:A:PHE:H	12	0.34
(1,160)	1:686:A:ILE:HD13	1:685:A:PHE:H	12	0.34
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	10	0.34
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	10	0.34
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	7	0.34
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.34
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	11	0.34
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	11	0.34
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	11	0.34
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	11	0.34
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	11	0.34
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	11	0.34
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	14	0.34
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	14	0.34
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	14	0.34
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	14	0.34
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	14	0.34
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	14	0.34
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	10	0.34
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	10	0.34
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	10	0.34
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.34
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.34
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.34
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.34
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.33
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.33
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.33
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.33
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.33
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.33
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	6	0.33
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	6	0.33
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	6	0.33
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	6	0.33
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	6	0.33
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	6	0.33
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.33
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.33
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.33
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.33
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.33
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.33
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.33
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.33
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.33
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.33
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.33
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	6	0.33
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	6	0.33
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	6	0.33
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	6	0.33
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	6	0.33
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	6	0.33
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.33
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.33
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.33
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.33
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.33
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.33
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.33
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.33
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.33
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.33
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.33
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.33
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	6	0.33
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	6	0.33
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	6	0.33
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	6	0.33
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	6	0.33
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	6	0.33
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.33
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.33
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.33
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.33
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.33
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.33
(1,614)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	14	0.33
(1,614)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	14	0.33
(1,614)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	14	0.33
(1,614)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	14	0.33
(1,614)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	14	0.33
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	10	0.33
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	10	0.33
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	10	0.33
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.33
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.33
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	6	0.33
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	11	0.33
(1,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	15	0.33
(1,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	15	0.33
(1,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	15	0.33
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	13	0.33
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	13	0.33
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	13	0.33
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	13	0.33
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	13	0.33
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	13	0.33
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.33
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.33
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.33
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	15	0.33
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	15	0.33
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	15	0.33
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	15	0.33
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	15	0.33
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	15	0.33
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	1	0.33
(1,456)	1:666:A:TRP:HE1	1:662:A:GLU:H	13	0.33
(1,400)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	14	0.33
(1,400)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	14	0.33
(1,400)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	14	0.33
(1,400)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	14	0.33
(1,400)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	14	0.33
(1,400)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	14	0.33
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	10	0.33
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	10	0.33
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	10	0.33
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.33
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.33
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	6	0.33
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	11	0.33
(1,340)	1:704:A:LEU:HD11	1:707:A:ARG:HE	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:704:A:LEU:HD12	1:707:A:ARG:HE	15	0.33
(1,340)	1:704:A:LEU:HD13	1:707:A:ARG:HE	15	0.33
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	13	0.33
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	13	0.33
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	13	0.33
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	13	0.33
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	13	0.33
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	13	0.33
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.33
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.33
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.33
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	15	0.33
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	15	0.33
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	15	0.33
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	15	0.33
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	15	0.33
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	15	0.33
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	1	0.33
(1,242)	1:666:A:TRP:HE1	1:662:A:GLU:H	13	0.33
(1,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	14	0.33
(1,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	14	0.33
(1,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	14	0.33
(1,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	14	0.33
(1,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	14	0.33
(1,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	14	0.33
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	10	0.33
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	10	0.33
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	10	0.33
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	12	0.33
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	12	0.33
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	6	0.33
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	11	0.33
(1,126)	1:704:A:LEU:HD11	1:707:A:ARG:HE	15	0.33
(1,126)	1:704:A:LEU:HD12	1:707:A:ARG:HE	15	0.33
(1,126)	1:704:A:LEU:HD13	1:707:A:ARG:HE	15	0.33
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	13	0.33
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	13	0.33
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	13	0.33
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	13	0.33
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	13	0.33
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	13	0.33
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.33
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.33
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	15	0.33
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	15	0.33
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	15	0.33
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	15	0.33
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	15	0.33
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	15	0.33
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	1	0.33
(1,28)	1:666:A:TRP:HE1	1:662:A:GLU:H	13	0.33
(1,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	3	0.32
(1,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	3	0.32
(1,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	3	0.32
(1,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	3	0.32
(1,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	3	0.32
(1,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	3	0.32
(1,610)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	6	0.32
(1,610)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	6	0.32
(1,610)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	6	0.32
(1,610)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	6	0.32
(1,610)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	6	0.32
(1,610)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	6	0.32
(1,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	2	0.32
(1,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	2	0.32
(1,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	2	0.32
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	3	0.32
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.32
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.32
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.32
(1,492)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.32
(1,492)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.32
(1,492)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.32
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	5	0.32
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	5	0.32
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	5	0.32
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.32
(1,407)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	3	0.32
(1,407)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	3	0.32
(1,407)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	3	0.32
(1,407)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	3	0.32
(1,407)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	3	0.32
(1,407)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	6	0.32
(1,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	6	0.32
(1,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	6	0.32
(1,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	6	0.32
(1,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	6	0.32
(1,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	6	0.32
(1,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	2	0.32
(1,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	2	0.32
(1,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	2	0.32
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	3	0.32
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.32
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.32
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.32
(1,278)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.32
(1,278)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.32
(1,278)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.32
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	5	0.32
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	5	0.32
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	5	0.32
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.32
(1,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	3	0.32
(1,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	3	0.32
(1,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	3	0.32
(1,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	3	0.32
(1,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	3	0.32
(1,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	3	0.32
(1,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	6	0.32
(1,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	6	0.32
(1,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	6	0.32
(1,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	6	0.32
(1,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	6	0.32
(1,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	6	0.32
(1,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	2	0.32
(1,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	2	0.32
(1,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	2	0.32
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	3	0.32
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.32
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.32
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.32
(1,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.32
(1,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.32
(1,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	5	0.32
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	5	0.32
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	5	0.32
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.32
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	13	0.31
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	13	0.31
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	13	0.31
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	13	0.31
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	13	0.31
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	13	0.31
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	13	0.31
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	13	0.31
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	13	0.31
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	13	0.31
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	13	0.31
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	13	0.31
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	13	0.31
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	13	0.31
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	13	0.31
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	13	0.31
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	13	0.31
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	13	0.31
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.31
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	6	0.31
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	6	0.31
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	6	0.31
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	8	0.31
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	8	0.31
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	8	0.31
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.31
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.31
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.31
(1,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	10	0.31
(1,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	10	0.31
(1,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	10	0.31
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	9	0.31
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	10	0.31
(1,564)	1:705:A:VAL:HG21	1:701:A:VAL:HA	5	0.31
(1,564)	1:705:A:VAL:HG22	1:701:A:VAL:HA	5	0.31
(1,564)	1:705:A:VAL:HG23	1:701:A:VAL:HA	5	0.31
(1,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	5	0.31
(1,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	5	0.31
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	14	0.31
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	14	0.31
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	14	0.31
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	14	0.31
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	14	0.31
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	14	0.31
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	9	0.31
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	9	0.31
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	9	0.31
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	9	0.31
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	9	0.31
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	9	0.31
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	11	0.31
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	15	0.31
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	15	0.31
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	15	0.31
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	4	0.31
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.31
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.31
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.31
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	6	0.31
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	6	0.31
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	6	0.31
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	8	0.31
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	8	0.31
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	8	0.31
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.31
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.31
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.31
(1,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	10	0.31
(1,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	10	0.31
(1,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	10	0.31
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	9	0.31
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	10	0.31
(1,350)	1:705:A:VAL:HG21	1:701:A:VAL:HA	5	0.31
(1,350)	1:705:A:VAL:HG22	1:701:A:VAL:HA	5	0.31
(1,350)	1:705:A:VAL:HG23	1:701:A:VAL:HA	5	0.31
(1,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	5	0.31
(1,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	5	0.31
(1,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	5	0.31
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	14	0.31
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	14	0.31
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	14	0.31
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	14	0.31
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	14	0.31
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	9	0.31
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	9	0.31
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	9	0.31
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	9	0.31
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	9	0.31
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	9	0.31
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	11	0.31
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	15	0.31
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	15	0.31
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	15	0.31
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	4	0.31
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.31
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.31
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	14	0.31
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	6	0.31
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	6	0.31
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	6	0.31
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	8	0.31
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	8	0.31
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	8	0.31
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.31
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.31
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.31
(1,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	10	0.31
(1,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	10	0.31
(1,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	10	0.31
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	9	0.31
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	10	0.31
(1,136)	1:705:A:VAL:HG21	1:701:A:VAL:HA	5	0.31
(1,136)	1:705:A:VAL:HG22	1:701:A:VAL:HA	5	0.31
(1,136)	1:705:A:VAL:HG23	1:701:A:VAL:HA	5	0.31
(1,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	5	0.31
(1,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	5	0.31
(1,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	5	0.31
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	14	0.31
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	14	0.31
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	14	0.31
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	14	0.31
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	14	0.31
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	9	0.31
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	9	0.31
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	9	0.31
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	9	0.31
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	9	0.31
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	9	0.31
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	11	0.31
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	15	0.31
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	15	0.31
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	15	0.31
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	4	0.31
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.31
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	15	0.31
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	12	0.3
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	12	0.3
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	12	0.3
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	12	0.3
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	12	0.3
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	12	0.3
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	12	0.3
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	12	0.3
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	12	0.3
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	12	0.3
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	12	0.3
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	12	0.3
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	12	0.3
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	12	0.3
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	12	0.3
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	12	0.3
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	12	0.3
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	12	0.3
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	11	0.3
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	11	0.3
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	11	0.3
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	11	0.3
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	11	0.3
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	11	0.3
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	11	0.3
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	11	0.3
(1,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.3
(1,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.3
(1,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.3
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.3
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	11	0.3
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	11	0.3
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	11	0.3
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	11	0.3
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	11	0.3
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	11	0.3
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	12	0.3
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	12	0.3
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	12	0.3
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	12	0.3
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	12	0.3
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	12	0.3
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	15	0.3
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	15	0.3
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	15	0.3
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	15	0.3
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	15	0.3
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	15	0.3
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	12	0.3
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	12	0.3
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	12	0.3
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	5	0.3
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	5	0.3
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	5	0.3
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	5	0.3
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	5	0.3
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	5	0.3
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	7	0.3
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	9	0.3
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	14	0.3
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	11	0.3
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	11	0.3
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	11	0.3
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	11	0.3
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	11	0.3
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	11	0.3
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	11	0.3
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	11	0.3
(1,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.3
(1,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.3
(1,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.3
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.3
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	11	0.3
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	11	0.3
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	11	0.3
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	11	0.3
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	11	0.3
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	11	0.3
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	12	0.3
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	12	0.3
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	12	0.3
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	12	0.3
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	12	0.3
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	12	0.3
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	15	0.3
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	15	0.3
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	15	0.3
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	15	0.3
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	15	0.3
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	15	0.3
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	12	0.3
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	12	0.3
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	12	0.3
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	5	0.3
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	5	0.3
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	5	0.3
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	5	0.3
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	5	0.3
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	5	0.3
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	7	0.3
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	9	0.3
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	14	0.3
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	11	0.3
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	11	0.3
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	11	0.3
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	11	0.3
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	11	0.3
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	11	0.3
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	11	0.3
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	11	0.3
(1,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.3
(1,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.3
(1,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.3
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.3
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	11	0.3
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	11	0.3
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	11	0.3
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	11	0.3
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	11	0.3
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	11	0.3
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	12	0.3
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	12	0.3
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	12	0.3
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	12	0.3
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	12	0.3
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	12	0.3
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	15	0.3
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	15	0.3
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	15	0.3
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	15	0.3
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	15	0.3
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	15	0.3
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	12	0.3
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	12	0.3
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	12	0.3
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	5	0.3
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	5	0.3
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	5	0.3
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	5	0.3
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	5	0.3
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	5	0.3
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	7	0.3
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	9	0.3
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	14	0.3
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	3	0.29
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	3	0.29
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	3	0.29
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	3	0.29
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	3	0.29
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	3	0.29
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	3	0.29
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	3	0.29
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	4	0.29
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	4	0.29
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	4	0.29
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	4	0.29
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	4	0.29
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	4	0.29
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	10	0.29
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	10	0.29
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	10	0.29
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	10	0.29
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	10	0.29
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	10	0.29
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	8	0.29
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.29
(1,615)	1:695:A:LEU:HD21	1:698:A:VAL:HB	3	0.29
(1,615)	1:695:A:LEU:HD22	1:698:A:VAL:HB	3	0.29
(1,615)	1:695:A:LEU:HD23	1:698:A:VAL:HB	3	0.29
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	1	0.29
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	1	0.29
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	1	0.29
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	1	0.29
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	1	0.29
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	1	0.29
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	5	0.29
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	5	0.29
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	5	0.29
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	5	0.29
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	5	0.29
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	5	0.29
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.29
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.29
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.29
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.29
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.29
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.29
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.29
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.29
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.29
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.29
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.29
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.29
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.29
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.29
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.29
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	3	0.29
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	3	0.29
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	3	0.29
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	11	0.29
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	11	0.29
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	11	0.29
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	1	0.29
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	1	0.29
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	1	0.29
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	1	0.29
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	1	0.29
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	1	0.29
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	1	0.29
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	1	0.29
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	1	0.29
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	1	0.29
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	1	0.29
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	1	0.29
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	1	0.29
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	1	0.29
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	1	0.29
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	1	0.29
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	1	0.29
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	1	0.29
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.29
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.29
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.29
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.29
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.29
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.29
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.29
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.29
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.29
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.29
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.29
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	4	0.29
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	4	0.29
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	4	0.29
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	4	0.29
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	4	0.29
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	4	0.29
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	10	0.29
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	10	0.29
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	10	0.29
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	10	0.29
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	10	0.29
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	10	0.29
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	8	0.29
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.29
(1,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	3	0.29
(1,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	3	0.29
(1,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	3	0.29
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	1	0.29
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	1	0.29
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	1	0.29
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	1	0.29
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	1	0.29
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	1	0.29
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	5	0.29
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	5	0.29
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	5	0.29
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	5	0.29
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	5	0.29
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	5	0.29
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.29
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.29
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.29
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.29
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.29
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.29
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.29
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.29
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	6	0.29
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.29
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.29
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.29
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.29
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.29
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.29
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	3	0.29
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	3	0.29
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	3	0.29
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	11	0.29
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	11	0.29
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	11	0.29
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	1	0.29
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	1	0.29
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	1	0.29
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	1	0.29
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	1	0.29
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	1	0.29
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	1	0.29
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	1	0.29
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	1	0.29
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	1	0.29
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	1	0.29
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	1	0.29
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	1	0.29
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	1	0.29
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	1	0.29
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	1	0.29
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	1	0.29
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	1	0.29
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.29
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.29
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.29
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.29
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.29
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.29
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.29
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.29
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.29
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.29
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.29
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.29
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	4	0.29
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	4	0.29
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	4	0.29
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	4	0.29
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	4	0.29
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	10	0.29
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	10	0.29
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	10	0.29
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	10	0.29
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	10	0.29
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	10	0.29
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	8	0.29
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	11	0.29
(1,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	3	0.29
(1,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	3	0.29
(1,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	3	0.29
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	1	0.29
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	1	0.29
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	1	0.29
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	1	0.29
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	1	0.29
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	1	0.29
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	5	0.29
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	5	0.29
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	5	0.29
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	5	0.29
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	5	0.29
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	5	0.29
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.29
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.29
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.29
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.29
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.29
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.29
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.29
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.29
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	6	0.29
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.29
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.29
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.29
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.29
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.29
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.29
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	3	0.29
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	3	0.29
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	3	0.29
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	11	0.29
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	11	0.29
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	11	0.29
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	1	0.29
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	1	0.29
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	1	0.29
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	1	0.29
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	1	0.29
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	1	0.29
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	1	0.29
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	1	0.29
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	1	0.29
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	1	0.29
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	1	0.29
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	1	0.29
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	1	0.29
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	1	0.29
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	1	0.29
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	1	0.29
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	1	0.29
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	1	0.29
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.29
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.29
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.29
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.29
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.29
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.29
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.29
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.29
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.29
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.29
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.29
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.29
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.28
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	7	0.28
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	7	0.28
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	7	0.28
(1,615)	1:695:A:LEU:HD21	1:698:A:VAL:HB	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:695:A:LEU:HD22	1:698:A:VAL:HB	9	0.28
(1,615)	1:695:A:LEU:HD23	1:698:A:VAL:HB	9	0.28
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	6	0.28
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	6	0.28
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	6	0.28
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	6	0.28
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	6	0.28
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	6	0.28
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.28
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.28
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.28
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.28
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.28
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.28
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	14	0.28
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	14	0.28
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	14	0.28
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	14	0.28
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	14	0.28
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	14	0.28
(1,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.28
(1,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.28
(1,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.28
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	1	0.28
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	1	0.28
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	1	0.28
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	9	0.28
(1,565)	1:705:A:VAL:HG21	1:702:A:LEU:HG	7	0.28
(1,565)	1:705:A:VAL:HG22	1:702:A:LEU:HG	7	0.28
(1,565)	1:705:A:VAL:HG23	1:702:A:LEU:HG	7	0.28
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	11	0.28
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	11	0.28
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	11	0.28
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	11	0.28
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	11	0.28
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	11	0.28
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	4	0.28
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	4	0.28
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	4	0.28
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	11	0.28
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	11	0.28
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	12	0.28
(1,443)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.28
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.28
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	7	0.28
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	7	0.28
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	7	0.28
(1,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	9	0.28
(1,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	9	0.28
(1,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	9	0.28
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	6	0.28
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	6	0.28
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	6	0.28
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	6	0.28
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	6	0.28
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	6	0.28
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.28
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.28
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.28
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.28
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.28
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.28
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	14	0.28
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	14	0.28
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	14	0.28
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	14	0.28
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	14	0.28
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	14	0.28
(1,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.28
(1,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.28
(1,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.28
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	1	0.28
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	1	0.28
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	1	0.28
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	9	0.28
(1,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	7	0.28
(1,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	7	0.28
(1,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	7	0.28
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	11	0.28
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	11	0.28
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	11	0.28
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	11	0.28
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	11	0.28
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	4	0.28
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	4	0.28
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	4	0.28
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	11	0.28
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	11	0.28
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	11	0.28
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	12	0.28
(1,229)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.28
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	10	0.28
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	7	0.28
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	7	0.28
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	7	0.28
(1,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	9	0.28
(1,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	9	0.28
(1,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	9	0.28
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	6	0.28
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	6	0.28
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	6	0.28
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	6	0.28
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	6	0.28
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	6	0.28
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.28
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.28
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.28
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.28
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.28
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.28
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	14	0.28
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	14	0.28
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	14	0.28
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	14	0.28
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	14	0.28
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	14	0.28
(1,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.28
(1,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.28
(1,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.28
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	1	0.28
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	1	0.28
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	1	0.28
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	9	0.28
(1,137)	1:705:A:VAL:HG21	1:702:A:LEU:HG	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:705:A:VAL:HG22	1:702:A:LEU:HG	7	0.28
(1,137)	1:705:A:VAL:HG23	1:702:A:LEU:HG	7	0.28
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	11	0.28
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	11	0.28
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	11	0.28
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	11	0.28
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	11	0.28
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	11	0.28
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	4	0.28
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	4	0.28
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	4	0.28
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	11	0.28
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	11	0.28
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	11	0.28
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	12	0.28
(1,15)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.28
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.27
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	12	0.27
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	12	0.27
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	12	0.27
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	12	0.27
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	12	0.27
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	12	0.27
(1,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.27
(1,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.27
(1,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.27
(1,522)	1:684:A:ILE:HG21	1:688:A:ILE:H	11	0.27
(1,522)	1:684:A:ILE:HG22	1:688:A:ILE:H	11	0.27
(1,522)	1:684:A:ILE:HG23	1:688:A:ILE:H	11	0.27
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	4	0.27
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	4	0.27
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	4	0.27
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	4	0.27
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	4	0.27
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	4	0.27
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	12	0.27
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	12	0.27
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	12	0.27
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	12	0.27
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	12	0.27
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	12	0.27
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	14	0.27
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	14	0.27
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	14	0.27
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	14	0.27
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	14	0.27
(1,502)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	9	0.27
(1,502)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	9	0.27
(1,502)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	9	0.27
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.27
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.27
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	15	0.27
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	15	0.27
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	15	0.27
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	15	0.27
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	15	0.27
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	15	0.27
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	10	0.27
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	10	0.27
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	10	0.27
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	8	0.27
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	8	0.27
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	8	0.27
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.27
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	9	0.27
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.27
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.27
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	12	0.27
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	12	0.27
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	12	0.27
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	12	0.27
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	12	0.27
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	12	0.27
(1,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.27
(1,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.27
(1,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.27
(1,308)	1:684:A:ILE:HG21	1:688:A:ILE:H	11	0.27
(1,308)	1:684:A:ILE:HG22	1:688:A:ILE:H	11	0.27
(1,308)	1:684:A:ILE:HG23	1:688:A:ILE:H	11	0.27
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	4	0.27
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	4	0.27
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	4	0.27
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	4	0.27
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	4	0.27
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	12	0.27
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	12	0.27
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	12	0.27
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	12	0.27
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	12	0.27
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	12	0.27
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	14	0.27
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	14	0.27
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	14	0.27
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	14	0.27
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	14	0.27
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	14	0.27
(1,288)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	9	0.27
(1,288)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	9	0.27
(1,288)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	9	0.27
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.27
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.27
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	15	0.27
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	15	0.27
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	15	0.27
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	15	0.27
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	15	0.27
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	15	0.27
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	10	0.27
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	10	0.27
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	10	0.27
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	8	0.27
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	8	0.27
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	8	0.27
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.27
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	9	0.27
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.27
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.27
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	12	0.27
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	12	0.27
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	12	0.27
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	12	0.27
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	12	0.27
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	12	0.27
(1,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.27
(1,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.27
(1,94)	1:684:A:ILE:HG21	1:688:A:ILE:H	11	0.27
(1,94)	1:684:A:ILE:HG22	1:688:A:ILE:H	11	0.27
(1,94)	1:684:A:ILE:HG23	1:688:A:ILE:H	11	0.27
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	4	0.27
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	4	0.27
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	4	0.27
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	4	0.27
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	4	0.27
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	4	0.27
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	12	0.27
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	12	0.27
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	12	0.27
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	12	0.27
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	12	0.27
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	12	0.27
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	14	0.27
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	14	0.27
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	14	0.27
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	14	0.27
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	14	0.27
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	14	0.27
(1,74)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	9	0.27
(1,74)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	9	0.27
(1,74)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	9	0.27
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.27
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.27
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	15	0.27
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	15	0.27
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	15	0.27
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	15	0.27
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	15	0.27
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	15	0.27
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	10	0.27
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	10	0.27
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	10	0.27
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	8	0.27
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	8	0.27
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	8	0.27
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.27
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.27
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	7	0.26
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	7	0.26
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	7	0.26
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	7	0.26
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	7	0.26
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	7	0.26
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	7	0.26
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	7	0.26
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	7	0.26
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	7	0.26
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	7	0.26
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	7	0.26
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	7	0.26
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	7	0.26
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	7	0.26
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	7	0.26
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	7	0.26
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	7	0.26
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	3	0.26
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	3	0.26
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	3	0.26
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	3	0.26
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	3	0.26
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	3	0.26
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	2	0.26
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	2	0.26
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	2	0.26
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	2	0.26
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.26
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.26
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.26
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.26
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.26
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.26
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	10	0.26
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	10	0.26
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	10	0.26
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	10	0.26
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	10	0.26
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	10	0.26
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	10	0.26
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	10	0.26
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	13	0.26
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	9	0.26
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	9	0.26
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	9	0.26
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	9	0.26
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	9	0.26
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	9	0.26
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	6	0.26
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	6	0.26
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	6	0.26
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.26
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	3	0.26
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	3	0.26
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	3	0.26
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	3	0.26
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	3	0.26
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	3	0.26
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	2	0.26
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	2	0.26
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	2	0.26
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	2	0.26
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.26
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.26
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.26
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.26
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.26
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.26
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	10	0.26
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	10	0.26
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	10	0.26
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	10	0.26
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	10	0.26
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	10	0.26
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	10	0.26
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	10	0.26
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	10	0.26
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	13	0.26
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	9	0.26
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	9	0.26
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	9	0.26
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	9	0.26
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	9	0.26
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	6	0.26
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	6	0.26
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	6	0.26
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.26
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	3	0.26
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	3	0.26
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	3	0.26
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	3	0.26
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	3	0.26
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	3	0.26
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	2	0.26
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	2	0.26
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	2	0.26
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	2	0.26
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.26
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.26
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.26
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.26
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.26
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.26
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	10	0.26
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	10	0.26
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	10	0.26
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	10	0.26
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	10	0.26
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	10	0.26
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	10	0.26
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	10	0.26
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	10	0.26
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	13	0.26
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	9	0.26
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	9	0.26
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	9	0.26
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	9	0.26
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	9	0.26
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	9	0.26
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	6	0.26
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	6	0.26
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.26
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	12	0.25
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	12	0.25
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	12	0.25
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	12	0.25
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	12	0.25
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	12	0.25
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.25
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.25
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.25
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.25
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.25
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.25
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	4	0.25
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	4	0.25
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	4	0.25
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	4	0.25
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	4	0.25
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	4	0.25
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	3	0.25
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	3	0.25
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	3	0.25
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	3	0.25
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	3	0.25
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	3	0.25
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	7	0.25
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	7	0.25
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	7	0.25
(1,590)	1:686:A:ILE:HD11	1:686:A:ILE:H	12	0.25
(1,590)	1:686:A:ILE:HD12	1:686:A:ILE:H	12	0.25
(1,590)	1:686:A:ILE:HD13	1:686:A:ILE:H	12	0.25
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	4	0.25
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.25
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	4	0.25
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	4	0.25
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	4	0.25
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	4	0.25
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	4	0.25
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	4	0.25
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	11	0.25
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	5	0.25
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	5	0.25
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	5	0.25
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	5	0.25
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	5	0.25
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.25
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.25
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.25
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.25
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.25
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.25
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	11	0.25
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	5	0.25
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	8	0.25
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	8	0.25
(1,462)	1:667:A:ALA:HB1	1:664:A:ASP:HA	6	0.25
(1,462)	1:667:A:ALA:HB2	1:664:A:ASP:HA	6	0.25
(1,462)	1:667:A:ALA:HB3	1:664:A:ASP:HA	6	0.25
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.25
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.25
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	12	0.25
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	12	0.25
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	12	0.25
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	12	0.25
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	12	0.25
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	12	0.25
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.25
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.25
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.25
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.25
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.25
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.25
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	4	0.25
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	4	0.25
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	4	0.25
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	4	0.25
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	4	0.25
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	4	0.25
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	3	0.25
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	3	0.25
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	3	0.25
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	3	0.25
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	3	0.25
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	7	0.25
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	7	0.25
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	7	0.25
(1,376)	1:686:A:ILE:HD11	1:686:A:ILE:H	12	0.25
(1,376)	1:686:A:ILE:HD12	1:686:A:ILE:H	12	0.25
(1,376)	1:686:A:ILE:HD13	1:686:A:ILE:H	12	0.25
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	4	0.25
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.25
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	4	0.25
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	4	0.25
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	4	0.25
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	4	0.25
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	4	0.25
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	4	0.25
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	11	0.25
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	5	0.25
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	5	0.25
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	5	0.25
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	5	0.25
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	5	0.25
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	5	0.25
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.25
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.25
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.25
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.25
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.25
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.25
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	11	0.25
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	5	0.25
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	8	0.25
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	8	0.25
(1,248)	1:667:A:ALA:HB1	1:664:A:ASP:HA	6	0.25
(1,248)	1:667:A:ALA:HB2	1:664:A:ASP:HA	6	0.25
(1,248)	1:667:A:ALA:HB3	1:664:A:ASP:HA	6	0.25
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.25
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.25
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	12	0.25
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	12	0.25
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	12	0.25
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	12	0.25
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	12	0.25
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.25
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.25
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.25
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.25
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.25
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.25
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	4	0.25
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	4	0.25
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	4	0.25
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	4	0.25
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	4	0.25
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	4	0.25
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	3	0.25
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	3	0.25
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	3	0.25
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	3	0.25
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	3	0.25
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	3	0.25
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	7	0.25
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	7	0.25
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	7	0.25
(1,162)	1:686:A:ILE:HD11	1:686:A:ILE:H	12	0.25
(1,162)	1:686:A:ILE:HD12	1:686:A:ILE:H	12	0.25
(1,162)	1:686:A:ILE:HD13	1:686:A:ILE:H	12	0.25
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	4	0.25
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	15	0.25
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	4	0.25
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	4	0.25
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	4	0.25
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	4	0.25
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	4	0.25
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	4	0.25
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	11	0.25
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	5	0.25
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	5	0.25
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	5	0.25
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	5	0.25
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	5	0.25
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	5	0.25
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.25
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.25
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.25
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.25
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.25
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	11	0.25
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	5	0.25
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	8	0.25
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	8	0.25
(1,34)	1:667:A:ALA:HB1	1:664:A:ASP:HA	6	0.25
(1,34)	1:667:A:ALA:HB2	1:664:A:ASP:HA	6	0.25
(1,34)	1:667:A:ALA:HB3	1:664:A:ASP:HA	6	0.25
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.25
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.25
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	3	0.24
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	3	0.24
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	3	0.24
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	3	0.24
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	3	0.24
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	3	0.24
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	3	0.24
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	3	0.24
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	3	0.24
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	3	0.24
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	3	0.24
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	3	0.24
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	3	0.24
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	3	0.24
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	3	0.24
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	3	0.24
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	3	0.24
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	3	0.24
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	12	0.24
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	15	0.24
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	2	0.24
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	2	0.24
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	2	0.24
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	9	0.24
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	9	0.24
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	9	0.24
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	9	0.24
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	9	0.24
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	9	0.24
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	9	0.24
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	9	0.24
(1,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	12	0.24
(1,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	12	0.24
(1,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	12	0.24
(1,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	12	0.24
(1,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	12	0.24
(1,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	12	0.24
(1,615)	1:695:A:LEU:HD21	1:698:A:VAL:HB	6	0.24
(1,615)	1:695:A:LEU:HD22	1:698:A:VAL:HB	6	0.24
(1,615)	1:695:A:LEU:HD23	1:698:A:VAL:HB	6	0.24
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	2	0.24
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	2	0.24
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	2	0.24
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	2	0.24
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	2	0.24
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	2	0.24
(1,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	13	0.24
(1,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	13	0.24
(1,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	13	0.24
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	8	0.24
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	13	0.24
(1,550)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.24
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	14	0.24
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	2	0.24
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	3	0.24
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	6	0.24
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	11	0.24
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	7	0.24
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	7	0.24
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	7	0.24
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	7	0.24
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	7	0.24
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	7	0.24
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	15	0.24
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	15	0.24
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	15	0.24
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	15	0.24
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	15	0.24
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	15	0.24
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.24
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.24
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	14	0.24
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	14	0.24
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	14	0.24
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	1	0.24
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	4	0.24
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	6	0.24
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	2	0.24
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	2	0.24
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	2	0.24
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	7	0.24
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	8	0.24
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	8	0.24
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	10	0.24
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	13	0.24
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.24
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.24
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.24
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.24
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	11	0.24
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	11	0.24
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	11	0.24
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	11	0.24
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	11	0.24
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	11	0.24
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	11	0.24
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	11	0.24
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	11	0.24
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	11	0.24
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	11	0.24
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	11	0.24
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	12	0.24
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	15	0.24
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	2	0.24
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	2	0.24
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	2	0.24
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	9	0.24
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	9	0.24
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	9	0.24
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	9	0.24
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	9	0.24
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	9	0.24
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	9	0.24
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	9	0.24
(1,407)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	12	0.24
(1,407)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	12	0.24
(1,407)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	12	0.24
(1,407)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	12	0.24
(1,407)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	12	0.24
(1,407)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	12	0.24
(1,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	6	0.24
(1,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	6	0.24
(1,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	6	0.24
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	2	0.24
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	2	0.24
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	2	0.24
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	2	0.24
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	2	0.24
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	2	0.24
(1,386)	1:692:A:LEU:HD11	1:689:A:VAL:HA	13	0.24
(1,386)	1:692:A:LEU:HD12	1:689:A:VAL:HA	13	0.24
(1,386)	1:692:A:LEU:HD13	1:689:A:VAL:HA	13	0.24
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	8	0.24
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	13	0.24
(1,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.24
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	14	0.24
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	2	0.24
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	3	0.24
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	6	0.24
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	11	0.24
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	7	0.24
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	7	0.24
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	7	0.24
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	7	0.24
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	7	0.24
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	7	0.24
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	15	0.24
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	15	0.24
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	15	0.24
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	15	0.24
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	15	0.24
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.24
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.24
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.24
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	14	0.24
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	14	0.24
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	14	0.24
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	1	0.24
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	4	0.24
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	6	0.24
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	2	0.24
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	2	0.24
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	2	0.24
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	7	0.24
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	8	0.24
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	8	0.24
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	10	0.24
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	13	0.24
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.24
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.24
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.24
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.24
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	11	0.24
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	11	0.24
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	11	0.24
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	11	0.24
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	11	0.24
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	11	0.24
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	11	0.24
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	11	0.24
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	11	0.24
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	11	0.24
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	11	0.24
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	11	0.24
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	12	0.24
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	15	0.24
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	2	0.24
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	2	0.24
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	2	0.24
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	9	0.24
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	9	0.24
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	9	0.24
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	9	0.24
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	9	0.24
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	9	0.24
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	9	0.24
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	9	0.24
(1,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	12	0.24
(1,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	12	0.24
(1,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	12	0.24
(1,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	12	0.24
(1,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	12	0.24
(1,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	12	0.24
(1,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	6	0.24
(1,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	6	0.24
(1,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	6	0.24
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	2	0.24
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	2	0.24
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	2	0.24
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	2	0.24
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	2	0.24
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	2	0.24
(1,172)	1:692:A:LEU:HD11	1:689:A:VAL:HA	13	0.24
(1,172)	1:692:A:LEU:HD12	1:689:A:VAL:HA	13	0.24
(1,172)	1:692:A:LEU:HD13	1:689:A:VAL:HA	13	0.24
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	8	0.24
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	13	0.24
(1,122)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.24
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	14	0.24
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	2	0.24
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	3	0.24
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	6	0.24
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	11	0.24
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	7	0.24
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	7	0.24
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	7	0.24
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	7	0.24
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	7	0.24
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	7	0.24
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	15	0.24
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	15	0.24
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	15	0.24
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	15	0.24
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	15	0.24
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.24
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.24
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.24
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	14	0.24
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	14	0.24
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	14	0.24
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	1	0.24
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	4	0.24
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	6	0.24
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	2	0.24
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	2	0.24
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	2	0.24
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	7	0.24
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	8	0.24
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	8	0.24
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	10	0.24
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	13	0.24
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.24
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.24
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.24
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.24
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	11	0.24
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	11	0.24
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	11	0.24
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	11	0.24
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	11	0.24
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	11	0.24
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	11	0.24
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	11	0.24
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	11	0.24
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	11	0.24
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	11	0.24
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	11	0.24
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	1	0.23
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	1	0.23
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	1	0.23
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	1	0.23
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	1	0.23
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	1	0.23
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.23
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.23
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.23
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.23
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.23
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	1	0.23
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	1	0.23
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	1	0.23
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	1	0.23
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	1	0.23
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	1	0.23
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.23
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.23
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.23
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.23
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.23
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.23
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	1	0.23
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	1	0.23
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	1	0.23
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	1	0.23
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	1	0.23
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	1	0.23
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	14	0.23
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	14	0.23
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	14	0.23
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	14	0.23
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	14	0.23
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	14	0.23
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.23
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	1	0.23
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	1	0.23
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	1	0.23
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	1	0.23
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	1	0.23
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	1	0.23
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	7	0.23
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	7	0.23
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	7	0.23
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	7	0.23
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	7	0.23
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	7	0.23
(1,625)	1:698:A:VAL:HG11	1:695:A:LEU:HG	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:698:A:VAL:HG12	1:695:A:LEU:HG	12	0.23
(1,625)	1:698:A:VAL:HG13	1:695:A:LEU:HG	12	0.23
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	4	0.23
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	4	0.23
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	4	0.23
(1,615)	1:695:A:LEU:HD21	1:698:A:VAL:HB	5	0.23
(1,615)	1:695:A:LEU:HD22	1:698:A:VAL:HB	5	0.23
(1,615)	1:695:A:LEU:HD23	1:698:A:VAL:HB	5	0.23
(1,614)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	13	0.23
(1,614)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	13	0.23
(1,614)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	13	0.23
(1,614)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	13	0.23
(1,614)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	13	0.23
(1,614)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	13	0.23
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	4	0.23
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	4	0.23
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	4	0.23
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	3	0.23
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	10	0.23
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	10	0.23
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	10	0.23
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	10	0.23
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	10	0.23
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	10	0.23
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	7	0.23
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	13	0.23
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	2	0.23
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	12	0.23
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.23
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.23
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.23
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.23
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.23
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.23
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.23
(1,492)	1:676:A:THR:HG21	1:669:A:LEU:HA	11	0.23
(1,492)	1:676:A:THR:HG22	1:669:A:LEU:HA	11	0.23
(1,492)	1:676:A:THR:HG23	1:669:A:LEU:HA	11	0.23
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	11	0.23
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	11	0.23
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	11	0.23
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	11	0.23
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	11	0.23
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	5	0.23
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	5	0.23
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	5	0.23
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	5	0.23
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	5	0.23
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	5	0.23
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	2	0.23
(1,449)	1:666:A:TRP:H	1:663:A:LEU:HA	3	0.23
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	12	0.23
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.23
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.23
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.23
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	14	0.23
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	14	0.23
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	14	0.23
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	14	0.23
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	14	0.23
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	14	0.23
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	14	0.23
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	14	0.23
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	14	0.23
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	14	0.23
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	14	0.23
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	14	0.23
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.23
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	1	0.23
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	1	0.23
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	1	0.23
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	1	0.23
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	1	0.23
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	1	0.23
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	7	0.23
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	7	0.23
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	7	0.23
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	7	0.23
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	7	0.23
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	7	0.23
(1,411)	1:698:A:VAL:HG11	1:695:A:LEU:HG	12	0.23
(1,411)	1:698:A:VAL:HG12	1:695:A:LEU:HG	12	0.23
(1,411)	1:698:A:VAL:HG13	1:695:A:LEU:HG	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	4	0.23
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	4	0.23
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	4	0.23
(1,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	5	0.23
(1,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	5	0.23
(1,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	5	0.23
(1,400)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	13	0.23
(1,400)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	13	0.23
(1,400)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	13	0.23
(1,400)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	13	0.23
(1,400)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	13	0.23
(1,400)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	13	0.23
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	4	0.23
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	4	0.23
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	4	0.23
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	3	0.23
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	10	0.23
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	10	0.23
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	10	0.23
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	10	0.23
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	10	0.23
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	10	0.23
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	7	0.23
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	13	0.23
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	2	0.23
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	12	0.23
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.23
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.23
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.23
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.23
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.23
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.23
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.23
(1,278)	1:676:A:THR:HG21	1:669:A:LEU:HA	11	0.23
(1,278)	1:676:A:THR:HG22	1:669:A:LEU:HA	11	0.23
(1,278)	1:676:A:THR:HG23	1:669:A:LEU:HA	11	0.23
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	11	0.23
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	11	0.23
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	11	0.23
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	11	0.23
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	11	0.23
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	5	0.23
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	5	0.23
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	5	0.23
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	5	0.23
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	5	0.23
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	5	0.23
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	2	0.23
(1,235)	1:666:A:TRP:H	1:663:A:LEU:HA	3	0.23
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	12	0.23
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.23
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.23
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.23
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	14	0.23
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	14	0.23
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	14	0.23
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	14	0.23
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	14	0.23
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	14	0.23
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	14	0.23
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	14	0.23
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	14	0.23
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	14	0.23
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	14	0.23
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	14	0.23
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.23
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	1	0.23
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	1	0.23
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	1	0.23
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	1	0.23
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	1	0.23
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	1	0.23
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	7	0.23
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	7	0.23
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	7	0.23
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	7	0.23
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	7	0.23
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	7	0.23
(1,197)	1:698:A:VAL:HG11	1:695:A:LEU:HG	12	0.23
(1,197)	1:698:A:VAL:HG12	1:695:A:LEU:HG	12	0.23
(1,197)	1:698:A:VAL:HG13	1:695:A:LEU:HG	12	0.23
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	4	0.23
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	4	0.23
(1,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	5	0.23
(1,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	5	0.23
(1,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	5	0.23
(1,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	13	0.23
(1,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	13	0.23
(1,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	13	0.23
(1,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	13	0.23
(1,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	13	0.23
(1,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	13	0.23
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	4	0.23
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	4	0.23
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	4	0.23
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	3	0.23
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	10	0.23
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	10	0.23
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	10	0.23
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	10	0.23
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	10	0.23
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	10	0.23
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	7	0.23
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	13	0.23
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	2	0.23
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	12	0.23
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.23
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.23
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.23
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.23
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.23
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.23
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.23
(1,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	11	0.23
(1,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	11	0.23
(1,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	11	0.23
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	11	0.23
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	11	0.23
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	11	0.23
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	11	0.23
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	11	0.23
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	11	0.23
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	5	0.23
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	5	0.23
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	5	0.23
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	5	0.23
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	5	0.23
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	2	0.23
(1,21)	1:666:A:TRP:H	1:663:A:LEU:HA	3	0.23
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	12	0.23
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.23
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.23
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	15	0.23
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	14	0.23
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	14	0.23
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	14	0.23
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	14	0.23
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	14	0.23
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	14	0.23
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	14	0.23
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	14	0.23
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	14	0.23
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	14	0.23
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	14	0.23
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	14	0.23
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.22
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.22
(1,616)	1:695:A:LEU:HD21	1:698:A:VAL:H	9	0.22
(1,616)	1:695:A:LEU:HD22	1:698:A:VAL:H	9	0.22
(1,616)	1:695:A:LEU:HD23	1:698:A:VAL:H	9	0.22
(1,616)	1:695:A:LEU:HD21	1:698:A:VAL:H	14	0.22
(1,616)	1:695:A:LEU:HD22	1:698:A:VAL:H	14	0.22
(1,616)	1:695:A:LEU:HD23	1:698:A:VAL:H	14	0.22
(1,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	14	0.22
(1,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	14	0.22
(1,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	14	0.22
(1,588)	1:686:A:ILE:HD11	1:685:A:PHE:H	7	0.22
(1,588)	1:686:A:ILE:HD12	1:685:A:PHE:H	7	0.22
(1,588)	1:686:A:ILE:HD13	1:685:A:PHE:H	7	0.22
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	8	0.22
(1,522)	1:684:A:ILE:HG21	1:688:A:ILE:H	10	0.22
(1,522)	1:684:A:ILE:HG22	1:688:A:ILE:H	10	0.22
(1,522)	1:684:A:ILE:HG23	1:688:A:ILE:H	10	0.22
(1,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.22
(1,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.22
(1,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.22
(1,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.22
(1,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.22
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	9	0.22
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	9	0.22
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	9	0.22
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	9	0.22
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	9	0.22
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	9	0.22
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	6	0.22
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	6	0.22
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	6	0.22
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	4	0.22
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	4	0.22
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	4	0.22
(1,492)	1:676:A:THR:HG21	1:669:A:LEU:HA	4	0.22
(1,492)	1:676:A:THR:HG22	1:669:A:LEU:HA	4	0.22
(1,492)	1:676:A:THR:HG23	1:669:A:LEU:HA	4	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	1	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	1	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	1	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	1	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	1	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	1	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	11	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	11	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	11	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	11	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	11	0.22
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	11	0.22
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	9	0.22
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	9	0.22
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	9	0.22
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	3	0.22
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	1	0.22
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	15	0.22
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.22
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.22
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	13	0.22
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	13	0.22
(1,437)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	13	0.22
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	13	0.22
(1,437)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	13	0.22
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	13	0.22
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	13	0.22
(1,437)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	13	0.22
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.22
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.22
(1,402)	1:695:A:LEU:HD21	1:698:A:VAL:H	9	0.22
(1,402)	1:695:A:LEU:HD22	1:698:A:VAL:H	9	0.22
(1,402)	1:695:A:LEU:HD23	1:698:A:VAL:H	9	0.22
(1,402)	1:695:A:LEU:HD21	1:698:A:VAL:H	14	0.22
(1,402)	1:695:A:LEU:HD22	1:698:A:VAL:H	14	0.22
(1,402)	1:695:A:LEU:HD23	1:698:A:VAL:H	14	0.22
(1,386)	1:692:A:LEU:HD11	1:689:A:VAL:HA	14	0.22
(1,386)	1:692:A:LEU:HD12	1:689:A:VAL:HA	14	0.22
(1,386)	1:692:A:LEU:HD13	1:689:A:VAL:HA	14	0.22
(1,374)	1:686:A:ILE:HD11	1:685:A:PHE:H	7	0.22
(1,374)	1:686:A:ILE:HD12	1:685:A:PHE:H	7	0.22
(1,374)	1:686:A:ILE:HD13	1:685:A:PHE:H	7	0.22
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	8	0.22
(1,308)	1:684:A:ILE:HG21	1:688:A:ILE:H	10	0.22
(1,308)	1:684:A:ILE:HG22	1:688:A:ILE:H	10	0.22
(1,308)	1:684:A:ILE:HG23	1:688:A:ILE:H	10	0.22
(1,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.22
(1,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.22
(1,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.22
(1,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.22
(1,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.22
(1,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.22
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	9	0.22
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	9	0.22
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	9	0.22
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	9	0.22
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	9	0.22
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	9	0.22
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	6	0.22
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	6	0.22
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	6	0.22
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	4	0.22
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	4	0.22
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:676:A:THR:HG21	1:669:A:LEU:HA	4	0.22
(1,278)	1:676:A:THR:HG22	1:669:A:LEU:HA	4	0.22
(1,278)	1:676:A:THR:HG23	1:669:A:LEU:HA	4	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	1	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	1	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	1	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	1	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	1	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	1	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	11	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	11	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	11	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	11	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	11	0.22
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	11	0.22
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	9	0.22
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	9	0.22
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	9	0.22
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	3	0.22
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	1	0.22
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	15	0.22
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.22
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.22
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	13	0.22
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	13	0.22
(1,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	13	0.22
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	13	0.22
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	13	0.22
(1,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	13	0.22
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	13	0.22
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	13	0.22
(1,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	13	0.22
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.22
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.22
(1,188)	1:695:A:LEU:HD21	1:698:A:VAL:H	9	0.22
(1,188)	1:695:A:LEU:HD22	1:698:A:VAL:H	9	0.22
(1,188)	1:695:A:LEU:HD23	1:698:A:VAL:H	9	0.22
(1,188)	1:695:A:LEU:HD21	1:698:A:VAL:H	14	0.22
(1,188)	1:695:A:LEU:HD22	1:698:A:VAL:H	14	0.22
(1,188)	1:695:A:LEU:HD23	1:698:A:VAL:H	14	0.22
(1,172)	1:692:A:LEU:HD11	1:689:A:VAL:HA	14	0.22
(1,172)	1:692:A:LEU:HD12	1:689:A:VAL:HA	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:692:A:LEU:HD13	1:689:A:VAL:HA	14	0.22
(1,160)	1:686:A:ILE:HD11	1:685:A:PHE:H	7	0.22
(1,160)	1:686:A:ILE:HD12	1:685:A:PHE:H	7	0.22
(1,160)	1:686:A:ILE:HD13	1:685:A:PHE:H	7	0.22
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	8	0.22
(1,94)	1:684:A:ILE:HG21	1:688:A:ILE:H	10	0.22
(1,94)	1:684:A:ILE:HG22	1:688:A:ILE:H	10	0.22
(1,94)	1:684:A:ILE:HG23	1:688:A:ILE:H	10	0.22
(1,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.22
(1,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.22
(1,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.22
(1,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.22
(1,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.22
(1,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.22
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	9	0.22
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	9	0.22
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	9	0.22
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	9	0.22
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	9	0.22
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	9	0.22
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	6	0.22
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	6	0.22
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	6	0.22
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	4	0.22
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	4	0.22
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	4	0.22
(1,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	4	0.22
(1,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	4	0.22
(1,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	4	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	1	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	1	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	1	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	1	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	1	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	1	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	11	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	11	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	11	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	11	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	11	0.22
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	11	0.22
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	9	0.22
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	9	0.22
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	3	0.22
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	1	0.22
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	15	0.22
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.22
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.22
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	13	0.22
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	13	0.22
(1,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	13	0.22
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	13	0.22
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	13	0.22
(1,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	13	0.22
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	13	0.22
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	13	0.22
(1,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	13	0.22
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.21
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.21
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.21
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.21
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.21
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.21
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.21
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.21
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.21
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.21
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.21
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.21
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	15	0.21
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	15	0.21
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	15	0.21
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	15	0.21
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	15	0.21
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	15	0.21
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.21
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	5	0.21
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	5	0.21
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	5	0.21
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	5	0.21
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	5	0.21
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.21
(1,615)	1:695:A:LEU:HD21	1:698:A:VAL:HB	7	0.21
(1,615)	1:695:A:LEU:HD22	1:698:A:VAL:HB	7	0.21
(1,615)	1:695:A:LEU:HD23	1:698:A:VAL:HB	7	0.21
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	4	0.21
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	4	0.21
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	4	0.21
(1,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	10	0.21
(1,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	10	0.21
(1,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	10	0.21
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	3	0.21
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	6	0.21
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	10	0.21
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	15	0.21
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	7	0.21
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	7	0.21
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	7	0.21
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	7	0.21
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	7	0.21
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	7	0.21
(1,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	10	0.21
(1,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	10	0.21
(1,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	10	0.21
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	14	0.21
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	14	0.21
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	14	0.21
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	14	0.21
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	14	0.21
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	14	0.21
(1,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.21
(1,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.21
(1,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.21
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	8	0.21
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	8	0.21
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	8	0.21
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	8	0.21
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	8	0.21
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	8	0.21
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	10	0.21
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	10	0.21
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	10	0.21
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.21
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.21
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.21
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.21
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.21
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.21
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.21
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.21
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.21
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.21
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.21
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.21
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.21
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.21
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.21
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.21
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.21
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.21
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.21
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	1	0.21
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	3	0.21
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	3	0.21
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	11	0.21
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.21
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	5	0.21
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	5	0.21
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	5	0.21
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	5	0.21
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	5	0.21
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	5	0.21
(1,405)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.21
(1,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	7	0.21
(1,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	7	0.21
(1,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	7	0.21
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	4	0.21
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	4	0.21
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	4	0.21
(1,386)	1:692:A:LEU:HD11	1:689:A:VAL:HA	10	0.21
(1,386)	1:692:A:LEU:HD12	1:689:A:VAL:HA	10	0.21
(1,386)	1:692:A:LEU:HD13	1:689:A:VAL:HA	10	0.21
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	6	0.21
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	10	0.21
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	15	0.21
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	7	0.21
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	7	0.21
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	7	0.21
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	7	0.21
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	7	0.21
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	7	0.21
(1,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	10	0.21
(1,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	10	0.21
(1,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	10	0.21
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	14	0.21
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	14	0.21
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	14	0.21
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	14	0.21
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	14	0.21
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	14	0.21
(1,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.21
(1,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.21
(1,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.21
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	8	0.21
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	8	0.21
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	8	0.21
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	8	0.21
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	8	0.21
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	8	0.21
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	10	0.21
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	10	0.21
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	10	0.21
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.21
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.21
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.21
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.21
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.21
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.21
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.21
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.21
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.21
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.21
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.21
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.21
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.21
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.21
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.21
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.21
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.21
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.21
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.21
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	1	0.21
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	3	0.21
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	3	0.21
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	11	0.21
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.21
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	5	0.21
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	5	0.21
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	5	0.21
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	5	0.21
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	5	0.21
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	5	0.21
(1,191)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.21
(1,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	7	0.21
(1,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	7	0.21
(1,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	7	0.21
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	4	0.21
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	4	0.21
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	4	0.21
(1,172)	1:692:A:LEU:HD11	1:689:A:VAL:HA	10	0.21
(1,172)	1:692:A:LEU:HD12	1:689:A:VAL:HA	10	0.21
(1,172)	1:692:A:LEU:HD13	1:689:A:VAL:HA	10	0.21
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	3	0.21
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	6	0.21
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	10	0.21
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	15	0.21
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	7	0.21
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	7	0.21
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	7	0.21
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	7	0.21
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	7	0.21
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	7	0.21
(1,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	10	0.21
(1,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	10	0.21
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	14	0.21
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	14	0.21
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	14	0.21
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	14	0.21
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	14	0.21
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	14	0.21
(1,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.21
(1,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.21
(1,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.21
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	8	0.21
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	8	0.21
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	8	0.21
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	8	0.21
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	8	0.21
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	8	0.21
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	10	0.21
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	10	0.21
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	10	0.21
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.21
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.21
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.21
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.21
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.21
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.21
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.21
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.21
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.21
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.21
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.21
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.21
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.21
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.21
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.21
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.21
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.21
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.21
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.21
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.21
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	1	0.21
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	3	0.21
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	11	0.21
(1,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	2	0.2
(1,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	2	0.2
(1,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	2	0.2
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.2
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.2
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	1	0.2
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	1	0.2
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	1	0.2
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	1	0.2
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	3	0.2
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.2
(1,613)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.2
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.2
(1,613)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.2
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.2
(1,613)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.2
(1,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	2	0.2
(1,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	2	0.2
(1,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	2	0.2
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	5	0.2
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	5	0.2
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	5	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	2	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	2	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	2	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	2	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	2	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	2	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	2	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	2	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	2	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	13	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	13	0.2
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	13	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	13	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	13	0.2
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	13	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	13	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	13	0.2
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	13	0.2
(1,567)	1:706:A:ASN:H	1:703:A:SER:HA	1	0.2
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.2
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.2
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.2
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.2
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.2
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.2
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	11	0.2
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	4	0.2
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	4	0.2
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	4	0.2
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	4	0.2
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	4	0.2
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	4	0.2
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	4	0.2
(1,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	4	0.2
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	4	0.2
(1,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	4	0.2
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	4	0.2
(1,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	4	0.2
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	2	0.2
(1,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	2	0.2
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	2	0.2
(1,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	2	0.2
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	2	0.2
(1,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	2	0.2
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	5	0.2
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	5	0.2
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	5	0.2
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	5	0.2
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	5	0.2
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	5	0.2
(1,502)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	13	0.2
(1,502)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	13	0.2
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	1	0.2
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	1	0.2
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	1	0.2
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	15	0.2
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	15	0.2
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	15	0.2
(1,488)	1:675:A:ILE:H	1:674:A:ASP:H	12	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	14	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	14	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	14	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	14	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	14	0.2
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	14	0.2
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	15	0.2
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.2
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	10	0.2
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	7	0.2
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	12	0.2
(1,444)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.2
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.2
(1,427)	1:701:A:VAL:HG11	1:698:A:VAL:HA	2	0.2
(1,427)	1:701:A:VAL:HG12	1:698:A:VAL:HA	2	0.2
(1,427)	1:701:A:VAL:HG13	1:698:A:VAL:HA	2	0.2
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.2
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.2
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	1	0.2
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	1	0.2
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	1	0.2
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	1	0.2
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	3	0.2
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.2
(1,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.2
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.2
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.2
(1,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.2
(1,386)	1:692:A:LEU:HD11	1:689:A:VAL:HA	2	0.2
(1,386)	1:692:A:LEU:HD12	1:689:A:VAL:HA	2	0.2
(1,386)	1:692:A:LEU:HD13	1:689:A:VAL:HA	2	0.2
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	5	0.2
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	5	0.2
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	5	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	2	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	2	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	2	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	2	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	2	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	2	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	2	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	2	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	2	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	13	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	13	0.2
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	13	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	13	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	13	0.2
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	13	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	13	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	13	0.2
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	13	0.2
(1,353)	1:706:A:ASN:H	1:703:A:SER:HA	1	0.2
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.2
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.2
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.2
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.2
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.2
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	11	0.2
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	4	0.2
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	4	0.2
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	4	0.2
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	4	0.2
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	4	0.2
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	4	0.2
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	4	0.2
(1,306)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	4	0.2
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	4	0.2
(1,306)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	4	0.2
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	4	0.2
(1,306)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	4	0.2
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	2	0.2
(1,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	2	0.2
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	2	0.2
(1,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	2	0.2
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	2	0.2
(1,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	2	0.2
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	5	0.2
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	5	0.2
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	5	0.2
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	5	0.2
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	5	0.2
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	5	0.2
(1,288)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	13	0.2
(1,288)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	13	0.2
(1,288)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	13	0.2
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	1	0.2
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	1	0.2
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	1	0.2
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	15	0.2
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	15	0.2
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	15	0.2
(1,274)	1:675:A:ILE:H	1:674:A:ASP:H	12	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	14	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	14	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	14	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	14	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	14	0.2
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	14	0.2
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	15	0.2
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.2
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	10	0.2
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	7	0.2
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	12	0.2
(1,230)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.2
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.2
(1,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	2	0.2
(1,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	2	0.2
(1,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	2	0.2
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.2
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.2
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	1	0.2
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	1	0.2
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	1	0.2
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	1	0.2
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	3	0.2
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.2
(1,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.2
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.2
(1,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.2
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.2
(1,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.2
(1,172)	1:692:A:LEU:HD11	1:689:A:VAL:HA	2	0.2
(1,172)	1:692:A:LEU:HD12	1:689:A:VAL:HA	2	0.2
(1,172)	1:692:A:LEU:HD13	1:689:A:VAL:HA	2	0.2
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	5	0.2
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	5	0.2
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	5	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	2	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	2	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	2	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	2	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	2	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	2	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	2	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	2	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	13	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	13	0.2
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	13	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	13	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	13	0.2
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	13	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	13	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	13	0.2
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	13	0.2
(1,139)	1:706:A:ASN:H	1:703:A:SER:HA	1	0.2
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.2
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.2
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.2
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.2
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.2
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.2
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	11	0.2
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	4	0.2
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	4	0.2
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	4	0.2
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	4	0.2
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	4	0.2
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	4	0.2
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	4	0.2
(1,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	4	0.2
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	4	0.2
(1,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	4	0.2
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	4	0.2
(1,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	4	0.2
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	2	0.2
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	2	0.2
(1,84)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	2	0.2
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	2	0.2
(1,84)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	2	0.2
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	5	0.2
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	5	0.2
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	5	0.2
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	5	0.2
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	5	0.2
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	5	0.2
(1,74)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	13	0.2
(1,74)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	13	0.2
(1,74)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	13	0.2
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	1	0.2
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	1	0.2
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	1	0.2
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	15	0.2
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	15	0.2
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	15	0.2
(1,60)	1:675:A:ILE:H	1:674:A:ASP:H	12	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	14	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	14	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	14	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	14	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	14	0.2
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	14	0.2
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	15	0.2
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.2
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	10	0.2
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	7	0.2
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	12	0.2
(1,16)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.2
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.2
(1,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	5	0.19
(1,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	5	0.19
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.19
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.19
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	10	0.19
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	10	0.19
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	10	0.19
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	2	0.19
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	2	0.19
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	2	0.19
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	2	0.19
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	2	0.19
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	2	0.19
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	2	0.19
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	2	0.19
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	2	0.19
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.19
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.19
(1,573)	1:707:A:ARG:H	1:704:A:LEU:HA	12	0.19
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.19
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.19
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.19
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.19
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.19
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.19
(1,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	12	0.19
(1,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	12	0.19
(1,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	12	0.19
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	9	0.19
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	1	0.19
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	8	0.19
(1,525)	1:686:A:ILE:H	1:684:A:ILE:H	13	0.19
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.19
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.19
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.19
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.19
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.19
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.19
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	7	0.19
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	7	0.19
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	7	0.19
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	7	0.19
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	7	0.19
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	9	0.19
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	9	0.19
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	9	0.19
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	6	0.19
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	6	0.19
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	6	0.19
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	6	0.19
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	6	0.19
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	6	0.19
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.19
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.19
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.19
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	6	0.19
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	3	0.19
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.19
(1,449)	1:666:A:TRP:H	1:663:A:LEU:HA	4	0.19
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	9	0.19
(1,443)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.19
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.19
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.19
(1,428)	1:701:A:VAL:HG21	1:698:A:VAL:HA	5	0.19
(1,428)	1:701:A:VAL:HG22	1:698:A:VAL:HA	5	0.19
(1,428)	1:701:A:VAL:HG23	1:698:A:VAL:HA	5	0.19
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.19
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.19
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	10	0.19
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	10	0.19
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	10	0.19
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	2	0.19
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	2	0.19
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	2	0.19
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	2	0.19
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	2	0.19
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	2	0.19
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	2	0.19
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	2	0.19
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	2	0.19
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.19
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.19
(1,359)	1:707:A:ARG:H	1:704:A:LEU:HA	12	0.19
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.19
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.19
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.19
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.19
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.19
(1,340)	1:704:A:LEU:HD11	1:707:A:ARG:HE	12	0.19
(1,340)	1:704:A:LEU:HD12	1:707:A:ARG:HE	12	0.19
(1,340)	1:704:A:LEU:HD13	1:707:A:ARG:HE	12	0.19
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	9	0.19
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	1	0.19
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	8	0.19
(1,311)	1:686:A:ILE:H	1:684:A:ILE:H	13	0.19
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.19
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.19
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.19
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.19
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.19
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.19
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	7	0.19
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	7	0.19
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	7	0.19
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	7	0.19
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	7	0.19
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	7	0.19
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	9	0.19
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	9	0.19
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	9	0.19
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	6	0.19
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	6	0.19
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	6	0.19
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	6	0.19
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	6	0.19
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	6	0.19
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.19
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.19
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.19
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	6	0.19
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	3	0.19
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.19
(1,235)	1:666:A:TRP:H	1:663:A:LEU:HA	4	0.19
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	9	0.19
(1,229)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.19
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.19
(1,214)	1:701:A:VAL:HG21	1:698:A:VAL:HA	5	0.19
(1,214)	1:701:A:VAL:HG22	1:698:A:VAL:HA	5	0.19
(1,214)	1:701:A:VAL:HG23	1:698:A:VAL:HA	5	0.19
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.19
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.19
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	10	0.19
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	10	0.19
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	10	0.19
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	2	0.19
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	2	0.19
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	2	0.19
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	2	0.19
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	2	0.19
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	2	0.19
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	2	0.19
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	2	0.19
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	2	0.19
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.19
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.19
(1,145)	1:707:A:ARG:H	1:704:A:LEU:HA	12	0.19
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.19
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.19
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.19
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.19
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.19
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.19
(1,126)	1:704:A:LEU:HD11	1:707:A:ARG:HE	12	0.19
(1,126)	1:704:A:LEU:HD12	1:707:A:ARG:HE	12	0.19
(1,126)	1:704:A:LEU:HD13	1:707:A:ARG:HE	12	0.19
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	9	0.19
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	1	0.19
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	8	0.19
(1,97)	1:686:A:ILE:H	1:684:A:ILE:H	13	0.19
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.19
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.19
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.19
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.19
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.19
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.19
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	7	0.19
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	7	0.19
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	7	0.19
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	7	0.19
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	7	0.19
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	9	0.19
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	9	0.19
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	9	0.19
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	6	0.19
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	6	0.19
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	6	0.19
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	6	0.19
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	6	0.19
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	6	0.19
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.19
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.19
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.19
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	6	0.19
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	3	0.19
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.19
(1,21)	1:666:A:TRP:H	1:663:A:LEU:HA	4	0.19
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	9	0.19
(1,15)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.19
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.19
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.19
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	5	0.18
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	5	0.18
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	5	0.18
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	5	0.18
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	5	0.18
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	5	0.18
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	5	0.18
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	5	0.18
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	5	0.18
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	1	0.18
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	4	0.18
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.18
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.18
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.18
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	14	0.18
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	14	0.18
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	14	0.18
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	14	0.18
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	14	0.18
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	11	0.18
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	11	0.18
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	11	0.18
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	15	0.18
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	15	0.18
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	15	0.18
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	15	0.18
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	15	0.18
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	15	0.18
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	15	0.18
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	15	0.18
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	15	0.18
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.18
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.18
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.18
(1,588)	1:686:A:ILE:HD11	1:685:A:PHE:H	3	0.18
(1,588)	1:686:A:ILE:HD12	1:685:A:PHE:H	3	0.18
(1,588)	1:686:A:ILE:HD13	1:685:A:PHE:H	3	0.18
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.18
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.18
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.18
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.18
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.18
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.18
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	15	0.18
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	3	0.18
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	3	0.18
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	3	0.18
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	3	0.18
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	3	0.18
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	3	0.18
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	1	0.18
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	1	0.18
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	1	0.18
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	15	0.18
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	15	0.18
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	15	0.18
(1,494)	1:676:A:THR:HG21	1:679:A:LEU:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:676:A:THR:HG22	1:679:A:LEU:H	5	0.18
(1,494)	1:676:A:THR:HG23	1:679:A:LEU:H	5	0.18
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	3	0.18
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.18
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.18
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.18
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	1	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.18
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.18
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.18
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.18
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	6	0.18
(1,453)	1:666:A:TRP:H	1:666:A:TRP:HE1	11	0.18
(1,453)	1:666:A:TRP:H	1:666:A:TRP:HE1	13	0.18
(1,449)	1:666:A:TRP:H	1:663:A:LEU:HA	1	0.18
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	8	0.18
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.18
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.18
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	15	0.18
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	15	0.18
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	15	0.18
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	15	0.18
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	15	0.18
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	15	0.18
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	15	0.18
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	15	0.18
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	15	0.18
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	15	0.18
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	15	0.18
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	1	0.18
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	4	0.18
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.18
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.18
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.18
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	14	0.18
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	14	0.18
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	14	0.18
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	14	0.18
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	14	0.18
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	14	0.18
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	11	0.18
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	11	0.18
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	11	0.18
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	15	0.18
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	15	0.18
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	15	0.18
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	15	0.18
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	15	0.18
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	15	0.18
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	15	0.18
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	15	0.18
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	15	0.18
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.18
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.18
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.18
(1,374)	1:686:A:ILE:HD11	1:685:A:PHE:H	3	0.18
(1,374)	1:686:A:ILE:HD12	1:685:A:PHE:H	3	0.18
(1,374)	1:686:A:ILE:HD13	1:685:A:PHE:H	3	0.18
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.18
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.18
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.18
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.18
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.18
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.18
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	15	0.18
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	3	0.18
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	3	0.18
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	3	0.18
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	3	0.18
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	3	0.18
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	1	0.18
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	1	0.18
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	1	0.18
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	15	0.18
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	15	0.18
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	15	0.18
(1,280)	1:676:A:THR:HG21	1:679:A:LEU:H	5	0.18
(1,280)	1:676:A:THR:HG22	1:679:A:LEU:H	5	0.18
(1,280)	1:676:A:THR:HG23	1:679:A:LEU:H	5	0.18
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	3	0.18
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.18
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.18
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.18
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	1	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.18
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.18
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.18
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.18
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	6	0.18
(1,239)	1:666:A:TRP:H	1:666:A:TRP:HE1	11	0.18
(1,239)	1:666:A:TRP:H	1:666:A:TRP:HE1	13	0.18
(1,235)	1:666:A:TRP:H	1:663:A:LEU:HA	1	0.18
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	8	0.18
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.18
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	15	0.18
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	15	0.18
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	15	0.18
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	15	0.18
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	15	0.18
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	15	0.18
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	15	0.18
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	15	0.18
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	15	0.18
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	15	0.18
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	15	0.18
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	15	0.18
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	1	0.18
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	4	0.18
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.18
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.18
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.18
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	15	0.18
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	14	0.18
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	14	0.18
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	14	0.18
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	14	0.18
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	14	0.18
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	14	0.18
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	11	0.18
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	11	0.18
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	11	0.18
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	15	0.18
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	15	0.18
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	15	0.18
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	15	0.18
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	15	0.18
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	15	0.18
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	15	0.18
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	15	0.18
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	15	0.18
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.18
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.18
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.18
(1,160)	1:686:A:ILE:HD11	1:685:A:PHE:H	3	0.18
(1,160)	1:686:A:ILE:HD12	1:685:A:PHE:H	3	0.18
(1,160)	1:686:A:ILE:HD13	1:685:A:PHE:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.18
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.18
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.18
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.18
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.18
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.18
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	15	0.18
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	3	0.18
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	3	0.18
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	3	0.18
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	3	0.18
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	3	0.18
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	3	0.18
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	1	0.18
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	1	0.18
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	1	0.18
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	15	0.18
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	15	0.18
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	15	0.18
(1,66)	1:676:A:THR:HG21	1:679:A:LEU:H	5	0.18
(1,66)	1:676:A:THR:HG22	1:679:A:LEU:H	5	0.18
(1,66)	1:676:A:THR:HG23	1:679:A:LEU:H	5	0.18
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	3	0.18
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.18
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.18
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.18
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	1	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.18
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.18
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.18
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.18
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	6	0.18
(1,25)	1:666:A:TRP:H	1:666:A:TRP:HE1	11	0.18
(1,25)	1:666:A:TRP:H	1:666:A:TRP:HE1	13	0.18
(1,21)	1:666:A:TRP:H	1:663:A:LEU:HA	1	0.18
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	8	0.18
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.18
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.18
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	15	0.18
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	15	0.18
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	15	0.18
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	15	0.18
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	15	0.18
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	15	0.18
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	15	0.18
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	15	0.18
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	15	0.18
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	15	0.18
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	15	0.18
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	15	0.18
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	2	0.17
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	2	0.17
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	2	0.17
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	11	0.17
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	11	0.17
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	11	0.17
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	2	0.17
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	2	0.17
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	2	0.17
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	11	0.17
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	11	0.17
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	11	0.17
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	2	0.17
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	2	0.17
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	2	0.17
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	11	0.17
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	11	0.17
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	11	0.17
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.17
(1,690)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.17
(1,689)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.17
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.17
(1,688)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.17
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	3	0.17
(1,632)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.17
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	15	0.17
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	15	0.17
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	15	0.17
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	15	0.17
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	15	0.17
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	15	0.17
(1,625)	1:698:A:VAL:HG11	1:695:A:LEU:HG	5	0.17
(1,625)	1:698:A:VAL:HG12	1:695:A:LEU:HG	5	0.17
(1,625)	1:698:A:VAL:HG13	1:695:A:LEU:HG	5	0.17
(1,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	5	0.17
(1,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	5	0.17
(1,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	5	0.17
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	10	0.17
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	10	0.17
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	10	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	3	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	3	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	3	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	3	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	3	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	3	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	3	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	3	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	3	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	9	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	9	0.17
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	9	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	9	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	9	0.17
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	9	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	9	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	9	0.17
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	9	0.17
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	11	0.17
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	11	0.17
(1,563)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	12	0.17
(1,563)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	12	0.17
(1,563)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	12	0.17
(1,563)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	12	0.17
(1,563)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	12	0.17
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	11	0.17
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	11	0.17
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	11	0.17
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	1	0.17
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.17
(1,485)	1:672:A:TRP:HE1	1:671:A:ASN:H	7	0.17
(1,481)	1:671:A:ASN:H	1:672:A:TRP:HE1	7	0.17
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	8	0.17
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	8	0.17
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	8	0.17
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	4	0.17
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	4	0.17
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	4	0.17
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	4	0.17
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	4	0.17
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	4	0.17
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	4	0.17
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	4	0.17
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	4	0.17
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	4	0.17
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	4	0.17
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	4	0.17
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	4	0.17
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	4	0.17
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	4	0.17
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	4	0.17
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	4	0.17
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	4	0.17
(1,462)	1:667:A:ALA:HB1	1:664:A:ASP:HA	3	0.17
(1,462)	1:667:A:ALA:HB2	1:664:A:ASP:HA	3	0.17
(1,462)	1:667:A:ALA:HB3	1:664:A:ASP:HA	3	0.17
(1,456)	1:666:A:TRP:HE1	1:662:A:GLU:H	6	0.17
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.17
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.17
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.17
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	10	0.17
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	10	0.17
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	10	0.17
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	10	0.17
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	10	0.17
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	10	0.17
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	10	0.17
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	10	0.17
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	10	0.17
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	10	0.17
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	10	0.17
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	3	0.17
(1,418)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.17
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	15	0.17
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	15	0.17
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	15	0.17
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	15	0.17
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	15	0.17
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	15	0.17
(1,411)	1:698:A:VAL:HG11	1:695:A:LEU:HG	5	0.17
(1,411)	1:698:A:VAL:HG12	1:695:A:LEU:HG	5	0.17
(1,411)	1:698:A:VAL:HG13	1:695:A:LEU:HG	5	0.17
(1,386)	1:692:A:LEU:HD11	1:689:A:VAL:HA	5	0.17
(1,386)	1:692:A:LEU:HD12	1:689:A:VAL:HA	5	0.17
(1,386)	1:692:A:LEU:HD13	1:689:A:VAL:HA	5	0.17
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	10	0.17
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	10	0.17
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	10	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	3	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	3	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	3	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	3	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	3	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	3	0.17
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	3	0.17
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	3	0.17
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	3	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	9	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	9	0.17
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	9	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	9	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	9	0.17
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	9	0.17
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	9	0.17
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	9	0.17
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	11	0.17
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	11	0.17
(1,349)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	12	0.17
(1,349)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	12	0.17
(1,349)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	12	0.17
(1,349)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	12	0.17
(1,349)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	12	0.17
(1,349)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	12	0.17
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	11	0.17
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	11	0.17
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	11	0.17
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	1	0.17
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.17
(1,271)	1:672:A:TRP:HE1	1:671:A:ASN:H	7	0.17
(1,267)	1:671:A:ASN:H	1:672:A:TRP:HE1	7	0.17
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	8	0.17
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	8	0.17
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	8	0.17
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	4	0.17
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	4	0.17
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	4	0.17
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	4	0.17
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	4	0.17
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	4	0.17
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	4	0.17
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	4	0.17
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	4	0.17
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	4	0.17
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	4	0.17
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	4	0.17
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	4	0.17
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	4	0.17
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	4	0.17
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	4	0.17
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	4	0.17
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	4	0.17
(1,248)	1:667:A:ALA:HB1	1:664:A:ASP:HA	3	0.17
(1,248)	1:667:A:ALA:HB2	1:664:A:ASP:HA	3	0.17
(1,248)	1:667:A:ALA:HB3	1:664:A:ASP:HA	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:666:A:TRP:HE1	1:662:A:GLU:H	6	0.17
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.17
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.17
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.17
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	10	0.17
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	10	0.17
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	10	0.17
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	10	0.17
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	10	0.17
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	10	0.17
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	10	0.17
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	10	0.17
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	10	0.17
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	10	0.17
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	10	0.17
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	10	0.17
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	3	0.17
(1,204)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.17
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	15	0.17
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	15	0.17
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	15	0.17
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	15	0.17
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	15	0.17
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	15	0.17
(1,197)	1:698:A:VAL:HG11	1:695:A:LEU:HG	5	0.17
(1,197)	1:698:A:VAL:HG12	1:695:A:LEU:HG	5	0.17
(1,197)	1:698:A:VAL:HG13	1:695:A:LEU:HG	5	0.17
(1,172)	1:692:A:LEU:HD11	1:689:A:VAL:HA	5	0.17
(1,172)	1:692:A:LEU:HD12	1:689:A:VAL:HA	5	0.17
(1,172)	1:692:A:LEU:HD13	1:689:A:VAL:HA	5	0.17
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	10	0.17
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	10	0.17
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	10	0.17
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	3	0.17
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	3	0.17
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	3	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	3	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	3	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	3	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	3	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	3	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	9	0.17
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	9	0.17
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	9	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	9	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	9	0.17
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	9	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	9	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	9	0.17
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	9	0.17
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	11	0.17
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	11	0.17
(1,135)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	12	0.17
(1,135)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	12	0.17
(1,135)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	12	0.17
(1,135)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	12	0.17
(1,135)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	12	0.17
(1,135)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	12	0.17
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	11	0.17
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	11	0.17
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	11	0.17
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	1	0.17
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.17
(1,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	7	0.17
(1,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	7	0.17
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	8	0.17
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	8	0.17
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	8	0.17
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	4	0.17
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	4	0.17
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	4	0.17
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	4	0.17
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	4	0.17
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	4	0.17
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	4	0.17
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	4	0.17
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	4	0.17
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	4	0.17
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	4	0.17
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	4	0.17
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	4	0.17
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	4	0.17
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	4	0.17
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	4	0.17
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	4	0.17
(1,34)	1:667:A:ALA:HB1	1:664:A:ASP:HA	3	0.17
(1,34)	1:667:A:ALA:HB2	1:664:A:ASP:HA	3	0.17
(1,34)	1:667:A:ALA:HB3	1:664:A:ASP:HA	3	0.17
(1,28)	1:666:A:TRP:HE1	1:662:A:GLU:H	6	0.17
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.17
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.17
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	15	0.17
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	10	0.17
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	10	0.17
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	10	0.17
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	10	0.17
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	10	0.17
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	10	0.17
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	10	0.17
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	10	0.17
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	10	0.17
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	10	0.17
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	10	0.17
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	10	0.17
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.16
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.16
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.16
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.16
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.16
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.16
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.16
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.16
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.16
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.16
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.16
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.16
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.16
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.16
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.16
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.16
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.16
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.16
(1,687)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	0.16
(1,687)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	0.16
(1,686)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	0.16
(1,686)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	0.16
(1,686)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	0.16
(1,685)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	0.16
(1,685)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	0.16
(1,685)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	0.16
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	8	0.16
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	8	0.16
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	8	0.16
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	8	0.16
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	8	0.16
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	8	0.16
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	10	0.16
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	10	0.16
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	10	0.16
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	10	0.16
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	10	0.16
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	10	0.16
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	10	0.16
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	10	0.16
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	10	0.16
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	6	0.16
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	6	0.16
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	6	0.16
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.16
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.16
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.16
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	1	0.16
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	1	0.16
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	1	0.16
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	1	0.16
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	1	0.16
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	1	0.16
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	1	0.16
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	1	0.16
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	1	0.16
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	9	0.16
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	9	0.16
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.16
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.16
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.16
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.16
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.16
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	9	0.16
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	9	0.16
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	9	0.16
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	9	0.16
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	9	0.16
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	9	0.16
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	11	0.16
(1,539)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	11	0.16
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	11	0.16
(1,539)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	11	0.16
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	11	0.16
(1,539)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	11	0.16
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	3	0.16
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	3	0.16
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	3	0.16
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	3	0.16
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	3	0.16
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	3	0.16
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	11	0.16
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	11	0.16
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	11	0.16
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	11	0.16
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	11	0.16
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	11	0.16
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	12	0.16
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	12	0.16
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	12	0.16
(1,488)	1:675:A:ILE:H	1:674:A:ASP:H	10	0.16
(1,488)	1:675:A:ILE:H	1:674:A:ASP:H	15	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	3	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	3	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	3	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	3	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	3	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	3	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	8	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	8	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	8	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	8	0.16
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	8	0.16
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	10	0.16
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	10	0.16
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	10	0.16
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.16
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.16
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.16
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.16
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.16
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.16
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.16
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	2	0.16
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	4	0.16
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	12	0.16
(1,449)	1:666:A:TRP:H	1:663:A:LEU:HA	15	0.16
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	1	0.16
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	15	0.16
(1,436)	1:663:A:LEU:HD11	1:667:A:ALA:H	13	0.16
(1,436)	1:663:A:LEU:HD12	1:667:A:ALA:H	13	0.16
(1,436)	1:663:A:LEU:HD13	1:667:A:ALA:H	13	0.16
(1,436)	1:663:A:LEU:HD21	1:667:A:ALA:H	13	0.16
(1,436)	1:663:A:LEU:HD22	1:667:A:ALA:H	13	0.16
(1,436)	1:663:A:LEU:HD23	1:667:A:ALA:H	13	0.16
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	8	0.16
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	8	0.16
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	8	0.16
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	8	0.16
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	8	0.16
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	8	0.16
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	10	0.16
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	10	0.16
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	10	0.16
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	10	0.16
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	10	0.16
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	10	0.16
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	10	0.16
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	10	0.16
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	10	0.16
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	6	0.16
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	6	0.16
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.16
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.16
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.16
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	1	0.16
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	1	0.16
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	1	0.16
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	1	0.16
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	1	0.16
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	1	0.16
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	1	0.16
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	1	0.16
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	1	0.16
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	9	0.16
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	9	0.16
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.16
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.16
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.16
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.16
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.16
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.16
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	9	0.16
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	9	0.16
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	9	0.16
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	9	0.16
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	9	0.16
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	9	0.16
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	11	0.16
(1,325)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	11	0.16
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	11	0.16
(1,325)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	11	0.16
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	11	0.16
(1,325)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	11	0.16
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	3	0.16
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	3	0.16
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	3	0.16
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	3	0.16
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	3	0.16
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	3	0.16
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	11	0.16
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	11	0.16
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	11	0.16
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	11	0.16
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	11	0.16
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	12	0.16
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	12	0.16
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	12	0.16
(1,274)	1:675:A:ILE:H	1:674:A:ASP:H	10	0.16
(1,274)	1:675:A:ILE:H	1:674:A:ASP:H	15	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	3	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	3	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	3	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	3	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	3	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	3	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	8	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	8	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	8	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	8	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	8	0.16
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	8	0.16
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	10	0.16
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	10	0.16
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	10	0.16
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.16
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.16
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.16
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.16
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.16
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.16
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.16
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	2	0.16
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	4	0.16
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	12	0.16
(1,235)	1:666:A:TRP:H	1:663:A:LEU:HA	15	0.16
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	1	0.16
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	15	0.16
(1,222)	1:663:A:LEU:HD11	1:667:A:ALA:H	13	0.16
(1,222)	1:663:A:LEU:HD12	1:667:A:ALA:H	13	0.16
(1,222)	1:663:A:LEU:HD13	1:667:A:ALA:H	13	0.16
(1,222)	1:663:A:LEU:HD21	1:667:A:ALA:H	13	0.16
(1,222)	1:663:A:LEU:HD22	1:667:A:ALA:H	13	0.16
(1,222)	1:663:A:LEU:HD23	1:667:A:ALA:H	13	0.16
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	8	0.16
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	8	0.16
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	8	0.16
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	8	0.16
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	8	0.16
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	10	0.16
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	10	0.16
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	10	0.16
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	10	0.16
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	10	0.16
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	10	0.16
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	10	0.16
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	10	0.16
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	10	0.16
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	6	0.16
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	6	0.16
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	6	0.16
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.16
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.16
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.16
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	1	0.16
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	1	0.16
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	1	0.16
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	1	0.16
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	1	0.16
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	1	0.16
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	1	0.16
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	1	0.16
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	1	0.16
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	9	0.16
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	9	0.16
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.16
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.16
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.16
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.16
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.16
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.16
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	9	0.16
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	9	0.16
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	9	0.16
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	9	0.16
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	9	0.16
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB2	11	0.16
(1,111)	1:702:A:LEU:HD21	1:706:A:ASN:HB3	11	0.16
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB2	11	0.16
(1,111)	1:702:A:LEU:HD22	1:706:A:ASN:HB3	11	0.16
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB2	11	0.16
(1,111)	1:702:A:LEU:HD23	1:706:A:ASN:HB3	11	0.16
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	3	0.16
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	3	0.16
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	3	0.16
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	3	0.16
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	3	0.16
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	3	0.16
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	11	0.16
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	11	0.16
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	11	0.16
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	11	0.16
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	11	0.16
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	11	0.16
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	12	0.16
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	12	0.16
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	12	0.16
(1,60)	1:675:A:ILE:H	1:674:A:ASP:H	10	0.16
(1,60)	1:675:A:ILE:H	1:674:A:ASP:H	15	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	3	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	3	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	3	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	3	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	3	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	3	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	8	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	8	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	8	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	8	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	8	0.16
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	8	0.16
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	10	0.16
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	10	0.16
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	10	0.16
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.16
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.16
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.16
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.16
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.16
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.16
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	2	0.16
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	4	0.16
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	12	0.16
(1,21)	1:666:A:TRP:H	1:663:A:LEU:HA	15	0.16
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	1	0.16
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	15	0.16
(1,8)	1:663:A:LEU:HD11	1:667:A:ALA:H	13	0.16
(1,8)	1:663:A:LEU:HD12	1:667:A:ALA:H	13	0.16
(1,8)	1:663:A:LEU:HD13	1:667:A:ALA:H	13	0.16
(1,8)	1:663:A:LEU:HD21	1:667:A:ALA:H	13	0.16
(1,8)	1:663:A:LEU:HD22	1:667:A:ALA:H	13	0.16
(1,8)	1:663:A:LEU:HD23	1:667:A:ALA:H	13	0.16
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	9	0.15
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	9	0.15
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	9	0.15
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	9	0.15
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	9	0.15
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	9	0.15
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	9	0.15
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	9	0.15
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	9	0.15
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	9	0.15
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	9	0.15
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	9	0.15
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	9	0.15
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	9	0.15
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	9	0.15
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	9	0.15
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	9	0.15
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	9	0.15
(1,638)	1:701:A:VAL:H	1:698:A:VAL:HA	2	0.15
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	2	0.15
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	2	0.15
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	2	0.15
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	2	0.15
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	2	0.15
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	2	0.15
(1,626)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	9	0.15
(1,626)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	9	0.15
(1,626)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	9	0.15
(1,626)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	9	0.15
(1,626)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	9	0.15
(1,615)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.15
(1,615)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.15
(1,615)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.15
(1,612)	1:695:A:LEU:H	1:694:A:GLY:H	7	0.15
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.15
(1,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.15
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.15
(1,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.15
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.15
(1,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.15
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	5	0.15
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	5	0.15
(1,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	5	0.15
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	5	0.15
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	5	0.15
(1,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	5	0.15
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	5	0.15
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	5	0.15
(1,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	5	0.15
(1,587)	1:686:A:ILE:HD11	1:683:A:ARG:HA	1	0.15
(1,587)	1:686:A:ILE:HD12	1:683:A:ARG:HA	1	0.15
(1,587)	1:686:A:ILE:HD13	1:683:A:ARG:HA	1	0.15
(1,587)	1:686:A:ILE:HD11	1:683:A:ARG:HA	2	0.15
(1,587)	1:686:A:ILE:HD12	1:683:A:ARG:HA	2	0.15
(1,587)	1:686:A:ILE:HD13	1:683:A:ARG:HA	2	0.15
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	4	0.15
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	4	0.15
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	2	0.15
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	12	0.15
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	4	0.15
(1,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	4	0.15
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	4	0.15
(1,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	4	0.15
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	4	0.15
(1,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	4	0.15
(1,508)	1:682:A:ILE:HG21	1:679:A:LEU:H	11	0.15
(1,508)	1:682:A:ILE:HG22	1:679:A:LEU:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:682:A:ILE:HG23	1:679:A:LEU:H	11	0.15
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	7	0.15
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	7	0.15
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	7	0.15
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	7	0.15
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	7	0.15
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	7	0.15
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	12	0.15
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	12	0.15
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	12	0.15
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	12	0.15
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	12	0.15
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	12	0.15
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.15
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.15
(1,499)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.15
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	3	0.15
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	3	0.15
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	3	0.15
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	2	0.15
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	2	0.15
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	2	0.15
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	3	0.15
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	3	0.15
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	3	0.15
(1,488)	1:675:A:ILE:H	1:674:A:ASP:H	1	0.15
(1,488)	1:675:A:ILE:H	1:674:A:ASP:H	5	0.15
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	4	0.15
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	10	0.15
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	4	0.15
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	4	0.15
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	4	0.15
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	14	0.15
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	14	0.15
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	14	0.15
(1,462)	1:667:A:ALA:HB1	1:664:A:ASP:HA	1	0.15
(1,462)	1:667:A:ALA:HB2	1:664:A:ASP:HA	1	0.15
(1,462)	1:667:A:ALA:HB3	1:664:A:ASP:HA	1	0.15
(1,462)	1:667:A:ALA:HB1	1:664:A:ASP:HA	5	0.15
(1,462)	1:667:A:ALA:HB2	1:664:A:ASP:HA	5	0.15
(1,462)	1:667:A:ALA:HB3	1:664:A:ASP:HA	5	0.15
(1,443)	1:665:A:LYS:H	1:662:A:GLU:HA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.15
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.15
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.15
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.15
(1,424)	1:701:A:VAL:H	1:698:A:VAL:HA	2	0.15
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	2	0.15
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	2	0.15
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	2	0.15
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	2	0.15
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	2	0.15
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	2	0.15
(1,412)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	9	0.15
(1,412)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	9	0.15
(1,412)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	9	0.15
(1,412)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	9	0.15
(1,412)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	9	0.15
(1,412)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	9	0.15
(1,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.15
(1,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.15
(1,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.15
(1,398)	1:695:A:LEU:H	1:694:A:GLY:H	7	0.15
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.15
(1,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.15
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.15
(1,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.15
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.15
(1,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.15
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	5	0.15
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	5	0.15
(1,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	5	0.15
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	5	0.15
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	5	0.15
(1,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	5	0.15
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	5	0.15
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	5	0.15
(1,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	5	0.15
(1,373)	1:686:A:ILE:HD11	1:683:A:ARG:HA	1	0.15
(1,373)	1:686:A:ILE:HD12	1:683:A:ARG:HA	1	0.15
(1,373)	1:686:A:ILE:HD13	1:683:A:ARG:HA	1	0.15
(1,373)	1:686:A:ILE:HD11	1:683:A:ARG:HA	2	0.15
(1,373)	1:686:A:ILE:HD12	1:683:A:ARG:HA	2	0.15
(1,373)	1:686:A:ILE:HD13	1:683:A:ARG:HA	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	4	0.15
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	4	0.15
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	2	0.15
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	12	0.15
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	4	0.15
(1,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	4	0.15
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	4	0.15
(1,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	4	0.15
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	4	0.15
(1,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	4	0.15
(1,294)	1:682:A:ILE:HG21	1:679:A:LEU:H	11	0.15
(1,294)	1:682:A:ILE:HG22	1:679:A:LEU:H	11	0.15
(1,294)	1:682:A:ILE:HG23	1:679:A:LEU:H	11	0.15
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	7	0.15
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	7	0.15
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	7	0.15
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	7	0.15
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	7	0.15
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	7	0.15
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	12	0.15
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	12	0.15
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	12	0.15
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	12	0.15
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	12	0.15
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	12	0.15
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.15
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.15
(1,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.15
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	3	0.15
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	3	0.15
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	3	0.15
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	2	0.15
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	2	0.15
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	2	0.15
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	3	0.15
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	3	0.15
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	3	0.15
(1,274)	1:675:A:ILE:H	1:674:A:ASP:H	1	0.15
(1,274)	1:675:A:ILE:H	1:674:A:ASP:H	5	0.15
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	4	0.15
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	10	0.15
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	4	0.15
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	4	0.15
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	14	0.15
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	14	0.15
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	14	0.15
(1,248)	1:667:A:ALA:HB1	1:664:A:ASP:HA	1	0.15
(1,248)	1:667:A:ALA:HB2	1:664:A:ASP:HA	1	0.15
(1,248)	1:667:A:ALA:HB3	1:664:A:ASP:HA	1	0.15
(1,248)	1:667:A:ALA:HB1	1:664:A:ASP:HA	5	0.15
(1,248)	1:667:A:ALA:HB2	1:664:A:ASP:HA	5	0.15
(1,248)	1:667:A:ALA:HB3	1:664:A:ASP:HA	5	0.15
(1,229)	1:665:A:LYS:H	1:662:A:GLU:HA	8	0.15
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.15
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.15
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.15
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.15
(1,210)	1:701:A:VAL:H	1:698:A:VAL:HA	2	0.15
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	2	0.15
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	2	0.15
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	2	0.15
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	2	0.15
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	2	0.15
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	2	0.15
(1,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	9	0.15
(1,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	9	0.15
(1,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	9	0.15
(1,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	9	0.15
(1,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	9	0.15
(1,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	9	0.15
(1,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.15
(1,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.15
(1,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.15
(1,184)	1:695:A:LEU:H	1:694:A:GLY:H	7	0.15
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.15
(1,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.15
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.15
(1,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.15
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.15
(1,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.15
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	5	0.15
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	5	0.15
(1,165)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	5	0.15
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	5	0.15
(1,165)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	5	0.15
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	5	0.15
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	5	0.15
(1,165)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	5	0.15
(1,159)	1:686:A:ILE:HD11	1:683:A:ARG:HA	1	0.15
(1,159)	1:686:A:ILE:HD12	1:683:A:ARG:HA	1	0.15
(1,159)	1:686:A:ILE:HD13	1:683:A:ARG:HA	1	0.15
(1,159)	1:686:A:ILE:HD11	1:683:A:ARG:HA	2	0.15
(1,159)	1:686:A:ILE:HD12	1:683:A:ARG:HA	2	0.15
(1,159)	1:686:A:ILE:HD13	1:683:A:ARG:HA	2	0.15
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	4	0.15
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	4	0.15
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	2	0.15
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	12	0.15
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	4	0.15
(1,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	4	0.15
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	4	0.15
(1,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	4	0.15
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	4	0.15
(1,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	4	0.15
(1,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	11	0.15
(1,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	11	0.15
(1,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	11	0.15
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	7	0.15
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	7	0.15
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	7	0.15
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	7	0.15
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	7	0.15
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	7	0.15
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	12	0.15
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	12	0.15
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	12	0.15
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	12	0.15
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	12	0.15
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	12	0.15
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.15
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.15
(1,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.15
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	3	0.15
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	3	0.15
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	2	0.15
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	2	0.15
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	2	0.15
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	3	0.15
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	3	0.15
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	3	0.15
(1,60)	1:675:A:ILE:H	1:674:A:ASP:H	1	0.15
(1,60)	1:675:A:ILE:H	1:674:A:ASP:H	5	0.15
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	4	0.15
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	10	0.15
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	4	0.15
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	4	0.15
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	4	0.15
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	14	0.15
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	14	0.15
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	14	0.15
(1,34)	1:667:A:ALA:HB1	1:664:A:ASP:HA	1	0.15
(1,34)	1:667:A:ALA:HB2	1:664:A:ASP:HA	1	0.15
(1,34)	1:667:A:ALA:HB3	1:664:A:ASP:HA	1	0.15
(1,34)	1:667:A:ALA:HB1	1:664:A:ASP:HA	5	0.15
(1,34)	1:667:A:ALA:HB2	1:664:A:ASP:HA	5	0.15
(1,34)	1:667:A:ALA:HB3	1:664:A:ASP:HA	5	0.15
(1,15)	1:665:A:LYS:H	1:662:A:GLU:HA	8	0.15
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.15
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.15
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.15
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.15
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	4	0.14
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	4	0.14
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	4	0.14
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	4	0.14
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	4	0.14
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	4	0.14
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	4	0.14
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	4	0.14
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	4	0.14
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	4	0.14
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	4	0.14
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	4	0.14
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	4	0.14
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	4	0.14
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	4	0.14
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	4	0.14
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	4	0.14
(1,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	3	0.14
(1,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	3	0.14
(1,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	3	0.14
(1,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	5	0.14
(1,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	5	0.14
(1,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	5	0.14
(1,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	5	0.14
(1,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	5	0.14
(1,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	5	0.14
(1,618)	1:696:A:ARG:H	1:693:A:ILE:HA	4	0.14
(1,612)	1:695:A:LEU:H	1:694:A:GLY:H	12	0.14
(1,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.14
(1,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.14
(1,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.14
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.14
(1,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.14
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.14
(1,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.14
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.14
(1,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.14
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	1	0.14
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	1	0.14
(1,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	1	0.14
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	1	0.14
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	1	0.14
(1,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	1	0.14
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	1	0.14
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	1	0.14
(1,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	1	0.14
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	4	0.14
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	7	0.14
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	15	0.14
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	15	0.14
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	15	0.14
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	15	0.14
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	15	0.14
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	15	0.14
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	7	0.14
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	7	0.14
(1,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	7	0.14
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	7	0.14
(1,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	7	0.14
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	8	0.14
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	8	0.14
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	8	0.14
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	8	0.14
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	8	0.14
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	8	0.14
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	13	0.14
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	13	0.14
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	13	0.14
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	13	0.14
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	13	0.14
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	13	0.14
(1,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	3	0.14
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	7	0.14
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	7	0.14
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	7	0.14
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	12	0.14
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	14	0.14
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	14	0.14
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	14	0.14
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	14	0.14
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	14	0.14
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	14	0.14
(1,464)	1:668:A:SER:H	1:665:A:LYS:HA	3	0.14
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	7	0.14
(1,453)	1:666:A:TRP:H	1:666:A:TRP:HE1	12	0.14
(1,450)	1:666:A:TRP:H	1:665:A:LYS:HA	13	0.14
(1,449)	1:666:A:TRP:H	1:663:A:LEU:HA	5	0.14
(1,449)	1:666:A:TRP:H	1:663:A:LEU:HA	9	0.14
(1,449)	1:666:A:TRP:H	1:663:A:LEU:HA	12	0.14
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.14
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	7	0.14
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	10	0.14
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	1	0.14
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	1	0.14
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	1	0.14
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	1	0.14
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	1	0.14
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	1	0.14
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	1	0.14
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	1	0.14
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	1	0.14
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	1	0.14
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	1	0.14
(1,427)	1:701:A:VAL:HG11	1:698:A:VAL:HA	3	0.14
(1,427)	1:701:A:VAL:HG12	1:698:A:VAL:HA	3	0.14
(1,427)	1:701:A:VAL:HG13	1:698:A:VAL:HA	3	0.14
(1,407)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	5	0.14
(1,407)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	5	0.14
(1,407)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	5	0.14
(1,407)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	5	0.14
(1,407)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	5	0.14
(1,407)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	5	0.14
(1,404)	1:696:A:ARG:H	1:693:A:ILE:HA	4	0.14
(1,398)	1:695:A:LEU:H	1:694:A:GLY:H	12	0.14
(1,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.14
(1,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.14
(1,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.14
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.14
(1,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.14
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.14
(1,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.14
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.14
(1,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.14
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	1	0.14
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	1	0.14
(1,341)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	1	0.14
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	1	0.14
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	1	0.14
(1,341)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	1	0.14
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	1	0.14
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	1	0.14
(1,341)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	1	0.14
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	4	0.14
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	7	0.14
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	15	0.14
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	15	0.14
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	15	0.14
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	15	0.14
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	15	0.14
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	7	0.14
(1,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	7	0.14
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	7	0.14
(1,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	7	0.14
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	7	0.14
(1,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	7	0.14
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	8	0.14
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	8	0.14
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	8	0.14
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	8	0.14
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	8	0.14
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	8	0.14
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	13	0.14
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	13	0.14
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	13	0.14
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	13	0.14
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	13	0.14
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	13	0.14
(1,287)	1:678:A:TRP:HE1	1:682:A:ILE:H	3	0.14
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	7	0.14
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	7	0.14
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	7	0.14
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	12	0.14
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	14	0.14
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	14	0.14
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	14	0.14
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	14	0.14
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	14	0.14
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	14	0.14
(1,250)	1:668:A:SER:H	1:665:A:LYS:HA	3	0.14
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	7	0.14
(1,239)	1:666:A:TRP:H	1:666:A:TRP:HE1	12	0.14
(1,236)	1:666:A:TRP:H	1:665:A:LYS:HA	13	0.14
(1,235)	1:666:A:TRP:H	1:663:A:LEU:HA	5	0.14
(1,235)	1:666:A:TRP:H	1:663:A:LEU:HA	9	0.14
(1,235)	1:666:A:TRP:H	1:663:A:LEU:HA	12	0.14
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.14
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	7	0.14
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	1	0.14
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	1	0.14
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	1	0.14
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	1	0.14
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	1	0.14
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	1	0.14
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	1	0.14
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	1	0.14
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	1	0.14
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	1	0.14
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	1	0.14
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	1	0.14
(1,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	3	0.14
(1,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	3	0.14
(1,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	3	0.14
(1,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	5	0.14
(1,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	5	0.14
(1,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	5	0.14
(1,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	5	0.14
(1,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	5	0.14
(1,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	5	0.14
(1,190)	1:696:A:ARG:H	1:693:A:ILE:HA	4	0.14
(1,184)	1:695:A:LEU:H	1:694:A:GLY:H	12	0.14
(1,164)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.14
(1,164)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.14
(1,164)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.14
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.14
(1,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.14
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.14
(1,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.14
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.14
(1,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.14
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	1	0.14
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	1	0.14
(1,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	1	0.14
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	1	0.14
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	1	0.14
(1,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	1	0.14
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	1	0.14
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	1	0.14
(1,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	1	0.14
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	7	0.14
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	15	0.14
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	15	0.14
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	15	0.14
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	15	0.14
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	15	0.14
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	15	0.14
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	7	0.14
(1,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	7	0.14
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	7	0.14
(1,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	7	0.14
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	7	0.14
(1,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	7	0.14
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	8	0.14
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	8	0.14
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	8	0.14
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	8	0.14
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	8	0.14
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	8	0.14
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	13	0.14
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	13	0.14
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	13	0.14
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	13	0.14
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	13	0.14
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	13	0.14
(1,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	3	0.14
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	7	0.14
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	7	0.14
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	7	0.14
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	12	0.14
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	14	0.14
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	14	0.14
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	14	0.14
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	14	0.14
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	14	0.14
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	14	0.14
(1,36)	1:668:A:SER:H	1:665:A:LYS:HA	3	0.14
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	7	0.14
(1,25)	1:666:A:TRP:H	1:666:A:TRP:HE1	12	0.14
(1,22)	1:666:A:TRP:H	1:665:A:LYS:HA	13	0.14
(1,21)	1:666:A:TRP:H	1:663:A:LEU:HA	5	0.14
(1,21)	1:666:A:TRP:H	1:663:A:LEU:HA	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:666:A:TRP:H	1:663:A:LEU:HA	12	0.14
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.14
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	7	0.14
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	10	0.14
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	1	0.14
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	1	0.14
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	1	0.14
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	1	0.14
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	1	0.14
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	1	0.14
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	1	0.14
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	1	0.14
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	1	0.14
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	1	0.14
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	1	0.14
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	1	0.14
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	10	0.13
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	10	0.13
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	10	0.13
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	10	0.13
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	10	0.13
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	10	0.13
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	10	0.13
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	10	0.13
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	10	0.13
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	10	0.13
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	10	0.13
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	10	0.13
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	10	0.13
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	10	0.13
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	10	0.13
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	10	0.13
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	10	0.13
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	10	0.13
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD11	12	0.13
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD12	12	0.13
(1,702)	1:696:A:ARG:H	1:693:A:ILE:HD13	12	0.13
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD11	12	0.13
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD12	12	0.13
(1,701)	1:696:A:ARG:H	1:693:A:ILE:HD13	12	0.13
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD11	12	0.13
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD12	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:696:A:ARG:H	1:693:A:ILE:HD13	12	0.13
(1,625)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.13
(1,625)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.13
(1,625)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.13
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	13	0.13
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	13	0.13
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	13	0.13
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	13	0.13
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	13	0.13
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	13	0.13
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	13	0.13
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	13	0.13
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	13	0.13
(1,618)	1:696:A:ARG:H	1:693:A:ILE:HA	2	0.13
(1,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	6	0.13
(1,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	6	0.13
(1,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	6	0.13
(1,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	6	0.13
(1,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	6	0.13
(1,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	6	0.13
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.13
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.13
(1,565)	1:705:A:VAL:HG21	1:702:A:LEU:HG	12	0.13
(1,565)	1:705:A:VAL:HG22	1:702:A:LEU:HG	12	0.13
(1,565)	1:705:A:VAL:HG23	1:702:A:LEU:HG	12	0.13
(1,563)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	5	0.13
(1,563)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	5	0.13
(1,563)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	5	0.13
(1,563)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	5	0.13
(1,563)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	5	0.13
(1,563)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	5	0.13
(1,546)	1:704:A:LEU:H	1:703:A:SER:HA	15	0.13
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	2	0.13
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	2	0.13
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	2	0.13
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	2	0.13
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	2	0.13
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	2	0.13
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	8	0.13
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	8	0.13
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	8	0.13
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	8	0.13
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	8	0.13
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	7	0.13
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	15	0.13
(1,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.13
(1,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.13
(1,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.13
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	7	0.13
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	7	0.13
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	7	0.13
(1,502)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	2	0.13
(1,502)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	2	0.13
(1,502)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	2	0.13
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	5	0.13
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	5	0.13
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	5	0.13
(1,492)	1:676:A:THR:HG21	1:669:A:LEU:HA	6	0.13
(1,492)	1:676:A:THR:HG22	1:669:A:LEU:HA	6	0.13
(1,492)	1:676:A:THR:HG23	1:669:A:LEU:HA	6	0.13
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	12	0.13
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	12	0.13
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	12	0.13
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	9	0.13
(1,462)	1:667:A:ALA:HB1	1:664:A:ASP:HA	4	0.13
(1,462)	1:667:A:ALA:HB2	1:664:A:ASP:HA	4	0.13
(1,462)	1:667:A:ALA:HB3	1:664:A:ASP:HA	4	0.13
(1,439)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.13
(1,411)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.13
(1,411)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.13
(1,411)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.13
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	13	0.13
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	13	0.13
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	13	0.13
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	13	0.13
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	13	0.13
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	13	0.13
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	13	0.13
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	13	0.13
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	13	0.13
(1,404)	1:696:A:ARG:H	1:693:A:ILE:HA	2	0.13
(1,386)	1:692:A:LEU:HD11	1:689:A:VAL:HA	6	0.13
(1,386)	1:692:A:LEU:HD12	1:689:A:VAL:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:692:A:LEU:HD13	1:689:A:VAL:HA	6	0.13
(1,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	6	0.13
(1,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	6	0.13
(1,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	6	0.13
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.13
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.13
(1,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	12	0.13
(1,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	12	0.13
(1,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	12	0.13
(1,349)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	5	0.13
(1,349)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	5	0.13
(1,349)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	5	0.13
(1,349)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	5	0.13
(1,349)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	5	0.13
(1,349)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	5	0.13
(1,332)	1:704:A:LEU:H	1:703:A:SER:HA	15	0.13
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	2	0.13
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	2	0.13
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	2	0.13
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	2	0.13
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	2	0.13
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	2	0.13
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	8	0.13
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	8	0.13
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	8	0.13
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	8	0.13
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	8	0.13
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	8	0.13
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	7	0.13
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	15	0.13
(1,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.13
(1,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.13
(1,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.13
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	7	0.13
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	7	0.13
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	7	0.13
(1,288)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	2	0.13
(1,288)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	2	0.13
(1,288)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	2	0.13
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	5	0.13
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	5	0.13
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:676:A:THR:HG21	1:669:A:LEU:HA	6	0.13
(1,278)	1:676:A:THR:HG22	1:669:A:LEU:HA	6	0.13
(1,278)	1:676:A:THR:HG23	1:669:A:LEU:HA	6	0.13
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	12	0.13
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	12	0.13
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	12	0.13
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	9	0.13
(1,248)	1:667:A:ALA:HB1	1:664:A:ASP:HA	4	0.13
(1,248)	1:667:A:ALA:HB2	1:664:A:ASP:HA	4	0.13
(1,248)	1:667:A:ALA:HB3	1:664:A:ASP:HA	4	0.13
(1,225)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.13
(1,197)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.13
(1,197)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.13
(1,197)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.13
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	13	0.13
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	13	0.13
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	13	0.13
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	13	0.13
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	13	0.13
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	13	0.13
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	13	0.13
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	13	0.13
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	13	0.13
(1,190)	1:696:A:ARG:H	1:693:A:ILE:HA	2	0.13
(1,172)	1:692:A:LEU:HD11	1:689:A:VAL:HA	6	0.13
(1,172)	1:692:A:LEU:HD12	1:689:A:VAL:HA	6	0.13
(1,172)	1:692:A:LEU:HD13	1:689:A:VAL:HA	6	0.13
(1,164)	1:687:A:ILE:HG21	1:691:A:SER:HG	6	0.13
(1,164)	1:687:A:ILE:HG22	1:691:A:SER:HG	6	0.13
(1,164)	1:687:A:ILE:HG23	1:691:A:SER:HG	6	0.13
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.13
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.13
(1,137)	1:705:A:VAL:HG21	1:702:A:LEU:HG	12	0.13
(1,137)	1:705:A:VAL:HG22	1:702:A:LEU:HG	12	0.13
(1,137)	1:705:A:VAL:HG23	1:702:A:LEU:HG	12	0.13
(1,135)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	5	0.13
(1,135)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	5	0.13
(1,135)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	5	0.13
(1,135)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	5	0.13
(1,135)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	5	0.13
(1,135)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	5	0.13
(1,118)	1:704:A:LEU:H	1:703:A:SER:HA	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	2	0.13
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	2	0.13
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	2	0.13
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	2	0.13
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	2	0.13
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	2	0.13
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	8	0.13
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	8	0.13
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	8	0.13
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	8	0.13
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	8	0.13
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	8	0.13
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	7	0.13
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	15	0.13
(1,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.13
(1,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.13
(1,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.13
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	7	0.13
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	7	0.13
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	7	0.13
(1,74)	1:679:A:LEU:HD11	1:666:A:TRP:HZ3	2	0.13
(1,74)	1:679:A:LEU:HD12	1:666:A:TRP:HZ3	2	0.13
(1,74)	1:679:A:LEU:HD13	1:666:A:TRP:HZ3	2	0.13
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	5	0.13
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	5	0.13
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	5	0.13
(1,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	6	0.13
(1,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	6	0.13
(1,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	6	0.13
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	12	0.13
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	12	0.13
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	12	0.13
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	9	0.13
(1,34)	1:667:A:ALA:HB1	1:664:A:ASP:HA	4	0.13
(1,34)	1:667:A:ALA:HB2	1:664:A:ASP:HA	4	0.13
(1,34)	1:667:A:ALA:HB3	1:664:A:ASP:HA	4	0.13
(1,11)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.13
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	11	0.12
(1,708)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	11	0.12
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	11	0.12
(1,708)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	11	0.12
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	11	0.12
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	11	0.12
(1,707)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	11	0.12
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	11	0.12
(1,707)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	11	0.12
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	11	0.12
(1,707)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	11	0.12
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	11	0.12
(1,706)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	11	0.12
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	11	0.12
(1,706)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	11	0.12
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	11	0.12
(1,706)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	11	0.12
(1,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	12	0.12
(1,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	12	0.12
(1,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	12	0.12
(1,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	8	0.12
(1,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	8	0.12
(1,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	8	0.12
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	7	0.12
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	7	0.12
(1,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	7	0.12
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	7	0.12
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	7	0.12
(1,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	7	0.12
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	7	0.12
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	7	0.12
(1,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	7	0.12
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	9	0.12
(1,620)	1:696:A:ARG:H	1:696:A:ARG:HE	10	0.12
(1,618)	1:696:A:ARG:H	1:693:A:ILE:HA	7	0.12
(1,616)	1:695:A:LEU:HD21	1:698:A:VAL:H	6	0.12
(1,616)	1:695:A:LEU:HD22	1:698:A:VAL:H	6	0.12
(1,616)	1:695:A:LEU:HD23	1:698:A:VAL:H	6	0.12
(1,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	9	0.12
(1,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	9	0.12
(1,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	9	0.12
(1,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	14	0.12
(1,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	14	0.12
(1,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	14	0.12
(1,588)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.12
(1,588)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.12
(1,582)	1:708:A:VAL:H	1:707:A:ARG:HA	10	0.12
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	11	0.12
(1,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	11	0.12
(1,563)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	3	0.12
(1,563)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	3	0.12
(1,563)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	3	0.12
(1,563)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	3	0.12
(1,563)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	3	0.12
(1,563)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	3	0.12
(1,541)	1:703:A:SER:H	1:700:A:ALA:HA	9	0.12
(1,540)	1:702:A:LEU:HD21	1:706:A:ASN:HD21	7	0.12
(1,540)	1:702:A:LEU:HD21	1:706:A:ASN:HD22	7	0.12
(1,540)	1:702:A:LEU:HD22	1:706:A:ASN:HD21	7	0.12
(1,540)	1:702:A:LEU:HD22	1:706:A:ASN:HD22	7	0.12
(1,540)	1:702:A:LEU:HD23	1:706:A:ASN:HD21	7	0.12
(1,540)	1:702:A:LEU:HD23	1:706:A:ASN:HD22	7	0.12
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.12
(1,524)	1:685:A:PHE:H	1:686:A:ILE:H	13	0.12
(1,522)	1:684:A:ILE:HG21	1:688:A:ILE:H	12	0.12
(1,522)	1:684:A:ILE:HG22	1:688:A:ILE:H	12	0.12
(1,522)	1:684:A:ILE:HG23	1:688:A:ILE:H	12	0.12
(1,507)	1:681:A:TYR:H	1:682:A:ILE:H	4	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	2	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	2	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	2	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	3	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	3	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	3	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	9	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	9	0.12
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	9	0.12
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	10	0.12
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	10	0.12
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	10	0.12
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	10	0.12
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	10	0.12
(1,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	10	0.12
(1,494)	1:676:A:THR:HG21	1:679:A:LEU:H	10	0.12
(1,494)	1:676:A:THR:HG22	1:679:A:LEU:H	10	0.12
(1,494)	1:676:A:THR:HG23	1:679:A:LEU:H	10	0.12
(1,492)	1:676:A:THR:HG21	1:669:A:LEU:HA	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:676:A:THR:HG22	1:669:A:LEU:HA	14	0.12
(1,492)	1:676:A:THR:HG23	1:669:A:LEU:HA	14	0.12
(1,488)	1:675:A:ILE:H	1:674:A:ASP:H	6	0.12
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	9	0.12
(1,487)	1:674:A:ASP:H	1:677:A:ASN:H	13	0.12
(1,485)	1:672:A:TRP:HE1	1:671:A:ASN:H	2	0.12
(1,481)	1:671:A:ASN:H	1:672:A:TRP:HE1	2	0.12
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.12
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.12
(1,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.12
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	11	0.12
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.12
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.12
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.12
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.12
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.12
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.12
(1,468)	1:669:A:LEU:H	1:666:A:TRP:HA	12	0.12
(1,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.12
(1,457)	1:667:A:ALA:H	1:664:A:ASP:HA	14	0.12
(1,456)	1:666:A:TRP:HE1	1:662:A:GLU:H	1	0.12
(1,456)	1:666:A:TRP:HE1	1:662:A:GLU:H	15	0.12
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	4	0.12
(1,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	5	0.12
(1,428)	1:701:A:VAL:HG21	1:698:A:VAL:HA	12	0.12
(1,428)	1:701:A:VAL:HG22	1:698:A:VAL:HA	12	0.12
(1,428)	1:701:A:VAL:HG23	1:698:A:VAL:HA	12	0.12
(1,427)	1:701:A:VAL:HG11	1:698:A:VAL:HA	8	0.12
(1,427)	1:701:A:VAL:HG12	1:698:A:VAL:HA	8	0.12
(1,427)	1:701:A:VAL:HG13	1:698:A:VAL:HA	8	0.12
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	7	0.12
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	7	0.12
(1,409)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	7	0.12
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	7	0.12
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	7	0.12
(1,409)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	7	0.12
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	7	0.12
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	7	0.12
(1,409)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	7	0.12
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	9	0.12
(1,406)	1:696:A:ARG:H	1:696:A:ARG:HE	10	0.12
(1,404)	1:696:A:ARG:H	1:693:A:ILE:HA	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:695:A:LEU:HD21	1:698:A:VAL:H	6	0.12
(1,402)	1:695:A:LEU:HD22	1:698:A:VAL:H	6	0.12
(1,402)	1:695:A:LEU:HD23	1:698:A:VAL:H	6	0.12
(1,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	9	0.12
(1,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	9	0.12
(1,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	9	0.12
(1,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	14	0.12
(1,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	14	0.12
(1,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	14	0.12
(1,374)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.12
(1,374)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.12
(1,374)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.12
(1,368)	1:708:A:VAL:H	1:707:A:ARG:HA	10	0.12
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	11	0.12
(1,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	11	0.12
(1,349)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	3	0.12
(1,349)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	3	0.12
(1,349)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	3	0.12
(1,349)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	3	0.12
(1,349)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	3	0.12
(1,349)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	3	0.12
(1,327)	1:703:A:SER:H	1:700:A:ALA:HA	9	0.12
(1,326)	1:702:A:LEU:HD21	1:706:A:ASN:HD21	7	0.12
(1,326)	1:702:A:LEU:HD21	1:706:A:ASN:HD22	7	0.12
(1,326)	1:702:A:LEU:HD22	1:706:A:ASN:HD21	7	0.12
(1,326)	1:702:A:LEU:HD22	1:706:A:ASN:HD22	7	0.12
(1,326)	1:702:A:LEU:HD23	1:706:A:ASN:HD21	7	0.12
(1,326)	1:702:A:LEU:HD23	1:706:A:ASN:HD22	7	0.12
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.12
(1,310)	1:685:A:PHE:H	1:686:A:ILE:H	13	0.12
(1,308)	1:684:A:ILE:HG21	1:688:A:ILE:H	12	0.12
(1,308)	1:684:A:ILE:HG22	1:688:A:ILE:H	12	0.12
(1,308)	1:684:A:ILE:HG23	1:688:A:ILE:H	12	0.12
(1,293)	1:681:A:TYR:H	1:682:A:ILE:H	4	0.12
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	2	0.12
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	2	0.12
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	2	0.12
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	3	0.12
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	3	0.12
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	3	0.12
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	9	0.12
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	9	0.12
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	10	0.12
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	10	0.12
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	10	0.12
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	10	0.12
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	10	0.12
(1,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	10	0.12
(1,280)	1:676:A:THR:HG21	1:679:A:LEU:H	10	0.12
(1,280)	1:676:A:THR:HG22	1:679:A:LEU:H	10	0.12
(1,280)	1:676:A:THR:HG23	1:679:A:LEU:H	10	0.12
(1,278)	1:676:A:THR:HG21	1:669:A:LEU:HA	14	0.12
(1,278)	1:676:A:THR:HG22	1:669:A:LEU:HA	14	0.12
(1,278)	1:676:A:THR:HG23	1:669:A:LEU:HA	14	0.12
(1,274)	1:675:A:ILE:H	1:674:A:ASP:H	6	0.12
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	9	0.12
(1,273)	1:674:A:ASP:H	1:677:A:ASN:H	13	0.12
(1,271)	1:672:A:TRP:HE1	1:671:A:ASN:H	2	0.12
(1,267)	1:671:A:ASN:H	1:672:A:TRP:HE1	2	0.12
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.12
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.12
(1,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.12
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	11	0.12
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.12
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.12
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.12
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.12
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.12
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.12
(1,254)	1:669:A:LEU:H	1:666:A:TRP:HA	12	0.12
(1,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.12
(1,243)	1:667:A:ALA:H	1:664:A:ASP:HA	14	0.12
(1,242)	1:666:A:TRP:HE1	1:662:A:GLU:H	1	0.12
(1,242)	1:666:A:TRP:HE1	1:662:A:GLU:H	15	0.12
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	4	0.12
(1,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	5	0.12
(1,214)	1:701:A:VAL:HG21	1:698:A:VAL:HA	12	0.12
(1,214)	1:701:A:VAL:HG22	1:698:A:VAL:HA	12	0.12
(1,214)	1:701:A:VAL:HG23	1:698:A:VAL:HA	12	0.12
(1,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	8	0.12
(1,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	8	0.12
(1,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	8	0.12
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	7	0.12
(1,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	7	0.12
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	7	0.12
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	7	0.12
(1,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	7	0.12
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	7	0.12
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	7	0.12
(1,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	7	0.12
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	9	0.12
(1,192)	1:696:A:ARG:H	1:696:A:ARG:HE	10	0.12
(1,190)	1:696:A:ARG:H	1:693:A:ILE:HA	7	0.12
(1,188)	1:695:A:LEU:HD21	1:698:A:VAL:H	6	0.12
(1,188)	1:695:A:LEU:HD22	1:698:A:VAL:H	6	0.12
(1,188)	1:695:A:LEU:HD23	1:698:A:VAL:H	6	0.12
(1,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	9	0.12
(1,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	9	0.12
(1,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	9	0.12
(1,164)	1:687:A:ILE:HG21	1:691:A:SER:HG	14	0.12
(1,164)	1:687:A:ILE:HG22	1:691:A:SER:HG	14	0.12
(1,164)	1:687:A:ILE:HG23	1:691:A:SER:HG	14	0.12
(1,160)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.12
(1,160)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.12
(1,160)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.12
(1,154)	1:708:A:VAL:H	1:707:A:ARG:HA	10	0.12
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	11	0.12
(1,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	11	0.12
(1,135)	1:705:A:VAL:HG11	1:709:A:ARG:HD2	3	0.12
(1,135)	1:705:A:VAL:HG11	1:709:A:ARG:HD3	3	0.12
(1,135)	1:705:A:VAL:HG12	1:709:A:ARG:HD2	3	0.12
(1,135)	1:705:A:VAL:HG12	1:709:A:ARG:HD3	3	0.12
(1,135)	1:705:A:VAL:HG13	1:709:A:ARG:HD2	3	0.12
(1,135)	1:705:A:VAL:HG13	1:709:A:ARG:HD3	3	0.12
(1,113)	1:703:A:SER:H	1:700:A:ALA:HA	9	0.12
(1,112)	1:702:A:LEU:HD21	1:706:A:ASN:HD21	7	0.12
(1,112)	1:702:A:LEU:HD21	1:706:A:ASN:HD22	7	0.12
(1,112)	1:702:A:LEU:HD22	1:706:A:ASN:HD21	7	0.12
(1,112)	1:702:A:LEU:HD22	1:706:A:ASN:HD22	7	0.12
(1,112)	1:702:A:LEU:HD23	1:706:A:ASN:HD21	7	0.12
(1,112)	1:702:A:LEU:HD23	1:706:A:ASN:HD22	7	0.12
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	13	0.12
(1,96)	1:685:A:PHE:H	1:686:A:ILE:H	13	0.12
(1,94)	1:684:A:ILE:HG21	1:688:A:ILE:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:684:A:ILE:HG22	1:688:A:ILE:H	12	0.12
(1,94)	1:684:A:ILE:HG23	1:688:A:ILE:H	12	0.12
(1,79)	1:681:A:TYR:H	1:682:A:ILE:H	4	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	2	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	2	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	2	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	3	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	3	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	3	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	9	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	9	0.12
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	9	0.12
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	10	0.12
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	10	0.12
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	10	0.12
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	10	0.12
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	10	0.12
(1,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	10	0.12
(1,66)	1:676:A:THR:HG21	1:679:A:LEU:H	10	0.12
(1,66)	1:676:A:THR:HG22	1:679:A:LEU:H	10	0.12
(1,66)	1:676:A:THR:HG23	1:679:A:LEU:H	10	0.12
(1,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	14	0.12
(1,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	14	0.12
(1,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	14	0.12
(1,60)	1:675:A:ILE:H	1:674:A:ASP:H	6	0.12
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	9	0.12
(1,59)	1:674:A:ASP:H	1:677:A:ASN:H	13	0.12
(1,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	2	0.12
(1,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	2	0.12
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.12
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.12
(1,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.12
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	11	0.12
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.12
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.12
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.12
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.12
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.12
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.12
(1,40)	1:669:A:LEU:H	1:666:A:TRP:HA	12	0.12
(1,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.12
(1,29)	1:667:A:ALA:H	1:664:A:ASP:HA	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:666:A:TRP:HE1	1:662:A:GLU:H	1	0.12
(1,28)	1:666:A:TRP:HE1	1:662:A:GLU:H	15	0.12
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	4	0.12
(1,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	5	0.12
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	9	0.11
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	9	0.11
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	9	0.11
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	9	0.11
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	9	0.11
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	9	0.11
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.11
(1,627)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.11
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.11
(1,627)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.11
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.11
(1,627)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.11
(1,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	15	0.11
(1,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	15	0.11
(1,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	15	0.11
(1,618)	1:696:A:ARG:H	1:693:A:ILE:HA	9	0.11
(1,606)	1:693:A:ILE:HD11	1:697:A:ILE:H	9	0.11
(1,606)	1:693:A:ILE:HD12	1:697:A:ILE:H	9	0.11
(1,606)	1:693:A:ILE:HD13	1:697:A:ILE:H	9	0.11
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	5	0.11
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	5	0.11
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	5	0.11
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	5	0.11
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	5	0.11
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	5	0.11
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	5	0.11
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	5	0.11
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	5	0.11
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	15	0.11
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	15	0.11
(1,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	15	0.11
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	15	0.11
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	15	0.11
(1,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	15	0.11
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	15	0.11
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	15	0.11
(1,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	15	0.11
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	10	0.11
(1,550)	1:704:A:LEU:H	1:704:A:LEU:HB3	1	0.11
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	1	0.11
(1,545)	1:704:A:LEU:H	1:701:A:VAL:HA	4	0.11
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	1	0.11
(1,538)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	1	0.11
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	1	0.11
(1,538)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	1	0.11
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	1	0.11
(1,538)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	1	0.11
(1,536)	1:702:A:LEU:H	1:704:A:LEU:H	15	0.11
(1,524)	1:685:A:PHE:H	1:686:A:ILE:H	11	0.11
(1,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	6	0.11
(1,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	6	0.11
(1,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	6	0.11
(1,508)	1:682:A:ILE:HG21	1:679:A:LEU:H	7	0.11
(1,508)	1:682:A:ILE:HG22	1:679:A:LEU:H	7	0.11
(1,508)	1:682:A:ILE:HG23	1:679:A:LEU:H	7	0.11
(1,507)	1:681:A:TYR:H	1:682:A:ILE:H	12	0.11
(1,495)	1:676:A:THR:HG21	1:681:A:TYR:HH	8	0.11
(1,495)	1:676:A:THR:HG22	1:681:A:TYR:HH	8	0.11
(1,495)	1:676:A:THR:HG23	1:681:A:TYR:HH	8	0.11
(1,494)	1:676:A:THR:HG21	1:679:A:LEU:H	9	0.11
(1,494)	1:676:A:THR:HG22	1:679:A:LEU:H	9	0.11
(1,494)	1:676:A:THR:HG23	1:679:A:LEU:H	9	0.11
(1,492)	1:676:A:THR:HG21	1:669:A:LEU:HA	2	0.11
(1,492)	1:676:A:THR:HG22	1:669:A:LEU:HA	2	0.11
(1,492)	1:676:A:THR:HG23	1:669:A:LEU:HA	2	0.11
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	7	0.11
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	7	0.11
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	7	0.11
(1,491)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	14	0.11
(1,491)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	14	0.11
(1,491)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	14	0.11
(1,488)	1:675:A:ILE:H	1:674:A:ASP:H	14	0.11
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	15	0.11
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	15	0.11
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	15	0.11
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	15	0.11
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	15	0.11
(1,484)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	15	0.11
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	12	0.11
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	12	0.11
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	12	0.11
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	12	0.11
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	12	0.11
(1,474)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.11
(1,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.11
(1,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.11
(1,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.11
(1,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.11
(1,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.11
(1,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.11
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	9	0.11
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	9	0.11
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	9	0.11
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	9	0.11
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	9	0.11
(1,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	9	0.11
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	9	0.11
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	9	0.11
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	9	0.11
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	9	0.11
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	9	0.11
(1,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	9	0.11
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	9	0.11
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	9	0.11
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	9	0.11
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	9	0.11
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	9	0.11
(1,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	9	0.11
(1,450)	1:666:A:TRP:H	1:665:A:LYS:HA	5	0.11
(1,443)	1:665:A:LYS:H	1:662:A:GLU:HA	10	0.11
(1,443)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.11
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.11
(1,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.11
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.11
(1,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.11
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.11
(1,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.11
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.11
(1,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.11
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.11
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.11
(1,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.11
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	9	0.11
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	9	0.11
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	9	0.11
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	9	0.11
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	9	0.11
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	9	0.11
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.11
(1,413)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.11
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.11
(1,413)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.11
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.11
(1,413)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.11
(1,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	15	0.11
(1,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	15	0.11
(1,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	15	0.11
(1,404)	1:696:A:ARG:H	1:693:A:ILE:HA	9	0.11
(1,392)	1:693:A:ILE:HD11	1:697:A:ILE:H	9	0.11
(1,392)	1:693:A:ILE:HD12	1:697:A:ILE:H	9	0.11
(1,392)	1:693:A:ILE:HD13	1:697:A:ILE:H	9	0.11
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	5	0.11
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	5	0.11
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	5	0.11
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	5	0.11
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	5	0.11
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	5	0.11
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	5	0.11
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	5	0.11
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	5	0.11
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	15	0.11
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	15	0.11
(1,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	15	0.11
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	15	0.11
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	15	0.11
(1,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	15	0.11
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	15	0.11
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	15	0.11
(1,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	15	0.11
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	10	0.11
(1,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	1	0.11
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	1	0.11
(1,331)	1:704:A:LEU:H	1:701:A:VAL:HA	4	0.11
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	1	0.11
(1,324)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	1	0.11
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	1	0.11
(1,324)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	1	0.11
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	1	0.11
(1,324)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	1	0.11
(1,322)	1:702:A:LEU:H	1:704:A:LEU:H	15	0.11
(1,310)	1:685:A:PHE:H	1:686:A:ILE:H	11	0.11
(1,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	6	0.11
(1,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	6	0.11
(1,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	6	0.11
(1,294)	1:682:A:ILE:HG21	1:679:A:LEU:H	7	0.11
(1,294)	1:682:A:ILE:HG22	1:679:A:LEU:H	7	0.11
(1,294)	1:682:A:ILE:HG23	1:679:A:LEU:H	7	0.11
(1,293)	1:681:A:TYR:H	1:682:A:ILE:H	12	0.11
(1,281)	1:676:A:THR:HG21	1:681:A:TYR:HH	8	0.11
(1,281)	1:676:A:THR:HG22	1:681:A:TYR:HH	8	0.11
(1,281)	1:676:A:THR:HG23	1:681:A:TYR:HH	8	0.11
(1,280)	1:676:A:THR:HG21	1:679:A:LEU:H	9	0.11
(1,280)	1:676:A:THR:HG22	1:679:A:LEU:H	9	0.11
(1,280)	1:676:A:THR:HG23	1:679:A:LEU:H	9	0.11
(1,278)	1:676:A:THR:HG21	1:669:A:LEU:HA	2	0.11
(1,278)	1:676:A:THR:HG22	1:669:A:LEU:HA	2	0.11
(1,278)	1:676:A:THR:HG23	1:669:A:LEU:HA	2	0.11
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	7	0.11
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	7	0.11
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	7	0.11
(1,277)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	14	0.11
(1,277)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	14	0.11
(1,277)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	14	0.11
(1,274)	1:675:A:ILE:H	1:674:A:ASP:H	14	0.11
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	15	0.11
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	15	0.11
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	15	0.11
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	15	0.11
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	15	0.11
(1,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	15	0.11
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	12	0.11
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	12	0.11
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	12	0.11
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	12	0.11
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	12	0.11
(1,260)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.11
(1,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.11
(1,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.11
(1,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.11
(1,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.11
(1,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.11
(1,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.11
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	9	0.11
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	9	0.11
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	9	0.11
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	9	0.11
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	9	0.11
(1,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	9	0.11
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	9	0.11
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	9	0.11
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	9	0.11
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	9	0.11
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	9	0.11
(1,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	9	0.11
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	9	0.11
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	9	0.11
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	9	0.11
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	9	0.11
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	9	0.11
(1,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	9	0.11
(1,236)	1:666:A:TRP:H	1:665:A:LYS:HA	5	0.11
(1,229)	1:665:A:LYS:H	1:662:A:GLU:HA	10	0.11
(1,229)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.11
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.11
(1,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.11
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.11
(1,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.11
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.11
(1,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.11
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.11
(1,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.11
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.11
(1,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.11
(1,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.11
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	9	0.11
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	9	0.11
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	9	0.11
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	9	0.11
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	9	0.11
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	9	0.11
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.11
(1,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.11
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.11
(1,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.11
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.11
(1,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.11
(1,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	15	0.11
(1,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	15	0.11
(1,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	15	0.11
(1,190)	1:696:A:ARG:H	1:693:A:ILE:HA	9	0.11
(1,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	9	0.11
(1,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	9	0.11
(1,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	9	0.11
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	5	0.11
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	5	0.11
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	5	0.11
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	5	0.11
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	5	0.11
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	5	0.11
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	5	0.11
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	5	0.11
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	5	0.11
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	15	0.11
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	15	0.11
(1,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	15	0.11
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	15	0.11
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	15	0.11
(1,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	15	0.11
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	15	0.11
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	15	0.11
(1,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	15	0.11
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	10	0.11
(1,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	10	0.11
(1,122)	1:704:A:LEU:H	1:704:A:LEU:HB3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	1	0.11
(1,117)	1:704:A:LEU:H	1:701:A:VAL:HA	4	0.11
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE1	1	0.11
(1,110)	1:702:A:LEU:HD11	1:699:A:PHE:HE2	1	0.11
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE1	1	0.11
(1,110)	1:702:A:LEU:HD12	1:699:A:PHE:HE2	1	0.11
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE1	1	0.11
(1,110)	1:702:A:LEU:HD13	1:699:A:PHE:HE2	1	0.11
(1,108)	1:702:A:LEU:H	1:704:A:LEU:H	15	0.11
(1,96)	1:685:A:PHE:H	1:686:A:ILE:H	11	0.11
(1,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	6	0.11
(1,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	6	0.11
(1,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	6	0.11
(1,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	7	0.11
(1,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	7	0.11
(1,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	7	0.11
(1,79)	1:681:A:TYR:H	1:682:A:ILE:H	12	0.11
(1,67)	1:676:A:THR:HG21	1:681:A:TYR:HH	8	0.11
(1,67)	1:676:A:THR:HG22	1:681:A:TYR:HH	8	0.11
(1,67)	1:676:A:THR:HG23	1:681:A:TYR:HH	8	0.11
(1,66)	1:676:A:THR:HG21	1:679:A:LEU:H	9	0.11
(1,66)	1:676:A:THR:HG22	1:679:A:LEU:H	9	0.11
(1,66)	1:676:A:THR:HG23	1:679:A:LEU:H	9	0.11
(1,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	2	0.11
(1,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	2	0.11
(1,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	2	0.11
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	7	0.11
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	7	0.11
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	7	0.11
(1,63)	1:676:A:THR:HG21	1:666:A:TRP:HZ3	14	0.11
(1,63)	1:676:A:THR:HG22	1:666:A:TRP:HZ3	14	0.11
(1,63)	1:676:A:THR:HG23	1:666:A:TRP:HZ3	14	0.11
(1,60)	1:675:A:ILE:H	1:674:A:ASP:H	14	0.11
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	15	0.11
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	15	0.11
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	15	0.11
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	15	0.11
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	15	0.11
(1,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	15	0.11
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	12	0.11
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	12	0.11
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	12	0.11
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	12	0.11
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	12	0.11
(1,46)	1:670:A:TRP:H	1:667:A:ALA:HA	14	0.11
(1,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.11
(1,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.11
(1,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.11
(1,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.11
(1,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.11
(1,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.11
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	9	0.11
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	9	0.11
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	9	0.11
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	9	0.11
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	9	0.11
(1,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	9	0.11
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	9	0.11
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	9	0.11
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	9	0.11
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	9	0.11
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	9	0.11
(1,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	9	0.11
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	9	0.11
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	9	0.11
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	9	0.11
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	9	0.11
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	9	0.11
(1,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	9	0.11
(1,22)	1:666:A:TRP:H	1:665:A:LYS:HA	5	0.11
(1,15)	1:665:A:LYS:H	1:662:A:GLU:HA	10	0.11
(1,15)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.11
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.11
(1,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.11
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.11
(1,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.11
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.11
(1,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.11
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.11
(1,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.11
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.11
(1,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.11
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.11
(1,626)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	14	0.1
(1,626)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	14	0.1
(1,626)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	14	0.1
(1,626)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	14	0.1
(1,626)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	14	0.1
(1,626)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	14	0.1
(1,585)	1:708:A:VAL:H	1:709:A:ARG:H	5	0.1
(1,532)	1:702:A:LEU:H	1:699:A:PHE:HA	6	0.1
(1,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	8	0.1
(1,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	8	0.1
(1,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	8	0.1
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	5	0.1
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	5	0.1
(1,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	5	0.1
(1,503)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	1	0.1
(1,503)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	1	0.1
(1,503)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	1	0.1
(1,503)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	1	0.1
(1,503)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	1	0.1
(1,503)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	1	0.1
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	9	0.1
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	9	0.1
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	9	0.1
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	9	0.1
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	9	0.1
(1,479)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	9	0.1
(1,469)	1:669:A:LEU:H	1:668:A:SER:HA	8	0.1
(1,469)	1:669:A:LEU:H	1:668:A:SER:HA	14	0.1
(1,450)	1:666:A:TRP:H	1:665:A:LYS:HA	6	0.1
(1,443)	1:665:A:LYS:H	1:662:A:GLU:HA	2	0.1
(1,412)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	14	0.1
(1,412)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	14	0.1
(1,412)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	14	0.1
(1,412)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	14	0.1
(1,412)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	14	0.1
(1,412)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	14	0.1
(1,371)	1:708:A:VAL:H	1:709:A:ARG:H	5	0.1
(1,318)	1:702:A:LEU:H	1:699:A:PHE:HA	6	0.1
(1,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	8	0.1
(1,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	8	0.1
(1,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	5	0.1
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	5	0.1
(1,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	5	0.1
(1,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	1	0.1
(1,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	1	0.1
(1,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	1	0.1
(1,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	1	0.1
(1,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	1	0.1
(1,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	1	0.1
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	9	0.1
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	9	0.1
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	9	0.1
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	9	0.1
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	9	0.1
(1,265)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	9	0.1
(1,255)	1:669:A:LEU:H	1:668:A:SER:HA	8	0.1
(1,255)	1:669:A:LEU:H	1:668:A:SER:HA	14	0.1
(1,236)	1:666:A:TRP:H	1:665:A:LYS:HA	6	0.1
(1,229)	1:665:A:LYS:H	1:662:A:GLU:HA	2	0.1
(1,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	14	0.1
(1,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	14	0.1
(1,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	14	0.1
(1,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	14	0.1
(1,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	14	0.1
(1,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	14	0.1
(1,157)	1:708:A:VAL:H	1:709:A:ARG:H	5	0.1
(1,104)	1:702:A:LEU:H	1:699:A:PHE:HA	6	0.1
(1,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	8	0.1
(1,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	8	0.1
(1,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	8	0.1
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	5	0.1
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	5	0.1
(1,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	5	0.1
(1,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	1	0.1
(1,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	1	0.1
(1,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	1	0.1
(1,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	1	0.1
(1,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	1	0.1
(1,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	1	0.1
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	9	0.1
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	9	0.1
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	9	0.1
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	9	0.1
(1,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	9	0.1
(1,41)	1:669:A:LEU:H	1:668:A:SER:HA	8	0.1
(1,41)	1:669:A:LEU:H	1:668:A:SER:HA	14	0.1
(1,22)	1:666:A:TRP:H	1:665:A:LYS:HA	6	0.1
(1,15)	1:665:A:LYS:H	1:662:A:GLU:HA	2	0.1

10 Dihedral-angle violation analysis

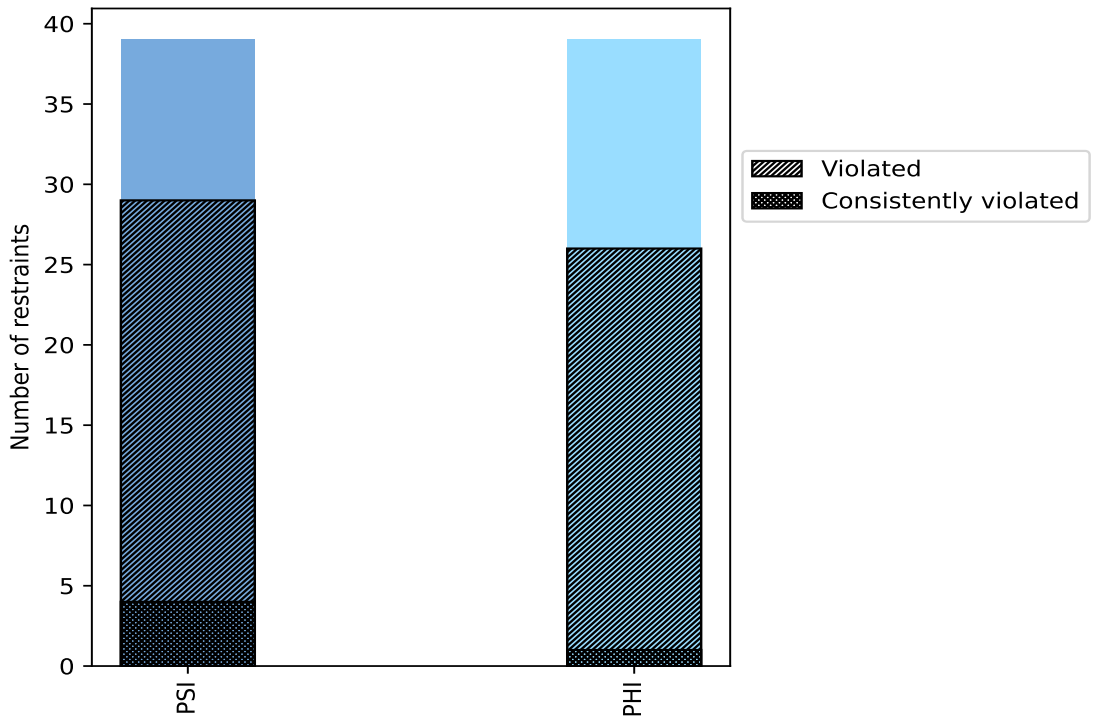
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	39	50.0	29	74.4	37.2	4	10.3	5.1
PHI	39	50.0	26	66.7	33.3	1	2.6	1.3
Total	78	100.0	55	70.5	70.5	5	6.4	6.4

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



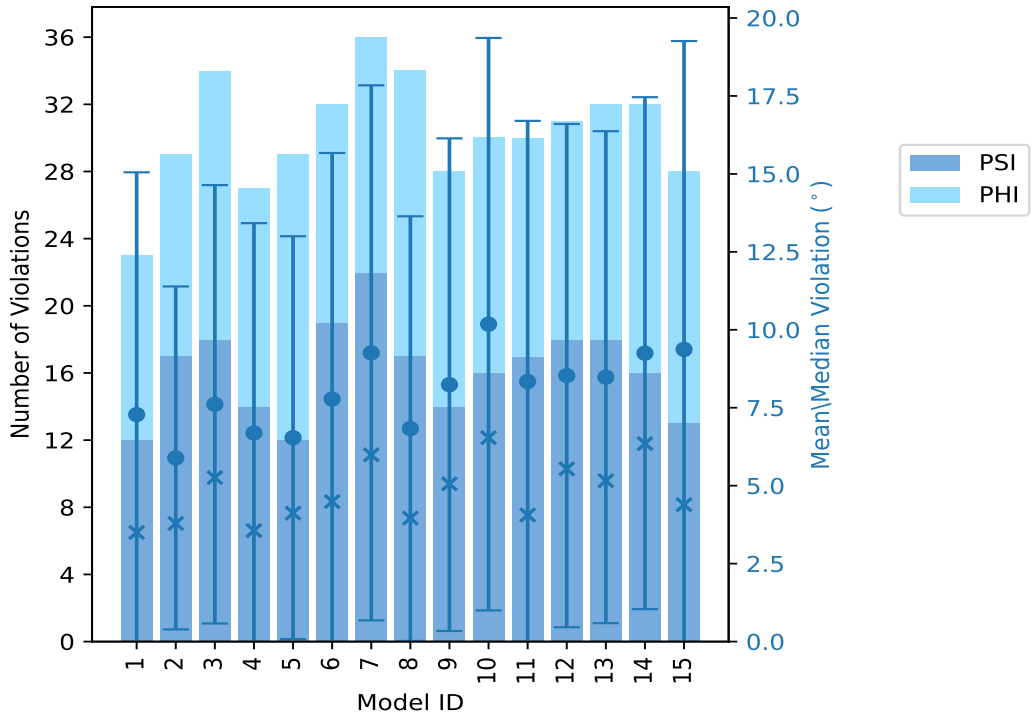
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	12	11	23	7.28	31.49	7.77	3.5
2	17	12	29	5.89	22.34	5.5	3.79
3	18	16	34	7.61	27.21	7.03	5.26
4	14	13	27	6.69	31.08	6.73	3.56
5	12	17	29	6.54	28.32	6.46	4.12
6	19	13	32	7.78	39.54	7.89	4.49
7	22	14	36	9.26	37.77	8.58	5.99
8	17	17	34	6.83	33.34	6.81	3.96
9	14	14	28	8.24	31.14	7.9	5.06
10	16	14	30	10.18	40.6	9.18	6.54
11	17	13	30	8.34	33.95	8.36	4.06
12	18	13	31	8.53	33.24	8.07	5.54
13	18	14	32	8.48	32.33	7.89	5.16
14	16	16	32	9.25	33.0	8.21	6.35
15	13	15	28	9.37	42.15	9.89	4.39

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



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

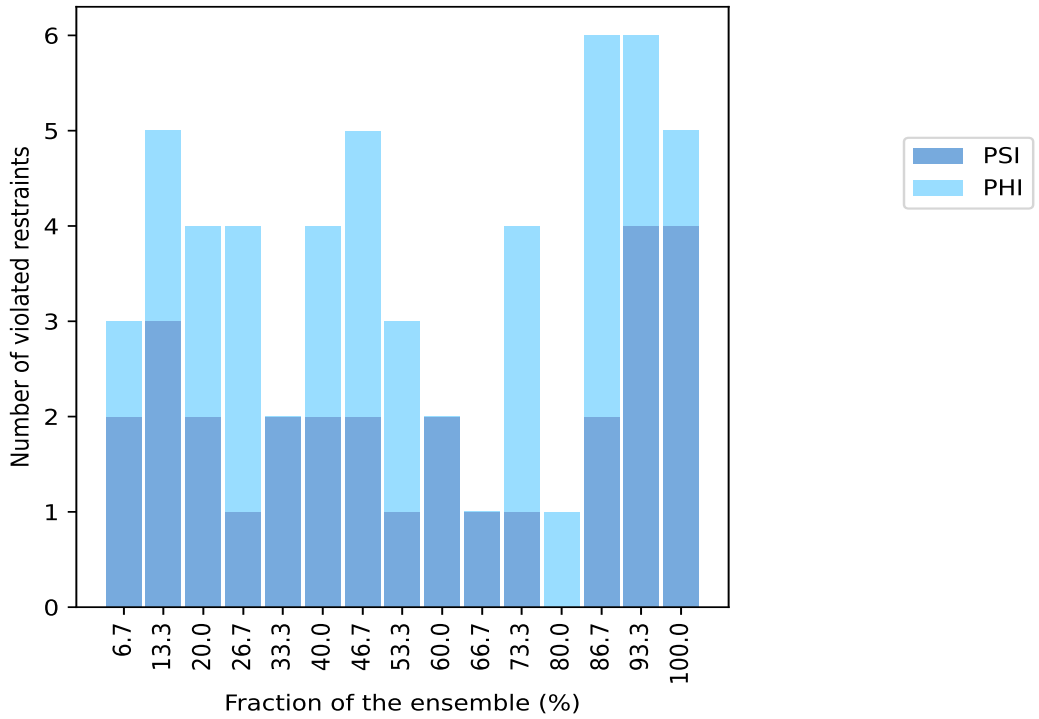
10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
2	1	3	1	6.7
3	2	5	2	13.3
2	2	4	3	20.0
1	3	4	4	26.7
2	0	2	5	33.3
2	2	4	6	40.0
2	3	5	7	46.7
1	2	3	8	53.3
2	0	2	9	60.0
1	0	1	10	66.7
1	3	4	11	73.3
0	1	1	12	80.0
2	4	6	13	86.7
4	2	6	14	93.3
4	1	5	15	100.0

[1] Number of models with violations

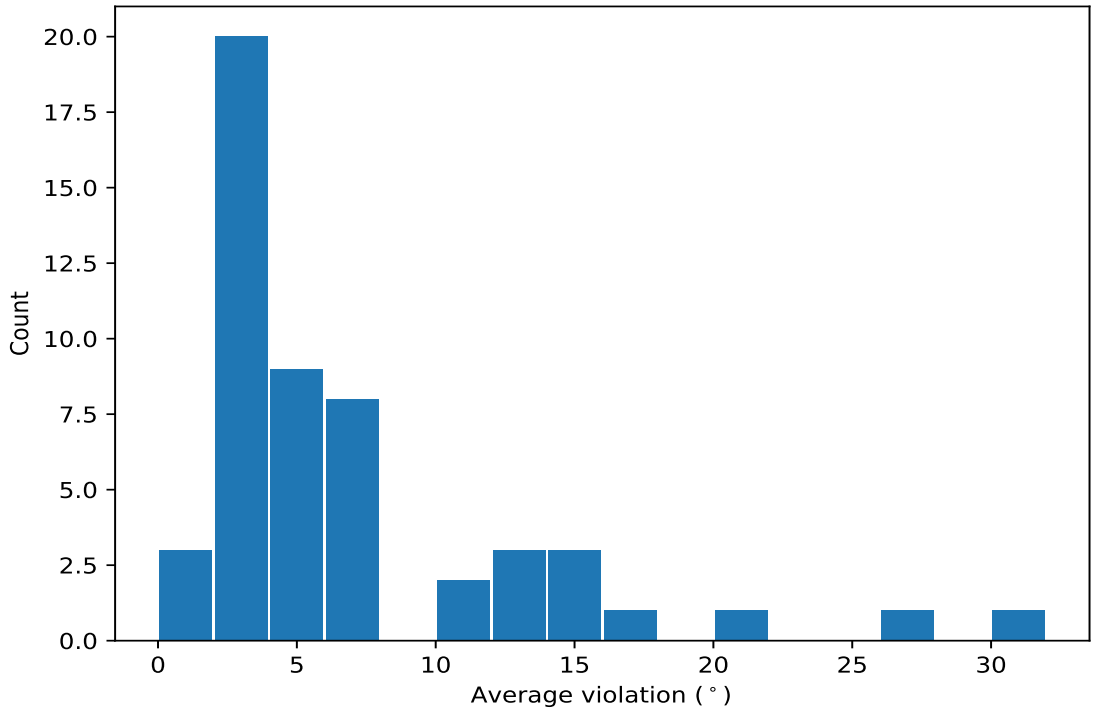
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	15	30.41	6.25	30.93
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	15	26.52	8.09	28.32
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	15	12.93	0.75	12.85
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	15	7.45	4.39	4.92
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	15	7.19	2.72	6.29
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	14	15.72	0.51	15.59
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	14	15.05	5.0	15.97
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	14	12.21	1.06	12.58
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	14	5.53	3.84	3.3
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	14	3.56	1.33	3.48
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	14	2.78	0.53	2.66
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	13	7.45	8.28	1.83
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	13	6.24	3.48	6.35
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	13	5.61	3.3	5.15
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	13	5.3	0.39	5.45
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	13	3.16	0.94	3.23
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	13	3.0	0.98	3.42
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	12	2.81	1.34	2.29
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	11	17.42	6.51	17.46
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	11	6.6	1.9	7.31
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	11	3.52	0.76	3.56

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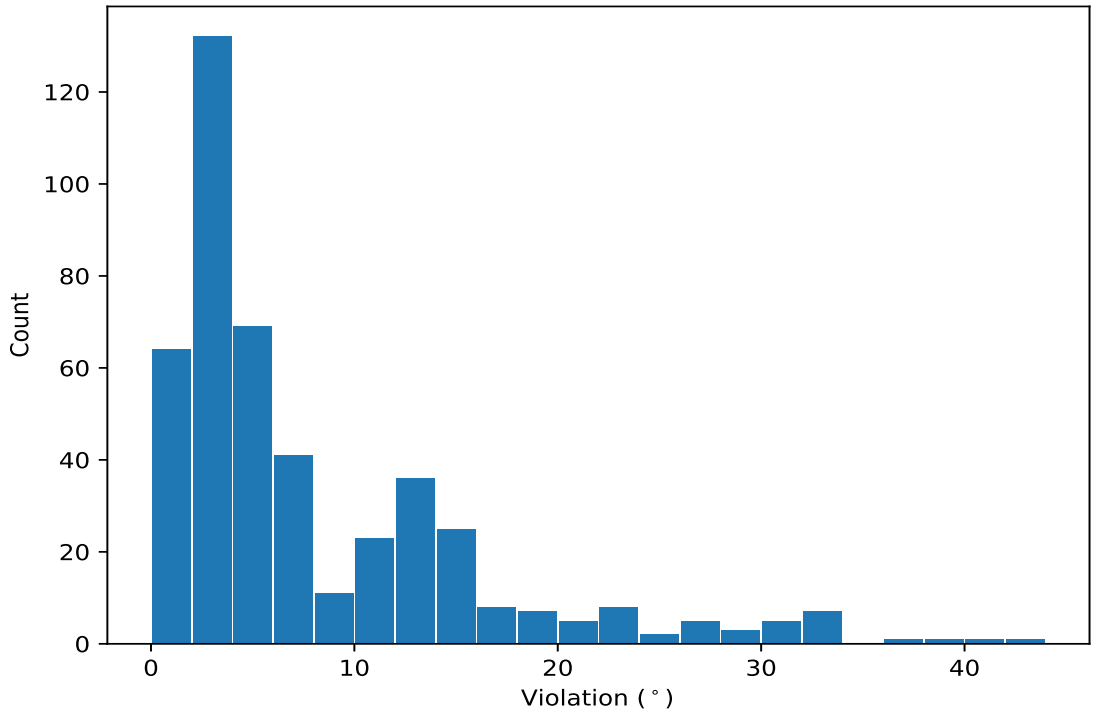
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	11	2.51	0.29	2.56
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	10	12.6	6.35	12.6
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	9	5.68	3.24	5.07
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	9	2.51	0.91	2.37
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	8	14.0	6.89	12.74
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	8	5.26	4.44	4.2
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	8	2.83	2.69	1.42
(1,33)	1:684:A:ILE:C	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	7	5.19	2.31	6.41
(1,47)	1:691:A:SER:C	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	7	3.82	1.34	3.75
(1,28)	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	1:683:A:ARG:N	7	3.31	2.18	2.16
(1,66)	1:701:A:VAL:N	1:701:A:VAL:CA	1:701:A:VAL:C	1:702:A:LEU:N	7	2.19	0.49	2.15
(1,17)	1:674:A:ASP:C	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	7	1.77	0.46	1.93
(1,8)	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	1:668:A:SER:N	6	5.52	4.41	4.72
(1,16)	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	1:672:A:TRP:N	6	4.99	0.31	5.08
(1,7)	1:666:A:TRP:C	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	6	2.15	1.54	1.66
(1,41)	1:688:A:ILE:C	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	6	2.14	0.92	1.92
(1,72)	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	1:705:A:VAL:N	5	10.69	5.04	13.14
(1,54)	1:695:A:LEU:N	1:695:A:LEU:CA	1:695:A:LEU:C	1:696:A:ARG:N	5	6.67	2.27	5.82
(1,2)	1:664:A:ASP:N	1:664:A:ASP:CA	1:664:A:ASP:C	1:665:A:LYS:N	4	6.66	3.58	6.99
(1,39)	1:687:A:ILE:C	1:688:A:ILE:N	1:688:A:ILE:CA	1:688:A:ILE:C	4	2.41	0.17	2.46
(1,67)	1:701:A:VAL:C	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	4	2.36	0.65	2.68
(1,9)	1:667:A:ALA:C	1:668:A:SER:N	1:668:A:SER:CA	1:668:A:SER:C	4	1.15	0.1	1.16
(1,50)	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	1:694:A:GLY:N	3	10.47	3.5	10.19
(1,73)	1:704:A:LEU:C	1:705:A:VAL:N	1:705:A:VAL:CA	1:705:A:VAL:C	3	4.48	2.43	4.71
(1,64)	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	1:701:A:VAL:N	3	3.92	1.28	3.84
(1,11)	1:668:A:SER:C	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	3	2.7	1.4	1.82
(1,22)	1:677:A:ASN:N	1:677:A:ASN:CA	1:677:A:ASN:C	1:678:A:TRP:N	2	20.49	17.29	20.49
(1,52)	1:694:A:GLY:N	1:694:A:GLY:CA	1:694:A:GLY:C	1:695:A:LEU:N	2	6.15	0.85	6.15
(1,29)	1:682:A:ILE:C	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	2	3.24	0.82	3.24
(1,20)	1:676:A:THR:N	1:676:A:THR:CA	1:676:A:THR:C	1:677:A:ASN:N	2	2.28	0.17	2.28
(1,15)	1:670:A:TRP:C	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	2	1.15	0.14	1.15

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	15	42.15
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	10	40.6
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	6	39.54
(1,22)	1:677:A:ASN:N	1:677:A:ASN:CA	1:677:A:ASN:C	1:678:A:TRP:N	7	37.77
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	11	33.95
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	8	33.34
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	12	33.24
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	15	33.12
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	14	33.0
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	14	32.6
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	13	32.33
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	7	31.99
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	1	31.49
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	9	31.14
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	4	31.08
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	11	30.93
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	13	29.7
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	12	29.65
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	5	28.32
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	9	27.55
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	7	27.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	3	27.21
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	10	26.45
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	15	26.31
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	14	25.43
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	1	24.72
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	3	23.92
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	5	23.75
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	3	23.68
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	13	23.55
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	6	23.55
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	10	22.75
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	8	22.35
(1,42)	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	1:690:A:GLY:N	2	22.34
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	9	21.54
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	7	21.44
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	10	21.25
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	3	20.77
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	9	20.12
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	10	19.83
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	14	19.16
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	2	19.14
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	11	19.02
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	2	18.24
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	13	18.1
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	10	18.09
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	12	17.6
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	7	17.5
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	10	17.46
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	11	17.35
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	10	17.26
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	12	16.68
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	5	16.27
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	15	16.13
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	13	15.95
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	3	15.85
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	12	15.81
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	12	15.75
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	12	15.72
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1	15.67
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	15	15.64
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	4	15.54
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	6	15.53
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	9	15.52
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	1	15.48
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	6	15.44
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	8	15.44
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	7	15.42
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	11	15.24
(1,77)	1:706:A:ASN:C	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	14	15.15
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	7	15.09
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	4	15.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	15	14.93
(1,50)	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	1:694:A:GLY:N	6	14.89
(1,72)	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	1:705:A:VAL:N	10	14.69
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	14	14.66
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	6	14.57
(1,72)	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	1:705:A:VAL:N	15	14.21
(1,8)	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	1:668:A:SER:N	13	14.05
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	8	13.72
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	4	13.67
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	14	13.52
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	4	13.44
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	7	13.4
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	10	13.38
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	5	13.31
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	10	13.27
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	11	13.21
(1,72)	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	1:705:A:VAL:N	12	13.14
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	3	13.14
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	4	13.06
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	7	13.01
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	3	12.88
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	14	12.85
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	11	12.85
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	6	12.78
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	6	12.78
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	7	12.77
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	13	12.7
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	15	12.64
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	9	12.63
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	4	12.53
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	2	12.49
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	15	12.47
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	11	12.28
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	12	12.23
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	14	12.19
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	13	12.18
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	1	12.16
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	8	12.15
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	9	12.09
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	11	12.08
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	3	12.05
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	11	12.05
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	8	12.0
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	5	11.76
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	8	11.62
(1,60)	1:698:A:VAL:N	1:698:A:VAL:CA	1:698:A:VAL:C	1:699:A:PHE:N	12	11.41
(1,2)	1:664:A:ASP:N	1:664:A:ASP:CA	1:664:A:ASP:C	1:665:A:LYS:N	13	11.35
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	15	11.32
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	4	11.27
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	8	11.24
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	13	11.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	12	11.09
(1,54)	1:695:A:LEU:N	1:695:A:LEU:CA	1:695:A:LEU:C	1:696:A:ARG:N	6	11.03
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	14	10.95
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	14	10.88
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	7	10.81
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	6	10.68
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	13	10.48
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	12	10.46
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	11	10.38
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	8	10.36
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	2	10.36
(1,72)	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	1:705:A:VAL:N	11	10.32
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	5	10.21
(1,50)	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	1:694:A:GLY:N	7	10.19
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	3	10.12
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	9	9.88
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	7	9.44
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	14	9.4
(1,68)	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	1:703:A:SER:N	1	9.24
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	2	9.04
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	8	8.83
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	2	8.65
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	7	8.63
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1	8.57
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	8	8.49
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	10	8.45
(1,28)	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	1:683:A:ARG:N	14	7.95
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	5	7.83
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	10	7.82
(1,74)	1:705:A:VAL:N	1:705:A:VAL:CA	1:705:A:VAL:C	1:706:A:ASN:N	5	7.76
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	9	7.73
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	14	7.69
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	3	7.63
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	8	7.6
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	1	7.59
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	3	7.54
(1,33)	1:684:A:ILE:C	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	8	7.41
(1,33)	1:684:A:ILE:C	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	3	7.39
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	3	7.37
(1,73)	1:704:A:LEU:C	1:705:A:VAL:N	1:705:A:VAL:CA	1:705:A:VAL:C	10	7.33
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	9	7.31
(1,2)	1:664:A:ASP:N	1:664:A:ASP:CA	1:664:A:ASP:C	1:665:A:LYS:N	10	7.31
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	14	7.22
(1,33)	1:684:A:ILE:C	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	11	7.11
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	12	7.07
(1,52)	1:694:A:GLY:N	1:694:A:GLY:CA	1:694:A:GLY:C	1:695:A:LEU:N	7	7.0
(1,8)	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	1:668:A:SER:N	7	6.98
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	6	6.88
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	13	6.82
(1,2)	1:664:A:ASP:N	1:664:A:ASP:CA	1:664:A:ASP:C	1:665:A:LYS:N	9	6.68
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	6	6.62

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,43)	1:689:A:VAL:C	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	13	6.55
(1,54)	1:695:A:LEU:N	1:695:A:LEU:CA	1:695:A:LEU:C	1:696:A:ARG:N	7	6.54
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	1	6.51
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	5	6.51
(1,33)	1:684:A:ILE:C	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	15	6.41
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	8	6.38
(1,8)	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	1:668:A:SER:N	14	6.35
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	14	6.35
(1,50)	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	1:694:A:GLY:N	12	6.34
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	7	6.31
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	2	6.29
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	15	6.24
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	14	6.2
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	9	6.07
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	3	6.06
(1,47)	1:691:A:SER:C	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	12	6.05
(1,54)	1:695:A:LEU:N	1:695:A:LEU:CA	1:695:A:LEU:C	1:696:A:ARG:N	9	5.82
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	10	5.77
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	13	5.73
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	7	5.67
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	13	5.66
(1,26)	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	1:680:A:TRP:N	7	5.6
(1,7)	1:666:A:TRP:C	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	3	5.56
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	12	5.54
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	2	5.53
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	15	5.53
(1,64)	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	1:701:A:VAL:N	3	5.52
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	8	5.5
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	12	5.46
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	11	5.45
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	6	5.43
(1,54)	1:695:A:LEU:N	1:695:A:LEU:CA	1:695:A:LEU:C	1:696:A:ARG:N	12	5.39
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	5	5.39
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	5	5.38
(1,16)	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	1:672:A:TRP:N	3	5.36
(1,52)	1:694:A:GLY:N	1:694:A:GLY:CA	1:694:A:GLY:C	1:695:A:LEU:N	6	5.3
(1,16)	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	1:672:A:TRP:N	13	5.25
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	6	5.19
(1,47)	1:691:A:SER:C	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	9	5.19
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	3	5.15
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	1	5.15
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	3	5.12
(1,16)	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	1:672:A:TRP:N	7	5.1
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	13	5.07
(1,16)	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	1:672:A:TRP:N	4	5.06
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	2	4.97
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	5	4.94
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	9	4.92
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	9	4.91
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	3	4.78
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	5	4.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	14	4.77
(1,16)	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	1:672:A:TRP:N	9	4.75
(1,73)	1:704:A:LEU:C	1:705:A:VAL:N	1:705:A:VAL:CA	1:705:A:VAL:C	15	4.71
(1,11)	1:668:A:SER:C	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	13	4.67
(1,54)	1:695:A:LEU:N	1:695:A:LEU:CA	1:695:A:LEU:C	1:696:A:ARG:N	11	4.57
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	6	4.56
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	10	4.55
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	13	4.53
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	10	4.52
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	5	4.49
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	8	4.49
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	8	4.48
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	14	4.46
(1,16)	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	1:672:A:TRP:N	2	4.44
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	6	4.43
(1,27)	1:681:A:TYR:C	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	7	4.32
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	14	4.3
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	9	4.3
(1,28)	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	1:683:A:ARG:N	10	4.25
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	9	4.25
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	14	4.21
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	13	4.21
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	13	4.21
(1,78)	1:707:A:ARG:N	1:707:A:ARG:CA	1:707:A:ARG:C	1:708:A:VAL:N	6	4.2
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	7	4.2
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	2	4.18
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	6	4.15
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	5	4.12
(1,45)	1:690:A:GLY:C	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	14	4.11
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	15	4.08
(1,31)	1:683:A:ARG:C	1:684:A:ILE:N	1:684:A:ILE:CA	1:684:A:ILE:C	14	4.08
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	3	4.07
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	10	4.06
(1,29)	1:682:A:ILE:C	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	14	4.06
(1,28)	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	1:683:A:ARG:N	7	3.99
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	9	3.98
(1,41)	1:688:A:ILE:C	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	13	3.98
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	2	3.95
(1,47)	1:691:A:SER:C	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1	3.93
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	7	3.89
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	10	3.85
(1,64)	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	1:701:A:VAL:N	2	3.84
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	6	3.83
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	2	3.79
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	7	3.77
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	7	3.76
(1,47)	1:691:A:SER:C	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	2	3.75
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	4	3.74
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	5	3.72
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	3	3.71
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	15	3.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	13	3.68
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	4	3.64
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	4	3.63
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	6	3.63
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	7	3.63
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	15	3.61
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	15	3.58
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	4	3.58
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	4	3.56
(1,46)	1:691:A:SER:N	1:691:A:SER:CA	1:691:A:SER:C	1:692:A:LEU:N	11	3.55
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	1	3.5
(1,33)	1:684:A:ILE:C	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	5	3.48
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	15	3.47
(1,47)	1:691:A:SER:C	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	5	3.46
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	10	3.46
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	10	3.45
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	12	3.44
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	8	3.44
(1,33)	1:684:A:ILE:C	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	14	3.43
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	1	3.42
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	11	3.42
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	4	3.38
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	2	3.36
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	3	3.36
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	4	3.31
(1,34)	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	1:686:A:ILE:N	12	3.3
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	2	3.25
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1	3.23
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	1	3.22
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	6	3.21
(1,22)	1:677:A:ASN:N	1:677:A:ASN:CA	1:677:A:ASN:C	1:678:A:TRP:N	14	3.2
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	4	3.2
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	11	3.16
(1,23)	1:677:A:ASN:C	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	13	3.14
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	5	3.12
(1,8)	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	1:668:A:SER:N	6	3.08
(1,71)	1:703:A:SER:C	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	6	3.06
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	13	3.06
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	8	3.05
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	8	3.04
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	2	3.0
(1,66)	1:701:A:VAL:N	1:701:A:VAL:CA	1:701:A:VAL:C	1:702:A:LEU:N	8	2.98
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	11	2.96
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	15	2.93
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	4	2.9
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	7	2.87
(1,67)	1:701:A:VAL:C	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	7	2.85
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	2	2.84
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	1	2.84
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	15	2.83
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	4	2.83

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	15	2.8
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	5	2.79
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	7	2.75
(1,67)	1:701:A:VAL:C	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	4	2.73
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	3	2.72
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	5	2.69
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	15	2.65
(1,67)	1:701:A:VAL:C	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	3	2.63
(1,66)	1:701:A:VAL:N	1:701:A:VAL:CA	1:701:A:VAL:C	1:702:A:LEU:N	2	2.63
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	9	2.62
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	8	2.6
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	4	2.6
(1,39)	1:687:A:ILE:C	1:688:A:ILE:N	1:688:A:ILE:CA	1:688:A:ILE:C	8	2.57
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	10	2.56
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	12	2.54
(1,39)	1:687:A:ILE:C	1:688:A:ILE:N	1:688:A:ILE:CA	1:688:A:ILE:C	5	2.52
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	15	2.51
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	3	2.49
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	8	2.47
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	14	2.46
(1,44)	1:690:A:GLY:N	1:690:A:GLY:CA	1:690:A:GLY:C	1:691:A:SER:N	6	2.45
(1,41)	1:688:A:ILE:C	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	15	2.45
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	8	2.44
(1,20)	1:676:A:THR:N	1:676:A:THR:CA	1:676:A:THR:C	1:677:A:ASN:N	4	2.44
(1,47)	1:691:A:SER:C	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	3	2.42
(1,29)	1:682:A:ILE:C	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	10	2.42
(1,39)	1:687:A:ILE:C	1:688:A:ILE:N	1:688:A:ILE:CA	1:688:A:ILE:C	9	2.4
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	1	2.4
(1,64)	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	1:701:A:VAL:N	8	2.39
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	13	2.37
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	15	2.37
(1,17)	1:674:A:ASP:C	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	2	2.37
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	6	2.35
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	2	2.34
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	2	2.33
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	9	2.33
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	10	2.32
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	11	2.32
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	5	2.29
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	7	2.29
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	5	2.27
(1,17)	1:674:A:ASP:C	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	13	2.25
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	4	2.24
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	10	2.24
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	2	2.21
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	7	2.18
(1,66)	1:701:A:VAL:N	1:701:A:VAL:CA	1:701:A:VAL:C	1:702:A:LEU:N	6	2.17
(1,28)	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	1:683:A:ARG:N	3	2.16
(1,28)	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	1:683:A:ARG:N	11	2.16
(1,66)	1:701:A:VAL:N	1:701:A:VAL:CA	1:701:A:VAL:C	1:702:A:LEU:N	10	2.15
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	10	2.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	11	2.15
(1,39)	1:687:A:ILE:C	1:688:A:ILE:N	1:688:A:ILE:CA	1:688:A:ILE:C	4	2.14
(1,20)	1:676:A:THR:N	1:676:A:THR:CA	1:676:A:THR:C	1:677:A:ASN:N	11	2.11
(1,66)	1:701:A:VAL:N	1:701:A:VAL:CA	1:701:A:VAL:C	1:702:A:LEU:N	13	2.08
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	11	2.06
(1,41)	1:688:A:ILE:C	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	11	2.06
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	12	2.05
(1,17)	1:674:A:ASP:C	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	12	2.05
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	12	2.04
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	8	2.03
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	13	2.03
(1,66)	1:701:A:VAL:N	1:701:A:VAL:CA	1:701:A:VAL:C	1:702:A:LEU:N	7	2.02
(1,35)	1:685:A:PHE:C	1:686:A:ILE:N	1:686:A:ILE:CA	1:686:A:ILE:C	1	2.02
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	12	1.99
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	14	1.97
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	6	1.95
(1,17)	1:674:A:ASP:C	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	5	1.93
(1,24)	1:678:A:TRP:N	1:678:A:TRP:CA	1:678:A:TRP:C	1:679:A:LEU:N	12	1.92
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	15	1.91
(1,47)	1:691:A:SER:C	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	8	1.91
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	13	1.83
(1,11)	1:668:A:SER:C	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	5	1.82
(1,63)	1:699:A:PHE:C	1:700:A:ALA:N	1:700:A:ALA:CA	1:700:A:ALA:C	7	1.79
(1,41)	1:688:A:ILE:C	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	6	1.78
(1,56)	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1:697:A:ILE:N	12	1.73
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	5	1.73
(1,7)	1:666:A:TRP:C	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	5	1.71
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	1	1.68
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	11	1.67
(1,7)	1:666:A:TRP:C	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	8	1.67
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	4	1.65
(1,7)	1:666:A:TRP:C	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	9	1.65
(1,55)	1:695:A:LEU:C	1:696:A:ARG:N	1:696:A:ARG:CA	1:696:A:ARG:C	10	1.64
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	3	1.63
(1,48)	1:692:A:LEU:N	1:692:A:LEU:CA	1:692:A:LEU:C	1:693:A:ILE:N	13	1.63
(1,11)	1:668:A:SER:C	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	15	1.6
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	11	1.58
(1,8)	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	1:668:A:SER:N	8	1.56
(1,18)	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	1:676:A:THR:N	2	1.52
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	9	1.49
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	6	1.45
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	2	1.45
(1,41)	1:688:A:ILE:C	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	3	1.44
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	3	1.42
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	1	1.41
(1,28)	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	1:683:A:ARG:N	12	1.41
(1,73)	1:704:A:LEU:C	1:705:A:VAL:N	1:705:A:VAL:CA	1:705:A:VAL:C	11	1.4
(1,17)	1:674:A:ASP:C	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	11	1.4
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	9	1.38
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	11	1.37
(1,66)	1:701:A:VAL:N	1:701:A:VAL:CA	1:701:A:VAL:C	1:702:A:LEU:N	4	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:664:A:ASP:N	1:664:A:ASP:CA	1:664:A:ASP:C	1:665:A:LYS:N	8	1.3
(1,15)	1:670:A:TRP:C	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	6	1.29
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	2	1.28
(1,28)	1:682:A:ILE:N	1:682:A:ILE:CA	1:682:A:ILE:C	1:683:A:ARG:N	2	1.28
(1,9)	1:667:A:ALA:C	1:668:A:SER:N	1:668:A:SER:CA	1:668:A:SER:C	14	1.28
(1,17)	1:674:A:ASP:C	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	3	1.26
(1,25)	1:678:A:TRP:C	1:679:A:LEU:N	1:679:A:LEU:CA	1:679:A:LEU:C	3	1.25
(1,67)	1:701:A:VAL:C	1:702:A:LEU:N	1:702:A:LEU:CA	1:702:A:LEU:C	5	1.24
(1,30)	1:683:A:ARG:N	1:683:A:ARG:CA	1:683:A:ARG:C	1:684:A:ILE:N	12	1.23
(1,12)	1:669:A:LEU:N	1:669:A:LEU:CA	1:669:A:LEU:C	1:670:A:TRP:N	3	1.23
(1,7)	1:666:A:TRP:C	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	12	1.22
(1,6)	1:666:A:TRP:N	1:666:A:TRP:CA	1:666:A:TRP:C	1:667:A:ALA:N	9	1.22
(1,9)	1:667:A:ALA:C	1:668:A:SER:N	1:668:A:SER:CA	1:668:A:SER:C	7	1.21
(1,61)	1:698:A:VAL:C	1:699:A:PHE:N	1:699:A:PHE:CA	1:699:A:PHE:C	13	1.19
(1,17)	1:674:A:ASP:C	1:675:A:ILE:N	1:675:A:ILE:CA	1:675:A:ILE:C	4	1.14
(1,41)	1:688:A:ILE:C	1:689:A:VAL:N	1:689:A:VAL:CA	1:689:A:VAL:C	8	1.13
(1,33)	1:684:A:ILE:C	1:685:A:PHE:N	1:685:A:PHE:CA	1:685:A:PHE:C	1	1.13
(1,9)	1:667:A:ALA:C	1:668:A:SER:N	1:668:A:SER:CA	1:668:A:SER:C	6	1.12
(1,8)	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	1:668:A:SER:N	9	1.12
(1,7)	1:666:A:TRP:C	1:667:A:ALA:N	1:667:A:ALA:CA	1:667:A:ALA:C	1	1.1
(1,72)	1:704:A:LEU:N	1:704:A:LEU:CA	1:704:A:LEU:C	1:705:A:VAL:N	8	1.08
(1,58)	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	1:698:A:VAL:N	1	1.08
(1,57)	1:696:A:ARG:C	1:697:A:ILE:N	1:697:A:ILE:CA	1:697:A:ILE:C	14	1.03
(1,49)	1:692:A:LEU:C	1:693:A:ILE:N	1:693:A:ILE:CA	1:693:A:ILE:C	14	1.01
(1,15)	1:670:A:TRP:C	1:671:A:ASN:N	1:671:A:ASN:CA	1:671:A:ASN:C	12	1.01
(1,9)	1:667:A:ALA:C	1:668:A:SER:N	1:668:A:SER:CA	1:668:A:SER:C	8	1.0